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SORPTION MODELING FOR HLW PERFORMANCE ASSESSMENT - TASK 2,

CNWRA
CONTROLLED
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SORPTION MODELING FOR HIGH-LEVEL WASTE PERFORMANCE ASSESSMENT
TASK 2 - David R. Turner

6/2/92 DRT

SORPTION MODELING USING THE MINTEQA2 Code.

- The MINTEQA2, Version 3.0 geochemical equilibrium code is being used to model radionuclide sorption. The code (executable) being used is compiled for the IBM PC/XT/AT. The objectives of this research are outlined in the Sorption Modeling for HLW Performance Assessment Project Plan, and in the Task 2 Workplan for Hydrogeochemical Modeling.

- Version 3.0, MINTEQA2 is described in the User's Manual (Allison et al., 1990). A Hardcopy is available through DRT and is under configuration control. The preprocessor PRODEFA2 is also described in the manual.

- Magnetic copies of MINTEQA2/PRODEFA2 as distributed from the U.S. EPA are available on the directory C:\MINTEQA2 on the IBM PS/2 model 70 of DRT. Copies are also under configuration control.

- MINTEQA2 uses extensive thermodynamic databases. These are described in the user's manual (Allison et al., 1990). Original magnetic copies are under configuration control at CNWRA. Hardcopies of all original databases are stored as quality assurance documents. Magnetic copies are also stored on DRT's IBM PS/2 under the directory C:\MINTEQA2\OLDDATA

- To model radionuclide sorption, it is necessary to construct an appropriate database. This was undertaken to add Pu, Np, Am, Tc, Th, Sn, Cs, Co, Ru, Zr, Ra, Eu and update uranium in the appropriate databases.

- Data sources (and the references therein) included:

EQ3/6 Data ϕ. Com. R7 (Wolery et al, 1990)
Phillips et al. (1988) Sandia Aqueous Solutions Database
Berner (1991) MINEQL/PSI (Paul Scherrer Institute, Switzerland)
CHEMVAL

- The data was formatted for MINTEQA2 as described in user's manual (Allison et al., 1990). Altered files are: Thermo.dbs, Type6.dbs, Redox.dbs, Comp.dbs.
- LogK data from EQ3/6 except:
  $HTcO_4^-$, $H_2TcO_4^0$, $HTcO_4^0$ Phillips et al. (1988)
  $Th(OH)_3$ Berner (1991)
  DRJ 6/4/92
- ΔH_r calculated using ~~QUATTRO PRO~~ LOTUS-123 spreadsheet program designed by Tim Griffin and ΔH_f° values from EQ3/6 and Phillips et al. (1988). Phillips et al. (1988) used esp. for Np, Pu, Th, U ΔH_r calculations.

See sample hand calculations pg 92, this volume. DRJ 8/10/94

- The current versions of the MINTEQA2 radionuclide database are found as hardcopy and computer files on C:\MINTEQA2 on DRT's IBM PS/2 Model 70. A CNWRA Memorandum from DRT dated 5/7/92 was sent to the Element Manager (J. Russell), Technical Director (W. Patrick) and QA Director (B. Mabrito) to petition for exemption from qualification for MINTEQA2 data. Approval of petition granted 5/8/92.

6/12/92 Initial Entry DRJ 1/17/97
DRJ

In order to "translate" thermodynamic data from EQ3/6 (Data ϕ.com.R7) into MINTEQA2 components, the following reactions are used:

		Log K	ΔH_f° (kcal/mol)	Source
1)	$PO_4^{3-} + H^+ = HPO_4^{2-}$	+12.3218	-305.3	EQ3/6
2)	$HPO_4^{2-} + H^+ = H_2PO_4^-$	+7.2054	-369.82	EQ3/6
3)	$CO_3^{2-} + H^+ = HCO_3^-$	+10.3288	-164.898	EQ3/6
4)	$4H^+ + 4e^- + O_2 = 2H_2O$	+83.12		MINTEQA2
5)	$SiO_{2(aq)} + 2H_2O = H_4SiO_4$	+0.1184	-348.98	EQ3/6 + MINTEQA2
6)	$VO_2^+ + 2H_2O = 4H^+ + VO_4^{3-}$	-28.4475		EQ3/6
7)	$H_2AsO_4^- + 2H^+ = H_3AsO_4^0$	+2.2492	-215.70	EQ3/6
8)	$Zr^{4+} + 2H_2O = Zr(OH)_2^{2+} + 2H^+$	+0.2385		EQ3/6

6/22/92
DRJ

Tim Griffin and D. Turner upgraded MINTEQA2 to include data from Data ϕ. Com. R12 release of EQ3/6 database. With the exception of CsBr, CsCl, + CsI aqueous species, Δgk values (@ 25°C) remained unchanged from Data ϕ. Com. R7 release.

ΔH_f° values more complete in Data ϕ. Com. R12. Sources listed in EQ3/6 database. Only the following species include ΔH_f° from Phillips et al. (1988). The rest are from Data ϕ. Com. R12

ΔH_f° From Phillips et al. (1988):

① Am:
$Am(CO_3)_2^-$; $AmCO_3^+$; $Am(OH)^{2+}$; $Am(OH)_2^+$; $Am(OH)_3^0$; $Am(SO_4)^+$; $Am(SO_4)_2^-$; $AmCl^{2+}$; $AmCl_2^+$; AmF_2^+

② Eu:
$EuCl^{+2}$

③ Np:
$Np(HPO_4)_3^{-2}$; $NpO_2(H_2PO_4)^0$; NpO_2Cl^+

④ Pu:
$Pu(H_2PO_4)^{+2}$; $Pu(SO_4)_2^0$; $PuCl^{+3}$; PuF^{+3}; $Pu(HPO_4)^{+2}$; $Pu(HPO_4)_2^0$; $Pu(HPO_4)_3^{-2}$; $Pu(HPO_4)^{-4}$; $PuO_2(CO_3)_3^{-4}$; $(PuO_2)_2OH^+$; $PuO_2(H_2PO_4)^+$

⑤ Th:
$Th(H_3PO_4)^{+4}$; $Th(H_2PO_4)^{+3}$; $Th(H_2PO_4)_2^{+2}$; $Th(HPO_4)_3^{-2}$; $Th(OH)_3^+$; $Th(SO_4)_3^{-2}$; $Th(SO_4)_4^{-4}$; $ThCl_2^{+2}$; $ThCl_3^+$

⑥ U

Solids – K-Autunite; Na-Autunite; Sr-Autunite; U_4O_9; U_3O_8; $U(SO_4)_2 \cdot 8H_2O$; Coffinite {$USiO_4$}; Gummite (UO_3 (am));

Aqueous – $U(OH)_2^{+2}$; $U(OH)_3^{+}$; $U(OH)_4^{0}$; $U(OH)_5^{-}$; UF_5^{-}; UF_6^{-2}; $UO_2(OH)_2^{0}$; $(UO_2)_2CO_3(OH)_3^{-}$; $UO_2HPO_4^{0}$; $UO_2(HPO_4)_2^{0}$; $UO_2(H_2PO_4)^{+}$; $UO_2(H_2PO_4)_2^{0}$; $UO_2(H_2PO_4)_3^{0}$

7/30/92 (JLR)

FITEQL Data used in Jan 1 – June 30, 1992 Semi-Annual Report

FITEQL, Version 2 – Input Data From Tripathi (1984). 1.05×10^{-6} M, NO CO_2

Input File – Example:

Monodentate TLM: $SOH + UO_2^{2+} = (SO^- \cdot UO_2^{2+})^+ + H^+ \quad -PSI0 + 2PSIB$

```
        1
        1
        1
        1
        1
       90
        5          1          3          1
00001  -3.5    3.40E-4   XOH      }
00160  -1.0    0.00E00   PSI0     }
00161  -0.5    0.00E00   PSIB     }
00162  -0.1    0.00E00   PSID     } components
00032  -6.0    1.05E-6   UO2+2    }
00033   0.0    0.00E00   UO2ads   }
00050   0.0    0.00E00   H+       }
00003  -1.0    0.00E00   NA+      }
00005  -1.0    0.00E00   NO3-     }

00050     0.00  050  1
00032     0.00  032  1
03201    -5.21  032  1 050 -1
03202   -10.32  032  1 050 -2
03203   -19.22  032  1 050 -3
03204   -33.03  032  1 050 -4
03205    -2.71  032  2 050 -1
03206    -5.64  032  2 050 -2
03207   -11.93  032  3 050 -4
03208   -15.59  032  3 050 -5              Geochem.
03209   -31.05  032  3 050 -7              Model
03210   -21.95  032  4 050 -7              (NEA, 1990)
03211     0.28  032  1 005  1
00100   -14.00  050 -1
01050     5.00  001  1 160  1 050  1
01100   -10.90  001  1 160 -1 050 -1
01103    -8.33  001  1 160 -1 161  1 050 -1 003  1
01055     8.74  001  1 160  1 161 -1 050  1 005  1
00001     0.00  001  1
01233    -7.60  001  1 160 -1 161  2 050 -1 032  1 033  1
          SA     Cs     C1    C2
00004    50.0  0.410   0.8   0.2
0.1      1.0  <-- Background valence
I          1
        1233
          25         1          1          0
          33
1.017E-7   }
1.638E-7   }
2.091E-7   }
2.630E-7   }
2.857E-7   }
3.096E-7   }
3.216E-7   }
3.282E-7   }
3.689E-7   }
4.213E-7   }
4.846E-7   }
5.526E-7   }
5.647E-7   } Sorbed U(VI)
6.216E-7   } (Molarity)
6.333E-7   }
6.690E-7   }
6.901E-7   }
7.545E-7   }
8.320E-7   }
8.619E-7   }

9.384E-7   }
1.019E-6   }
1.030E-6   }
1.039E-6   }
1.031E-6   }
            50                          Digitized from
-5.230     }                            Tripathi (1984)
-5.423     }
-5.611     }
-5.738     }
-5.822     }
-5.874     }
-5.769     }
-5.904     }
-5.884     }
-5.997     }
-6.054     }
-6.170     } log a_H+
-6.105     }
-6.146     }
-6.162     }
-6.203     }
-6.264     }
-6.264     }
-6.364     }
-6.379     }
-6.469     }
-6.853     }
-8.121     }
-8.859     }
-9.217     }
            00          00
```


Example of Output: $(SO^- \cdot UO_2^{2+})$

```
VALUES OF ADJUSTABLE PARAMETERS AT EACH ITERATION: LOG K, T, LOG X
 I   V(Y): SOS/DF       1233

 0       4.324E-01 -7.600E+00
 1       4.121E-01 -4.709E+00
 2       3.956E-01 -4.269E+00
 3       3.829E-01 -3.984E+00
 4       3.738E-01 -3.774E+00
 5       3.675E-01 -3.614E+00
 6       3.634E-01 -3.491E+00
 7       3.609E-01 -3.396E+00
 8       3.594E-01 -3.324E+00
 9       3.585E-01 -3.270E+00
10       3.580E-01 -3.230E+00
11       3.578E-01 -3.200E+00
12       3.577E-01 -3.179E+00
13       3.576E-01 -3.164E+00
14       3.576E-01 -3.152E+00
15       3.575E-01 -3.145E+00
16       3.575E-01 -3.139E+00
17       3.575E-01 -3.135E+00
18       3.575E-01 -3.132E+00
19       3.575E-01 -3.130E+00
20       3.575E-01 -3.129E+00
21       3.575E-01 -3.128E+00
22       3.575E-01 -3.127E+00
23       3.575E-01 -3.127E+00
24       3.575E-01 -3.126E+00
25       3.575E-01 -3.126E+00
26       3.575E-01 -3.126E+00
27       3.575E-01 -3.126E+00
28       3.575E-01 -3.126E+00
29       3.575E-01 -3.126E+00

**** OPTIMIZATION PROCEDURE CONVERGED

29       3.575E-01 (-3.126E+00) — Log K_SO-·UO2^2+
```

For TLM:

Input Parameters

		Reference
$\log K^{+}$	5.0	Smith + Jenne (1991)
$\log K^{-}$	−10.9	Smith + Jenne (1991)
C_1	0.8 F/m^2	Hayes et al. (1991)
C_2	0.2 F/m^2	Hayes et al. (1991)
$\log K_{Na^+}$	−8.33	Hayes et al. (1991)
$\log K_{NO_3^-}$	8.74	Hayes et al. (1991)
N_s	10 sites/nm^2	Hayes et al. (1991)

Note: Hayes et al. (1991) recommend ΔpK_a ≥ 4.0 (JLR 7/30/92)

Output (FITEQL, Version 2.0)

$\log K_{UO_2^{2+}}$	$SO^- \cdot UO_2^{2+}$	−3.126
$\log K_{UO_2OH^+}$	$SO^- \cdot UO_2OH^+$	−9.063
$\log K_{UO_2(OH)_2}$	$SOH^0 \cdot UO_2(OH)_2^0$	−6.532
$\log K_{UO_2(OH)_3^-}$	$SOH_2^+ \cdot UO_2(OH)_3^-$	−4.298
$\log K_{UO_2(OH)_4^{2-}}$	$SOH_2^+ \cdot UO_2(OH)_4^{2-}$	−10.02

10/12/92
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SCM Comparison (CCM, DLM, TLM) for U(VI)-goethite sorption

- FITEQL Input slightly modified from earlier FITEQL Runs (see pg. 4-5, this volume).
- Log K values for chemical equilibrium modified for I = 0.1 M according to sheme outlined in Dzombak + Morel (1990). Log K values corrected using Davies Eqn. and assuming that all activity coefficients are equal for charged species. (See section 2.9 and Table 2.13, Dzombak and Morel, 1990)
- Log K values for complexation rxns (i.e. K_+, K_-, K_{cat}, K_{An}) not corrected for ionic strength, since these were determined for dilute solutions with ionic strength ≈ 0.1 (Hayes et al., 1991) Table VI.
- Also, TLM parameters for K_+ and K_- are from Smith and Jenne (1991), and are based on a detailed survey of TLM values reported in the literature.
- Still fitting data with monodentate UO_2 monomer of form $UO_2(OH)_n^{2-n}$

INDEPENDENTLY FIXED SCM PARAMETERS USED IN THE PRESENT STUDY.

Parameter	$TLM_{a,b}$	CCM_b	DLM_b
Log K_+	5.0	6.8	7.1
Log K_-	-10.9	-10.2	-10.2
C_1	0.8 F/m²	1.0 F/m²	--
C_2	0.2 F/m²	--	--
Log K_{Na^+}	-8.33	--	--
Log K_{NO3^-}	8.74	--	--
N_s	10 sites/nm²	10 sites/nm²	10 sites/nm²

(a) Smith and Jenne (1991)
(b) Hayes et al. (1991)

Terminology:
$XOH^\circ = SOH^\circ = MOH^\circ$

SAMPLE INPUT FOR FITEQL

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```
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        1
        1
        1
        1
        1
       40
        3        1        3        1
00001  -3.5   3.40E-4   XOH
00160  -1.0   0.00E00   PSI0
00032  -6.0   1.05E-6   UO2+2
00033   0.0   0.00E00   UO2ads - Dummy variable
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
00100  -13.78  050 -1
01050    7.10  001  1 160  1 050  1
01100  -10.24  001  1 160 -1 050 -1
00001    0.00  001  1
03301  -10.00  001  1 160  1 050 -1 032  1 033  1

00002   50.0  0.410     1.0
           0        0
           1
        3301
          25        1        1        0
          33
1.015E-7
1.624E-7
2.081E-7
2.630E-7
2.859E-7
3.089E-7
3.217E-7
3.274E-7
3.694E-7
4.200E-7
4.845E-7
5.513E-7
5.660E-7
6.225E-7
6.335E-7
```

should be 6.8 + 10.2 for CCM

should be 1 for CCM

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```
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                 6.691E-7
00000020         6.913E-7
00000030         7.549E-7
00000040         8.353E-7
00000050         8.639E-7
00000060         9.385E-7
00000070         1.020E-6
00000080         1.031E-6
00000090         1.041E-6
00000098         1.033E-6
00000100               50
00000102         -5.23
00000104         -5.43
00000106         -5.61
00000110         -5.73
00000120         -5.83
00000124         -5.87
00000126         -5.77
00000127         -5.91
00000128         -5.89
00000129         -5.99
00000130         -6.05
00000131         -6.17
00000132         -6.10
00000133         -6.14
00000134         -6.15
00000135         -6.20
00000137         -6.25
00000139         -6.25
00000140         -6.35
00000145         -6.38
00000150         -6.46
xouo2            -6.84
00000174         -8.12
00000175         -8.84
00000180         -9.20
00000185               00      00
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000440
00000460
00000480
00000500
00000520
00000540

00000560
00000580
00000600
00000610
00000620
00000630
00000640
00000650
00000660
00000670
00000680
00000690
00000700
00000710
00000720
00000730
00000740
00000760
00000780
00000800
00000820
00000840
00000860
00000880
00000900
00000920
00000940
00000960
00000980
00001010
00001030
00001050
00001070
00001090
00001110
00001130
00001370
```

$XO \cdot UO_2^+$

~~CCM~~ DLM DEJ 1/28/93

```
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        1
        1
        1
        1
        1
       90
        5        1        3        1
00001  -3.5   3.40E-4   XOH
00160  -1.0   0.00E00   PSI0
00161  -0.5   0.00E00   PSIB
00162  -0.1   0.00E00   PSID
00032  -6.0   1.05E-6   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
00100  -13.78  050 -1
01050    5.00  001  1 160  1 050  1
01100  -10.90  001  1 160 -1 050 -1
01103   -8.33  001  1 160 -1 161  1 050 -1 003  1
01055    8.74  001  1 160  1 161 -1 050  1 005  1
00001    0.00  001  1
03301   -7.60  001  1 160 -1 161  2 050 -1 032  1 033  1

00004   50.0  0.410   0.8   0.2
0.1     1.0
          1
       3301
         25        1        1        0
         33
1.015E-7
1.624E-7
2.081E-7
2.630E-7
2.859E-7
3.089E-7
3.217E-7
3.274E-7
3.694E 7
4.200E 7
4.845E-7
```

$XO \cdot UO_2^+$

TLM

```
00000020
00000030
00000040
00000050
00000060     Oct 16 15:08 1992  xouo2.tlm Page 2
00000070
00000080
00000090         5.513E-7
00000092         5.660E-7
00000094         6.225E-7
00000098         6.335E-7
00000100         6.691E-7
00000102         6.913E-7
00000104         7.549E-7
00000106         8.353E-7
00000110         8.639E-7
00000120         9.385E-7
00000124         1.020E-6
00000126         1.031E-6
00000127         1.041E-6
00000128         1.033E-6
00000129               50
00000130         -5.23
00000131         -5.43
00000132         -5.61
00000133         -5.73
00000134         -5.83
00000135         -5.87
00000137         -5.77
00000139         -5.91
00000140         -5.89
00000145         -5.99
00000146         -6.05
00000147         -6.17
00000150         -6.10
xouo2            -6.14
00000174         -6.15
00000175         -6.20
00000180         -6.25
00000185         -6.25
00000190         -6.35
00000195         -6.38
00000230         -6.46
00000240         -6.84
00000260         -8.12
00000280         -8.84
00000300         -9.20
00000320               00      00
00000340
00000360
00000380
00000400
00000420
00000440
00000460

00000480
00000500
00000520
00000540
00000560
00000580
00000600
00000610
00000620
00000630
00000640
00000650
00000660
00000670
00000680
00000690
00000700
00000710
00000720
00000730
00000740
00000760
00000780
00000800
00000820
00000840
00000860
00000880
00000900
00000920
00000940
00000960
00000980
00001010
00001030
00001050
00001070
00001090
00001110
00001130
00001370
```

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```
            1
            1
            1
            1
            1
           40
            3          1          3          1
00001   -3.5    3.40E-4   XOH
00160   -1.0    0.00E00   PSI0
00032   -6.0    1.05E-6   UO2+2
00033    0.0    0.00E00   UO2ads
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   NO3-

00050    0.00   050  1
00032    0.00   032  1
03201   -5.43   032  1 050 -1
03202  -10.54   032  1 050 -2
03203  -19.22   032  1 050 -3
03204  -32.59   032  1 050 -4
03205   -2.49   032  2 050 -1
03206   -5.42   032  2 050 -2
03207  -12.37   032  3 050 -4
03208  -16.25   032  3 050 -5
03209  -31.49   032  3 050 -7
03210  -22.83   032  4 050 -7
03211   -0.05   032  1 005  1
00100  -13.78   050 -1
01050    7.10   001  1 160  1 050  1
01100  -10.24   001  1 160 -1 050 -1
00001    0.00   001  1
03301  -10.00   001  1 160  1 050 -1 032  1 033  1


00002   50.0  0.410
0.1     1.0
           1
        3301
          25          1          1          0
          33
1.015E-7
1.624E-7
2.081E-7
2.630E-7
2.859E-7
3.089E-7
3.217E-7
3.274E-7
3.694E-7
4.200E-7
4.845E-7
5.513E-7
5.660E-7
6.225E-7
6.335E-7
```

Dummy variable

$XO{\cdot}UO_2^+$

DLM

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```
00000020    6.691E-7
00000030    6.913E-7
00000040    7.549E-7
00000050    8.353E-7
00000060    8.639E-7
00000070    9.385E-7
00000080    1.020E-6
00000090    1.031E-6
00000098    1.041E-6
00000100    1.033E-6
00000102           50
00000104   -5.23
00000106   -5.43
00000110   -5.61
00000120   -5.73
00000124   -5.83
00000126   -5.87
00000127   -5.77
00000128   -5.91
00000129   -5.89
00000130   -5.99
00000131   -6.05
00000132   -6.17
00000133   -6.10
00000134   -6.14
00000135   -6.15
00000137   -6.20
00000139   -6.25
00000140   -6.25
00000145   -635
00000150    638
xouo2+      646
00000174    784
00000175   -8.12
00000180   -8.84
00000185   -9.20
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000440
00000460
00000480
00000500
00000520
00000540
00000560
00000580
00000600
00000610
00000620
00000630
00000640
00000650
00000660
00000670
00000680
00000690
00000700
00000710
00000720
00000730
00000740
00000760
00000780
00000800
00000820
00000840
00000860
00000880
00000900
00000920
00000940
00000960
00000980
00001010
00001030
00001050
00001070
00001090
00001110
00001130
00001370
          00        00
```

INPUT FILES:

XOUO2.* = $XO{\cdot}UO_2^+$ where '*' is DLM, CCM, or TLM depending on the model.
XOHUO2.* = $XOH{\cdot}UO_2^{2+}$
XOUO2OH.* = $XO{\cdot}UO_2OH^0$
XOHUO2OH.* = $XOH{\cdot}UO_2OH^+$
XOUO2OH2.* = $XO{\cdot}UO_2(OH)_2^-$
XOHUOOH2.* = $XOH{\cdot}UO_2(OH)_2^0$
XOH2UOH2.* = $XOH_2{\cdot}UO_2(OH)_2^+$
XOHUOOH3.* = $XOH{\cdot}UO_2(OH)_3^-$
XOH2UOH3.* = $XOH_2{\cdot}UO_2(OH)_3^0$
XOHUOOH4.* = $XOH{\cdot}UO_2(OH)_4^{-2}$
XOH2UOH4.* = $XOH_2{\cdot}UO_2(OH)_4^-$

These files are stored on CNWRA LAN on:
K:\TURNER\FITEQL\INPUT* (i.e. DLM, CCM, TLM)
and supercede the earlier FITURAN input files

10/16/92
DRJ

RESULTS OF FITEQL RUNS ($\log K_{UO_2(OH)_n}$)

	CCM LOG K	SOS/DF	DLM LOG K	SOS/DF	TLM LOG K	SOS/DF
*						
$XO{\cdot}UO_2^+$	1.85	.09	1.15	.17	-3.36	.35
$XOH{\cdot}UO_2^{2+}$	10.56	.09	9.1	.23	5.23	.32
$XO{\cdot}UO_2(OH)_2^-$	-15.5	.09	-14.87	.03	-14.78	.08
$XOH{\cdot}UO_2(OH)_2^0$	-6.84	.09	-6.81	.09	-6.74	.09
$XOH_2{\cdot}UO_2(OH)_2^+$	1.85	.09	1.15	.17	1.65	.10
$XO{\cdot}UO_2OH$	-6.84	.09	-6.81	.09	-9.28	.27
$XOH{\cdot}UO_2OH^+$	1.85	.09	1.15	.17	4.56	.32
$XOH{\cdot}UO_2(OH)_3^-$	-15.5	.09	-14.87	.03	-12.57	.008
$XOH_2{\cdot}UO_2(OH)_3^0$	-6.84	.09	-6.81	.09	-4.51	.006
$XOH{\cdot}UO_2(OH)_4^{-2}$	-24.1	.09	-22.89	.01	-17.96	.004
$XOH_2{\cdot}UO_2(OH)_4^-$	-15.5	.09	-14.87	.03	-10.23	.003

OUTPUT FILES:

UO2CCM1 = $XO{\cdot}UO_2^+$ -CCM
UO2CCM2 = $XOH{\cdot}UO_2^{2+}$ "
UOH1CCM1 = $XO{\cdot}UO_2OH^0$ "
UOH1CCM2 = $XOH{\cdot}UO_2OH^+$ "
UOH2CCM1 = $XO{\cdot}UO_2(OH)_2^-$ "
UOH2CCM2 = $XOH{\cdot}UO_2(OH)_2^0$ "
UOH2CCM3 = $XOH_2{\cdot}UO_2(OH)_2^+$ "
UOH3CCM1 = $XOH{\cdot}UO_2(OH)_3^-$ "
UOH3CCM2 = $XOH_2{\cdot}UO_2(OH)_3^0$ "
UOH4CCM1 = $XOH{\cdot}UO_2(OH)_4^{-2}$ "
UOH4CCM2 = $XOH_2{\cdot}UO_2(OH)_4^-$ "

Also UO2DLM1, etc... and UO2TLM1, etc...

CNWRA LAN
K:\TURNER\FITEQL\OUTPUT*
where * is DLM, CCM, or TLM

10/19/92 DRJ

Added Sr (strontium) log K values from Data0.com.R12 release of EQ3/EQ6 database to MINTEQA2 database.

References for radionuclides compiled in files:

K:\TURNER\MINTEQA2\SPECIES.REF
K:\TURNER\MINTEQA2\RADREFS.DAT

10/20/92 DRJ

BEGIN TO MODEL U(VI)-CO_2 SORPTION DATA OF Tripathi (1984)

1) USED DLM MODEL. FITEQL WITH DLM Parameters (K_+, K_-, N_S) from § Hayes et al. (1991) (See table on pg. 6)

Monodentate complexes, recast for CO_2 as component, according to:

$$XOH + UO_2^{2+} + CO_3^{2-} = XOH\cdot UO_2CO_3^0 + \cancel{2H^+}$$ DRJ 10/20

$$CO_2 + H_2O = CO_3^{2-} + 2H^+$$

$$\boxed{XOH + UO_2^{2+} + CO_2 + H_2O = XOH\cdot UO_2CO_3^0 + 2H^+}$$

Also correct/recast chemical equilibria for CO_2 as component:

	Log K
$UO_2^{2+} + CO_3^{2-} = UO_2CO_3^0$	9.6147
$CO_2 + H_2O = CO_3^{2-} + 2H^+$	−18.16
$\boxed{UO_2^{2+} + CO_2 + H_2O = UO_2CO_3^0 + 2H^+}$	−8.545

COMPLEXES FIT TO DATA USING FITEQL:

	Input FILE	Output File
$XOH\cdot UO_2CO_3^0$	XOHUC1.DLM	UC1DLM1.OUT
$XOH_2\cdot UO_2(CO_3)_2^-$	XOH2UC2.DLM	UC2DLM1.OUT
$XOH_2\cdot UO_2(CO_3)_3^{-3}$	XOH2UC3.DLM	UC3DLM1.OUT
$XOH_2\cdot (UO_2)_2CO_3(OH)_3^0$	XOH2UCO.DLM	UCO1DLM1.OUT
$XOH_4\cdot UO_2(OH)_4^{-2}$	XOHUOH4C.DLM	UOH4DLMC.OUT

10/23/92 DRJ

FITEQL INPUT - WITH $p(CO_2) = 10^{-3.5}$ atm; I = 0.1 M; DLM; 1.05×10^{-6} M U(VI) U(VI)-SORPTION DATA FROM TRIPATHI (1984)

EXAMPLE:

Oct 23 08:55 1992 xohuc1.dlm Page 1

```
     1
     1
     1
     1
     1
    30
     4          2          3          1
00001  -3.5    3.40E-4   XOH
00160  -1.0    0.00E00   PSI0
00032  -6.0    1.05E-6   UO2+2
00140  -3.5    3.16E-4   CO2g
00141   0.0    0.00E00   CO3ads
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   Na+
00005  -1.0    0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
00140    0.00  140  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -8.77  032  1 140  1 050 -2
03212  -19.35  032  1 140  2 050 -4
03213  -30.81  032  1 140  3 050 -6
03214  -51.09  032  3 140  6 050-12
03215  -70.09  032 11 140  6 050-24
03216  -19.28  032  2 140  1 050 -5
03217  -18.11  032  3 140  1 050 -5
03218   -0.05  032  1 005  1
00100  -13.78  050 -1
01401  -17.50  140  1 050 -2
01402   -7.61  140  1 050 -1
01403   -1.48  140  1
01404  -16.67  140  1 003  1 050 -2
01405   -8.08  140  1 003  1 050 -1
01050    7.10  001  1 160  1 050  1
00001    0.00  001  1
01100  -10.24  001  1 160 -1 050 -1
03301    0.00  001  1 160  0 050 -2 032  1 033  1 140  1 141  1


00002   50.0  0.410
0.1    1.0
       1
    3301
      40          2          1          0
      33
```

= Dummy variables

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```
00000010  1.015E-7
00000020  1.629E-7
00000030  2.092E-7
00000040  2.638E-7
00000050  2.868E-7
00000060  3.105E-7
00000070  3.072E-7
00000080  3.228E-7
00000090  3.292E-7
00000097  3.688E-7
00000098  4.217E-7
00000099  4.851E-7
00000100  5.522E-7
00000102  5.659E-7
00000104  6.030E-7
00000106  6.689E-7
00000110  6.921E-7
00000120  7.555E-7
00000122  8.344E-7
00000124  8.635E-7
00000126  9.390E-7
00000128  1.021E-6
00000130  1.013E-6
00000132  1.024E-6
00000134  9.962E-7
00000136  9.579E-7
00000138  9.185E-7
00000140  8.720E-7
00000142  8.161E-7
00000144  7.645E-7
00000146  7.027E-7
00000148  6.730E-7
00000150  6.016E-7
00000152  5.401E-7
00000154  4.431E-7
00000156  3.543E-7
00000158  3.261E-7
00000159  2.980E-7
00000160  2.375E-7
00000161  1.801E-7
00000162        141
00000163  1.015E-7
00000164  1.629E-7
00000165  2.092E-7
00000166  2.638E-7
00000168  2.868E-7
00000170  3.105E-7
xohuc1    3.228E-7
00000180  3.292E-7
00000182  3.688E-7
00000184  4.217E-7
00000185  4.851E-7
00000190  5.522E-7
00000195  5.659E-7
00000230  6.300E-7
00000240  6.689E-7
```

$XOH\cdot UO_2CO_3^0$

141 M CO_3(ads) = UO_2(ads)

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```
6.921E-7
7.555E-7
8.344E-7
8.635E-7
9.390E-7
1.021E-6
1.013E-6
1.024E-6
9.962E-7
9.579E-7
9.185E-7
8.720E-7
8.160E-7
7.645E-7
7.027E-7
6.730E-7
6.324E-7
6.016E-7
5.401E-7
4.431E-7
3.543E-7
3.261E-7
2.980E-7
2.375E-7
1.801E-7
      50
-5.23
-5.42
-5.60
-5.73
-5.82
-5.87
-5.76
-5.90
-5.88
-5.99
-6.04
-6.16
-6.10
-6.14
-6.19
-6.26
-6.25
-6.35
-6.37
-6.46
-6.84
-6.98
-7.08
-7.11
-7.22
-7.34
-7.40
-7.45
-7.50
-7.62
```

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```
00000820  -7.53
00000830  -7.62
00000840  -7.58
00000850  -7.65
00000860  -7.69
00000870  -7.76
00000880  -7.84
00000890  -7.86
00000900  -7.93
00000910  -8.11
00000920
00000930
00000940
00000950
00000960
00000970
00000980
00000990
00001000
00001010
00001020
00001030
00001040
00001050
00001060
00001070
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001150
00001160
00001170
00001180
00001190
00001200
00001210
00001220
00001230
00001240
00001250
00001260
00001270
00001280
00001290
00001300
00001310
00001320
00001330
00001340
00001350
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00001370
00001380
00001390
00001400
00001410
00001420
00001430
00001440
00001450
00001460
00001470
00001480
```

00 00

00000260 00000270 00000280 00000290 00000300 00000310 00000320 00000330 00000340 00000350 00000360 00000370 00000380 00000390 00000400 00000410 00000420 00000430 00000440 00000450 00000460 00000470 00000480 00000490 00000500 00000510 00000520 00000530 00000540 00000550 00000560 00000570 00000580 00000590 00000600 00000610 00000620 00000630 00000640 00000650 00000660 00000670 00000680 00000690 00000700 00000710 00000720 00000730 00000740 00000750 00000760 00000770 00000780 00000790 00000800 00000810

10/23/92
DRJ

LOGK VALUES FROM FITEQL RUNS (CORRECTED TO $CO_3^{2-} + 2H^+ = H_2O + CO_2$)

	Rxn w/ CO_2 → LOGK^a	SOS/DF	LOGK^c (= LOGK^a + 18.16)	
$XOH \cdot UO_2CO_3^0$	-3.125	.07	15.04	Converting CO_2 to CO_3^{2-} for MINTEQA2 RUNS
$XOH_2 \cdot UO_2(CO_3)_2^-$	-7.6668	.09	28.65	
$XOH_2 \cdot UO_2(CO_3)_3^{-3}$	-20.36	.08	34.12	
$XOH_2 \cdot (UO_2)_2CO_3(OH)_3$	-7.491	.04	10.67	
$XOH \cdot UO_2(OH)_4^{-2}$	-23.11	1.82	-23.11 * (No CO_2, so no change)	

10/29/92
DRJ

FITEQL + MINTEQA2 RUNS USING CNWRA data for U(VI)-SORPTION on Clinoptilolite

Using only 14 forward reactions @ 2×10^{-6} M $UO_2(NO_3)_2$ from Pabalan + Turner (1992).

Assuming a specific surface area of 700 m^2/g; DLM; Corrected for I=0.1 M

Modeled data using 5 species:

	LogK	INPUT FILE (K:\TURNER\FITEQL\DLM\)
$XOH \cdot UO_2CO_3^0$	~~15.0~~	GZEOLUC1.DLM
$XOH_2 \cdot UO_2(CO_3)_2^-$	~~28.7~~	GZEOLUC2.DLM
$XOH_2 \cdot UO_2(CO_3)_3^{-3}$	~~34.1~~	GZEOLUC3.DLM
$XOH_2 \cdot (UO_2)_2CO_3(OH)_3^0$	~~10.7~~	GZIOLUCO.DLM
$XOH \cdot UO_2(OH)_4^{-2}$	~~-23.1~~	GZEOLUOH.DLM

Entered wrong LogK here.

Rxn w/ CO_2 →

FOR ZEOLITES:

	LogK^a	SOS/DF	LOGK^c (Correcting CO_2 to CO_3^{2-})
$XOH \cdot UO_2CO_3^0$	-4.23	.14	13.94
$XOH_2 \cdot UO_2(CO_3)_2^-$	-8.95	.50	27.37
$XOH_2 \cdot UO_2(CO_3)_3^{-3}$	-21.82	1.30	32.66
$XOH_2 \cdot (UO_2)_2CO_3(OH)_3$	-8.58	0.14	9.58
$XOH \cdot UO_2(OH)_4^{-2}$	-24.68	0.81	-24.68 No $CO_2 \rightarrow CO_3^{2-}$ correction necessary

ZEOLITE DATA:

$\Sigma U = 2.0 \times 10^{-6}$ m $UO_2(NO_3)_2$

Forward pH equil	Forward %U lost	Reverse pH equil	Reverse %Ulost	UO_2CO_3	$(UO_2)_2(OH)_3CO_3$
2.93,	22.248, 4.450×10^{-7} m	2.55,	22.574	1.335×10^{-6}	2.225×10^{-7}
3.71,	24.769, 4.954×10^{-7}	3.21,	16.397	1.486×10^{-6}	2.477×10^{-7}
4.65,	75.294, 1.506×10^{-6}	3.92,	48.603	4.518×10^{-6}	7.53×10^{-7}
6.05,	94.79, 1.896×10^{-6}	4.77,	83.169	5.688×10^{-6}	9.48×10^{-7}
6.5,	97.038, 1.941×10^{-6}	6.01,	94.882	5.823×10^{-6}	9.705×10^{-7}
6.72,	96.66, 1.933×10^{-6}	6.27,	94.221	5.799×10^{-6}	9.667×10^{-7}
6.76,	96.366, 1.927×10^{-6}	6.42,	95.213	5.781×10^{-6}	9.635×10^{-7}
6.9,	94.769, 1.895×10^{-6}	6.67,	92.368	5.685×10^{-6}	9.475×10^{-7}
6.89,	94.118, 1.882×10^{-6}	6.89,	90.228	5.646×10^{-6}	9.410×10^{-7}
7.07,	91.387, 1.828×10^{-6}	7.1,	81.846	5.484×10^{-6}	9.140×10^{-7}
7.31,	71.324, 1.426×10^{-6}	7.35,	72.426	4.278×10^{-6}	7.130×10^{-7}
7.85,	38.298, 7.660×10^{-7}	7.8,	26.765	2.298×10^{-6}	3.830×10^{-7}
8.35,	7.5, 1.5×10^{-7}	8.3,	0	4.5×10^{-7}	7.5×10^{-8}
8.94,	0.14706, 2.941×10^{-9}	8.91,	0	8.823×10^{-9}	1.471×10^{-9}

$\Sigma U = 2.0 \times 10^{-5}$ m $UO_2(NO_3)_2$

Forward pHeq	Forward %Ulost.	Reverse pH eq	Reverse %Ulost
2.81,	10.504, 2.101×10^{-6}	2.06,	23.109
3.68,	11.134, 2.227×10^{-6}	2.96,	5.2521
4.61,	53.992, 1.080×10^{-5}	3.82,	9.4538
5.49,	89.307, 1.786×10^{-5}	5.26,	76.05
6.52,	93.634, 1.873×10^{-5}	6.24,	91.807
6.76,	83.445, 1.669×10^{-5}	6.36,	87.92
6.9,	81.071, 1.621×10^{-5}	6.51,	85.609
6.98,	79.79, 1.596×10^{-5}	6.68,	81.534
6.98,	81.282, 1.626×10^{-5}	6.7,	82.206
7.18,	77.311, 1.546×10^{-5}	7.05,	80.651
7.4,	68.697, 1.374×10^{-5}	6.82,	88.824
7.89,	20.798, 4.160×10^{-6}	7.66,	29.832
8.44,	0, 0	8.26,	0
8.94,	1.0504, 2.101×10^{-7}	8.85,	0

MINTEQA2 OUTPUT FILES Include (all on K:\TURNER\MINTEQA2\OUTPUT):

- UO_2TLM.OUT, UO2DLM.OUT, UO2SCM.OUT — TRIPATH1 (1984), 10^{-6} m U(vi), NO CO_2
- GZDLMUC.OUT - Pabalan zeolite Data. Forward rxn only. 10^{-6} M.
- UCO2DLM.OUT - TRIPATH1 (1984), DLM, 10^{-6} m U(vi), Atmos. CO_2
- UOH4DLM.OUT - VARIABLE LOG K for mon $UO_2(OH)_4^{-2}$ complex
- SITECONC.OUT - NO UO_2, Goethite site conc. of varible pH.

11/13/92 XRJ

GRAPHING SITE DISTRIBUTION FOR CCM, DLM, TLM.

SIGMAPLOT FILES INCLUDE:

SITEDLM.SPS
SITECCM.SPS
SITETLM.SPS

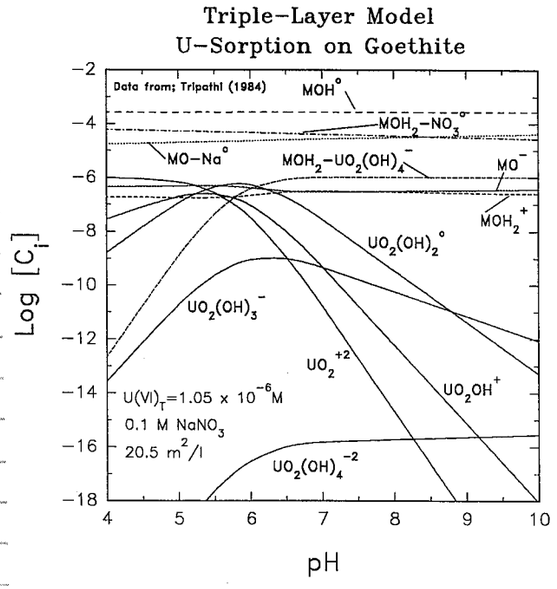
of interest are concentrations of:

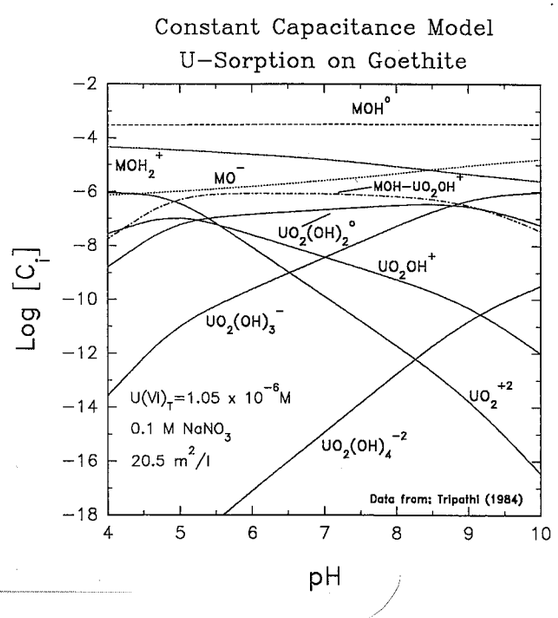
MOH^o, MOH_2^+, MO^-, $MOUO_2(OH)_n$, UO_2OH^+, UO_2^{2+}, $UO_2(OH)_2^o$, $UO_2(OH)_3^-$, $UO_2(OH)_4^{-2}$.

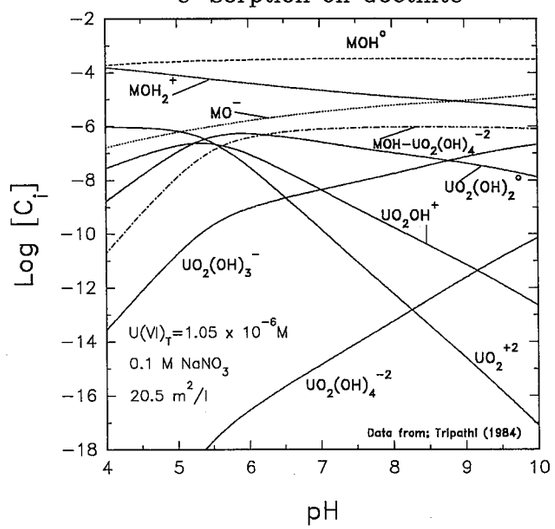
Data gathered from appropriate MINTEQA2 output files:

UO_2DLM.OUT
UO2CCM.OUT
UO2TLM.OUT

Resultant Graphs:







12/15/92 XRJ

Adopted CNWRA Radionuclide database to MINTEQA2, Ver. 3.11 database. Version 3.11 database is the same as 3.0 THERMP.DBS, only it has been modified to standardize formatting (i.e., all of the columns line up)

CNWRA data modified to match standardized formatting (i.e., lining up columns). In addition, data entry was modified to alphabetize the data in THERMO.DBS. This was done to simplify finding data in the database.

12/16/92 XRJ

Checked CNWRA database against Data0.com.R16 (26 June 92) release of EQ3/6. Corrected minor mistakes in CNWRA data. Modifications on Data0.com.R12 data involved recasting rxns in terms of HCO_3^- (from CO_3^{2-}), HPO_4^{2-} (from PO_4^{3-}), H^+ (from OH^-). No other significant changes in more recent EQ3/6 release. Added several solid phases from EQ3/6 database. These are not new to EQ3/6, but were missed the first time around. Subsequent reordering of EQ3/6 data (re-alphabetized) made them easier to find: $CoCO_3$, Co_2SiO_4, $KTcO_4$, $NaTcO_4$, $NaUO_3$, $Na_4UO_2(CO_3)_3$, $NaNpO_2(CO_3):3.5H_2O$, Rb_2UO_4, Sn_2S_3, SrI_2

1/8/93 DRJ

Directory structure on K: drive (LAN) modified to give better idea of data location. This involved creation of element specific subdirectories for FITEQL runs. All file names remain unchanged. But, for example, location of all DLM uranium runs are located in:

K:\TURNER\FITEQL\INPUT\DLM\URANIUM.

Separate subdirectories for plutonium + Np are prepared in anticipation of FITEQL runs for sorption data

e.g. K:\TURNER\FITEQL\INPUT\DLM\PLUTONUM
K:\TURNER\FITEQL\INPUT\DLM\NEPTUNUM

Similar directory structures adopted for TLM + CCM.

1/26/93 DRJ

Corrected previous FITEQL runs for data (U(VI)-goethite) of Tripathi (1984) Mistake was made in using the default error estimates (1×10^{-6} M) for an extremely dilute solution (also 1×10^{-6} m $U(VI)_T$). Using the experimental error of the order of the solution concentration resulted in erroneously low values of V_y = SOS/DF in the FITEQL runs.

The runs were redone using the estimated error of ±8% due to sorption on the container walls reported by Tripathi (1984). All other parameters, values, and file name/locations are the same as reported previously (pg. 046/6; 046/8 (1/26 DRJ) through 12) all files are located as described above in 1/8/93 entry.

An example of the revised FITEQL input + resultant output is shown here:

No CO_2

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```
     1
     1
     1
     1
     1
    90
     5          1          3          1
00001  -3.5    3.40E-4   XOH
00160  -1.0    0.00E00   PSI0
00161  -0.5    0.00E00   PSIB
00162  -0.1    0.00E00   PSID
00032  -6.0    1.05E-6   UO2+2
00033   0.0    0.00E00   UO2ads  — dummy variables
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   NA+
00005  -1.0    0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
00100  -13.78  050 -1
01050    5.00  001  1 160  1 050  1
01100  -10.90  001  1 160 -1 050 -1
01103   -8.33  001  1 160 -1 161  1 050 -1 003  1
01055    8.74  001  1 160  1 161 -1 050  1 005  1
00001    0.00  001  1
03301   -7.60  001  1 160 -1 161  2 050 -1 032  1 033  1

00004   50.0  0.410   0.8   0.2
0.1    1.0
         1
      3301
        25          1          1          0
        33
1.015E-7
1.624E-7
2.081E-7
2.630E-7
2.859E-7
3.089E-7
3.217E-7
3.274E-7
3.694E-7
4.200E-7
4.845E-7
5.513E-7
5.660E-7
6.225E-7
6.335E-7
6.691E-7
6.913E-7
7.549E-7
8.353E-7
8.639E-7
9.385E-7
1.020E-6
1.031E-6
1.041E-6
1.033E-6
```

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```
00000020
00000030
00000040
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000137
00000139
00000140
00000145
00000146
00000147
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000440
00000460
     50
-5.23
-5.43
-5.61
-5.73
-5.83
-5.87
-5.77
-5.91
-5.89
-5.99
-6.05
-6.17
-6.10
-6.14
-6.15
-6.20
-6.25
-6.25
-6.35
-6.38
-6.46
-6.84
-9.12
-8.84
-9.20
     1     1
    33    0.08   8.0E-08
    50    0.05   0.0E-00
00000480
00000500
00000520
00000540
00000560
00000580
00000600
00000610
00000620
00000630
00000640
00000650
00000660
00000670
00000680
00000690
00000700
00000710
00000720
00000730
00000740
00000760
00000780
00000800
00000820
00000840
00000860
00000880
00000900
00000920
00000940
00000960
00000980
00001010
00001030
00001050
00001070
00001090
00001110
00001130
00001170
00001180
00001190
```

Input file
Stored K:\TURNER\FITEQL\INPUT\TLM\URANIUM

Forming $XO\text{-}UO_2^+$

TLM

} Tripathi's error ±8%

$.08 \times 1 \times 10^{-6}$
$= 8 \times 10^{-8}$

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VALUES OF ADJUSTABLE PARAMETERS AT EACH ITERATION: LOG K, T, LOG X

I	V(Y): SOS/DF	3301	
0	2.179E+01	-7.600E+00	← initial guess
1	2.023E+01	-4.951E+00	
2	1.943E+01	-4.595E+00	
3	1.907E+01	-4.405E+00	
4	1.892E+01	-4.293E+00	
5	1.886E+01	-4.226E+00	
6	1.883E+01	-4.185E+00	
7	1.882E+01	-4.160E+00	
8	1.882E+01	-4.146E+00	
9	1.882E+01	-4.137E+00	
10	1.882E+01	-4.131E+00	
11	1.882E+01	-4.128E+00	
12	1.882E+01	-4.126E+00	
13	1.882E+01	-4.125E+00	
14	1.882E+01	-4.124E+00	
15	1.882E+01	-4.124E+00	
16	1.882E+01	-4.123E+00	
17	1.882E+01	-4.123E+00	
18	1.882E+01	-4.123E+00	
19	1.882E+01	-4.123E+00	

$\log K_{XO\text{-}UO_2^+} = -4.123$

SOS/DF = 18.82

Partial output showing resultant log K output

**** OPTIMIZATION PROCEDURE CONVERGED

19 1.882E+01 -4.123E+00

Resultant Parameters and error estimates from FITEQL runs

Tripathi (1984) U(VI)-goethite sorption data, 1.05×10^{-6} M $UO_2(NO_3)_2$, NO CO_2, 0.1 M $NaNO_3$

FOR CCM, DLM, TLM

	Log K CCM	SOS/DF	DLM	SOS/DF	TLM	SOS/DF
$XO\text{-}UO_2^+$	0.87 ~~1.69~~	7.427 ~~4.434~~	0.95	8.32	-4.12	18.92
$XOH\text{-}UO_2^{+2}$	8.74 ~~10.39~~	9.147 ~~4.446~~	8.84	11.31	4.62	16.97
$XO\text{-}UO_2OH^0$	-6.98 ~~-7.00~~	4.813 ~~4.93~~	-6.96	4.64	-9.56	13.61
$XOH\text{-}UO_2OH^+$	0.87 ~~1.69~~	7.427 ~~4.434~~	0.95	8.32	-1.21	13.21
$XO\text{-}UO_2(OH)_2^-$	-14.89 ~~-15.69~~	2.30 ~~4.433~~	-14.95	1.68	-14.97	4.61
$XOH\text{-}UO_2(OH)_2^0$	-6.98 ~~-7.00~~	4.813 ~~4.93~~	-6.96	4.64	-6.89	4.90
$XOH_2\text{-}UO_2(OH)_2^+$	0.87 ~~1.69~~	7.427 ~~4.434~~	0.95	8.32	1.46	5.24
$XOH\text{-}UO_2(OH)_3^-$	-14.89 ~~-15.69~~	2.30 ~~4.433~~	-14.95	1.68	-12.61	0.45
$XOH_2\text{-}UO_2(OH)_3^0$	-6.98 ~~-7.00~~	4.813 ~~4.93~~	-6.96	4.64	-4.53	0.33
$XOH\text{-}UO_2(OH)_4^{-2}$	-22.79 ~~-24.79~~	1.33 ~~4.446~~	-22.94	0.64	-17.49	0.25
$XOH_2\text{-}UO_2(OH)_4^-$	-14.89 ~~-15.69~~	2.30 ~~4.933~~	-14.95	1.68	-10.22	0.23

Corrections to CCM values - DLM 1/28/93

Note: Westall (1982) states that SOS/DF values between 0.1 & 20 are indicative of a reasonable fit. The smaller the number, the better the 'fit' to the data.

FOR U(VI)-CO_2-H_2O-goethite system (DLM model only)

	w/ CO_2 as component Log K	SOS/DF	Corrected/Changed to CO_3^{-2} Log K
$XOH\cdot UO_2CO_3$	-3.27	4.29	+14.89
$XOH_2\text{-}UO_2(CO_3)_2^-$	-7.78	1.77	+28.54
$XOH_2\text{-}UO_2(CO_3)_3^{-3}$	-20.43	0.66	+34.05
$XOH_2\cdot(UO_2)_2CO_3(OH)_3^0$	-7.62	4.61	+10.54
$XOH\cdot UO_2(OH)_4^{-2}$	-23.27	32.29	-23.27

Change to CO_3 as component described above on pg. 12 (046/12)

1/28/93 DLJ Discovered errors in CCM input files. Forgot to change the FITEQL flag indicating which SCM should be used (see pg. 7, corrections on sample output). Also, used DLM parameters for K_+ + K_-. This problem has been corrected and the FITEQL calculations redone. correct values listed below and on Table on pg. 18.

MINTEQA2 calculations rerun using correct log K values. and 12/17/92 CNLWRA radionuclide database. Resultant graphs shown below

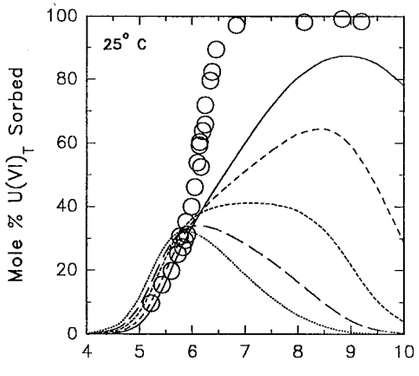
CCM

	Log K	SOS/DF
$XO\text{-}UO_2^+$	0.87	7.427
$XOH\text{-}UO_2^{+2}$	8.74	9.147
$XO\text{-}UO_2OH^0$	-6.98	4.813
$XOH\text{-}UO_2OH^+$	0.87	7.427
$XO\text{-}UO_2(OH)_2^-$	-14.89	2.30
$XOH\text{-}UO_2(OH)_2^0$	-6.98	4.813
$XOH_2\text{-}UO_2(OH)_2^+$	0.87	7.427
$XOH\text{-}UO_2(OH)_3^-$	-14.89	2.30
$XOH_2\text{-}UO_2(OH)_3^0$	-6.98	4.813
$XOH\text{-}UO_2(OH)_4^{-2}$	-22.79	1.33
$XOH_2\text{-}UO_2(OH)_4^-$	-14.89	2.30

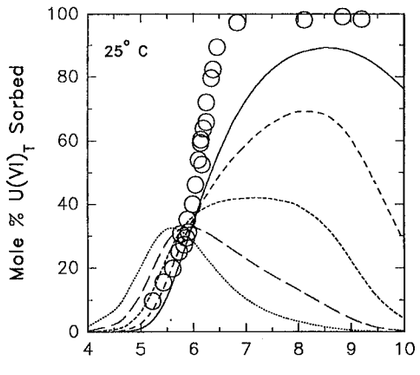
File names remain unchanged. Corrected FITEQL runs replace earlier runs. DLM + TLM values unchanged.

RESULTS OF MINTEQA2 calculations made using parameters for DLM, CCM, TLM listed in tables on pg. 6, pg. 18.
%U sorbed vs pH data stored on K:\TURNER\MINTEQA2\OUTPUT\UO2DLM.OUT
K:\ * \ * \ * \UO2TLM.OUT
K:\ * \ * \ * \UO2CCM.OUT

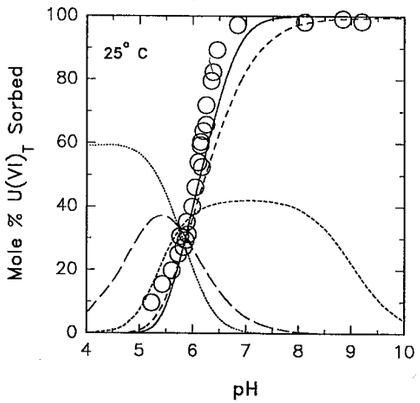
Constant Capacitance Model (CCM)

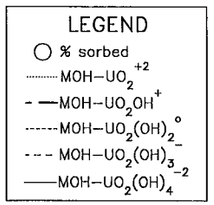


Diffuse-Layer Model (DLM)



Triple-Layer Model (TLM)





2/4/93 SRL FITEQL runs with Pu^{+4}-goethite sorption data of Sanchez et al. (1985). The approach taken is identical to that used for uranium sorption data of Tripathi (1984). DLM, CCM, TLM surface complexation models, using parameters on pg. 6

Pu^{+4} hydrolysis constants, corrected for I = 0.1

		Log k; I=0	I = 0.1
4101	$Pu^{+4} + H_2O = Pu(OH)^{+3} + H^+$	-0.50	-1.17
4102	$Pu^{+4} + 2H_2O = Pu(OH)_2^{+2} + 2H^+$	-2.32	-3.42
4103	$Pu^{+4} + 3H_2O = Pu(OH)_3^{+} + 3H^+$	-5.28	-6.60
4104	$Pu^{+4} + 4H_2O = Pu(OH)_4^{0} + 4H^+$	-9.52	-10.84
4105	$Pu^{+4} + 5H_2O = Pu(OH)_5^{-} + 5H^+$	-14.98	-16.08
00100	$H_2O = H^+ + OH^-$	-14.00	-13.78

Sorption data are digitized from Fig. 1(a) in Sanchez et al. (1985)
1×10^{-4} m Pu^{+4} ; 0.1 m $NaNO_3$; A_{sp} = 51.8 m^2/g ; no CO_2

	pH	% sorbed	U sorbed (m/L)
1 hr contact	2.44	26.92	2.69×10^{-12}
	2.83	37.91	3.79×10^{-12}
	3.15	50.50	5.05×10^{-12}
	2.53	54.26	5.43×10^{-12}
	3.96	80.42	8.04×10^{-12}
	4.75	96.38	9.64×10^{-12}
	6.36	99.48	9.95×10^{-12}
	7.94	99.41	9.94×10^{-12}
	8.50	99.99	9.99×10^{-12}
	8.97	99.99	9.99×10^{-12}
	9.21	99.99	9.99×10^{-12}
	9.46	99.99	9.99×10^{-12}
24 hr contact	2.41	25.56	2.56×10^{-12}
	2.57	34.88	3.49×10^{-12}
	2.93	45.89	4.59×10^{-12}
	3.15	45.19	4.52×10^{-12}
	3.99	81.59	8.16×10^{-12}
	6.13	96.94	9.69×10^{-12}
	8.11	99.99	9.99×10^{-12}
	8.91	99.99	9.99×10^{-12}
96 hr contact	2.26	21.04	2.10×10^{-12}
	2.39	29.97	3.00×10^{-12}
	3.01	40.16	4.62×10^{-12}
	3.84	73.97	7.40×10^{-12}
	5.81	99.99	9.99×10^{-12}
	6.86	99.99	9.99×10^{-12}
	7.46	99.99	9.99×10^{-12}

Sanchez et al. (1985) indicate that equilibrium is achieved in one hour. This is much less than that reported for other actinides, so only the longer experiments were used in fitting exercise. This gives 15 data points

DLM:

Initial FITEQL runs did not converge. Gradually increased estimated error in an effort to relax convergence criteria. This does not have a large effect on log K value for binding constants, but it does affect the goodness-of-fit parameter. The effect on log K ~0.1 or less (observed). However, the standard deviation reported by FITEQL is larger, in the range of 0.2-0.5. Prior to increasing estimated error, the runs would converge towards a value, but not quite meet convergence criteria. This gave an idea what value was being approached and what might be valid. Slow convergence suggests an ill-conditioned system using the conceptual model. 2/4/93 DW

The sorption data is heavily weighted towards complete sorption. Because the sorption edge is of most interest due to rapid changes in % sorbed over a narrow pH range, we first dropped the 100% sorbed data at high pH. This improved the convergence characteristics of the model, and again, the effect on calculated/estimated log K is fairly small (±0.1-0.2). This was done only for $XOPu(OH)_3^0$; ~~$XOPu(OH)_4^0$~~; $XOH_2Pu(OH)_5^0$ 2/4/93 DW

Given this difficulty in getting the DLM to converge under these conditions, the resultant log K values should be viewed with skepticism and used with caution. This is especially true given the relatively large standard deviations calculated for the binding constants.

DLM Constants: 1×10^{-11} M $Pu(NO_3)_4$; No CO_2; 0.1 M $NaNO_3$

Reaction	Log K	V_y (SOS/DF)	σ_{LogK}	Error Used *
$XO\text{-}Pu^{+3}$	14.62	0.93	0.30	
$XOH\text{-}PuOH^{+2}$ 2/4/93 DW	8.13	4.68	0.15	
$XO\text{-}Pu(OH)_2^+$	2.47	0.97	0.41	
$XOH\text{-}Pu(OH)_2^{+2}$	8.13	4.68	0.15	
$XO\text{-}Pu(OH)_3^0$	-5.35	0.14	0.55	
$XOH\text{-}Pu(OH)_3^+$	2.47	0.97	0.41	
$XO\text{-}Pu(OH)_4^-$	-11.98	0.13	0.54	
$XOH\text{-}Pu(OH)_4^0$	-5.35	0.14	0.55	
$XOH_2\text{-}Pu(OH)_4^+$	2.47	0.97	0.41	
$XOH\text{-}Pu(OH)_5^-$	-11.98	0.13	0.54	
$XOH_2\text{-}Pu(OH)_5^0$	-5.35	0.14	0.55	

Errors Used:	$S_{T,rel}$	$S_{T,abs}$	$S_{X,rel}$	$S_{X,abs}$
$XO\text{-}Pu^{+3}$	0.35	3.5×10^{-12}	0.05	0
$XOPuOH^{+2}$; $XOH\text{-}Pu(OH)_2^{+2}$	0.20	1.0×10^{-12}	0.10	0
$XO\text{-}Pu(OH)_2^+$; $XOH\text{-}Pu(OH)_3^+$; $XOH_2\text{-}Pu(OH)_4^+$	0.03	5.0×10^{-12}	0.10	0
$XO\text{-}Pu(OH)_3^0$; $XOH\text{-}Pu(OH)_4^0$; $XOH_2Pu(OH)_5^0$	0.05	5.0×10^{-12}	0.10	0
$XO\text{-}Pu(OH)_4^-$; $XOH\text{-}Pu(OH)_5^-$	0.03	5.0×10^{-12}	0.10	0

3/2/93

DR

Back to Pu^{+4} - sorption

Conditional Equilibrium Constants have been determined for DLM, CCM, TLM models at I = 0.1 m and using the data of Sanchez et al. (1985) for Pu(IV)-Goethite sorption. Both data for $Pu(IV)_T = 1 \times 10^{-11}$ M and $Pu(IV)_T = 1 \times 10^{-10}$ M have been fit using fitting program FITEQL

Results: I = 0.1 m, $Pu(IV)_T = 10^{-11}$ M

10^{-11} M	DLM			CCM			TLM		
Surface Species	LogK	SOS/DF	σ_{logK} (std. dev.)	LogK	SOS/DF	σ_{logK}	LogK	SOS/DF	σ_{logK}
XO-Pu^{+3}	14.62	0.93	0.30	17.17	8.71	0.11	-3.84	15.03	0.14
XOPuOH^{+2}	8.13	4.68	0.15	9.71	3.47	0.18	-5.96	14.24	0.11
XO-$Pu(OH)_2^+$	2.47	0.97	0.41	2.38	6.57	0.12	-8.22	12.49	0.09
XOH-$Pu(OH)_2^{+2}$	8.13	4.68	0.15	9.71	3.47	0.18	-0.10	5.59	0.09
XO-$Pu(OH)_3^0$	-5.35	0.14	0.55	-5.74	1.50	0.15	-10.86	10.42	0.10
XOH-$Pu(OH)_3^+$	2.47	0.97	0.41	2.38	6.57	0.12	-2.73	3.37	0.10
XO-$Pu(OH)_4^-$	-11.98	0.13	0.54	-12.61	1.51	0.19	-13.23	1.38	0.20
XOH-$Pu(OH)_4^0$	-5.35	0.14	0.55	-5.74	1.50	0.15	n.c.	—	—
XOH_2-$Pu(OH)_4^+$	2.47	0.97	0.41	2.38	6.57	0.12	3.17	5.11	0.12
XOH-$Pu(OH)_5^-$	-11.98	0.13	0.54	-12.61	1.51	0.19	n.c.	—	—
XOH_2-$Pu(OH)_5^0$	-5.35	0.14	0.55	-5.74	1.50	0.15	n.c.	—	—

n.c. = no convergence

3/2/93 (cont'd)

$Pu(IV)_T = 10^{-10}$ M ; I = 0.1 M $NaNO_3$

	DLM			CCM			TLM		
Surface Species	LogK	SOS/DF	σ_{logK}	LogK	SOS/DF	σ_{logK}	LogK	SOS/DF	σ_{logK}
XO-Pu^{+3}	14.58	7.17	0.10	16.38	2.52	0.12	-4.47	14.06	0.44
XO-PuOH^{+2}	7.80	14.10	0.04	8.83	1.87	0.13	-6.29	13.67	0.24
XO-$Pu(OH)_2^+$	1.00	1.99	0.13	1.23	1.35	0.13	-8.23	10.69	0.12
XOH-$Pu(OH)_2^{+2}$	7.80	14.10	0.04	8.83	1.87	0.13	-0.11	10.75	0.12
XO-$Pu(OH)_3^0$	-6.20	1.27	0.16	-6.41	1.05	0.14	-11.06	5.09	0.10
XOH-$Pu(OH)_3^+$	1.00	1.99	0.13	1.23	1.35	0.13	-2.92	5.14	0.10
XO-$Pu(OH)_4^-$	-13.45	1.58	0.17	-14.05	0.46	0.14	-14.50	1.05	0.14
XOH-$Pu(OH)_4^0$	-6.20	1.27	0.16	-6.41	1.05	0.14	-6.33	1.08	0.14
XOH_2-$Pu(OH)_4^+$	1.00	1.99	0.13	1.23	1.35	0.13	+1.83	1.11	0.13
XOH-$Pu(OH)_5^-$	-13.45	1.58	0.17	-14.05	0.46	0.14	-10.17	1.76	0.17
XOH_2-$Pu(OH)_5^0$	-6.20	1.27	0.16	-6.41	1.05	0.14	-2.02	1.73	0.17

Note: In general, the 10^{-10} M data set was much easier to reach convergence, given the constraints of a single, mononuclear surface species. This seems to be due to the fact that the 10^{-11} M data set includes a number of points where %sorption ≈ 100%. The smaller 10^{-10} M data set did not include these points, allowing more "flexibility" in trying to fit the data.

3/2/93 (cont'd)

Once $\log k$ + $\sigma_{\log k}$ values were obtained for two concentrations, it is possible to use the weighting scheme proposed by Dzombak + Morel (1990) to develop a single data set.

$\log k = \sum_i w_i (\log k)_i$ where the weighting factor w_i is:

$$w_i = \frac{(1/\sigma_{\log k})_i}{\sum_i (1/\sigma_{\log k})_i}$$

Therefore:

Surface Species	DLM 10^{-10} + 10^{-11} = Log k	CCM 10^{-10} + 10^{-11} = Log k	TLM 10^{-10} + 10^{-11} = Log k
XO-Pu^{+3}	$(0.24)^{0.75}(14.58) + (0.25)(14.62) = 14.59$	$(.48)(16.38) + (.52)(17.17) = 16.79$	$(.24)(-4.47) + (.76)(-3.84) = -3.99$
XO-$PuOH^{+2}$	$(0.79)(7.86) + (.21)(8.13) = 7.87$	$(.58)(8.83) + (.42)(9.7) = 9.20$	$(.31)(-6.29) + (.69)(-5.46) = -6.06$
XO-$Pu(OH)_2^+$	$(0.76)(1.00) + (.24)(2.47) = 1.35$	$(.48)(1.23) + (.52)(2.38) = 1.83$	$(.42)(-8.23) + (.58)(-8.22) = -8.22$
XOH-$Pu(OH)_2^{+2}$	$(0.79)(7.86) + (.21)(8.13) = 7.87$	$(.58)(8.83) + (.42)(17.17) = 9.20$	$(.42)(-0.11) + (.58)(-0.10) = -0.10$
XO-$Pu(OH)_3^0$	$(0.77)(-6.20) + (0.23)(-5.35) = -6.01$	$(.52)(-6.41) + (.48)(-5.74) = -6.09$	$(.5)(-11.04) + (.5)(-10.86) = -10.96$
XOH-$Pu(OH)_3^+$	$(0.76)(1.00) + (0.24)(2.47) = 1.35$	$(.48)(1.23) + (.52)(2.38) = 1.83$	$(.5)(-2.42) + (.5)(-2.73) = -2.83$
XO-$Pu(OH)_4^-$	$(0.76)(-13.45) + (0.24)(-11.98) = -13.10$	$(.58)(-14.05) + (.42)(-12.61) = -13.44$	$(.59)(-14.56) + (.41)(-13.23) = -13.98$
XOH-$Pu(OH)_4^0$	$(0.77)(-6.20) + (0.23)(-5.35) = -6.01$	$(.52)(-6.41) + (.48)(-5.74) = -6.09$	-6.33 *
XOH_2-$Pu(OH)_4^+$	$(0.76)(1.00) + (0.24)(2.47) = 1.35$	$(.48)(1.23) + (.52)(2.38) = 1.83$	$(.48)(1.83) + (.52)(3.17) = 2.53$
XOH-$Pu(OH)_5^-$	$(0.76)(-13.45) + (0.24)(-11.98) = -13.10$	$(.58)(-14.05) + (.42)(-12.61) = -13.44$	-10.17 *
XOH_2-$Pu(OH)_5^0$	$(0.77)(-6.20) + (0.23)(-5.35) = -6.01$	$(.52)(-6.41) + (.48)(-5.74) = -6.09$	-2.02 *

* 10^{-11} M did not converge

Note: A spreadsheet program has been developed to calculated the weighted avg. log k 95% confidence limits based on Dzombak and Morel (1990). See pp. 95 for sample hand calculations. DJ 8/12/94

3/2/93 (cont'd)

Note: These equilibrium constants are conditional constants as determined by FITEQL, and valid for I = 0.1 M. Prior to use in MINTEQA2, they need to be "retrofitted" or corrected to I = 0 M. This was done using Davies Eqn. and Table 2.13 from Dzombak + Morel (1990):

Information potentially subject to copyright protection was redacted from this location. The redacted material (Table 2.13: Activity coefficients...) is from the following reference.

Dzombak, D.A. and F.M.M. Morel. "Surface Complexation Modeling: Hydrous Ferric Oxide." New York City, New York: John Wiley and Sons. 1990.

	DLM I=0.1	DLM I=0	CCM I=0.1	CCM I=0	TLM I=0.1	TLM I=0
		DJ 3/8/93		DJ 3/8/93		DJ 3/8/93
XO-Pu^{+3}	14.59	16.24 ~~15.95~~	16.79	18.44 ~~17.45~~	-3.99	-2.34 ~~-3.53~~
XO-$PuOH^{+2}$	7.87	9.41 ~~8.97~~	9.20	10.74 ~~10.30~~	-6.06	-4.52 ~~-4.96~~
XO-$Pu(OH)_2^+$	1.35	2.78 ~~2.67~~	1.83	3.26 ~~2.82~~	-8.22	-6.79 ~~-6.90~~
XOH-$Pu(OH)_2^{+2}$	7.87	9.41 ~~8.97~~	9.20	10.74 ~~10.38~~	-0.10	1.44 ~~1.00~~
XO-$Pu(OH)_3^0$	-6.01	-4.69 ~~-4.69~~	-6.09	-4.77 ~~-4.77~~	-10.96	-9.64 ~~-9.64~~
XOH-$Pu(OH)_3^+$	1.35	2.78 ~~2.67~~	1.83	3.26 ~~2.82~~	-2.83	-1.40 ~~-1.51~~
XO-$Pu(OH)_4^-$	-13.10	-11.89 ~~-12.06~~	-13.44	-12.23 ~~-12.34~~	-13.98	-12.77 ~~-12.88~~
XOH-$Pu(OH)_4^0$	-6.01	-4.69 ~~-4.69~~	-6.09	-4.77 ~~-4.77~~	-6.33	-5.01 ~~-5.01~~
XOH_2-$Pu(OH)_4^+$	1.35	2.78 ~~2.67~~	1.83	3.26 ~~2.82~~	2.53	3.96 ~~3.85~~
XOH-$Pu(OH)_5^-$	-13.10	-11.89 ~~-12.06~~	-13.44	-12.23 ~~-12.34~~	-10.17	-8.96 ~~-9.07~~
XOH_2-$Pu(OH)_5^0$	-6.01	-4.69 ~~-4.69~~	-6.09	-4.77 ~~-4.77~~	-2.02	-0.70 ~~-0.70~~

Note: changes in corrected values because should not have included surface species in original ionic strength calculations. DJ 3/8/93

3/8/93 (KN)

Correcting Uranium Logk values to I=0 m (Pg. 18)

$Logk^{\circ} = Logk^{0.1M} + \log\gamma_{prod} - \log\gamma_{reactants}$

	DLM		CCM		TLM	
	I=0.1 M	I=0 M	I=0.1 M	I=0M	I=0.1 m	I=0m
$XOHUO_2^{+}$	0.95	1.28	0.87	1.20	-4.12	-3.79
$XOHUO_2^{+2}$	8.84	9.38	8.74	9.18	4.62	5.06
$XOHUO_2OH^{\circ}$	-6.96	-6.74	-6.98	-6.76	-9.56	-9.34
$XOHUO_2OH^{+}$	0.95	1.28	0.87	1.20	-1.21	-0.88
$XOHUO_2(OH)_2^{-}$	-14.95	-14.84	-14.89	-14.78	-14.97	-14.86
$XOHUO_2(OH)_2^{\circ}$	-6.96	-6.74	-6.98	-6.76	-6.89	-6.67
$XOH_2UO_2(OH)_2^{+}$	0.95	1.28	0.87	1.20	1.46	1.79
$XOHUO_2(OH)_3^{-}$	-14.95	-14.84	-14.89	-14.78	-12.61	-12.50
$XOH_2UO_2(OH)_3^{+}$	-6.96	-6.74	-6.98	-6.76	-4.53	-4.31
$XOH\text{-}UO_2(OH)_4^{-2}$	-22.79	-22.94	-22.79	-22.79	-17.99	-17.99
$XOH_2UO_2(OH)_4^{-}$	-14.95	-14.84	-14.89	-14.78	-10.22	-10.11

For CO_2-U(VI) complexation reactions:

	Log K I=0.1 m	Log K I=0 m
$XOH + UO_2^{+2} + CO_2 + H_2O = XOH\cdot UO_2CO_3^{\circ} + 2H^{+}$	-3.27	-3.05
$XOH + UO_2^{+2} + 2CO_2 + 2H_2O = XOH_2\cdot UO_2(CO_3)_2^{-} + 3H^{+}$	-7.78	-7.67
$XOH + UO_2^{+2} + 3CO_2 + 3H_2O = XOH_2\cdot UO_2(CO_3)_3^{-3} + 5H^{+}$	-20.43	-20.54
$XOH + 2UO_2^{+2} + CO_2 + 4H_2O = XOH_2(UO_2)_2CO_3(OH)_3^{\circ} + 4H^{+}$	-7.62	-7.18
$XOH + UO_2^{+2} + 4H_2O = XOH\cdot UO_2(OH)_4^{-2} + 4H^{+}$	-23.27	-23.27

3/8/93 (cont'd)

Corrected to CO_3^{-2} using

$CO_3^{-2} + 2H^{+} = CO_2 + H_2O$ $\quad Logk = 18.16$

	I = 0
$XOH\cdot UO_2CO_3^{-}$	+15.11
$XOH_2\cdot UO_2(CO_3)_2^{-}$	+28.65
$XOH_2\cdot UO_2(CO_3)_3^{-3}$	+33.94
$XOH_2(UO_2)_2CO_3(OH)_3$	+10.98
$XOH\cdot UO_2(OH)_4^{-2}$	-23.27

3/17/93

(DEV)

The work of Mesuere (1992; Ph.D. Diss.), site density for goethite is less than the 10 sites/nm² proposed by Hayes et al. (1991). Lower values are also proposed for ferrihydrite in the extensive compilation in 'Surface Complexation Modeling' by Dzombak + Morel (1990).

— Therefore, we have used FITEQL to reinterpret the potentiometric titration data used by Hayes et al. (1991), assuming a lower value for site density (N_s). The titration data is tabulated in Hayes et al. (1990), NUREG/CR-5547. This is a more complete version of the results presented in Hayes et al. (1991). The value chosen for N_s = 2.3 sites/nm². This is the value of Dzombak + Morel and is in the range (0.5-16) of Mesuere (1992).

— Five different ionic strengths were modeled for $NaNO_3$ background electrolyte: 0.005; 0.0095; 0.0275; 0.054; 0.087 (moles/liter). The DLM + TLM models are theoretically applicable at any ionic strength, and only one set of parameters is necessary. The CCM, however, is strictly speaking, valid only for one ionic strength, and the parameters must be redetermined for each new set of experimental conditions:

DLM (N_s = 2.3 sites/nm²)

I (M)	$\log K_+$	$\log K_-$	SOS/DF	$\sigma_{\log K_+}$	$\sigma_{\log K_-}$
0.005	NC	NC	NC	NC	NC
0.0095	8.50	-8.86	173.2	3.974×10^{-2}	4.844×10^{-2}
0.0275	8.00	-9.08	65.0	1.758×10^{-2}	2.379×10^{-2}
0.054	7.70	-9.24	36.5	1.081×10^{-2}	1.621×10^{-2}
0.087	7.49	-9.37	24.8	8.544×10^{-3}	1.353×10^{-2}

Using weighting method of Dzombak + Morel (1990) [see pg. 26], the values are

$\log K_+ = (.086)(8.5) + (.195)(8.00) + (.318)(7.70) + (.401)(7.49) = \boxed{7.74}$ DLM

$\log K_- = (.164)(-8.86) + (.209)(-9.08) + (.310)(-9.24) + (.377)(-9.37) = \boxed{-9.22}$

CCM $C_1 = 1.0$ F/m²

$N_s = 2.3$ sites/nm²

I (m)	$\log K_+$	$\log K_-$	SOS/DF	$\sigma_{\log K_+}$	$\sigma_{\log K_-}$
0.005	6.95	-10.22	2.58	6.106×10^{-3}	1.173×10^{-2}
0.0095	7.09	-10.07	3.87	6.934×10^{-3}	1.179×10^{-2}
0.0275	7.29	-9.76	4.55	7.982×10^{-3}	1.259×10^{-2}
0.054	7.46	-9.51	6.21	9.067×10^{-3}	1.358×10^{-2}
0.087	7.55	-9.36	6.52	1.014×10^{-2}	1.463×10^{-2}

A plot of $\log K$ vs. $\log(I)$ allows easy extrapolation to other ionic strengths (see attached graph, next page).

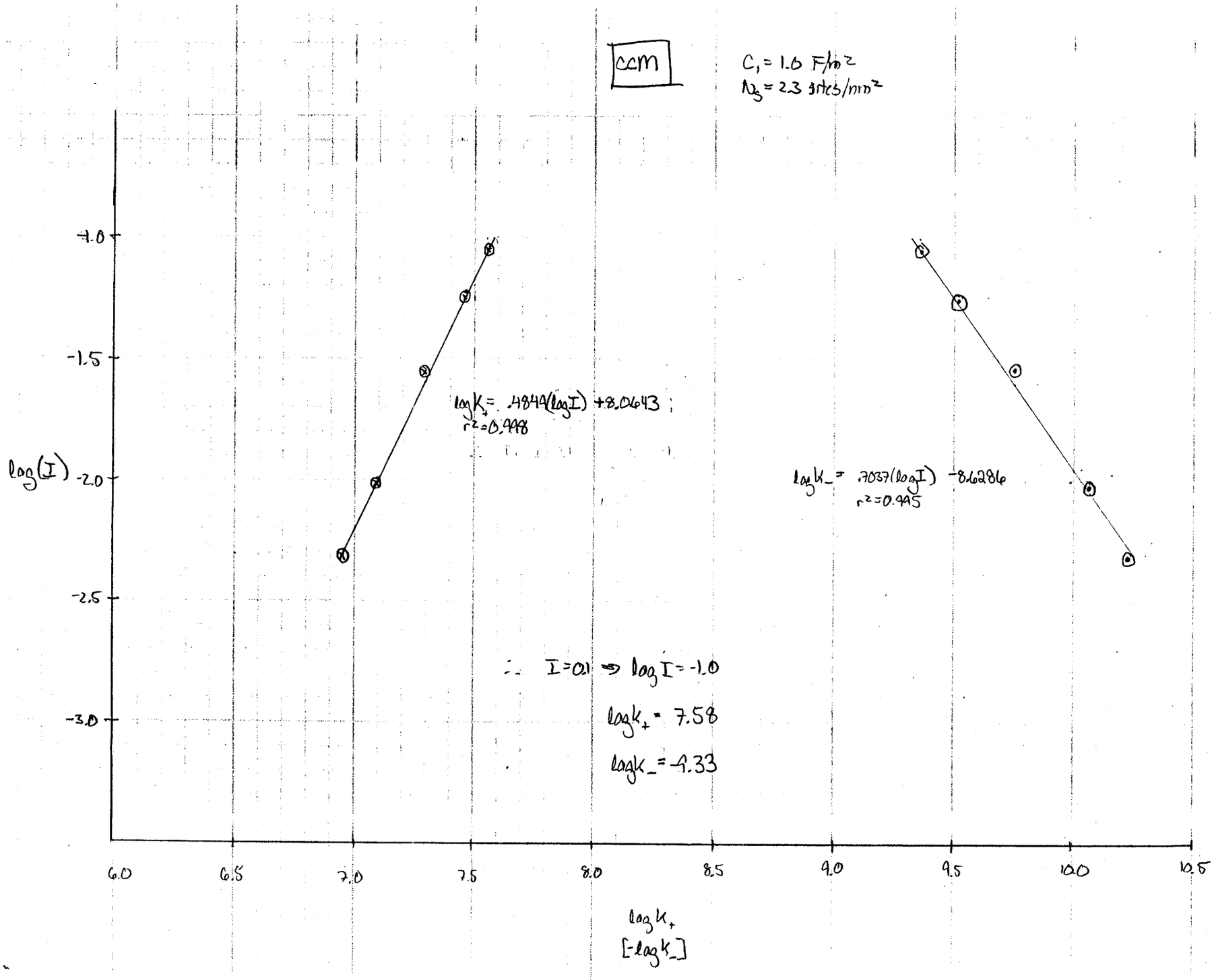
A simple L.R. results in

$\log K_+ = .4849(\log I) + 8.0643$ $\quad r^2 = 0.998$

$\log K_- = .7037(\log I) - 8.6286$ $\quad r^2 = 0.995$

∴ for I = 0.1 M (common to most radionuclide sorption experiments)

$\log K_+ = 7.58$
$\log K_- = -9.33$ ccm


ccm
$C_1 = 1.6$ F/m²
$N_s = 2.3$ sites/nm²
$\log K_+ = .4849(\log I) + 8.0643$
$r^2 = 0.998$
$\log K_- = .7037(\log I) - 8.6286$
$r^2 = 0.995$
$\therefore I = 0.1 \Rightarrow \log I = -1.0$
$\log k_+ = 7.58$
$\log k_- = 4.33$
log(I)
-1.0
-1.5
-2.0
-2.5
-3.0
6.0
6.5
7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5
$\log k_+$
$[-\log k_-]$

TLM $C_1 = 0.8$ F/m² $C_2 = 0.2$ F/m² $\log k_+ = 5.0$ $\log k_- = -10.9$ } from Smith and Jenne (1991)

I (m)	$\log k_{Na^+}$	$\log k_{NO_3^-}$	SOS/DF	$\sigma_{\log k_{Na^+}}$	$\sigma_{\log k_{NO_3^-}}$
0.005	-9.26	7.94	2.85	6.154×10^{-3}	1.253×10^{-2}
0.0095	-9.10	8.09	3.34	6.977×10^{-3}	1.239×10^{-2}
0.0275	-8.78	8.29	4.57	8.006×10^{-3}	1.297×10^{-2}
0.054	-8.52	8.46	6.22	9.085×10^{-3}	1.384×10^{-2}
0.087	-8.37	8.55	6.52	1.015×10^{-2}	1.485×10^{-2}

$\log k_{Na^+} = (.25)(-9.26) + (.22)(-9.10) + (.20)(-8.78) + (.17)(-8.52) + (.16)(-8.37) =$ **-8.86** TLM

$\log k_{NO_3^-} = (.21)(7.94) + (.21)(8.09) + (.21)(8.29) + (.19)(8.46) + (.18)(8.55) =$ **8.25**

These values for $\log k_+$, $\log k_-$, $\log k_{Na^+}$, $\log k_{NO_3^-}$ are then substituted in the FITEQL input files for uranium

K:\TURNER\FITEQL\INPUT\CCM\URANIUM*.CDZ (DZ = Dzombak + Morel)
K:\TURNER\FITEQL\INPUT\DLM\URANIUM*.DDZ
K:\TURNER\FITEQL\INPUT\TLM\URANIUM*.TDZ

The results are given on the next page: (Note: these are conditional constants for I=0.1 m; see pgs. 27-28)

U(VI) sorption on goethite; no CO_2; 1.05×10^{-6} M $U(VI)_T$; N_s=2.3 sites/nm^2

3/18/93
(DJ)

Log K

	CCM			DLM					
	Log K	SOS/DF	$\sigma_{\log K}$	Log K	SOS/DF	$\sigma_{\log K}$	Log K	SOS/DF	$\sigma_{\log K}$
$XOUO_2^+$	1.66	7.17	.042	1.68	7.74	.042	-2.31	17.06	.065
$XOHUO_2^{+2}$	9.50	9.18	.044	9.40	11.47	.044	6.15	15.06	.092
$XOUO_2OH^0$	-6.19	4.38	.041	-6.09 (3/17/93 DJ)	3.76	.042	-8.20	11.85	.045
$XOHUO_2OH^+$	1.66	7.17	.042	1.68	7.74	.042	-0.26	12.53	.056
$XOUO_2(OH)_2^-$	-14.08	1.98	.043	-13.95 (3/17/93 DJ)	1.16	.045	-13.86	2.43	.053
$XOHUO_2(OH)_2^0$	-6.19	4.38	.041	-6.09	3.76	.042	-6.26	4.46	.041
$XOH_2UO_2(OH)_2^+$	1.66	7.17	.042	1.68	7.74	.042	1.72	7.09	.052
$XOHUO_2(OH)_3^-$	-14.08	1.98	.043	-13.95	1.16	.045	-12.13	0.48	.059
$XOH_2UO_2(OH)_3^0$	-6.19	4.38	.041	-6.09	3.76	.042	-4.53	0.47	.048
$XOHUO_2(OH)_4^{-2}$	-21.96	1.06	.047	-21.79	0.41	.051	-17.56	0.32	.091
$XOH_2UO_2(OH)_4^-$	-14.08	1.98	.043	-13.95	1.16	.045	-10.37	0.20	.065

- In most cases, it is worth noting that the "goodness-of-fit" measure SOS/DF is lower for these values compared to pg. 18. This indicates that the fit is "better" assuming a lower value for N_s, in agreement with observations of Mesuere (1992).

- Also note that calculated log K values are generally higher to compensate for the reduced number of available sites.

Corrected for I=0

	CCM		DLM		TLM	
	I=0.1	I=0	I=0.1	I=0	I=0.1	I=0
$XOUO_2^+$	1.66	1.99	1.68	2.01	-2.31	-1.98
$XOHUO_2^{+2}$	9.50	9.94	9.40	9.84	6.15	6.59
$XOUO_2OH^0$	-6.19	-5.97	-6.09	-5.87	-8.20	-7.98
$XOHUO_2OH^+$	1.66	1.99	1.68	2.01	-0.26	+0.07
$XOUO_2(OH)_2^-$	-14.08	-13.97	-13.95	-13.84	-13.86	-13.75
$XOHUO_2(OH)_2^0$	-6.19	-5.97	-6.09	-5.87	-6.26	-6.04
$XOH_2UO_2(OH)_2^+$	1.66	1.99	1.68	2.01	1.72	2.05
$XOHUO_2(OH)_3^-$	-14.08	-13.97	-13.95	-13.84	-12.13	-12.02
$XOH_2UO_2(OH)_3^0$	-6.19	-5.97	-6.09	-5.87	-4.53	-4.31
$XOHUO_2(OH)_4^{-2}$	-21.96	-21.96	-21.79	-21.79	-17.56	-17.56
$XOH_2UO_2(OH)_4^-$	-14.08	-13.97	-13.95	-13.84	-10.37	-10.26

3/19/93 DR

Continue work of reexamining U(VI)-goethite sorption data assuming a smaller site density (N_s = 2.3 sites/nm^2)

This work considers U(VI)-H_2O-CO_2 system with $p(CO_2) = 10^{-3.48}$ atm. Data is from Tripathi (1984),

$U(VI)_T = 1.05 \times 10^{-6}$ M
N_s = 2.3 sites/nm^2
C_s = 0.410 g FeOOH/L
A_{sp} = 50 m^2/g
I = 0.1 M $NaNO_3$

log K - DLM

		log k	SOS/DF	$\sigma_{log k}$	Extrapolate to I=0
reaction written w/ CO_2	$XOH \cdot UO_2CO_3^0$	-2.44	3.26	0.023	-2.22
	$XOH_2 \cdot UO_2(CO_3)_2^-$	-6.81	1.14	0.027	-6.70
	$XOH_2 \cdot UO_2(CO_3)_3^{-3}$	-19.23	0.83	0.035	-19.34
	$XOH_2 \cdot (UO_2)_2CO_3(OH)_3^0$	-6.81	3.87	0.031	-6.37
	$XOH \cdot UO_2(OH)_4^{-2}$	-22.21	32.51	0.045	-22.21

Extrapolation to I=0 from I=0.1 using method outlined on pg. 27-28

Converting $CO_2 + H_2O = CO_3^{-2} + 2H^+$

	I=0.1 M	I=0 M
$XOH \cdot UO_2CO_3^0$	15.72	15.94
$XOH_2 \cdot UO_2(CO_3)_2^-$	29.51	29.62
$XOH_2 \cdot UO_2(CO_3)_3^{-3}$	35.25	35.14
$XOH_2(UO_2)_2CO_3(OH)_3^0$	11.35	11.79
$XOH \cdot UO_2(OH)_4^{-2}$	-22.21	-22.21

4/1/93 DR

Re-analyze titration data of Hayes et al. (1990). Some mistakes found in FITEQL input files

i.e. DLM - C_1 changed from 1.0 to 0.8 F/m^2
- Also, ionic strength incorrectly entered as 0.005 in all files
All files - dissociation constant of water not corrected properly for ionic strength effects

Input files corrected; Following results supercede those reported on pp. 30-32

DLM N_s = 2.3 sites/nm^2

I(M)	log K_+	log K_-	SOS/DF	$\sigma_{log K_+}$	$\sigma_{log K_-}$
0.005	NC	NC	NC	NC	NC
0.0095	8.44 ~~8.50~~ 4/1/93	-8.96 ~~-8.86~~ 4/1/93	164.0	3.38×10^{-2}	4.25×10^{-2}
0.0275	7.96 ~~8.02~~	-9.16 ~~-9.08~~	59.2	1.62×10^{-2}	2.32×10^{-2}
0.054	7.67 ~~7.72~~	-9.32 ~~-9.24~~	32.2	1.03×10^{-2}	1.66×10^{-2}
0.087	7.47 ~~7.49~~	-9.45 ~~-9.37~~	21.7	8.34×10^{-3}	1.40×10^{-2}

weighted values:

$\log K_+ = (.096)(8.44) + (.200)(7.96) + (.316)(7.67) + (.389)(7.47) =$ **7.72**

$\log K_- = (.114)(-8.96) + (.217)(-9.16) + (.304)(-9.32) + (.360)(-9.45) =$ **-9.29**

CCM C_1 = 1.00 F/m^2
N_s = 2.3 sites/nm^2

I(M)	$\log K_+$	$\log K_-$	SOS/DF	$\sigma_{log K_+}$	$\sigma_{log K_-}$
0.005	6.95	-10.22	2.73	6.11×10^{-3}	1.17×10^{-2}
0.0095	7.08	-10.09	3.05	6.92×10^{-3}	1.20×10^{-2}
0.0275	7.28	-9.80	3.54	7.90×10^{-3}	1.30×10^{-2}
0.054	7.43	-9.58	3.83	8.81×10^{-3}	1.40×10^{-2}
0.087	7.52	-9.45	3.66	9.16×10^{-3}	1.49×10^{-2}

Linear Regression (see next page):

$\log K_+ = 0.4607 (\log I) + 8.0085$

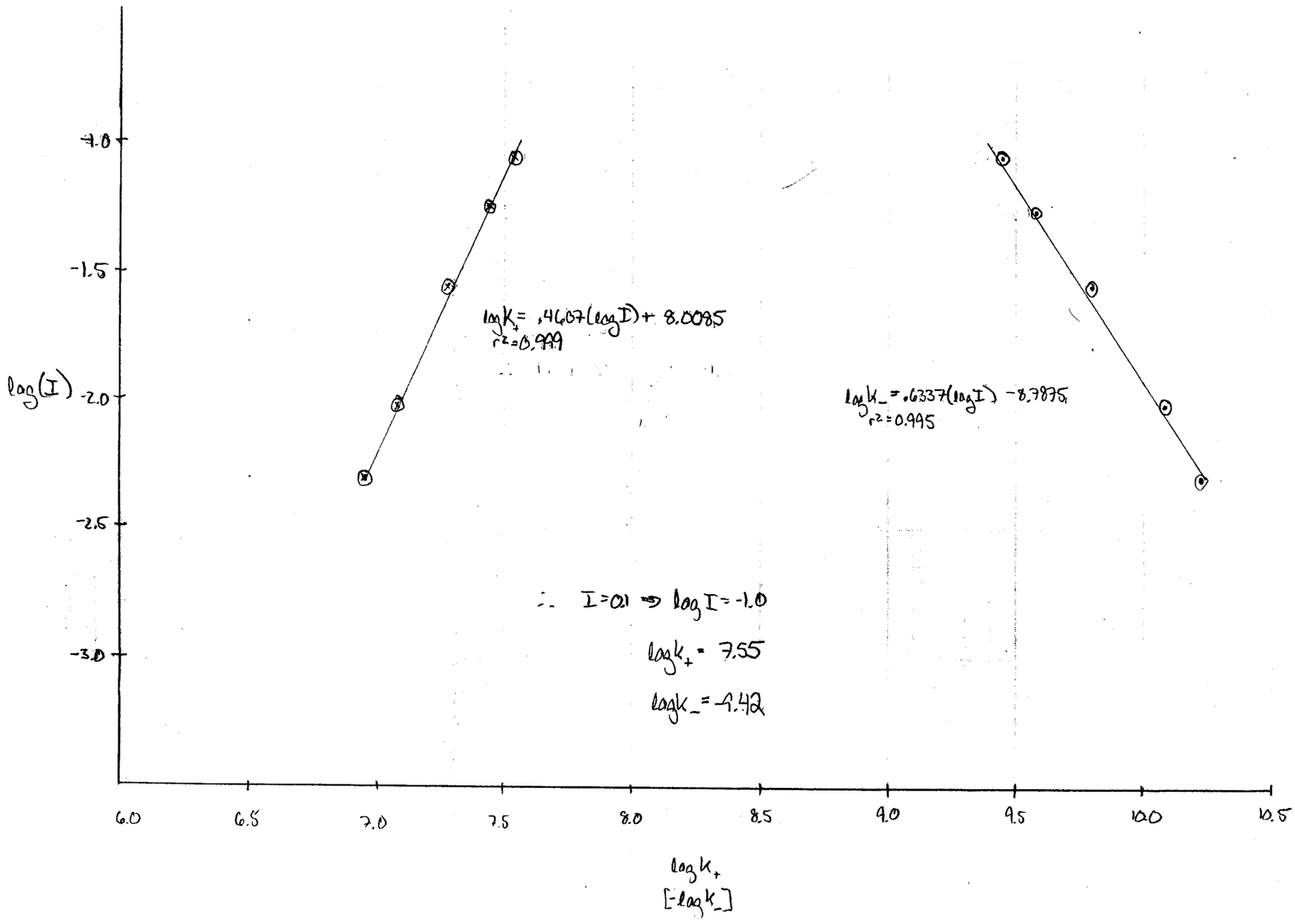
$\log K_- = .6337 (\log I) - 8.7875$

@ I=0.1
$\log K_+ = 7.55$
$\log K_- = -9.42$

ccm

$C_1 = 1.0$ F/m²

$N_s = 2.3$ sites/nm²



$\therefore$ $I = 0.1 \Rightarrow \log I = -1.0$

$\log k_+ = 7.55$

$\log k_- = -1.42$

Note: 4/13/93 (LD)

discovered one more error in input files for TLM only

TLM $C_1 = 0.8$ F/m² $\quad \log k_+ = 5.0$

$C_2 = 0.2$ F/m² $\quad \log k_- = -10.9$

I (m)	$\log K_{Na^+}$	$\log k_{NO_3^-}$	SOS/DF	$\sigma_{\log k_{Na^+}}$	$\sigma_{\log k_{NO_3^-}}$
0.005	-7.71 ~~-8.01~~	9.51 ~~8.21~~	14.4	1.37×10^{-2}	7.01×10^{-3}
0.0095	-7.81 ~~-8.83~~	9.41 ~~8.39~~	16.9	1.47×10^{-2}	8.51×10^{-3}
0.0275	-7.82 ~~-8.38~~	9.28 ~~8.72~~	11.9	1.95×10^{-2}	1.35×10^{-2}
0.054	-7.54 ~~-7.86~~	9.41 ~~9.14~~	8.1	3.72×10^{-2}	3.11×10^{-2}
0.087	-7.20 ~~-7.86~~	9.74 ~~9.70~~	6.1	1.28×10^{-1}	1.16×10^{-1}

weighting

$\log K_{Na^+} = (.321)(-8.01) + (.299)(-8.83) + (.226)(-8.38) + (.118)(-7.86) + (.036)(-7.86) =$ ~~-8.02~~ -7.73

$\log k_{NO_3^-} = (.380)(8.21) + (.313)(8.39) + (.198)(8.72) + (.086)(9.14) + (.023)(9.70) =$ 8.48

9.51 9.41 9.28 9.41 9.74 9.43

Of course, these changes will filter through the uranium data reported on pp. 34-36:

	CCM			DLM			TLM		
SJT 4/13/93	log k	SOS/DF	$\sigma_{\log k}$	log k	SOS/DF	$\sigma_{\log k}$	log k	SOS/DF	$\sigma_{\log k}$
$XO\cdot UO_2^{+2}$	1.63	7.26	.042	1.66	7.81	.042	~~-2.48~~ -2.76	~~19.18~~ 17.93	~~.046~~ .061
$XOH\cdot UO_2^{+2}$	9.46	9.31	.044	9.37	11.56	.044	~~6.42~~ 6.30	~~15.09~~ 13.36	~~.041~~ .041
$XO\cdot UO_2OH^0$	-6.20	4.36	.041	-6.10	3.75	.042	~~-8.34~~ -8.54	~~12.04~~ 13.66	~~.045~~ .046
$XOH\cdot UO_2OH^+$	1.63	7.26	.042	1.66	7.81	.042	~~-2.62~~ -0.26 -2.03 4/13/93 LD	~~12.64~~ 12.76	~~.052~~ .052
$XO\cdot UO_2(OH)_2^-$	-14.08	1.89	.043	-13.95	1.11	.046	~~-13.95~~ -14.04	~~2.71~~ 3.90	~~.053~~ .052
$XOH\cdot UO_2(OH)_2^0$	-6.20	4.36	.041	-6.10	3.75	.042	~~-6.23~~ -5.96	~~4.48~~ 4.65	~~.041~~ .041
$XOH_2\cdot UO_2(OH)_2^+$	1.63	7.26	.042	1.66	7.81	.042	~~1.88~~ 2.57	~~6.71~~ 5.66	~~.052~~ .052
$XOH\cdot UO_2(OH)_3^-$	-14.08	1.89	.043	-13.95	1.11	.046	~~-12.08~~ -11.75	~~0.48~~ .50	~~.054~~ .046
$XOH_2\cdot UO_2(OH)_3^0$	-6.20	4.36	.041	-6.10	3.75	.042	~~-4.36~~ -3.66	~~0.44~~ .35	~~.048~~ .044
$XOH\cdot UO_2(OH)_4^{-2}$	-21.94	1.01	.047	-21.79	0.39	.051	~~-17.46~~ -17.04	~~0.33~~ .38	~~.093~~ .095
$XOH_2\cdot UO_2(OH)_4^-$	-14.08	1.89	.043	-13.95	1.11	.046	~~-10.46~~ -9.42	~~0.20~~ .21	~~.066~~ .067

All changes in red 4/13/93 (LD)

log k

	CCM I=.1	CCM I=0	DLM I=0.1	DLM I=0	TLM I=0.1	TLM I=0
$XO{\cdot}UO_2^+$	1.63	1.96	1.66	1.99	~~-3.48~~ -2.76	~~-2.15~~ -2.49
$XOH{\cdot}UO_2^{+2}$	9.46	9.90	9.37	9.81	~~6.12~~ 6.30	6.56 6.74
$XO{\cdot}UO_2OH^0$	-6.20	-5.98	-6.10	-5.88	~~-8.34~~ ~~-8.34~~ w/113	-8.12 -8.32
$XOH{\cdot}UO_2OH^+$	1.63	1.96	1.66	1.99	~~-2.26~~ ~~-2.63~~ -2.23	+0.07 +.30
$XO{\cdot}UO_2(OH)_2^-$	-14.08	-13.97	-13.95	-13.84	-13.95 -14.04	-13.84 -13.93
$XOH{\cdot}UO_2(OH)_2^0$	-6.20	-5.98	-6.10	-5.88	~~-6.23~~ -5.96	-6.01 -5.74
$XOH_2{\cdot}UO_2(OH)_2^+$	1.63	1.96	1.66	1.99	~~+1.88~~ 2.57	2.21 2.90
$XOH{\cdot}UO_2(OH)_3^-$	-14.08	-13.97	-13.95	-13.84	~~-12.08~~ -11.75	~~-11.97~~ -11.64
$XOH_2{\cdot}UO_2(OH)_3^0$	-6.20	-5.98	-6.10	-5.88	~~-4.36~~ -3.66	~~-4.14~~ -3.44
$XOH{\cdot}UO_2(OH)_4^{-2}$	-21.44	-21.44	-21.79	-21.79	~~-17.46~~ -17.04	~~-21.79~~ -17.84 -17.96 w/113
$XOH_2{\cdot}UO_2(OH)_4^-$	-14.08	-13.97	-13.95	-13.84	-10.26 ~~-9.42~~	-10.05 -9.31

Note: changes from values reported on pp. 34-36 are minor

	log k (I=0.1)	SOS/DF	$\sigma_{\log k}$	I=0	log k
$XOH{\cdot}UO_2CO_3^0$	-2.45	3.24	.023	-2.23	15.93
$XOH_2{\cdot}UO_2(CO_3)_2^-$	-6.82	1.10	.027	-6.71	29.61
$XOH_2{\cdot}UO_2(CO_3)_3^{-3}$	-19.25	0.95	.036	-19.36	35.12
$XOH_2(UO_2)_2CO_3(OH)_3^+$	-6.82	3.85	.031	-6.38	11.78
$XOH{\cdot}UO_2(OH)_4^{-2}$	-22.20	32.63	.046	-22.20	-22.20

8/3/93 (AL)

Checks for accuracy/precision of digitizing equipment

1) SummaGraphics Microgrid 2 Digitizing Tablet
Located in CNWRA computer room, run on IRIS workstation

Operator: Tim Griffin, D. Turner - Spring 1992

Software: getcoords.C program written by R. Martin, April 1992

```
Apr 10 09:21 1992  getcoords.c Page 1


#include <stdio.h>

main(argc,argv)   /* copy input to output; 2nd version */
int   argc;
char  *argv[];
{
  int  CarriageReturn = 13;
  int  LineFeed = 10;
  int  c;

/*  FILE  *fopen(),   *fclose(); */
  FILE  *tablet_fp, *myfile_fp;

  if (argc != 2) {
     printf(" Usage: %s outfile \n",argv[0]);
     exit (0);
  }

  tablet_fp = fopen("/dev/ttyd10","r");
  myfile_fp = fopen(argv[1],"w");

  while  ((c = fgetc(tablet_fp)) != EOF) {
    fputc(c,myfile_fp); fputc(c,stdout);
    if (c == LineFeed ) {
       fflush(myfile_fp);
    }
  }
  fclose(myfile_fp);
  fclose(tablet_fp);
}
```

Checks on data of Tripathi (1984) indicate precision of .2 to .5 mm. This will include digitizer nominal reproducibility and operator reproducibility. In the case of Tripathi data, this translates to ~ ± .02 pH and ~ ± .1 to .3 % sorbed. Reproduction distortion and figure enlargement are also included

DRJ 8/13/93

2) ~~Sigm~~ Numonics 2200 Accugrid Digitizing Tablet
Software: SigmaScan
Computer: IBM 486 Model 90 PS/2
Operator: Stephen Sassman, Summer 1993

In a test of reproducibility, Stephen Sassman was able to reproduce graph "corners" within ~.1 to .2 mm. Again, this includes nominal digitizer reproducibility and operator reproducibility.

Also - Check of spreadsheet developed by D.R. Turner to convert potentiometric data from $\mu C/cm^2$ to TOTH. This code is adapted from the Basic program ABDATZ.BAS reported in Appendix IV.B of: Dzombak, D. 1985. 'Toward a Uniform Model for the Sorption of Inorganic Ions on Hydrous oxides', Ph.D Dissertation, MIT
Spreadsheet: QUATTRO
Necessary input:

Ionic Strength, pH, Asp, $\mu C/cm^2$ serial data, solid concentration

Checking against sample problem reported in Appendix IV.B shows agreement

type of solid: HYDROUS FERRIC OXIDE
source of data: YATES (1975)

Output Example from Appendix IV.B1 Dzombak (1985)

IONIC STRENGTH (mol/L) = .01

SURFACE AREA (sq.m/g) = 257
SOLID CONC (g/L) = 1.4

pH	SURFACE CHARGE			TOTH (desired values)	Spreadsheet values:
	uC/sq.cm	ueqv/g	mol/L	mol/L	
4.025	30.644	816.245	1.143E-03	1.237E-03	→ 1.2371×10^{-3}
4.308	28.038	746.831	1.046E-03	1.095E-03	
4.621	24.731	658.744	9.222E-04	9.462E-04	
5.041	20.889	556.407	7.790E-04	7.891E-04	
5.344	18.412	490.429	6.866E-04	6.911E-04	
5.736	14.903	396.962	5.557E-04	5.576E-04	
6.220	10.815	288.072	4.033E-04	4.039E-04	→ 4.0388×10^{-4}
6.726	7.465	198.841	2.784E-04	2.785E-04	
7.236	4.497	119.784	1.677E-04	1.675E-04	
7.830	1.165	31.031	4.344E-05	4.263E-05	
8.185	-1.115	-29.700	-4.158E-05	-4.346E-05	→ -4.3460×10^{-5}
8.419	-2.836	-75.541	-1.058E-04	-1.090E-04	
8.892	-6.168	-164.293	-2.300E-04	-2.396E-04	
9.695	-13.672	-364.172	-5.098E-04	-5.708E-04	

8/13/93 DRJ
The spreadsheet consists of ~~file~~ Cell formulas that can be copied to different spreadsheets for different potentiometric titration data

Sample hand calculations on pp 43-44, this volume.
DRJ 8/18/94

8/4/93 DRJ

FITEQL code slightly modified to allow handling of slightly larger problems. This required redimensioning several matrices and increasing the limits of several variables as described in the Users' Manual for FITEQL, Version 1.2 (Westall, 1982)

The matrices increased were the number of components allowed (10 → 20) and the number of secial data points allowed (40 → 50)

Dimension variables affected include

		Old	New
#Data pts	NDPDIM	40	50
#components	NEC	10	20
	NTØDIM	10	20
	NWWDIM	10	20
	NAADIM	30	40
	NADIM	10	20
	NXØDIM	10	20
	NXXDIM	10	20

Once changed in the source code, FITEQL was recompiled on an IBM 486 PS/2 machine using the Lahey F77L-EM/32, Version 5.10 Fortran compiler. The new code is stored as FIT2DIM.FOR (Source Code) and FIT2DIM.Exe (Executable). Testing versus sample files show that the output is identical for the original and the newest/revised version of the code. In otherwords, output calculated using FIT2.EXE as the code is matched by using FIT2DIM.EXE, and both 8/4/93 output files agree with the output file included with the orginal distribution of FITEQL.

10/11/93 DRJ

Summary of SCM modeling activities using FITEQL and MINTEQA2

Step 1 - Determine acidity constants for DLM, CCM, & TLM This is done assuming $N_S = 2.31$ sites/nm^2; and generalized A_{SP}. Potentiometric titration data selected from open literature. Data sources are:

Mineral	Generalized A_{SP} (m^2/g)	pH_{ZPC} ($\pm 1\ \sigma$)	Reference(s)
Goethite	50	8.0±0.8 (n=11)	Hsi and Langmuir (1985); Hayes et al. (1990); Yates and Healy (1975); Balistrieri and Murray (1981); Mesuere (1992)
Ferrihydrite$_{(a)}$	600	8.0±0.1 (n=9)	Hsi and Langmuir (1985); Davis (1977); Swallow (1978); Yates (1975)
Magnetite	5	6.7±0.1 (n=2)	Regazzoni et al. (1983)
Pyro-SiO_2	175	2.8±0.3 (n=3)	Abendroth (1970); Bolt (1957)
α-Al_2O_3	12	8.9±0.4 (n=4)	Hayes et al. (1990)
γ-Al_2O_3	120	8.4±0.3 (n=3)	Huang and Stumm (1972); Sprycha (1989)
δ-MnO_2	270	1.9±0.5 (n=7)	Murray (1974); Catts and Langmuir (1986)
TiO_2(anatase)	(b)	6.1±0.2 (n=2)	Sprycha (1984); Berube and de Bruyn (1968)
TiO_2(rutile)	30	5.9±0.3 (n=4)	Berube and de Bruyn (1968); Yates (1975)

Full-references are listed in Oct Sept. 93 Topical report entitled "Mechanistic Approaches to Radionuclide Sorption Modeling" (Turner, 1993; CNWRA 93-019) 10/11

Data digitized using systems and methods outlined on pp. 41-43. Conversion of data to TOTH and pH accomplished using methods described in Dzombak (1985) and Dzombak + Morel (1990).

10/25/93 Turner

All Potentiometric Titration Data Is in the Keeping of D.R. Turner. Summary of the Acidity Constants (K_+, K_-, K_{Cation}, K_{Anion}) determined by combining the weighted values is given here:
These values are assumed to be for I=0m except for CCM where reference state I=0.1 M is used.

Table 1. Best Estimate Values for SCM Constants - Simple Hydroxides.

Mineral	Mineral Properties[a]	References	Model	Log K_+ (± 95%)[b]	Log K_- (± 95%)[b]	Log K_{Anion} (± 95%)[b]	Log K_{Cation} (± 95%)[b]
Goethite	pH_{ZPC}=8.0 A_{SP}=50m^2/g	Yates and Healy (1975); Balistrieri and Murray (1981); Hsi and Langmuir (1985); Hayes et al. (1990); Mesuere (1992)	CCM(0.1M)	6.47±0.72	-9.03±0.22	n.a.	n.a.
			DLM	7.35±0.11	-9.17±0.08	n.a.	n.a.
			TLM(d)	6.00	-10.00	8.78±0.13	-7.64±0.07
Ferrihydrite[c]	pH_{ZPC}=8.0 A_{SP}=600m^2/g	Yates (1975); Davis (1977); Swallow (1978); Hsi and Langmuir (1985)	CCM(0.1M)	7.35±1.08	-8.45±2.23	n.a.	n.a.
			DLM	7.29±0.10	-8.93±0.07	n.a.	n.a.
			TLM(d)	6.00	-10.00	8.43±0.04	-7.66±0.12
Magnetite	pH_{ZPC}=6.7 A_{SP}=5m^2/g	Regazzoni et al. (1983)	CCM(0.1M)(e)	6.26	-7.32	n.a.	n.a.
			DLM	6.72±0.02	-6.37±0.71	n.a.	n.a.
			TLM(d)	4.70	-8.70	7.95±0.11	-5.47±0.06
SiO_2	pH_{ZPC}=2.8 A_{SP}=175m^2/g	Abendroth (1970); Bolt (1957)	CCM(0.1M)	(f)	-7.04±0.09	n.a.	n.a.
			DLM	(f)	-7.20±0.05	n.a.	n.a.
			TLM(d)	0.90	-4.90	(f)	-6.22±0.05
α-Al_2O_3	pH_{ZPC}=8.9 A_{SP}=12m^2/g	Hayes et al. (1990)	CCM(0.1M)(e)	~~9.98~~ 8.12	~~-8.32~~ -9.54	n.a.	n.a.
			DLM	8.33±0.15	-9.73±0.12	n.a.	n.a.
			TLM(d)	6.90	-10.90	10.12±0.03	-7.73±0.07
γ-Al_2O_3	pH_{ZPC}=8.4 A_{SP}=120m^2/g	Huang and Stumm (1972); Sprycha (1989)	CCM(0.1M)	6.92±0.06	-9.00±0.15	n.a.	n.a.
			DLM	6.85±0.06	-9.05±0.09	n.a.	n.a.
			TLM(d)	6.40	-10.40	8.28±0.05	-7.95±0.11
δ-MnO_2	pH_{ZPC}=1.9 A_{SP}=270m^2/g	Murray (1974); Catts and Langmuir (1986)	CCM(0.1M)	(f)	-2.14±24.7	n.a.	n.a.
			DLM	(f)	-3.27±0.73	n.a.	n.a.
			TLM(d)	-0.10	-3.9	(f)	-0.75±0.84
TiO_2(anatase)	pH_{ZPC}=6.1 A_{SP}= (c)	Sprycha (1984); Berube and de Bruyn (1968)	CCM(0.1M)(e)	6.64	-5.60	n.a.	n.a.
			DLM	5.37±0.30	-5.92±0.12	n.a.	n.a.
			TLM(d)	4.10	-8.10	7.13±0.17	-4.59±0.10
TiO_2(rutile)	pH_{ZPC}=5.9 A_{SP}=30m^2/g	Berube and de Bruyn (1968); Yates (1975)	CCM(0.1M)(e)	3.91	-7.79	n.a.	n.a.
			DLM	4.23±0.09	-7.49±0.12	n.a.	n.a.
			TLM(d)	3.90	-7.90	5.24±0.08	-6.42±0.08

n.a. Parameters not applicable to CCM and DLM models.

(a)N_S=2.31 sites/nm^2 (from Dzombak and Morel, 1990) assumed for all minerals.
(b) 95 % confidence interval based on FITEQL standard deviation and defined using the methods of Dzombak and Morel (1990).
(c) Mineral properties and DLM parameters for ferrihydrite are from Dzombak and Morel (1990).
(d) For TLM, Log K_+ and Log K_- fixed by convention. See text for discussion.
(e) FITEQL did not converge at I = 0.1 M. Extrapolated from $Log_{10}(I)$ vs Log K_+ and Log K_-.
(f) Not considered for δ-MnO_2 and am-SiO_2.

11/8/93 D.R. Turner

U(VI)-Al_2O_3 sorption data

These data were received from J. Prikryl at CNWRA Lab and the results are given below

	pH	U (ppb)	pH	U (ppb) ave	CL correction	U (ppb) CL cor	U/107	Minus 1	%U sorbed	U (m) CL cor	U sorbed
1	1.990	106.430	1.990	106.525	0.100	106.625	0.996	-0.004	0.350	4.48e-7	$1.16\times10^{-[illegible]}$
2	1.990	106.620	2.180	107.815	0.100	107.915	1.009	0.009	-0.855	4.53e-7	0
3	2.180	108.330	2.460	105.990	0.100	106.090	0.991	-0.009	0.850	4.46e-7	$3.40\times10^{-[illegible]}$
4	2.180	107.300	2.770	107.100	0.100	107.200	1.002	0.002	-0.187	4.50e-7	0
5	2.460	105.690	2.940	105.780	0.100	105.880	0.990	-0.010	1.047	4.45e-7	$4.29\times10^{-[illegible]}$
6	2.460	106.290	2.990	105.805	0.150	105.955	0.990	-0.010	0.977	4.45e-7	$3.97\times10^{-[illegible]}$
7	2.770	107.340	3.140	105.395	0.150	105.545	0.986	-0.014	1.360	4.43e-7	$5.69\times10^{-[illegible]}$
8	2.770	106.860	3.240	105.920	0.200	106.120	0.992	-0.008	0.822	4.46e-7	3.28×10^{-9}
9	2.940	106.020	3.370	106.300	0.250	106.550	0.996	-0.004	0.421	4.48e-7	1.47×10^{-9}
10	2.940	105.540	3.550	106.150	0.250	106.400	0.994	-0.006	0.561	4.47e-7	2.10×10^{-9}
11	2.990	105.890	3.680	104.610	0.300	104.910	0.980	-0.020	1.953	4.41e-7	$8.36\times10^{-[illegible]}$
12	2.990	105.720	3.920	101.915	0.400	102.315	0.956	-0.044	4.379	4.30e-7	$1.93\times10^{-[illegible]}$
13	3.140	106.030	4.420	98.125	0.600	98.725	0.923	-0.077	7.734	4.15e-7	$3.43\times10^{-[illegible]}$
14	3.140	104.760	5.110	79.335	2.800	82.135	0.768	-0.232	23.238	3.45e-7	1.04×10^{-7}
15	3.240	106.260	5.580	61.205	4.800	66.005	0.617	-0.383	38.313	2.77e-7	1.72×10^{-7}
16	3.240	105.580	5.870	48.720	5.500	54.220	0.507	-0.493	49.327	2.28e-7	2.21×10^{-7}
17	3.370	105.940	6.300	36.910	5.400	42.310	0.395	-0.605	60.458	1.78e-7	2.71×10^{-7}
18	3.370	106.660	6.750	43.375	4.000	47.375	0.443	-0.557	55.724	1.99e-7	2.50×10^{-7}
19	3.550	105.910	6.890	45.690	4.300	49.990	0.467	-0.533	53.280	2.10e-7	2.39×10^{-7}
20	3.550	106.390	7.140	48.040	2.800	50.840	0.475	-0.525	52.486	2.14e-7	$2.36\times10^{-[illegible]}$
21	3.680	103.980	7.470	58.420	0.600	59.020	0.552	-0.448	44.841	2.48e-7	2.01×10^{-7}
22	3.680	105.240	7.710	77.140	-0.200	76.940	0.719	-0.281	28.093	3.23e-7	1.26×10^{-7}
23	3.920	101.920	8.180	98.960	-1.500	97.460	0.911	-0.089	8.916	4.09e-7	3.97×10^{-8}
24	3.920	101.910	8.340	103.890	-1.650	102.240	0.956	-0.044	4.449	4.29e-7	1.96×10^{-8}
25	4.420	98.450	8.460	106.010	-1.750	104.260	0.974	-0.026	2.561	4.38e-7	1.11×10^{-8}
26	4.420	97.800	8.670	106.120	-1.800	104.320	0.975	-0.025	2.505	4.38e-7	1.08×10^{-8}
27	5.110	79.920	8.860	105.210	-1.850	103.360	0.966	-0.034	3.402	4.34e-7	1.49×10^{-8}
28	5.110	78.750	8.510	106.245	-1.750	104.495	0.977	-0.023	2.341	4.39e-7	1.01×10^{-8}
29	5.580	60.860	8.710	105.940	-1.800	104.140	0.973	-0.027	2.673	4.37e-7	1.16×10^{-8}
30	5.580	61.550	8.830	105.690	-1.800	103.890	0.971	-0.029	2.907	4.36e-7	$1.27\times10^{-[illegible]}$
31	5.870	48.630	4.040	107.360	0.450	107.810			1.794	4.53e-7	$6.22\times10^{-[illegible]}$
32	5.870	48.810	4.560	98.310	0.680	98.990			9.829	4.16e-7	4.33×10^{-8}
33	6.300	36.830	4.940	89.540	1.800	91.340	$U_T = 109.24$		16.797	3.84e-7	7.54×10^{-8}
34	6.300	36.990	6.000	44.030	5.600	49.630	$= 4.59\times10^{-7}$		54.791	2.08e-7	2.51×10^{-7}
35	6.750	42.600	6.530	39.250	5.200	44.450			59.510	1.87e-7	2.32×10^{-7}
36	6.750	44.150									
37	6.890	45.790									
38	6.890	45.590									
39	7.140	47.900									
40	7.140	48.180									
41	7.470	58.610									
42	7.470	58.230									
43	7.710	77.700									
44	7.710	76.580									
45	8.180	99.650									
46	8.180	98.270									
47	8.340	103.870									
48	8.340	103.910									
49	8.460	105.990									
50	8.460	106.030									
51	8.670	106.090									
52	8.670	106.150									
53	8.860	105.210									
54	8.860	105.210									
55	8.510	106.080									
56	8.510	106.410									
57	8.710	105.920									
58	8.710	105.960									
59	8.830	105.540									
60	8.830	105.840									
61	4.040	107.630									
62	4.040	107.090									
63	4.560	98.940									
64	4.560	97.680									
65	4.940	89.140									
66	4.940	89.940									
67	6.000	44.260									
68	6.000	43.800									
69	6.530	38.980									
70	6.530	39.520									

mg/L

ug/L

Finall ~ 106.9 ppb

$U_T = 4.49\times10^{-7}$ m

= 106.9 ppb

1 mole U = 238,029 ppm = 238,029,000

M =

1m = 238,029,000 ppb

106.

106.99

8006 (.229 m2/g) data

Wed, Oct 20, 1993 12:01 PM

	pH	U (ppb)	pH	U (ppb) ave	CL correction	U (ppb) CL cor	U/113.8	Minus 1	%U sorbed	U (m) CL cor	U sorbed
1	1.980	112.940	1.980	112.545	0.100	112.645	0.990	-0.010	1.015	4.73e-7	4.85×10^{-9}
2	1.980	112.150	2.350	112.805	0.100	112.905	0.992	-0.008	0.786	4.74e-7	3.76×10^{-9}
3	2.350	112.980	2.690	113.375	0.100	113.475	0.997	-0.003	0.286	4.77e-7	1.37×10^{-9}
4	2.350	112.630	2.970	112.015	0.150	112.165	0.986	-0.014	1.437	4.71e-7	6.87×10^{-9}
5	2.690	113.310	3.070	112.255	0.150	112.405	0.988	-0.012	1.226	4.72e-7	5.86×10^{-9}
6	2.690	113.440	3.300	111.795	0.200	111.995	0.984	-0.016	1.586	4.71e-7	7.58×10^{-9}
7	2.970	111.860	3.460	112.075	0.250	112.325	0.987	-0.013	1.296	4.72e-7	6.14×10^{-9}
8	2.970	112.170	3.680	110.870	0.300	111.170	0.977	-0.023	2.311	4.67e-7	[illegible] $\times10^{-8}$
9	3.070	112.440	3.880	113.030	0.400	113.430	0.997	-0.003	0.325	4.77e-7	1.55×10^{-9}
10	3.070	112.070	4.140	112.780	0.470	113.250	0.995	-0.005	0.483	4.76e-7	2.31×10^{-9}
11	3.300	112.020	4.340	111.095	0.570	111.665	0.981	-0.019	1.876	4.69e-7	2.17×10^{-9}
12	3.300	111.570	4.610	108.135	0.670	108.805	0.956	-0.044	4.389	4.57e-7	2.10×10^{-8}
13	3.460	112.270	5.550	93.745	4.600	98.345	0.864	-0.136	13.581	4.13e-7	6.49×10^{-8}
14	3.460	111.880	5.780	88.810	5.400	94.210	0.828	-0.172	17.214	3.96e-7	8.23×10^{-8}
15	3.680	111.210	6.040	82.050	5.550	87.600	0.770	-0.230	23.023	3.68e-7	1.10×10^{-7}
16	3.680	110.530	6.190	78.955	5.500	84.455	0.742	-0.258	25.786	3.55e-7	1.23×10^{-7}
17	3.880	113.070	6.730	80.820	4.800	85.620	0.752	-0.248	24.763	3.60e-7	1.18×10^{-7}
18	3.880	112.990	6.850	82.380	4.450	86.830	0.763	-0.237	23.699	3.65e-7	1.13×10^{-7}
19	4.140	112.510	6.920	84.310	4.200	88.510	0.778	-0.222	22.223	3.72e-7	1.06×10^{-7}
20	4.140	113.050	6.970	84.545	4.000	88.545	0.778	-0.222	22.192	3.72e-7	1.06×10^{-7}
21	4.340	111.300	7.040	87.915	3.500	91.415	0.803	-0.197	19.670	3.84e-7	9.40×10^{-8}
22	4.340	110.890	7.170	91.235	2.700	93.935	0.825	-0.175	17.456	3.95e-7	8.34×10^{-8}
23	4.610	108.190	7.260	93.985	2.000	95.985	0.843	-0.157	15.655	4.03e-7	7.48×10^{-8}
24	4.610	108.080	7.530	99.870	0.600	100.470	0.883	-0.117	11.714	4.22e-7	5.60×10^{-8}
25	5.550	93.710	7.730	106.390	-0.200	106.190	0.933	-0.067	6.687	4.46e-7	3.20×10^{-8}
26	5.550	93.780	7.970	111.430	-1.150	110.280	0.969	-0.031	3.093	4.63e-7	1.48×10^{-8}
27	5.780	88.890	8.220	113.705	-1.500	112.205	0.986	-0.014	1.402	4.71e-7	6.70×10^{-9}
28	5.780	88.730	8.560	115.100	-1.770	113.330	0.996	-0.004	0.413	4.76e-7	1.97×10^{-9}
29	6.040	81.710	8.980	113.465	-1.850	111.615	0.981	-0.019	1.920	4.69e-7	9.18×10^{-9}
30	6.040	82.390									
31	6.190	78.600									
32	6.190	79.310									
33	6.730	80.870									
34	6.730	80.770									
35	6.850	82.210									
36	6.850	82.550									
37	6.920	84.230									
38	6.920	84.390									
39	6.970	84.540									
40	6.970	84.550									
41	7.040	87.950									
42	7.040	87.880									
43	7.170	91.340									
44	7.170	91.130									
45	7.260	94.060									
46	7.260	93.910									
47	7.530	100.030									
48	7.530	99.710									
49	7.730	106.310									
50	7.730	106.470									
51	7.970	111.140									
52	7.970	111.720									
53	8.220	113.750									
54	8.220	113.660									
55	8.560	114.450									
56	8.560	115.750									
57	8.980	114.390									
58	8.980	112.540									

$U(VI)_T = 113.7$ ppb
4.78×10^{-7} M

11/8/93
D.R. Turner

$U(VI)-Al_2O_3$ sorption data

These data were received from J. Prikryl at CNWRA Lab and the results are given below.

8007 (.0686 m2/g) data

Wed, Oct 20, 1993 12:13 PM

	pH	U(ppb)
1	1.950	114.540
2	1.950	114.540
3	2.340	116.560
4	2.340	115.020
5	2.730	116.270
6	2.730	116.740
7	3.000	115.340
8	3.000	115.330
9	3.240	115.740
10	3.240	116.130
11	3.510	114.960
12	3.510	114.380
13	3.750	112.450
14	3.750	114.600
15	4.050	113.540
16	4.050	113.360
17	4.250	113.050
18	4.250	113.770
19	4.500	113.370
20	4.500	113.760
21	4.880	110.680
22	4.880	111.450
23	4.990	110.910
24	4.990	109.870
25	5.300	108.590
26	5.300	107.830
27	5.600	100.180
28	5.600	99.450
29	5.700	101.860
30	5.700	101.730
31	5.990	99.260
32	5.990	99.990
33	6.040	100.690
34	6.040	101.790
35	6.180	100.310
36	6.180	100.160
37	5.920	95.540
38	5.920	96.310
39	6.390	95.560
40	6.390	96.610
41	6.730	96.760
42	6.730	97.350
43	7.020	99.790
44	7.020	98.010
45	7.380	101.260
46	7.380	102.120
47	7.540	104.880
48	7.540	105.210
49	7.690	106.220
50	7.690	106.450
51	7.980	112.540
52	7.980	113.690
53	8.240	115.550
54	8.240	115.660
55	8.630	115.220
56	8.630	115.360
57	8.940	117.940
58	8.940	117.230

pH	U (ppb) ave	CL correction	U (ppb) CL cor	U/115.93	Minus 1	%U sorbed	U (m) CL cor	U sorbed
1.950	114.540	0.100	114.640	0.989	-0.011	1.113	4.82e-7	5.42×10^{-9}
2.340	115.790	0.100	115.890	1.000	-0.000	0.035	4.87e-7	1.70×10^{-10}
2.730	116.505	0.100	116.605	1.006	0.006	-0.582	4.90e-7	0
3.000	115.335	0.150	115.485	0.996	-0.004	0.384	4.85e-7	1.87×10^{-9}
3.240	115.935	0.200	116.135	1.002	0.002	-0.177	4.88e-7	0
3.510	114.670	0.250	114.920	0.991	-0.009	0.871	4.83e-7	4.24×10^{-9}
3.750	113.525	0.350	113.875	0.982	-0.018	1.773	4.78e-7	8.63×10^{-9}
4.050	113.450	0.450	113.900	0.982	-0.018	1.751	4.79e-7	8.53×10^{-9}
4.250	113.410	0.520	113.930	0.983	-0.017	1.725	4.79e-7	8.40×10^{-9}
4.500	113.656	0.680	114.336	0.986	-0.014	1.375	4.80e-7	6.70×10^{-9}
4.880	111.065	1.670	112.735	0.972	-0.028	2.756	4.74e-7	1.34×10^{-8}
4.990	110.390	2.200	112.590	0.971	-0.029	2.881	4.73e-7	1.40×10^{-8}
5.300	108.210	3.800	112.010	0.966	-0.034	3.381	4.71e-7	1.65×10^{-8}
5.600	99.815	4.800	104.615	0.902	-0.098	9.760	4.40e-7	4.75×10^{-8}
5.700	101.795	5.100	106.895	0.922	-0.078	7.793	4.49e-7	3.80×10^{-8}
5.990	99.625	5.600	105.225	0.908	-0.092	9.234	4.42e-7	4.50×10^{-8}
6.040	101.240	5.550	106.790	0.921	-0.079	7.884	4.49e-7	3.84×10^{-8}
6.180	100.235	5.500	105.735	0.912	-0.088	8.794	4.44e-7	4.28×10^{-8}
5.920	95.925	5.500	101.425	0.875	-0.125	12.512	4.26e-7	6.09×10^{-8}
6.390	96.085	5.300	101.385	0.875	-0.125	12.546	4.26e-7	6.11×10^{-8}
6.730	97.055	4.800	101.855	0.879	-0.121	12.141	4.28e-7	5.91×10^{-8}
7.020	98.900	3.950	102.850	0.887	-0.113	11.283	4.32e-7	5.50×10^{-8}
7.380	101.190	1.100	102.290	0.882	-0.118	11.766	4.30e-7	5.73×10^{-8}
7.540	105.045	0.400	105.445	0.910	-0.090	9.044	4.43e-7	4.40×10^{-8}
7.690	106.335	-0.200	106.135	0.916	-0.084	8.449	4.46e-7	4.12×10^{-8}
7.980	113.115	-1.200	111.915	0.965	-0.035	3.463	4.70e-7	1.69×10^{-8}
8.240	115.605	-1.550	114.055	0.984	-0.016	1.617	4.79e-7	7.87×10^{-9}
8.630	115.290	-1.800	113.490	0.979	-0.021	2.105	4.77e-7	1.03×10^{-8}
8.940	117.585	-1.850	115.735	0.998	-0.002	0.168	4.86e-7	8.18×10^{-10}

115.9

$U(VI)_T = 4.87\times10^{-7}$

11/8/93 D.R. Turner

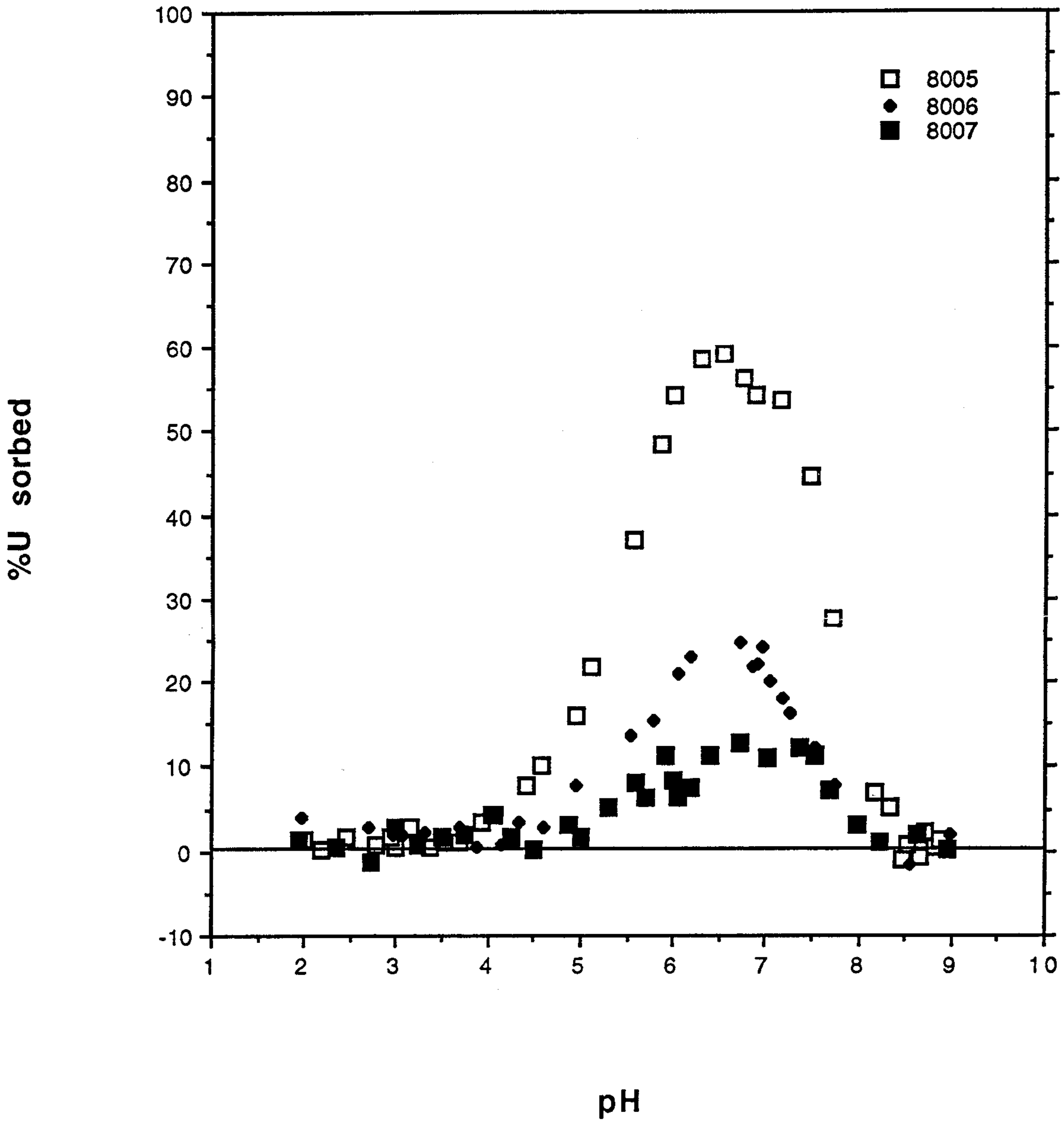
U(VI)-Al_2O_3 sorption data

These data were received from J. Prikryl at CNWRA Lab and the results are given below

MM

47

Uranium sorption on alpha alumina (corrected data)



11/8/93 D.R. Turner

U(VI)-Al_2O_3 sorption data

These data were received from J. Prikryl at CNWRA Lab and the results are given below.

DRT

mm

47

11/8/93
D.Turner

- Asp: 8005 = 2.09 m^2/g
  8006 = 0.229 m^2/g
  8007 = .0686 m^2/g

- N_S = 2.31 sites/nm^2
- K_+, K_- are taken from table on pg. 46 of this lab notebook and corrected to I=0.1 m

FITEQL results (assuming 1% error) are listed in a three-ring binder - "Binding Constants-Uranium" Number 046-A in the possession of D.R. Turner @ CNWRA

11/17/93
D.Turner

U(VI)-Sorption on Clinoptilolite

Data for 2 uranium ~~compost~~ concentrations: DRT 11/17

ΣU = 500 ppb = 2.1×10^{-6} M
ΣU = 50 ppb = 2.1×10^{-7} M

Data are from CNWRA laboratories, provided by R. Pabalan.

Reported Clinoptilolite concentration is:

$(Na_{1.807}K_{0.123}Ca_{.0031}Mg_{0.0349})(Al_{1.948}Fe_{.044})(Si_{10.044}Ti_{.004})O_{24}:7.23H_2O$

Assuming surface sites are stoichiometric ratios of $SiOH^0$: $AlOH^0$
This yields 10.044/1.948 = 5.156 : 1

Experimental Conditions:
I = 0.1 m $NaNO_3$
C_s = 2 g/l (.1 g/50 ml)
Assuming N_s = 2.31 sites/nm^2 (Dzombak + Morel, 1990)
A_{sp} = 16 m^2/g (LANL Monthly report, April 1993)

T_{XOH} = 1.23×10^{-4} moles sites / l H_2O

T_{SiOH} = 1.028×10^{-4} moles sites / l H_2O
T_{AlOH} = 1.994×10^{-5} moles sites / l H_2O
$\frac{SiOH^0}{AlOH^0}$ = 5.156/1

- FITEQL, Version 2.0 is used with NEA uranium data corrected to I=0.1 m.
- Single complexation reactions for each site are considered. Si + Al
- U-binding reactions are considered separately, but protonation/deprotonation reactions for both sites are considered in all chemical equilibrium models.

Models employed: DLM + TLM. Model parameters given in Table 1 on page 46.

$U(VI)_T$ = 500 ppb = 2.1×10^{-6} M

Clinoptilolite

CNWRA Data

pH fwd	%U lost zeol.
1.89	0.486126239
1.89	-0.122144491
2.18	0.056409336
2.18	0.09142675
2.45	0.358279784
2.45	-0.085891242
2.71	0.983086014
2.71	1.099278047
2.96	1.56529851
2.96	0.174763909
3.26	1.516708543
3.26	0.02900451
3.61	2.227414181
3.61	2.465137749
3.88	4.15696903
3.88	3.609530025
4.27	6.38434128
4.27	5.878612042
4.55	9.922313057
4.55	10.26318026
4.79	16.41092948
4.79	15.74407676
5.01	21.33614047
5.01	21.39376364
5.71	35.17397929
5.71	35.06309047
5.87	47.3193166
5.87	46.8523561
5.86	49.03616101
5.86	48.99846587
6.04	51.83729021
6.04	51.04605616
6.17	53.6314631
6.17	53.56873793
6.92	44.80317281
6.92	45.2126752
6.58	57.93998887
6.58	58.41471619
6.53	54.17080169
6.53	53.82199068
7.11	39.35598087
7.11	39.27673951
7.03	44.31052568
7.03	43.43336546
7.32	32.94692928
7.32	33.04970341
7.57	20.43030115
7.57	20.59446842
7.8	7.77229787
7.8	7.966601939
8.08	0.556747658
8.08	2.035994578
8.34	0.499067884
8.34	0.23005161
8.67	-0.287563509
8.67	0.398791595
8.9	-0.27422111
8.9	-0.098708559

$U(VI)_T = 50ppb = 2.1 \times 10^{-7}$ M

Clinoptilolite Data

CNLWRA

pH fwd	%U lost zeol.
2.04	-0.559393723
2.04	-0.887891792
2.28	1.902716472
2.28	0.90553147
2.5	-1.31872223
2.5	-1.575988446
2.74	-2.656107753
2.74	0.823078382
2.97	0.118370276
2.97	-0.680686044
3.24	2.740551649
3.24	2.478563153
3.52	2.522902973
3.52	4.698852434
3.82	7.581396179
3.82	7.189997924
4.12	10.19845806
4.12	8.109854643
4.44	17.67747964
4.44	19.79392277
4.69	18.31057502
4.69	17.75594733
4.97	29.23098851
4.97	27.43660056
5.17	35.09043137
5.17	35.61626068
5.27	40.83890651
5.27	41.37123558
5.42	43.84033175
5.42	38.78991458
5.49	52.71216497
5.49	52.5535139
5.61	52.07549714
5.61	51.68991579
5.89	69.19137568
5.89	69.76666968
6.07	72.32312425
6.07	71.72239252
6.36	71.91691883
6.36	71.74231686
6.6	69.52864866
6.6	68.87890755
6.79	58.15416091
6.79	57.50068191
7.16	47.30508801
7.16	46.34295332
7.35	33.26601912
7.35	33.47577145
7.78	12.83030137
7.78	14.87894512
8	4.591366668
8	2.721626861
8.28	0.331536355
8.28	0.720798516
8.59	0.562990793
8.59	-1.338678531
8.85	-0.656187639
8.85	2.936338348

U(VI)-Clinoptilolite Sorption Data corrected for container loss (CNWRA, 1993)

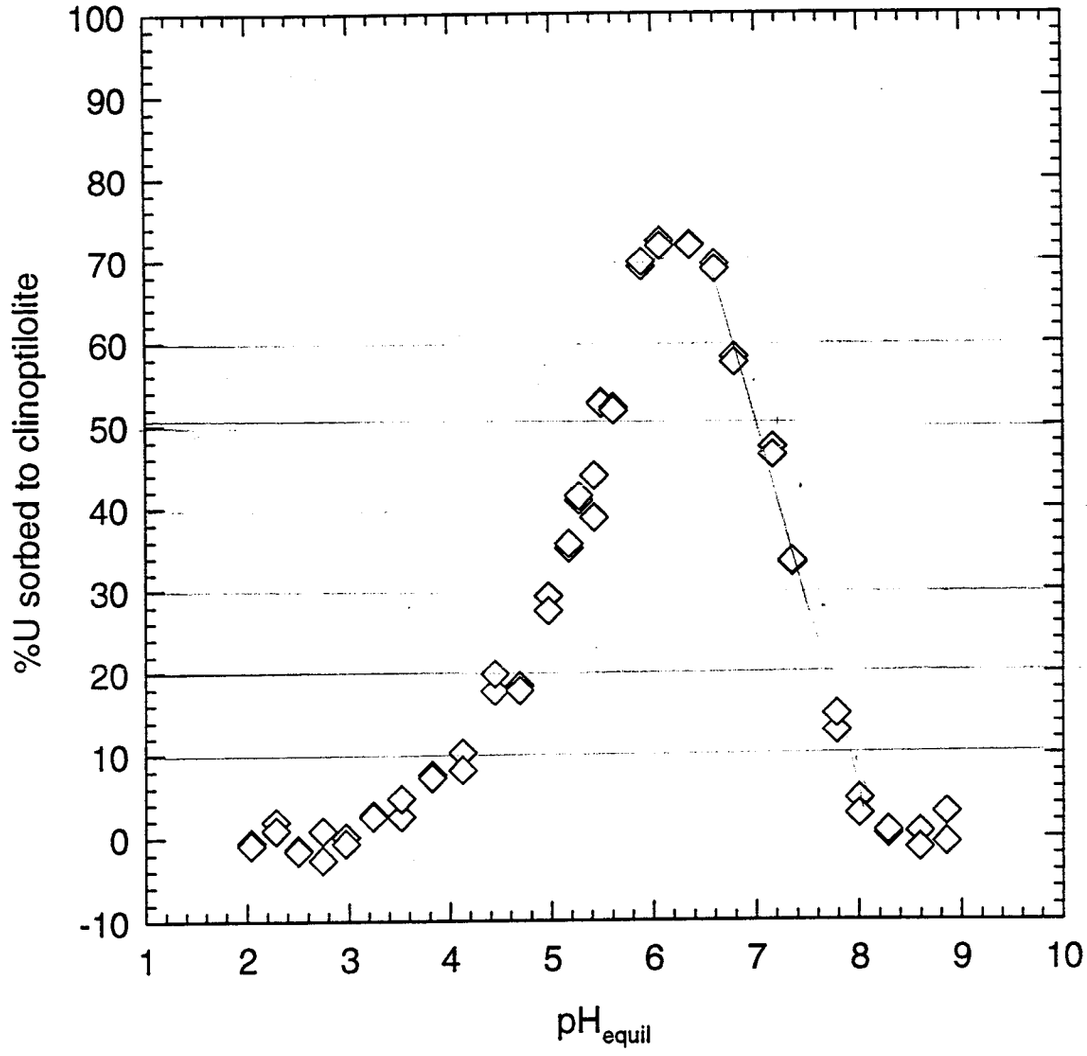
50ppb	50ppb	50ppb	50ppb	50ppb	50ppb	50ppb	50ppb	500ppb	500ppb	500ppb	500ppb	500ppb	500ppb	500ppb	500ppb
pH	% sorbed	conc. sorbed	avg sorbed	uco(*0.5)	uc1(1*)	uc2(*2.0)	uc3(*3.0)	pH	% sorbed	conc. sorbed	avg sorbed	uco(*0.5)	uc1(1*)	uc2(*2.0)	uc3(*3.0)
2.04	-0.559393723	-1.175e-09						1.89	0.486126239	1.021e-08					
2.04	-0.887891792	-1.865e-09	-1.520e-09	-7.600e-10	-1.520e-09	-3.040e-09	-4.560e-09	1.89	-0.122144491	-2.566e-09	3.823e-09	1.911e-09	3.823e-09	7.646e-09	1.147e-08
2.28	1.902716472	3.997e-09						2.18	0.056409336	1.185e-09					
2.28	0.905531470	1.902e-09	2.949e-09	1.475e-09	2.949e-09	5.899e-09	8.848e-09	2.18	0.091426750	1.920e-09	1.553e-09	7.764e-10	1.553e-09	3.105e-09	4.658e-09
2.50	-1.318722230	-2.770e-09						2.45	0.358279784	7.526e-09					
2.50	-1.575988446	-3.310e-09	-3.040e-09	-1.520e-09	-3.040e-09	-6.081e-09	-9.121e-09	2.45	-0.085891242	-1.804e-09	2.861e-09	1.430e-09	2.861e-09	5.722e-09	8.583e-09
2.74	-2.656107753	-5.579e-09						2.71	0.983086014	2.065e-08					
2.74	0.823078382	1.729e-09	-1.925e-09	-9.626e-10	-1.925e-09	-3.850e-09	-5.776e-09	2.71	1.099278047	2.309e-08	2.187e-08	1.094e-08	2.187e-08	4.374e-08	6.561e-08
2.97	0.118370276	2.486e-10						2.96	1.565298510	3.288e-08					
2.97	-0.680686044	-1.430e-09	-5.906e-10	-2.953e-10	-5.906e-10	-1.181e-09	-1.772e-09	2.96	0.174763909	3.671e-09	1.828e-08	9.138e-09	1.828e-08	3.655e-08	5.483e-08
3.24	2.740551649	5.757e-09						3.26	1.516708543	3.186e-08					
3.24	2.478563153	5.206e-09	5.482e-09	2.741e-09	5.482e-09	1.096e-08	1.644e-08	3.26	0.029004510	6.093e-10	1.623e-08	8.117e-09	1.623e-08	3.247e-08	4.870e-08
3.52	2.522902973	5.300e-09						3.61	2.227414181	4.679e-08					
3.52	4.698852434	9.870e-09	7.585e-09	3.792e-09	7.585e-09	1.517e-08	2.275e-08	3.61	2.465137749	5.178e-08	4.929e-08	2.464e-08	4.929e-08	9.857e-08	1.479e-07
3.82	7.581396179	1.593e-08						3.88	4.156969030	8.732e-08					
3.82	7.189997924	1.510e-08	1.551e-08	7.757e-09	1.551e-08	3.103e-08	4.654e-08	3.88	3.609530025	7.582e-08	8.157e-08	4.079e-08	8.157e-08	1.631e-07	2.447e-07
4.12	10.198458060	2.142e-08						4.27	6.384341280	1.341e-07					
4.12	8.109854643	1.704e-08	1.923e-08	9.615e-09	1.923e-08	3.846e-08	5.769e-08	4.27	5.878612042	1.235e-07	1.288e-07	6.440e-08	1.288e-07	2.576e-07	3.864e-07
4.44	17.677479640	3.713e-08						4.55	9.922313057	2.084e-07					
4.44	19.793922770	4.158e-08	3.936e-08	1.968e-08	3.936e-08	7.871e-08	1.181e-07	4.55	10.263180260	2.156e-07	2.120e-07	1.060e-07	2.120e-07	4.240e-07	6.360e-07
4.69	18.310575020	3.846e-08						4.79	16.410929480	3.447e-07					
4.69	17.755947330	3.730e-08	3.788e-08	1.894e-08	3.788e-08	7.576e-08	1.136e-07	4.79	15.744076760	3.307e-07	3.377e-07	1.689e-07	3.377e-07	6.754e-07	1.013e-06
4.97	29.230988510	6.140e-08						5.01	21.336140470	4.482e-07					
4.97	27.436600560	5.763e-08	5.952e-08	2.976e-08	5.952e-08	1.190e-07	1.786e-07	5.01	21.393763640	4.494e-07	4.488e-07	2.244e-07	4.488e-07	8.976e-07	1.346e-06
5.17	35.090431370	7.371e-08						5.71	35.173979290	7.389e-07					
5.17	35.616260680	7.481e-08	7.426e-08	3.713e-08	7.426e-08	1.485e-07	2.228e-07	5.71	35.063090470	7.365e-07	7.377e-07	3.688e-07	7.377e-07	1.475e-06	2.213e-06
5.27	40.838906510	8.579e-08						5.87	47.319316600	9.940e-07					
5.27	41.371235580	8.690e-08	8.634e-08	4.317e-08	8.634e-08	1.727e-07	2.590e-07	5.87	46.852356100	9.842e-07	9.891e-07	4.945e-07	9.891e-07	1.978e-06	2.967e-06
5.42	43.840331750	9.209e-08						5.86	49.036161010	1.030e-06					
5.42	38.789914580	8.148e-08	8.679e-08	4.339e-08	8.679e-08	1.736e-07	2.604e-07	5.86	48.998465870	1.029e-06	1.030e-06	5.148e-07	1.030e-06	2.059e-06	3.089e-06

5.49	52.712164970	1.107e-07						6.04	51.837290210	1.089e-06					
5.49	52.553513900	1.104e-07	1.106e-07	5.528e-08	1.106e-07	2.211e-07	3.317e-07	6.04	51.046056160	1.072e-06	1.081e-06	5.403e-07	1.081e-06	2.161e-06	3.242e-06
5.61	52.075497140	1.094e-07						6.17	53.631463100	1.127e-06					
5.61	51.689915790	1.086e-07	1.090e-07	5.449e-08	1.090e-07	2.180e-07	3.270e-07	6.17	53.568737930	1.125e-06	1.126e-06	5.630e-07	1.126e-06	2.252e-06	3.378e-06
5.89	69.191375680	1.453e-07						6.92	44.803172810	9.411e-07					
5.89	69.766669680	1.466e-07	1.459e-07	7.297e-08	1.459e-07	2.919e-07	4.378e-07	6.92	45.212675200	9.497e-07	9.454e-07	4.727e-07	9.454e-07	1.891e-06	2.836e-06
6.07	72.323124250	1.519e-07						6.58	57.939988870	1.217e-06					
6.07	71.722392520	1.507e-07	1.513e-07	7.564e-08	1.513e-07	3.026e-07	4.539e-07	6.58	58.414716190	1.227e-06	1.222e-06	6.110e-07	1.222e-06	2.444e-06	3.666e-06
6.36	71.916918830	1.511e-07						6.53	54.170801690	1.138e-06					
6.36	71.742316860	1.507e-07	1.509e-07	7.544e-08	1.509e-07	3.018e-07	4.527e-07	6.53	53.821990680	1.131e-06	1.134e-06	5.671e-07	1.134e-06	2.268e-06	3.403e-06
6.60	69.528648660	1.461e-07						7.11	39.355980870	8.267e-07					
6.60	68.878907550	1.447e-07	1.454e-07	7.268e-08	1.454e-07	2.907e-07	4.361e-07	7.11	39.276739510	8.250e-07	8.259e-07	4.129e-07	8.259e-07	1.652e-06	2.478e-06
6.79	58.154160910	1.222e-07						7.03	44.310525680	9.308e-07					
6.79	57.500681910	1.208e-07	1.215e-07	6.074e-08	1.215e-07	2.429e-07	3.644e-07	7.03	43.433365460	9.124e-07	9.216e-07	4.608e-07	9.216e-07	1.843e-06	2.765e-06
7.16	47.305088010	9.937e-08						7.32	32.946929280	6.921e-07					
7.16	46.342953320	9.735e-08	9.836e-08	4.918e-08	9.836e-08	1.967e-07	2.951e-07	7.32	33.049703410	6.942e-07	6.932e-07	3.466e-07	6.932e-07	1.386e-06	2.079e-06
7.35	33.266019120	6.988e-08						7.57	20.430301150	4.292e-07					
7.35	33.475771450	7.032e-08	7.010e-08	3.505e-08	7.010e-08	1.402e-07	2.103e-07	7.57	20.594468420	4.326e-07	4.309e-07	2.154e-07	4.309e-07	8.618e-07	1.293e-06
7.78	12.830301370	2.695e-08						7.80	7.772297870	1.633e-07					
7.78	14.878945120	3.125e-08	2.910e-08	1.455e-08	2.910e-08	5.821e-08	8.731e-08	7.80	7.966601939	1.673e-07	1.653e-07	8.265e-08	1.653e-07	3.306e-07	4.959e-07
8.00	4.591366668	9.645e-09						8.08	0.556747658	1.169e-08					
8.00	2.721626861	5.717e-09	7.681e-09	3.840e-09	7.681e-09	1.536e-08	2.304e-08	8.08	2.035994578	4.277e-08	2.723e-08	1.362e-08	2.723e-08	5.446e-08	8.169e-08
8.28	0.331536355	6.964e-10						8.34	0.499067884	1.048e-08					
8.28	0.720798516	1.514e-09	1.105e-09	5.526e-10	1.105e-09	2.211e-09	3.316e-09	8.34	0.230051610	4.832e-09	7.658e-09	3.829e-09	7.658e-09	1.532e-08	2.297e-08
8.59	0.562990793	1.183e-09						8.67	-0.287563509	-6.041e-09					
8.59	-1.338678531	-2.812e-09	-8.147e-10	-4.073e-10	-8.147e-10	-1.629e-09	-2.444e-09	8.67	0.398791595	8.377e-09	1.168e-09	5.841e-10	1.168e-09	2.336e-09	3.505e-09
8.85	-0.656187639	-1.378e-09						8.90	-0.274221110	-5.760e-09					
8.85	2.936338348	6.168e-09	2.395e-09	1.197e-09	2.395e-09	4.790e-09	7.184e-09	8.90	-0.098708559	-2.073e-09	-3.917e-09	-1.958e-09	-3.917e-09	-7.834e-09	-1.175e-08

T_{AlOH^o} = 1.994×10^{-5} moles sites/L H_2O

T_{SiOH^o} = 1.028×10^{-4} moles sites/L H_2O

%U sorbed vs. pH



$(Na_{1.837}K_{0.123}Ca_{0.0231}Mg_{0.0349})(Al_{1.948}Fe_{0.044})(Si_{10.044}Ti_{0.044})O_{24} \cdot 7.45\ H_2O$

$SiOH^o : AlOH^o = \frac{10.044}{1.948} =$

$= 5.156 : 1$

$\Sigma U = 50\ ppb$

$I = 0.1\ m\ NaNO_3$

$0.1\ g\ zeo / 50\ ml$ solution

$2\ g/l$

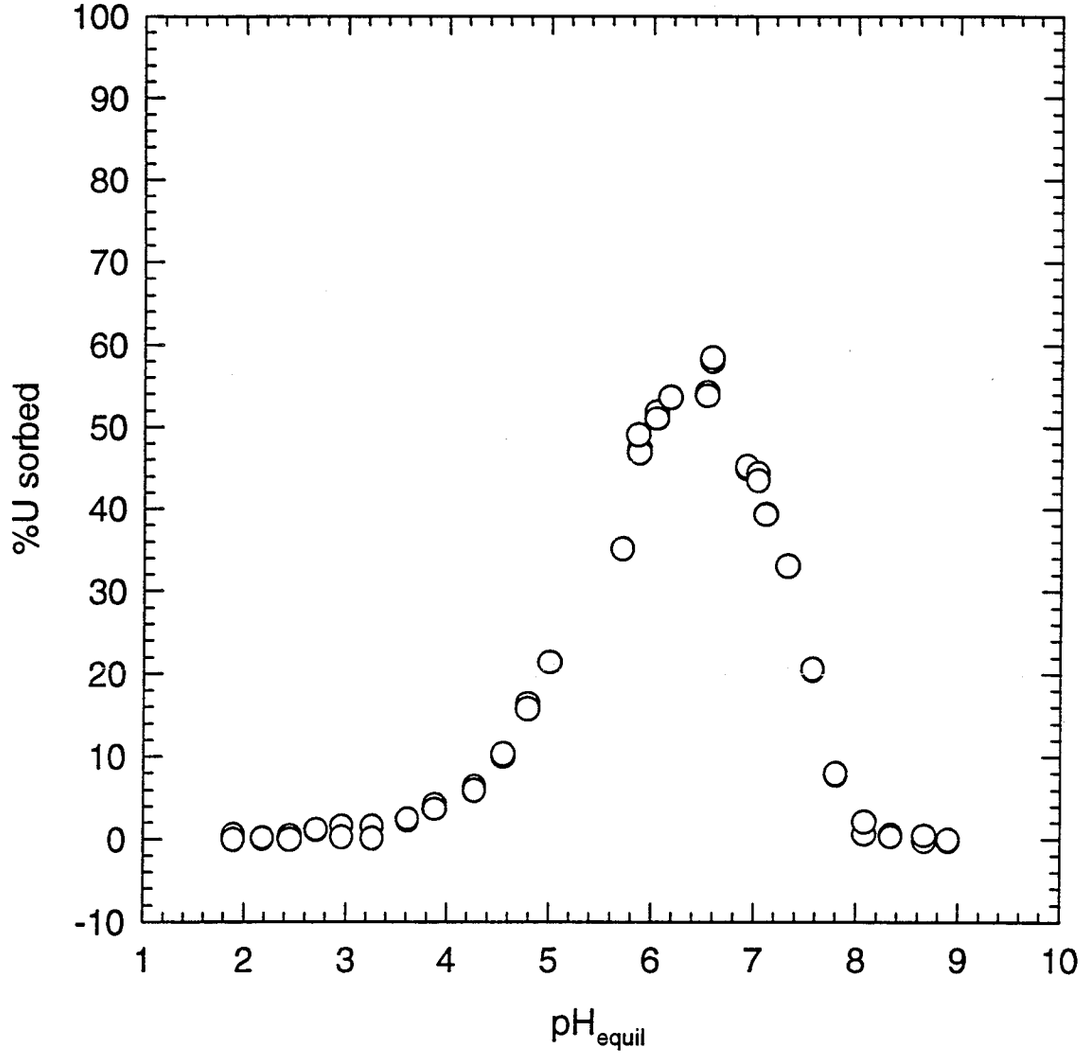
$T_{XOH} = 1.23 \times 10^{-4}$ moles/L

BIB

10 26 93

50

%U sorbed vs. pH



$\Sigma U = 500\ \mu M$

$I = 0.1\ m\ NaNO_3$

0.1 g goe/50 ml solution

$T_{XOH} = 1.23 \times 10^{-4}$ moles sites/L

$\Sigma U = 500\ \mu M$

U(VI)-Clinoptilolite Binding Constants†

Log K (I = 0M)	SiOH°		AlOH°	
	DLM	TLM	DLM	TLM
Model Parameters				
XO^-	-7.20	-4.90	-9.73	-10.80
XOH_2^+	n.a.	0.90	8.33	6.80
XO-Na°	n.a.	-6.22	n.a.	-7.73
XOH_2-NO_3°	n.a.	n.a.	n.a.	10.12
U(VI) Binding Constants				
XOH-UO_2^{++}	5.86	n.d.	9.23	n.d.
XO-UO_2^+	0.17	-2.71	2.66	1.73
XO-UO_2OH°	-6.35	-6.09	-4.24	-2.13
XOH-$UO_2(OH)_2$°	-6.35	-6.35	-4.24	-2.92
XOH-UO_2CO_3°	15.51	15.52	17.96	19.18

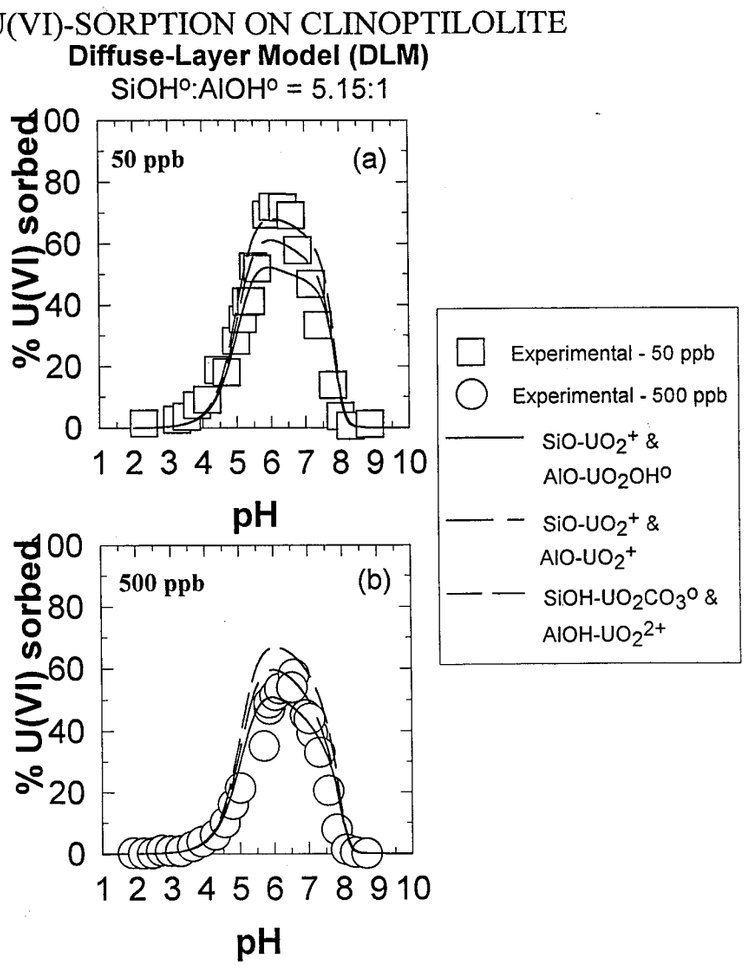
n.a. Not applicable to DLM
n.d. Not determined for TLM

† Binding constants determined using FITEQL, Version 2.0 (Westall, 1982) with data from NEA Thermodynamic Database for Uranium (Grenthe et al., 1992). $N_S = 2.31$ sites/nm^2; $A_{SP} = 16$ m^2/g. Values listed are weighted combination of values determined from the 50 ppb and 500 ppb datasets.

Some of the resulting binding constants include:

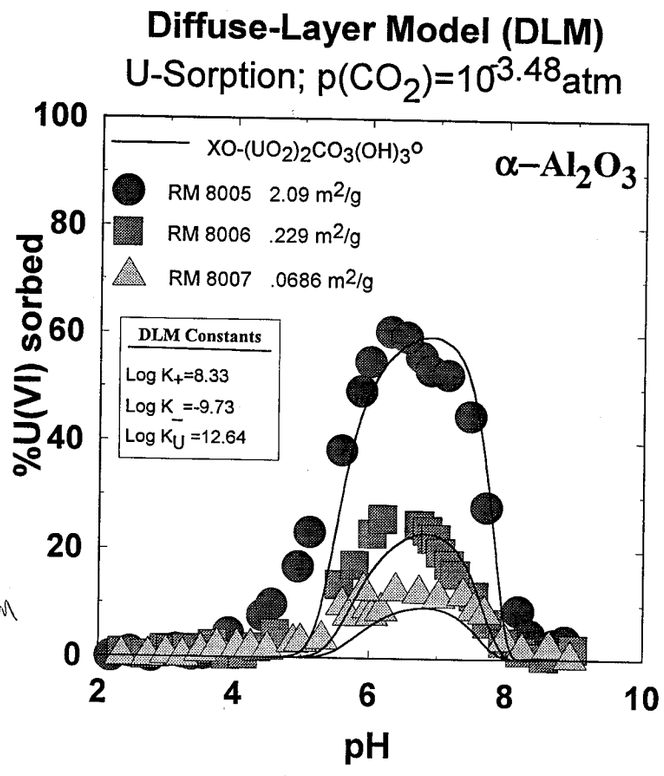
11/18/93
D. Turner

Using the binding constants determined from the clinoptilolite data (pg. 49-51 this book), MINTEQA2 was used to model the sorption behavior. The CNWRA database for MINTEQA2 (12/17/92 version) was used with uranium data from NEA database (Grenthe et al, 1992). The results are shown below.



12/3/93
D. Turner

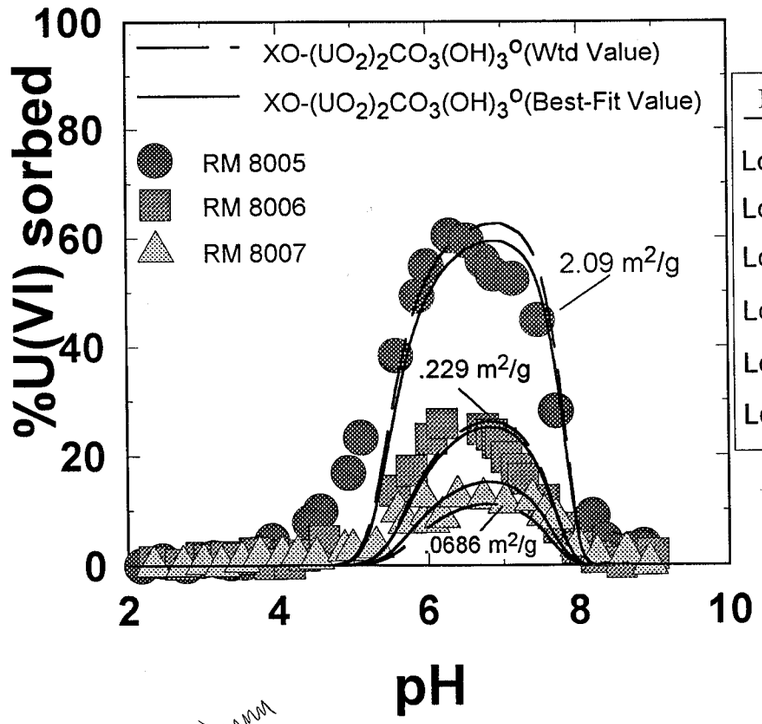
α-Al_2O_3 data from CNWRA. Attempt to fit/predict sorption data @ other Surface Area/Volume ratios using one data set. Fitting data for $A_{SP} = 2.09 m^2/g$ gives a binding constant for $XO\text{-}(UO_2)_2CO_3(OH)_3^-$ of $\log K = 12.64$. Using this data to model lower SA/Volume ratios (MINTEQA2, version 3.11 with 12/17/92 CNWRA database), the results are shown below.



Resultant fit is not too bad, but worsening of fit below pH ≈ 5 suggests may need non-carbonate species such as UO_2^{2+} or UO_2OH^+

α-Al_2O_3 modeling results using Best-Fit and weighted values as shown below:

Diffuse-Layer Model (DLM)
U-Sorption; $p(CO_2)=10^{-3.48}$atm



DLM Constants	
Log K_+	=8.33
Log K_-	=-9.73
Log K_{wtd}	=12.73
Log K_{8005}	=12.64
Log K_{8006}	=12.70
Log K_{8007}	=12.91

Best-Fit

DRJ 12/21

12/21/93 D. Turner

In response to concerns regarding scientific notebooks at CNWRA, at brief background of MINTEQA2 is include with the inclusion of radioelement thermodynamic data added to the MINTEQA2 databases and data sources.

The primary documentation for MINTEQA2, Ver 3.11 consists of the User's Manual prepared by EPA (Allison et al., 1991 - MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: Version 3.0 User's Manual, EPA/600/3-91/021) and internal documentation for modifications of 3.0 to 3.11 in the code itself.

Code Versions used have been and will continue to be documented in this book and in reports and articles in which model results are reported

MINTEQA2 and the preprocessor code PRODEFA2 have been under development at the EPA Center for Exposure Assessment Modeling in Athens, GA. The database as distributed is from WATEQ3, a USGS aqueous speciation code, and data sources from the documentation for WATEQ3 can be used to identify data sources for the more common elements such as Ca^{2+}, Mg^{2+}, CO_3^{2-}, etc.

DRJ 12/21

The version of MINTEQA2/PRODEFA2 ~~is~~ used at CNWRA is version 3.11 and was obtained by D.R. Turner from the CEAM staff in ~~Atlanta~~ Athens Georgia in August 1992 as compressed files on a single 3½" diskette. This diskette is attached to the back of this book.
This software has been installed as a PC version on the IBM PS/2 of David Turner at CNWRA.
Additional installation was on the CNWRA (12/21/DRJ) LAN server under K:\TURNER\MINTEQA2, although this may change as space is needed on the server. The only modifications to the code have been to the 4 databases COMP.DBS, THERMO.DBS, TYPE6.DBS, and REDOX.DBS, as described below and on pg. 15. Database modification methods are described in the user's manual.

Unfortunately, MINTEQA2 requires databases have the original names for use by the codes, and version numbers have not been added.
Petition for data exemption is attached below:
Radionuclide/Radioelement log k values are attached to the opposite page.

Memorandum

To: Wesley C. Patrick (Technical Director)
and Bruce E. Mabrito (Director of Quality Assurance)

From: David R. Turner DRT

Subject: Exemption for qualification of data in the MINTEQA2/PRODEFA2 software package

Date: May 7, 1992

The MINTEQA2/PRODEFA2 geochemical speciation code is under continuing development at the Environmental Research Laboratory of the U. S. Environmental Protection Agency in Athens, Georgia. Version 3.0 will be used in research and technical assistance activities at the Center for Nuclear Waste Regulatory Analyses, and it is anticipated that updated versions will be incorporated and evaluated as they become available. The PRODEFA2 code is the preprocessor used to prepare input files for the MINTEQA2 code, and as such does not directly use any geochemical data. As it is currently constructed, the MINTEQA2 code uses extensive databases to provide the information necessary in calculating equilibrium species distribution between liquid, solid, and gas phases from well established thermodynamic principles. The purpose of this memorandum is to petition for exclusion and exemption of these existing data from qualification requirements under Quality Assurance Procedure QAP-015.

Section 5.1.3 in QAP-015 provides for the exclusion of existing data from qualification if "The existing data were generated by the DOE or its contractors and the purpose of the Center activity or project is to provide an independent evaluation of that data" and/or "The existing data are being used as a basis of comparison in confirmatory research or other evaluations". The original MINTEQ code was developed at Pacific Northwest Laboratory and funded in part by the DOE. Much of the original data are based on the U. S. Geological Survey's WATEQ3 code, which has been used extensively in the scientific community and is well documented. At CNWRA, the MINTEQA2 database has also been expanded to include radioelement data from the EQ3/6 software package, also developed by the DOE. In addition, many of the data in the MINTEQA2 database (such as molecular weights and species charge) "... are accepted in the scientific and engineering community as established fact.", the third criteria justifying exclusion from qualification (Section 5.1.3).

Section 5.3 in QAP-015 also permits exemption of existing data from qualification where "In certain circumstances, programmatic requirements and constrains or other factors may make it necessary to use data which are not qualified". If such data are used in Center reports, a clear statement on the qualification status of the data is to be provided. Progress in numerous research and technical assistance activities at the CNWRA requires the use of geochemical data. While some of the data in the MINTEQA2 database are recognized by the scientific and engineering community as uncertain, they represent the current best estimates in the evolving state of geochemical data. Even though activities at CNWRA may address the state-of-the-art in geochemical data in narrowly defined areas, it is beyond the scope of the CNWRA program and resources to do so for all of the data in the MINTEQA2/PRODEFA2 package, which currently includes data for over 1200 species involving more than 125 components.

Concurrence	Approval	Approval
5/8/92	5/8/92	5/8/92
John L. Russell Element Manager	Wesley C. Patrick Technical Director	Bruce E. Mabrito Director of Quality Assurance

Radionuclide data added to MINTEQA2 database 12/17/92

```
0401400 Am(CO3)2-1        2.464     13.3000                  -1.   4.0  0.0  363.0184
 4.00 2      2.000 140      1.000  40
0401401 AmCO3+1           3.599      8.2600                   1.   4.0  0.0  303.0092
 2.00 2      1.000 140      1.000  40
0401402 Am(CO3)3-3                    14.9500                  -3.   4.0  0.0  423.0276
 6.00 2      3.000 140      1.000  40
0401800 AmCl+2           -3.703      1.1002                   2.   4.5  0.0  278.4527
       2      1.000 180      1.000  40
0401801 AmCl2+1          -7.65       1.5628                   1.   4.0  0.0  313.9054
       2      2.000 180      1.000  40
0402700 AmF+2             1.671      4.2881                   2.   4.5  0.0  261.9984
       2      1.000 270      1.000  40
0402701 AmF2+1            4.424      7.3740                   1.   4.0  0.0  280.9968
       2      2.000 270      1.000  40
0402702 AmF3                         10.5626                  0.   3.0  0.0  299.9952
       2      3.000 270      1.000  40
0404920 AmNO3+2                       1.1530                   2.   4.5  0.0  305.0049
       2      1.000 492      1.000  40
0404921 Am(NO3)2+1                    1.6610                   1.   4.0  0.0  367.0099
       2      2.000 492      1.000  40
0400020 Am(OH)+2         13.831      -6.5900                   2.   4.5  0.0  260.0073
       3      1.000   2      1.000  40    -1.000 330
0400021 Am(OH)2+1        18.758     -15.9902                   1.   4.0  0.0  277.0147
       3      2.000   2      1.000  40    -2.000 330
0400022 Am(OH)3          22.545     -23.7852                   0.   3.0  0.0  294.0220
       3      3.000   2      1.000  40    -3.000 330
0407320 Am(SO4)+1         5.124      3.6137                   1.   4.0  0.0  339.0636
       2      1.000 732      1.000  40
0407321 Am(SO4)2-1       10.764      5.0280                  -1.   4.0  0.0  435.1272
       2      2.000 732      1.000  40
0405800 Am(H2PO4)+2                   22.2760                  2.   4.5  0.0  339.9872
       3      1.000 580      1.000  40     2.000 330
0405801 Am(H2PO4)2+1                  42.8148                  1.   4.0  0.0  436.9745
       3      2.000 580      1.000  40     4.000 330
0405802 Am(H2PO4)3                    63.3391                  0.   3.0  0.0  533.9617
       3      3.000 580      1.000  40     6.000 330
0405803 Am(H2PO4)4-1                  83.4380                 -1.   4.0  0.0  630.9490
       3      4.000 580      1.000  40     8.000 330
0421400 Am(O2)HCO3                    12.629                   0.   3.0  0.0  336.0159
 1.00 3      1.000  42      1.000 140     1.000 330
1351300 CoBr2            -0.135      -0.0358                  0.   3.0  0.0  218.7412
       2      1.000 135      2.000 130
1351800 CoCl +1          41.066       0.1547                  1.   4.0  0.0   94.3859
       2      1.000 135      1.000 180
1357300 CoHS +1                       5.9813                  1.   4.0  0.0   92.0052
       2      1.000 135      1.000 730
1357301 Co(HS)2                       9.0306                  0.   3.0  0.0  125.0772
       2      1.000 135      2.000 730
1353800 CoI2              0.759      -0.0944                  0.   3.0  0.0  312.7421
       2      1.000 135      2.000 380
1354920 CoNO3 +1                      0.2000                  1.   4.0  0.0  120.9381
       2      1.000 135      1.000 492
1350020 CoOH +1          13.732      -10.0149                 1.   4.0  0.0   75.9405
       3      1.000 135      1.000 002    -1.000 330
1350021 Co(OH)2                      -18.8000                 0.   3.0  0.0   92.9479
       3      1.000 135      2.000 002    -2.000 330
1350022 Co(OH)4 -2                   -45.7804                -2.   4.0  0.0  126.9626
       3      1.000 135      4.000 002    -4.000 330
1350023 Co2(OH)3 +1                  -11.2000                 1.   4.0  0.0  168.8884
       3      2.000 135      3.000 002    -3.000 330
1350024 Co4(OH)4 +4                  -30.3804                 4.   5.5  0.0  303.7622
       3      4.000 135      4.000 002    -4.000 330
1357320 CoS2O3                        42.3035                 0.   3.0  0.0  171.0634
       5      1.000 135      2.000 732    10.000 330  8.000 001    -5.000 002
1357321 CoSO4             0.094       0.0436                  0.   3.0  0.0  154.9948
       2      1.000 135      1.000 732
1357620 CoSeO4                        2.7000                  0.   3.0  0.0  201.8908
       2      1.000 135      1.000 762
2201300 CsBr              2.62       -0.2712                  0.   3.0  0.0  212.8094
       2      1.000 220      1.000 130
2201800 CsCl              0.653      -0.1385                  0.   3.0  0.0  168.3581
       2      1.000 220      1.000 180
2203800 CsI              -1.57        0.2639                  0.   3.0  0.0  259.8099
       2      1.000 220      1.000 380
2611300 EuBr  +2                      0.5572                  2.   4.5  0.0  231.8690
       2      1.000 261      1.000 130
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2611301 EuBr2 +1                0.2145                  1.   4.0  0.0  311.7730
      2     1.000 261     2.000 130
2611302 EuBrO3 +2             -141.5895                 2.   4.5  0.0  279.8672
      5     1.000 261     1.000 130     3.000 002    -6.000 330    -6.000 001
2611400 EuCO3 +1                7.8005                  1.   4.0  0.0  211.9744
2.000 2     1.000 261     1.000 140
2611401 Eu(CO3)2 -1             12.2583                 -1.   4.0  0.0  271.9838
4.000 2     1.000 261     2.000 140
2611402 Eu(CO3)3 -3             14.1709                 -3.   4.0  0.0  331.9932
6.000 2     1.000 261     3.000 140
2611403 Eu(HCO3) +2             11.9225                  2.   4.5  0.0  212.9823
1.000 3     1.000 261     1.000 140     1.000 330
2611404 EuOHCO3                  1.8347                  0.   3.0  0.0  228.9817
3.000 4     1.000 261     1.000 002     1.000 140    -1.000 330
2611405 EuOH(CO3)2-2             5.4816                 -2.   4.0  0.0  288.9911
5.000 4     1.000 261     1.000 002    -1.000 330     2.000 140
2611406 Eu(OH)2CO3-1            -7.5174                 -1.   4.0  0.0  245.9891
4.000 4     1.000 261     2.000 002     1.000 140    -2.000 330
2611800 EuCl +2               0.023     0.6915                2.   4.5  0.0  187.4177
      2     1.000 261     1.000 180
2611801 EuCl2 +1                0.2553                  1.   4.0  0.0  222.8704
      2     1.000 261     2.000 180
2612700 EuF +2                  3.6416                  2.   4.5  0.0  170.9634
      2     1.000 261     1.000 270
2612701 EuF2 +1                 6.0854                  1.   4.0  0.0  189.9618
      2     1.000 261     2.000 270
2613800 EuIO3 +2              2.829     2.156                 2.   4.5  0.0  326.8677
      2     1.000 261     1.000 381
2614920 EuNO3 +2                1.0392                  2.   4.5  0.0  213.9699
      2     1.000 261     1.000 492
2613300 EuOH +2                -7.8214                  2.   4.5  0.0  168.9723
      3     1.000 261     1.000 002    -1.000 330
2613301 Eu(OH)2 +1             -14.8609                 1.   4.0  0.0  185.9797
      3     1.000 261     2.000 002    -2.000 330
2613302 Eu(OH)3                -24.1253                 0.   3.0  0.0  202.9870
      3     1.000 261     3.000 002    -3.000 330
2613303 Eu(OH)4 -1             -36.5958                -1.   4.0  0.0  219.9944
      3     1.000 261     4.000 002    -4.000 330
2613304 Eu2(OH)2 +4             -6.9182                 4.   5.5  0.0  337.9447
      3     2.000 261     2.000 002    -2.000 330
2617320 EuSO4 +1              4.192     3.9029                1.   4.0  0.0  248.0266
      2     1.000 261     1.000 732
2617321 Eu(SO4)2 -1           6.129     5.4693               -1.   4.0  0.0  344.0882
      2     1.000 261     2.000 732
5500020 Np(OH)+2             11.976    -7.0000                2.   4.5  0.0  254.0553
      3     1.000   2     1.000 550    -1.000 330
5505800 Np(H2PO4)+2         -11.888    21.9300                2.   4.5  0.0  334.0351
      3     1.000 580     1.000 550     2.000 330
5505801 Np(H2PO4)2+         -27.057    42.7500                1.   4.0  0.0  431.0222
      3     2.000 580     1.000 550     4.000 330
5505802 Np(H2PO4)3          -45.253    64.1800                0.   3.0  0.0  528.0093
      3     3.000 580     1.000 550     6.000 330
5511400 Np(CO3)5-6            4.599    38.3000               -6.   4.0  0.0  537.0940
10.00 2     5.000 140     1.000 551
5511800 NpCl+3                4.873     0.2000                3.   5.0  0.0  272.5007
      2     1.000 180     1.000 551
5511801 NpCl2+2              22.614    -0.1000                2.   4.5  0.0  307.9534
      2     2.000 180     1.000 551
5512700 NpF+3                -0.818     8.7000                3.   5.0  0.0  256.0464
      2     1.000 270     1.000 551
5512701 NpF2+2                1.449    15.4000                2.   4.5  0.0  275.0448
      2     2.000 270     1.000 551
5513300 Np(OH)+3             12.192    -1.0000                3.   5.0  0.0  254.0553
      3     1.000   2     1.000 551    -1.000 330
5513301 Np(OH)2+2            18.42     -2.8000                2.   4.5  0.0  271.0620
      3     2.000   2     1.000 551    -2.000 330
5513302 Np(OH)3+1            23.792    -5.8000                1.   4.0  0.0  288.0699
      3     3.000   2     1.000 551    -3.000 330
5513303 Np(OH)4              26.193    -9.6000                0.   3.0  0.0  305.0772
      3     4.000   2     1.000 551    -4.000 330
5513304 Np(OH)5-1            29.109   -14.3000               -1.   4.0  0.0  322.0847
      3     5.000   2     1.000 551    -5.000 330
5515800 Np(HPO4)+2           -1.71     25.2200                2.   4.5  0.0  333.0272
      3     1.000 580     1.000 551     1.000 330
5515801 Np(HPO4)2           -15.449    48.0400                0.   3.0  0.0  429.0064
      3     2.000 580     1.000 551     2.000 330
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5515802 Np(HPO4)3-2   -21.533    70.3700                -2.  4.0  0.0  524.9856
      3     3.000 580     1.000 551     3.000 330
5515803 Np(HPO4)4-4   -30.085    92.4900                -4.  4.0  0.0  620.9648
      3     4.000 580     1.000 551     4.000 330
5515804 Np(HPO4)5-6   -37.532   113.610                 -6.  4.0  0.0  716.9440
      3     5.000 580     1.000 551     5.000 330
5517320 Np(SO4)+2       4.959     5.5000                 2.  4.5  0.0  333.1116
      2     1.000 732     1.000 551
5517321 Np(SO4)2        9.565     9.9000                 0.  3.0  0.0  429.1752
      2     2.000 732     1.000 551
5521400 NpO2(CO3)-1    13.018     4.6000                -1.  4.0  0.0  329.0560
 2.00 2     1.000 140     1.000 552
5521401 NpO2(CO3)2-3    6.876     7.0000                -3.  4.0  0.0  389.0652
 4.00 2     2.000 140     1.000 552
5521402 NpO2(CO3)3-5    6.237     8.5000                -5.  4.0  0.0  449.0744
 6.00 2     3.000 140     1.000 552
5521800 NpO2Cl          3.696    -0.4000                 0.  3.0  0.0  304.4995
      2     1.000 180     1.000 552
5522700 NpO2F           8.19      1.0000                 0.  3.0  0.0  288.0452
      2     1.000 270     1.000 552
5523300 NpO2(OH)       10.427    -8.9000                 0.  3.0  0.0  286.0541
      3     1.000   2     1.000 552    -1.000 330
5525800 NpO2(H2PO4)    16.844    20.1300                 0.  3.0  0.0  366.0339
      3     1.000 580     1.000 552     2.000 330
5525801 NpO2(HPO4)-1    8.405    15.8200                -1.  4.0  0.0  365.0260
      3     1.000 580     1.000 552     1.000 330
5527320 NpO2(SO4)-1     4.576     0.4000                -1.  4.0  0.0  365.1104
      2     1.000 732     1.000 552
5531400 NpO2(CO3)2-2    6.662    14.0000                -2.  4.0  0.0  389.0652
 4.00 2     2.000 140     1.000 553
5531401 NpO2(CO3)3-4   -9.783    20.4000                -4.  4.0  0.0  449.0744
 6.00 2     3.000 140     1.000 553
5531800 NpO2Cl+1        2.871    -0.2000                 1.  4.0  0.0  304.4995
      2     1.000 180     1.000 553
5532700 NpO2F+1         0.215     4.6000                 1.  4.0  0.0  288.0452
      2     1.000 270     1.000 553
5532701 NpO2F2          0.63      7.8000                 0.  3.0  0.0  307.0436
      2     2.000 270     1.000 553
5533300 NpO2(OH)+1     10.368    -5.2000                 1.  4.0  0.0  286.0541
      3     1.000   2     1.000 553    -1.000 330
5533301 (NpO2)2(OH)2   10.921    -6.4000                 2.  4.5  0.0  572.1082
      3     2.000   2     2.000 553    -2.000 330
5533302 (NpO2)3(OH)5   26.937   -17.5000                 1.  4.0  0.0  892.1769
      3     5.000   2     3.000 553    -5.000 330
5535800 NpO2(H2PO4)   -36.956    21.8300                 1.  4.0  0.0  366.0339
      3     1.000 580     1.000 553     2.000 330
5535801 NpO2(HPO4)     -5.061    20.5200                 0.  3.0  0.0  365.0260
      3     1.000 580     1.000 553     1.000 330
5537320 NpO2(SO4)       4.753     3.3000                 0.  3.0  0.0  365.1104
      2     1.000 732     1.000 553
6401800 PuCl+2                    0.0017                 2.  4.5  0.0  279.4527
      2     1.000 180     1.000 640
6403300 Pu(OH)+2       12.79     -7.9680                 2.  4.5  0.0  261.0073
      3     1.000   2     1.000 640    -1.000 330
6405800 Pu(H2PO4)+2     3.322    22.0035                 2.  4.5  0.0  340.9871
      3     1.000 580     1.000 640     2.000 330
6407320 Pu(SO4)+        3.492     3.4935                 1.  4.0  0.0  340.0636
      2     1.000 732     1.000 640
6407321 Pu(SO4)2-                 3.39                  -1.  4.0  0.0  436.1272
      2     2.000 732     1.000 640
6411800 PuCl+3          3.984     0.1435                 3.  5.0  0.0  279.4527
      2     1.000 180     1.000 641
6412700 PuF+3           5.091     8.4600                 3.  5.0  0.0  262.9984
      2     1.000 270     1.000 641
6412701 PuF2+2                   15.4000                 2.  4.5  0.0  281.9968
      2     2.000 270     1.000 641
6412702 PuF3+                     5.3000                 1.  4.0  0.0  300.9952
      2     3.000 270     1.000 641
6412703 PuF4                      4.2000                 0.  3.0  0.0  319.9936
      2     4.000 270     1.000 641
6413300 Pu(OH)+3       11.516    -0.5048                 3.  5.0  0.0  261.0073
      3     1.000   2     1.000 641    -1.000 330
6413301 Pu(OH)2+2      17.77     -2.3235                 2.  4.5  0.0  278.0146
      3     2.000   2     1.000 641    -2.000 330
6413302 Pu(OH)3+1      23.084    -5.2810                 1.  4.0  0.0  295.0219
      3     3.000   2     1.000 641    -3.000 330
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6413303 Pu(OH)4         26.08      -9.5174                0.   3.0  0.0  312.0292
      3     4.000   2     1.000 641     -4.000 330
6413304 Pu(OH)5-1       30.037     -14.9802               -1.   4.0  0.0  329.0365
      3     5.000   2     1.000 641     -5.000 330
6415800 Pu(HPO4)+2       6.12       25.3321               2.   4.5  0.0  339.9792
      3     1.000 580     1.000 641      1.000 330
6415801 Pu(HPO4)2       -0.83       48.4919               0.   3.0  0.0  435.9583
      3     2.000 580     1.000 641      2.000 330
6415802 Pu(HPO4)3-2    -12.092      70.4253               -2.   4.0  0.0  531.9375
      3     3.000 580     1.000 641      3.000 330
6415803 Pu(HPO4)4-4    -32.572      92.5339               -4.   4.0  0.0  627.9166
      3     4.000 580     1.000 641      4.000 330
6417320 Pu(SO4)+2        2.95        5.7710               2.   4.5  0.0  340.0636
      2     1.000 732     1.000 641
6417321 Pu(SO4)2         9.806      10.2456               0.   3.0  0.0  436.1272
      2     2.000 732     1.000 641
6423300 PuO2(OH)        16.486      -9.6323               0.   3.0  0.0  293.0061
      3     1.000   2     1.000 642     -1.000 330
6431400 PuO2(CO3)(aq                12.7000               0.   0.0  0.0  336.0080
 2.00 2     1.000 140     1.000 643
6431401 PuO2(CO3)2-2     5.485      14.9148               -2.   4.0  0.0  396.0172
 4.00 2     2.000 140     1.000 643
6431402 PuO2(CO3)3-4    -9.304      18.5000               -4.   0.0  0.0  456.0264
 6.00 2     3.000 140     1.000 643
6431800 PuO2Cl+1         2.78       -0.2084               1.   4.0  0.0  311.4515
      2     1.000 180     1.000 643
6432700 PuO2F+1         -1.241       5.6674               1.   4.0  0.0  294.9972
      2     1.000 270     1.000 643
6432701 PuO2F2          -3.69       10.9669               0.   3.0  0.0  313.9956
      2     2.000 270     1.000 643
6432702 PuO2F3-1        -7.016      15.9160               -1.   4.0  0.0  332.9940
      2     3.000 270     1.000 643
6432703 PuO2F4-2        -9.54       18.7628               -2.   3.0  0.0  351.9924
      2     4.000 270     1.000 643
6433300 PuO2(OH)+1      10.823      -5.6379               1.   4.0  0.0  293.0061
      3     1.000   2     1.000 643     -1.000 330
6433301 (PuO2)2(OH)2    13.83       -8.2626               2.   4.5  0.0  586.0122
      3     2.000   2     2.000 643     -2.000 330
6433302 (PuO2)3(OH)5    33.335     -21.6550               1.   4.0  0.0  913.0329
      3     5.000   2     3.000 643     -5.000 330
6433303 PuO2(OH)2(aq                -11.9000               0.   0.0  0.0  310.0134
      3     2.000   2     1.000 643     -2.000 330
6433304 (PuO2)(OH)3-                -20.7000               -1.   0.0  0.0  327.0208
      3     3.000   2     1.000 643     -3.000 330
6433305 (PuO2)2(OH)+  207.367       -4.3000               3.   0.0  0.0  569.0049
      3     1.000   2     2.000 643     -1.000 330
6435800 PuO2(H2PO4)+    -5.1        23.5277               1.   4.0  0.0  372.9859
      3     1.000 580     1.000 643      2.000 330
6437320 PuO2(SO4)        4.8         3.2658               0.   3.0  0.0  372.0624
      2     1.000 732     1.000 643
6901800 RuCl +1                     -0.4887               1.   4.0  0.0  136.5227
      2     1.000 690     1.000 180
6907320 RuSO4                        2.3547               0.   3.0  0.0  197.1316
      2     1.000 690     1.000 732
6911800 RuCl +2                      2.1742               2.   4.5  0.0  136.5227
      2     1.000 691     1.000 180
6911801 RuCl2 +1                     3.7527               1.   4.0  0.0  171.9754
      2     1.000 691     2.000 180
6911802 RuCl3                        4.2976               0.   3.0  0.0  207.4281
      2     1.000 691     3.000 180
6911803 RuCl4 -1                     4.1418               -1.   4.0  0.0  242.8808
      2     1.000 691     4.000 180
6911804 RuCl5 -2                     3.8457               -2.   4.0  0.0  278.3335
      2     1.000 691     5.000 180
6911805 RuCl6 -3                     3.4446               -3.   4.0  0.0  313.7862
      2     1.000 691     6.000 180
6913300 RuOH +2                     -2.2392               2.   4.5  0.0  118.0773
      3     1.000 691     1.000 002     -1.000 330
6913301 Ru(OH)2 +1                  -3.5148               1.   4.0  0.0  135.0847
      3     1.000 691     2.000 002     -2.000 330
6917320 RuSO4 +1                     1.9518               1.   4.0  0.0  197.1316
      2     1.000 691     1.000 732
6917321 Ru(SO4)2 -1                  3.0627               -1.   4.0  0.0  293.1932
      2     1.000 691     2.000 732
6923300 Ru4(OH)12+4                  7.1960               4.   5.5  0.0  608.3681
      3     4.000 692     4.000 002     -4.000 330
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6921800 Ru(OH)2Cl+1                1.3858          1.   4.0  0.0  170.5374
     2     1.000 692      1.000 180
6921801 Ru(OH)2Cl2                 1.8081          0.   3.0  0.0  205.9901
     2     1.000 692      2.000 180
6921802 Ru(OH)2Cl3-1               1.6172         -1.   4.0  0.0  241.4428
     2     1.000 692      3.000 180
6921803 Ru(OH)2Cl4-2               2.7052         -2.   4.0  0.0  276.8955
     2     1.000 692      4.000 180
6927320 Ru(OH)2SO4                 1.7941          0.   3.0  0.0  231.1463
     2     1.000 692      1.000 732
7801800 SnCl +1         2.511      1.0500          1.   4.0  0.0  154.1627
     2     1.000 780      1.000 180
7801801 SnCl2           2.931      1.7100          0.   3.0  0.0  189.6154
     2     1.000 780      2.000 180
7801802 SnCl3 -1        5.173      1.6900         -1.   4.0  0.0  225.0681
     2     1.000 780      3.000 180
7802700 SnF +1         -1.056      4.0800          1.   4.0  0.0  137.7084
     2     1.000 780      1.000 270
7802701 SnF2           -0.063      6.6800          0.   3.0  0.0  156.7068
     2     1.000 780      2.000 270
7802702 SnF3 -1        -7.346      9.4600         -1.   4.0  0.0  175.7052
     2     1.000 780      3.000 270
7803300 SnOH +1         4.943     -3.9851          1.   4.0  0.0  135.7173
     3     1.000 780      1.000 002    -1.000 330
7803301 Sn(OH)2        10.05      -7.9102          0.   3.0  0.0  152.7247
     3     1.000 780      2.000 002    -2.000 330
7803302 Sn(OH)3 -1     22.633    -17.4053         -1.   4.0  0.0  169.7320
     3     1.000 780      3.000 002    -3.000 330
7813300 SnOH +3        -1.196      0.6049          3.   5.0  0.0  135.7173
     3     1.000 781      1.000 002    -1.000 330
7813301 Sn(OH)2 +2     -0.482     -0.1902          2.   4.5  0.0  152.7247
     3     1.000 781      2.000 002    -2.000 330
7813302 Sn(OH)3 +1     -1.887      0.5147          1.   4.0  0.0  169.7320
     3     1.000 781      3.000 002    -3.000 330
7813303 Sn(OH)4        -2.642      0.8496          0.   3.0  0.0  186.7394
     3     1.000 781      4.000 002    -4.000 330
7817320 Sn(SO4)2                  -0.8072          0.   3.0  0.0  310.8372
     2     1.000 781      2.000 732
7817321 SnSO4 +2                  -3.1094          2.   4.5  0.0  214.7736
     2     1.000 781      1.000 732
8001400 SrCO3(aq)                  2.8653          0.   0.0  0.0  147.6292
 2.00 2    1.000 800      1.000 140
8001800 SrCl+                     -0.2485          1.   4.0  0.0  123.0730
     2     1.000 800      1.000 180
8002700 SrF+                       0.1393          1.   4.0  0.0  106.6184
     2     1.000 800      1.000 270
8004920 SrNO3+                     0.800           1.   4.0  0.0  149.6249
     2     1.000 800      1.000 492
8003300 SrOH+                    -13.29            1.   4.0  0.0  104.6273
     3     1.000 800      1.000 002    -1.000 330
8005800 SrPO4-                     5.48           -1.   4.0  0.0  182.5914
     2     1.000 800      1.000 580
8005801 SrHPO4(aq)                14.406           0.   3.0  0.0  183.5993
     3     1.000 800      1.000 580     1.000 330
8005802 SrH2PO4+                  20.2834          1.   4.0  0.0  184.6073
     3     1.000 800      1.000 580     2.000 330
8005803 SrP2O7-2                   1.6561         -2.   4.0  0.0  261.5633
     4     1.000 800      2.000 580     2.000 330  -1.000 002
8007320 SrSO4(aq)                  2.30            0.   3.0  0.0  183.6776
     2     1.000 800      1.000 732
8001431 SrFe(CN)6-    -69.8300    55.6181   0.000  0.000-1.00 0.00 0.00 299.5734
 0.00 3    1.000 800      1.000 281     6.000 143
8610020 ((TcO(OH)2)2              -0.1271          0.   3.0  0.0  296.0282
     3     4.000    2     2.000 861    -4.000 330
8610021 TcO(OH)2                  -3.3221          0.   3.0  0.0  148.0140
     3     2.000    2     1.000 861    -2.000 330
8610022 TcO(OH)+                  -1.3355          1.   4.0  0.0  131.0067
     3     1.000    2     1.000 861    -1.000 330
8633300 HTcO4-                     8.7070         -1.   0.0  0.0  163.0055
     2     1.000 330      1.000 863
8633301 H2TcO4                     9.0050          0.   0.0  0.0  164.0135
     2     2.000 330      1.000 863
8643300 HTcO4                      1.1600          0.   0.0  0.0  163.0055
     2     1.000 330      1.000 864
8661800 ThCl +3         0.019      0.9533          3.   5.0  0.0  267.4908
     2     1.000 866      1.000 180
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8661801 ThCl2 +2        20.906     0.6755                2.   4.5  0.0  302.9435
      2     1.000 866     2.000 180
8661802 ThCl3 +1        15.769     1.4972                1.   4.0  0.0  338.3962
      2     1.000 866     3.000 180
8661803 ThCl4                      1.0728                0.   3.0  0.0  373.8489
      2     1.000 866     4.000 180
8662700 ThF +3          -1.161     7.8722                3.   5.0  0.0  251.0365
      2     1.000 866     1.000 270
8662701 ThF2 +2         -1.851    14.0881                2.   4.5  0.0  270.0349
      2     1.000 866     2.000 270
8662702 ThF3 +1         -2.787    18.7353                1.   4.0  0.0  289.0333
      2     1.000 866     3.000 270
8662703 ThF4            -3.533    22.1511                0.   3.0  0.0  308.0317
      2     1.000 866     4.000 270
8663300 ThOH +3          5.982    -3.8874                3.   5.0  0.0  249.0454
      3     1.000 866     1.000 002    -1.000 330
8663301 Th(OH)2 +2      14.023    -7.1071                2.   4.5  0.0  266.0528
      3     1.000 866     2.000 002    -2.000 330
8663302 Th(OH)3 +       20.348   -11.70                  1.   0.0  0.0  283.0602
      3     1.000 866     3.000 002    -3.000 330
8663303 Th(OH)4 aq      27.24    -15.9000                0.   3.0  0.0  300.0675
      3     1.000 866     4.000 002    -4.000 330
8663304 Th2(OH)2 +6     15.23     -6.4624                6.   6.0  0.0  498.0909
      3     2.000 866     2.000 002    -2.000 330
8663305 Th4(OH)8 +8     58.619   -21.7581                8.   6.0  0.0 1064.2111
      3     4.000 866     8.000 002    -8.000 330
8663306 Th6(OH)15+9    109.531   -37.7046                9.   6.0  0.0 1647.3387
      3     6.000 866    15.000 002  -15.000 330
8665800 Th(H2PO4)2+2    -6.44     47.8503                2.   4.5  0.0  426.0123
      3     1.000 866     2.000 580     4.000 330
8665801 Th(HPO4)2      -10.287    47.3372                0.   3.0  0.0  423.9964
      3     1.000 866     2.000 580     2.000 330
8665802 Th(HPO4)3 -2   -19.66     68.1545               -2.   4.0  0.0  519.9755
      3     1.000 866     3.000 580     3.000 330
8665803 ThH3PO4 +4      12.38     23.4412                4.   5.5  0.0  330.0331
      3     1.000 866     1.000 580     3.000 330
8665804 ThH2PO4 +3      11.59     24.0276                3.   5.0  0.0  329.0252
      3     1.000 866     1.000 580     2.000 330
8667320 ThSO4 +2         3.91      5.3140                2.   4.5  0.0  328.1017
      2     1.000 866     1.000 732
8667321 Th(SO4)2         7.709     9.6167                0.   3.0  0.0  424.1653
      2     1.000 866     2.000 732
8667322 Th(SO4)3 -2     11.88     10.4010               -2.   4.0  0.0  520.2289
      2     1.000 866     3.000 732
8667323 Th(SO4)4 -4     13.37      8.3999               -4.   4.0  0.0  616.2925
      2     1.000 866     4.000 732
8911300 UBr +3                     1.4250                3.   5.0  0.0  317.9329
      2     1.000 891     1.000 130
8911400 U(CO3)4 -4                32.8272               -4.   4.0  0.0  478.0665
 8.00 2     1.000 891     4.000 140
8911401 U(CO3)5 -6      -4.766    33.9269               -6.   4.0  0.0  538.0759
10.00 2     1.000 891     5.000 140
8911800 UCl +3          -4.537     1.7082                3.   5.0  0.0  273.4820
      2     1.000 891     1.000 180
8912700 UF +3           -1.336     9.2413                3.   5.0  0.0  257.0274
      2     1.000 891     1.000 270
8912701 UF2 +2          -0.903    16.1403                2.   4.5  0.0  276.0258
      2     1.000 891     2.000 270
8912702 UF3 +1           0.036    21.4818                1.   4.0  0.0  295.0242
      2     1.000 891     3.000 270
8912703 UF4 AQ          -0.972    25.3412                0.   3.0  0.0  314.0226
      2     1.000 891     4.000 270
8912704 UF5 -1           4.38     26.8110               -1.   4.0  0.0  333.0210
      2     1.000 891     5.000 270
8912705 UF6 -2           3.29     28.8414               -2.   4.0  0.0  352.0194
      2     1.000 891     6.000 270
8913800 UI +3                      1.2152                3.   5.0  0.0  364.9334
      2     1.000 891     1.000 380
8914920 UNO3 +3                    1.4514                3.   5.0  0.0  300.0338
      2     1.000 891     1.000 492
8914921 U(NO3)2 +2                 2.2617                2.   4.5  0.0  362.0387
      2     1.000 891     2.000 492
8913300 UOH +3          11.205    -0.5381                3.   5.0  0.0  255.0364
      3     1.000 891     1.000   2    -1.000 330
8913301 U(OH)2 +2       20.434    -2.270                 2.   0.0  0.0  272.0437
      3    -2.000 330     1.000 891     2.000   2
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8913302 U(OH)3 +1       26.651    -4.935                  1.   0.0  0.0  289.0511
      3     1.000 891     3.000   2    -3.000 330
8913303 U(OH)4 AQ       28.798    -4.5577                 0.   0.0  0.0  306.0586
      3     1.000 891     4.000   2    -4.000 330
8913304 U(OH)5 -1       30.245   -13.120                 -1.   0.0  0.0  323.0659
      3     1.000 891     5.000   2    -5.000 330
8913305 U6(OH)15+9              -17.229                  9.   0.0  0.0 1683.2846
      3     6.000 891    15.000   2   -15.000 330
8917320 USO4 +2         36.961     6.5016                 2.   4.5  0.0  334.0906
      2     1.000 891     1.000 732
8917321 U(SO4)2 AQ       7.946    10.3507                 0.   3.0  0.0  430.1522
      2     1.000 891     2.000 732
8921400 UO2(CO3)3 -5             7.3898                 -5.   4.0  0.0  450.0559
 6.00 2     1.000 893     3.000 140
8931300 UO2Br +1                 0.1731                  1.   4.0  0.0  349.9317
      2     1.000 893     1.000 130
8931400 UO2CO3 AQ        1.202    9.6147                 0.   3.0  0.0  330.0372
 2.00 2     1.000 893     1.000 140
8931401 UO2CO3)2-2       4.297   16.9698                -2.   4.0  0.0  390.0465
 4.00 2     1.000 893     2.000 140
8931402 UO2CO3)3-4      -9.281   21.5846                -4.   4.0  0.0  450.0559
 6.00 2     1.000 893     3.000 140
8931403 UO2)3CO3)6     -16.323   53.9127                -6.   4.0  0.0 1170.1395
12.00 2     3.000 893     6.000 140
8931404 UO2)CO3OH)               36.2277                -2.   4.0  0.0 3534.4492
12.00 4    11.000 893     6.000 140    12.000 002   -12.000 330
8931405 UO2)2CO3OH)3   -14.394   -0.8969                -1.   4.0  0.0  651.0868
 2.00 4     2.000 893     1.000 140     3.000 002    -3.000 330
8931406 UO2OHCO2                 0.7066                  1.   4.0  0.0  939.1296
 2.00 4     3.000 893     1.000 140     4.000 002    -3.000 330
8931800 UO2Cl +1         1.921    0.1567                 1.   4.0  0.0  305.4808
      2     1.000 893     1.000 180
8931801 UO2Cl2           3.593   -1.1257                 0.   3.0  0.0  340.9331
      2     1.000 893     2.000 180
8932700 UO2F +1          0.413    5.0497                 1.   4.0  0.0  289.0262
      2     1.000 893     1.000 270
8932701 UO2F2 AQ         0.513    8.5394                 0.   3.0  0.0  308.0246
      2     1.000 893     2.000 270
8932702 UO2F3 -1         0.575   10.7800                -1.   4.0  0.0  327.0230
      2     1.000 893     3.000 270
8932703 UO2F4 -2         0.088   11.5403                -2.   4.0  0.0  346.0214
      2     1.000 893     4.000 270
8934920 UO2NO3 +1                0.2801                  1.   4.0  0.0  332.0326
      2     1.000 893     1.000 492
8933300 UO2OH +1        10.325   -5.2080                 1.   0.0  0.0  287.0352
      3     1.000 893     1.000   2    -1.000 330
8933301 UO2(OH)2        18.094  -10.3221                 0.   3.0  0.0  304.0424
      3     1.000 893     2.000 002    -2.000 330
8933302 UO2(OH)3 -1             -19.2222                -1.   4.0  0.0  321.0497
      3     1.000 893     3.000 002    -3.000 330
8933303 UO2(OH)4 -2             -33.0294                -2.   4.0  0.0  338.0571
      3     1.000 893     4.000 002    -4.000 330
8933304 UO2)2OH +3               -2.7091                 3.   5.0  0.0  557.0627
      3     2.000 893     1.000 002    -1.000 330
8933305 UO2)2OH2+2       9.000   -5.6368                 2.   4.5  0.0  574.0703
      3     2.000 893     2.000   2    -2.000 330
8933306 UO2)3OH)4               -11.9312                 2.   4.5  0.0  878.1125
      3     3.000 893     4.000 002    -4.000 330
8933307 UO2)3OH5+1      23.224  -15.5895                 1.   4.0  0.0  895.1203
      3     3.000 893     5.000   2    -5.000 330
8933308 UO2)3OH)7               -31.0542                -1.   4.0  0.0  929.1345
      3     3.000 893     7.000 002    -7.000 330
8933309 UO2)4OH)7               -21.9540                 1.   4.0  0.0 1199.1622
      3     4.000 893     7.000 002    -7.000 330
8935800 UO2HPO4 AQ      -2.03    21.2298                 0.   3.0  0.0  366.0072
      3     1.000 893     1.000 580     1.000 330
8935801 UO2H2PO4+1      -3.66    23.9926                 1.   4.0  0.0  367.0151
      3     1.000 893     1.000 580     2.000 330
8935802 UO2H2PO4)2      79.15    46.6163                 0.   3.0  0    464.002
      3     1.000 893     2.000 580     4.000 330
8935803 UO2H2PH3P +1             47.4362                 1.   4.0  0.0  465.007
      3     1.000 893     2.000 580     5.000 330
8935804 UO2H3PO4 2               23.6405                 2.   4.5  0.0  368.0229
      3     1.000 893     1.000 580     3.000 330
8935805 UO2PO4 -1                14.8528                -1.   4.0  0.0  364.9991
      2     1.000 893     1.000 580
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8937320 UO2SO4 AQ       4.738     3.0632                    0.   3.0  0.0  366.0894
      2     1.000 893     1.000 732
8937321 UO2SO4)2-2      8.523     3.9796                   -2.   4.0  0.0  462.1510
      2     1.000 893     2.000 732
8937700 UO2H3SIO4                -2.4                       1.   0.0  0.0  365.135
      3     1.000 893     1.000 770    -1.000 330
9102700 ZrF +3                    8.5835                    3.   5.0  0.0  110.2224
      2     1.000 910     1.000 270
9102701 ZrF2 +2                  15.7377                    2.   4.5  0.0  129.2208
      2     1.000 910     2.000 270
9102702 ZrF3 +1                  21.2792                    1.   4.0  0.0  148.2192
      2     1.000 910     3.000 270
9102703 ZrF4                     25.9411                    0.   3.0  0.0  167.2176
      2     1.000 910     4.000 270
9102704 ZrF5  -1                 30.3098                   -1    4.0  0.0  186.2160
      2     1.000 910     5.000 270
9102705 ZrF6 -2                  34.0188                   -2.   4.0  0.0  205.2144
      2     1.000 910     6.000 270
9103300 ZrOH +3                   0.0457                    3.   5.0  0.0  108.2297
      2     1.000 910     1.000 002    -1.000 330
9103301 Zr(OH)2 +2                0.2385                    2.   4.5  0.0  125.2387
      3     1.000 910     2.000 002    -2.000 330
9103302 Zr(OH)3 +1               -0.6693                    1.   4.0  0.0  142.2460
      3     1.000 910     3.000 002    -3.000 330
9103303 Zr(OH)4                  -1.4666                    0.   3.0  0.0  159.2534
      3     1.000 910     4.000 002    -4.000 330
9107320 ZrSO4 +2                  3.6064                    2.   4.5  0.0  187.2876
      2     1.000 910     1.000 732
9107321 Zr(SO4)2                  6.2965                    0.   3.0  0.0  283.3512
      2     1.000 910     2.000 732
9107322 Zr(SO4)3 -2               7.3007                   -2.   4.0  0.0  379.4148
      2     1.000 910     3.000 732
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Data Sources
12/17/92 Database

AQUEOUS SPECIES	LOGK REF
Am(CO3)2-	86KER/SIL
AmCO3+	86KER/SIL
Am(CO3)3 -3	86KER/SIL
AmNO3 +2	84KER
Am(NO3)2+	84KER
Am(OH) +2	86KER/SIL
Am(OH)2+	86KER/SIL
Am(OH)3 (aq)	86KER/SIL
Am(SO4)+	84KER
Am(SO4)2-	84KER
AmCl +2	84KER
AmCl2+	84KER
AmF +2	84KER
AmF2+	84KER
AmF3 (aq)	84KER
Am(H2PO4) +2	84KER
Am(H2PO4)2+	84KER
Am(H2PO4)3 (aq)	84KER
Am(H2PO4)4-	84KER
AmO2HCO3	84KER
Co(HS)2 (aq)	74NAU/RYZ
Co(OH)2 (aq)	76BAE/MES
Co(OH)4 -2	76SMI/MAR
Co2(OH)3+	76BAE/MES
Co4(OH)4 +4	76SMI/MAR
CoBr2 (aq)	82WAG/EVA
CoCl+	74NAU/RYZ
CoHS+	74NAU/RYZ
CoI2 (aq)	82WAG/EVA
CoNO3+	76SMI/MAR
CoOH+	SUPCRT91
CoS2O3 (aq)	74NAU/RYZ
CoSeO4 (aq)	76SMI/MAR
CoSO4 (aq)	82WAG/EVA
CsBr	SUPCRT91
CsCl	SUPCRT91
CsI	SUPCRT91
Eu(CO3)-	87RAR2
Eu(CO3)3 -3	87RAR2
Eu(HCO3) +2	87RAR2
EuOH(CO3)2 -2	87RAR2
Eu(OH)2+	87RAR2
Eu(OH)2CO3 -1	87RAR2
Eu(OH)3 (aq)	87RAR2
Eu(OH)4-	87RAR2
EuOHCO3 (aq)	87RAR2
Eu(SO4)2-	85RAR2
Eu2(OH)2 +4	87RAR2
EuBr +2	85RAR2
EuBr2+	85RAR2
EuBrO3 +2	85RAR2
EuCl +2	85RAR2
EuCl2+	85RAR2
EuCO3+	87RAR2
EuF +2	85RAR2
EuF2+	85RAR2
EuIO3 +2	85RAR2
EuNO3 +2	85RAR2
EuOH +2	87RAR2
EuSO4+	85RAR2
Np(OH) +2	84LEM
Np(H2PO4) +2	84LEM
Np(H2PO4)2+	84LEM
Np(H3PO4)3 (aq)	84LEM
Np(CO3)5 -6	84LEM
Np(OH) +3	84LEM
Np(OH)2 +2	84LEM
Np(OH)3+	84LEM
Np(OH)4 (aq)	84LEM

Np(OH5)-	84LEM
Np(SO4) +2	84LEM
Np(SO4)2 (aq)	84LEM
NpCl +3	84LEM
NpCl2 +2	84LEM
NpF +3	84LEM
NpF2 +2	84LEM
Np(HPO4) +2	84LEM
Np(HPO4)2 (aq)	84LEM
Np(HPO4)3 -2	84LEM
Np(HPO4)4 -4	84LEM
Np(HPO4)5 -6	84LEM
NpO2(CO3)-	84LEM
NpO2(CO3)2 -3	84LEM
NpO2(CO3)3 -5	84LEM
NpO2OH (aq)	84LEM
NpO2(SO4)-	84LEM
NpO2Cl (aq)	84LEM
NpO2F (aq)	84LEM
NpO2(H2PO4) (aq)	84LEM
NpO2(HPO4)-	84LEM
NpO2(CO3)2 -2	84LEM
NpO2(CO3)3 -4	84LEM
NpO2OH+	84LEM
(NpO2)2(OH)2 +2	84LEM
(NpO2)3(OH)5+	84LEM
NpO2(SO4) (aq)	84LEM
NpO2Cl+	84LEM
NpO2F+	84LEM
NpO2F2 (aq)	84LEM
NpO2(H2PO4)+	84LEM
NpO2(HPO4) (aq)	84LEM
Pu(OH) +2	80LEM/TRE
PuSO4+	80LEM/TRE
Pu(SO4)2-	CHEMVAL
Pu(H2PO4) +2	80LEM/TRE
PuCl +2	82SCH/FEL
Pu(OH) +3	80LEM/TRE
Pu(OH)2 +2	80LEM/TRE
Pu(OH)3+	80LEM/TRE
Pu(OH)4 (aq)	80LEM/TRE
Pu(OH)5-	80LEM/TRE
PuSO4 +2	80LEM/TRE
Pu(SO4)2 (aq)	80LEM/TRE
PuCl +3	82SCH/FEL
PuF +3	84NAS/CLE
PuF2 +2	84NAS/CLE
PuF3+	84NAS/CLE
PuF4 (aq)	84NAS/CLE
Pu(HPO4) +2	80LEM/TRE
Pu(HPO4)2 (aq)	80LEM/TRE
Pu(HPO4)3 -2	80LEM/TRE
Pu(HPO4)4 -4	80LEM/TRE
PuO2(OH) (aq)	80LEM/TRE
PuO2(CO3) (aq)	80LEM/TRE
PuO2(CO3)2 -2	80LEM/TRE
PuO2(CO3)3 -4	80LEM/TRE
PuO2OH+	80LEM/TRE
(PuO2)2(OH)2 +2	80LEM/TRE
(PuO2)3(OH)5+	80LEM/TRE
PuO2(OH)2 (aq)	80LEM/TRE
PuO2(OH)3-	80LEM/TRE
(PuO2)2(OH) +3	80LEM/TRE
PuO2SO4 (aq)	80LEM/TRE
PuO2Cl+	80LEM/TRE
PuO2F+	80LEM/TRE
PuO2F2 (aq)	80LEM/TRE
PuO2F3-	80LEM/TRE
PuO2F4 -2	80LEM/TRE
PuO2(H2PO4)+	80LEM/TRE
RuCl +2	85RAR1
RuCl2+	85RAR1
RuCl3 (aq)	85RAR1
RuCl4-	85RAR1

RuCl5 -2	85RAR1
RuCl6 -3	85RAR1
RuOH +2	85RAR1
Ru(OH)2+	85RAR1
RuSO4+	85RAR1
Ru(SO4)2-	85RAR1
RuCl+	85RAR1
RuSO4 (aq)	85RAR1
Ru(OH)2Cl+	85RAR1
Ru(OH)2Cl2 (aq)	85RAR1
Ru(OH)2Cl3-	85RAR1
Ru(OH)2Cl4 -2	85RAR1
Ru(OH)2SO4 (aq)	85RAR1
Ru4(OH)12 +4	85RAR1
Sn(OH)2 (aq)	84JAC/HEL
Sn(OH)3-	84JAC/HEL
SnOH+	84JAC/HEL
SnCl+	84JAC/HEL
SnCl2 (aq)	84JAC/HEL
SnCL3-	84JAC/HEL
SnF +	84JAC/HEL
SnF2 (aq)	84JAC/HEL
SnF3-	84JAC/HEL
Sn(OH)2 +2	84JAC/HEL
Sn(OH)3+	84JAC/HEL
Sn(OH)4 (aq)	82WAG/EVA
SnOH +3	84JAC/HEL
SnSO4 +2	82WAG/EVA
SrCl+	SUPCRT91
SrCO3 (aq)	SUPCRT91
SrF+	SUPCRT91
SrH2PO4+	76SMI/MAR
SrHPO4	76SMI/MAR
SrNO3+	76SMI/MAR
SrOH+	76BAE/MES
SrP2O7 -2	76SMI/MAR
SrPO4-	76SMI/MAR
SrSO4 (aq)	83REA
(TcO(OH)2)2	83RAR
TcO(OH)2	83RAR
TcO(OH)+	83RAR
HTcO4-	83RAR
H2TcO4 (aq)	83RAR
HTcO4 (aq)	88PHI
ThH3PO4 +4	80LAN/HER
ThH2PO4 +3	80LAN/HER
Th(H2PO4)2 +2	80LAN/HER
Th(HPO4)2 (aq)	80LAN/HER
Th(HPO4)3 -2	80LAN/HER
Th(OH)2 +2	80LAN/HER
Th(OH)3+	80LAN/HER
Th(OH)4 (aq)	76BAE/MES
Th(SO4)2 (aq)	80LAN/HER
Th(SO4)3 -2	80LAN/HER
Th(SO4)4 -4	80LAN/HER
Th2(OH)2 +6	80LAN/HER
Th4(OH)8 +8	80LAN/HER
Th6(OH)15 +9	80LAN/HER
ThCl +3	80LAN/HER
ThCl2 +2	80LAN/HER
ThCl3+	80LAN/HER
ThCl4 (aq)	80LAN/HER
ThF +3	80LAN/HER
ThF2 +2	80LAN/HER
ThF3+	80LAN/HER
ThF4 (aq)	80LAN/HER
ThOH +3	82WAG/EVA
ThSO4 +2	80LAN/HER
UOH +3	92NEA
U(OH)2 +2	90NEA
U(OH)3+	90NEA

U(OH)4 (aq)	90NEA
U(OH)5-	90NEA
U6(OH)15	92NEA
UF +3	92NEA
UF2 +2	92NEA
UF3+	92NEA
UF4 (aq)	92NEA
UF5-	92NEA
UF6 -2	92NEA
UCl +3	92NEA
UBr +3	92NEA
UI +3	92NEA
U(CO3)4 -4	92NEA
U(CO3)5 -6	92NEA
UNO3 +3	92NEA
U(NO3)2 +2	92NEA
USO4 +2	92NEA
U(SO4)2 (aq)	92NEA
UO2(CO3)3 -5	92NEA
UO2OH+	92NEA
UO2(OH)2 (aq)	92NEA
UO2(OH)3-	92NEA
UO2(OH)4 -2	92NEA
(UO2)2OH +3	92NEA
(UO2)2(OH)2 +2	92NEA
(UO2)3(OH)4 +2	92NEA
(UO2)3(OH)5+	92NEA
(UO2)3(OH)7-	92NEA
(UO2)4(OH)7+	92NEA
UO2F+	92NEA
UO2F2 (aq)	92NEA
UO2F3-	92NEA
UO2F4 -2	92NEA
UO2CL+	92NEA
UO2Cl2 (aq)	92NEA
UO2Br+	92NEA
UO2CO3 (aq)	92NEA
UO2(CO3)2 -2	92NEA
UO2(CO3)4 -4	92NEA
(UO2)2(CO3)6 -6	92NEA
(UO2)11(CO3)6(OH)12 -2	90NEA
(UO2)2CO3(OH)3-	90NEA
UO2OHCO2+	90NEA
UO2NO3+	92NEA
UO2SO4 (aq)	92NEA
UO2(SO4)2 -2	92NEA
UO2HPO4 (aq)	90NEA
UO2H2PO4+	90NEA
UO2(H2PU4)2 (aq)	90NEA
UO2(H2PO4)(H3PO4)+	90NEA
UO2H3PO4 +2	90NEA
UO2PO4-	90NEA
UO2H3SiO4	90NEA
Zr(OH)3+	74NAU/RYZ
Zr(OH)4 (aq)	74NAU/RYZ
Zr(SO4)2 (aq)	74NAU/RYZ
Zr(SO4)3 -2	74NAU/RYZ
ZrF +3	74NAU/RYZ
ZrF2 +2	74NAU/RYZ
ZrF3+	74NAU/RYZ
ZrF4 (aq)	74NAU/RYZ
ZrF5-	74NAU/RYZ
ZrF6 -2	74NAU/RYZ
ZrOH +3	74NAU/RYZ
ZrSO4 +2	74NAU/RYZ
Zr(OH)2 +2	74NAU/RYZ

SOLIDS	LOGK REF
Am (c)	76OET/RAN
Am(OH)3 (s)	86KER/SIL
Am(OH)3 (am)	86KER/SIL
AmOHCO3 (s)	86KER/SIL

Co(c)	79ROB/HEM
CoS	74NAU/RYZ
Co(OH)2	76BAE/MES
CoFe2O4	74NAU/RYZ
CoO	82WAG/EVA
CoCO3	84SVE
CoCl2	82WAG/EVA
CoCl2:2H2O	82WAG/EVA
CoCl2:6H2O	82WAG/EVA
CoF2	82WAG/EVA
CoF3	79KUB/ALC
Co(NO3)2	65GAR/CHR
CoSO4	82WAG/EVA
CoSO4:3CoOH2	82WAG/EVA
CoSO4:6H2O	82WAG/EVA
CoSO4:H2O	74NAU/RYZ
CoSeO3	76SMI/MAR
Co2SiO4	82WAG/EVA,74NAU/RYZ
Co3(PO4)2	82WAG/EVA
CoHPO4	82WAG/EVA
Co3(AsO4)2	82WAG/EVA
Cs(c)	89COX/WAG
Cs2U2O7	90NEA
Cs2U4O12	90NEA
Eu(c)	85RAR2
EuS	85RAR2
Eu(OH)2Cl	85RAR2
Eu(OH)3	87RAR2
Eu2O3(cubic)	85RAR2
Eu2O3(mono)	85RAR2
Eu3O4	85RAR2
EuO	85RAR2
EuOCl	87RAR2
EuBr3	85RAR2
EuCl2	87RAR2
EuCl3	85RAR2
EuCl3:6H2O	85RAR2
EuF3:5H2O	85RAR2
Eu(IO3)3:2H2O	85RAR2
Eu2(CO3)3:3H2O	87RAR2
Eu(NO3)3:6H2O	85RAR2
Eu2(SO4)3:8H2O	85RAR2
EuSO4	85RAR2
Np(c)	84LEM
NaNpO2CO3:3.5H2O	84LEM
Np(OH)4	84LEM
NpO2	84LEM
Np(HPO4)2	84LEM
NpO2(OH) (am)	84LEM
Np2O5	84LEM
NpO2(OH)2	84LEM
Pu(OH)3	80LEM/TRE
Beta-Pu2O3	80LEM/TRE
PuF3	80LEM/TRE
Pu(c)	86MOR
Pu(OH)4	80LEM/TRE
PuO2	80LEM/TRE
PuF4	80LEM/TRE
Pu(HPO4)2	80LEM/TRE
PuO2(OH) (am)	80LEM/TRE
PuO2(OH)2	80LEM/TRE
PuO2(HPO4)	80LEM/TRE
Ra (c)	82WAG/EVA
Ra(NO3)2	82WAG/EVA
RaCl2:2H2O	82WAG/EVA
RaSO4	82WAG
Ru(c)	85RAR1
Ru(OH)3:H2O	85RAR1
RuO2:2H2O	85RAR1
RuO2	85RAR1

RuBr3	85RAR1
RuCl3	85RAR1
RuI3	85RAR1
Sn(c)	SUPCRT91
Sn2S3(Ottemanite)	79KUB/ALC
Sn3S4	79KUB/ALC
Sn(OH)2	82WAG/EVA
Romarchite(SnO)	SUPCRT91
Cassiterite(SnO2)	SUPCRT91
SnBr2	79KUB/ALC
SnBr4	82WAG/EVA
SnCl2	79KUB/ALC
Sn(SO4)2	79KUB/ALC
Sn(SO4)	79KUB/ALC
SnSe	79KUB/ALC
SnSe2	79KUB/ALC
Sr(c)	79ROB/HEM
Sr(NO3)2	79ROB/HEM
Sr(NO3)2:4H2O	82WAG/EVA
Sr(OH)2	85CHA/DAV
Sr2SIO4	77BAR/KNA
SrSiO3	82WAG/EVA
SrBr2	82WAG/EVA
SrBr2:H2O	82WAG/EVA
SrBr2:6H2O	82WAG/EVA
SrCl2	82WAG/EVA
SrCl2:H2O	82WAG/EVA
SrCl2:2H2O	82WAG/EVA
SrCl2:6H2O	82WAG/EVA
SrI2	79KUB/ALC
SrF2	76SMI/MAR
SrHPO4	82WAG/EVA
SrO	82WAG/EVA
SrS	82WAG/EVA
SrZrO3	74NAU/RYZ
Strontianite	SUPCRT91
Celestite	SUPCRT91
KTcO4	83RAR
NaTcO4	83RAR
Tc(OH)2	83RAR
Tc(OH)3	83RAR
Tc3O4	83RAR
TcS2	83RAR
TcOH	83RAR
TcO2:2H2O (am)	83RAR
Tc4O7	83RAR
TcS3	83RAR
TcO3	83RAR
Tc(c)	83RAR
Tc2S7	83RAR
Th(c)	89COX/WAG
Th2S3	82WAG/EVA
Th7S12	82WAG/EVA
ThS2	82WAG/EVA
Th(OH)4	74NAU/RYZ
ThO2	89COX/WAG
ThBr4	82WAG/EVA
ThCl4	80LAN/HER
ThF4	80LAN/HER
ThF4:2.5H2O	82WAG/EVA
ThI4	82WAG/EVA
Th(NO3)4:5H2O	82WAG/EVA
Th(SO4)2	82WAG/EVA
Th2Se3	74MIL
Autunite	90SVE
H-Autunite	90NEA
K-Autunite	90SVE
Na-Autunite	90SVE
Sr-Autunite	78LAN
USb2	
U3Sb4	

Ningoyite	78LAN
Uramphite	78LAN
Saleeite	90SVE
Uranocirite	78LAN
Bassetite	78LAN
Torbernite	90SVE
Przhevalskite	78LAN
Uranophane	78LAN
UBr2Cl	90NEA
UBr3	90NEA
UCl3	90NEA
UBrCl2	90NEA
UOCl	90NEA
UF3	90NEA
UI3	90NEA
UO2 (am)	90NEA
U4O9 (c)	78LAN
U3O8 (c)	90NEA
UBr4	90NEA
UOBr2	90NEA
UBr3Cl	90NEA
UBrCl3	90NEA
UCl4	90NEA
UBr2Cl2	90NEA
UOCl2	90NEA
U2O2Cl5	90NEA
UF4 (c)	90NEA
UF4:2.5H2O	90NEA
U2F9	90NEA
U4F17	89NEA
UClF3	90NEA
UCl2F2	90NEA
UCl3F	90NEA
UOF2	90NEA
UOF2:H2O	90NEA
UOFOH	90NEA
UI4	90NEA
UClI3	90NEA
UCl2I2	90NEA
UCl3I	90NEA
U(CO3)2	90NEA
U(OH)2SO4	90NEA
U(SO4)2	90NEA
U(SO4)2:4H2O	90NEA
U(SO4)2:8H2O	90NEA
U(HPO4)2:4H2O	90NEA
Coffinite	90NEA
Na3UO4	90NEA
UBr5	90NEA
UOBr3	90NEA
UCl5	90NEA
UOCl3	90NEA
UO2Cl	90NEA
U5O12Cl	90NEA
Alpha-UF5	90NEA
Beta-UF5	90NEA
UPO5	90NEA
Beta-UO2(OH)2	90NEA
Schoepite	90NEA
Dehyd-Schoep(.393)	88OHA/LEW
Dehyd-Schoep(.648)	88OHA/LEW
Dehyd-Schoep(.850)	88OHA/LEW
Dehyd-Schoep(.900)	90NEA
Dehyd-Schoep(1.00)	88OHA/LEW
Uraninite	90NEA
Alpha-UO3	90NEA
Beta-UO3	90NEA
Gamma-UO3	90NEA
Gummite	78LAN
K2UO4	90NEA
Li2UO4	90NEA
Na2U2O7	90NEA
Alpha-Na2UO4	90NEA
BaUO4	90NEA
CaUO4	90NEA
MgUO4	90NEA

NaUO3	90NEA
NaUO2(CO3)3	90NEA
Rb2UO4	90NEA
Alpha-SrUO4	90NEA
UO2Br2	90NEA
UO2Br2:H2O	90NEA
UO2Br2:3H2O	90NEA
UO2BrOH:2H2O	90NEA
UCl6	90NEA
UO2Cl2	90NEA
UO2Cl2:H2O	90NEA
UO2Cl2:3H2O	90NEA
UO2ClOH:2H2O	90NEA
(UO2)2Cl3	90NEA
UF6	90NEA
UO2FOH	90NEA
UO2FOH:H2O	90NEA
UO2FOH:2H2O	90NEA
UO2F2	90NEA
UO2F2:3H2O	90NEA
U2O3F6	90NEA
U3O5F8	90NEA
UOF4	90NEA
Rutherfordine	90NEA
UO2(NO3)2	90NEA
UO2(NO3)2:H2O	90NEA
UO2(NO3)2:2H2O	90NEA
UO2(NO3)2:3H2O	90NEA
UO2(NO3)2:6H2O	90NEA
UO2SO4	90NEA
UO2SO4:H2O	64OWE/MAY
UO2SO4:2.5H2O	64OWE/MAY
UO2SO4:3H2O	64OWE/MAY
UO2SO4:3.5H2O	64OWE/MAY
(UO2)3(PO4)2	90NEA
(UO2)3(PO4)2:4H2O	90NEA
(UO2)P2O7	90NEA
Parsonsite	78RIC/NRI
UO2(PO3)2	90NEA
UO2HPO4	84TRI
UO2HPO4:4H2O	90NEA
UP2O7:2OH2O	90NEA
UO2(AsO3)2	90NEA
(UO2)2As2O7	90NEA
(UO2)3(AsO4)2	90NEA
K(UO2)AsO4	82WAG/EVA
Boltwoodite	82HEM
Haiweeite	82HEM
Kasolite	82HEM
Sklodowskite	82HEM
Soddyite	82HEM
Weeksite	82HEM
Tyuyamunite	78LAN
Carnotite	78LAN
Zr(c)	79ROB/HEM
Baddelyite	79ROB/HEM
Zircon	79ROB/HEM

REDOX SPECIES	LOGK REF
Eu+3/Eu+2	SUPCRT91
U+3/UO2+2	90NEA
U+4/UO2+2	90NEA
UO2+/UO2+2	90NEA
Am+4/Am+3	84KER
AmO2+/Am+3	84KER
AmO2+2/Am+3	84KER
Np+3/Np+4	84LEM
NpO2+/Np+4	84LEM
NpO2+2/Np+4	76FUG/OET
Pu+3/Pu+4	80LEM/TRE
PuO2+/Pu+4	80LEM/TRE
PuO2+2/Pu+4	80LEM/TRE

Ru+2/RuO4-2	85RAR1
Ru+3/RuO4-2	85RAR1
Ru(OH)2+2/RuO4-2	85RAR1
RuO4-/RuO4-2	85RAR1
Sn+2/Sn+4	84JAC/HEL
Tc+3/TcO4-	83RAR/84RAR
TcO+2/TcO4-	83RAR/84RAR
TcO4-3/TcO4-	83RAR/84RAR
TcO4-2/TcO4-	83RAR/84RAR
Co+2/Co+3	SUPCRT91

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1/11/94 D.R. Turner — Minor change to MINTEQA2 file COMP.DBS - Zr mistakenly entered as Zr^{2+}. Changed to Zr^{4+} (this matches the charge assumed in the reactions used in THERMO.DBS and TYPE6.DBS) No other changes made at this time to other databases. Corrected versions on disk in back pocket.

1/14/94 D.R. Turner — Changes to databases for Co-solids. Formatting error in THERMO.DBS and TYPE6.DBS. These changes were made so that the stoichiometrics and component IDs were in the appropriate column. UNFRMT program then run to produce THERMO.UNF + TYPE6.UNF. Corrected databases on disk in back pocket. Only cobalt solids data affected

2/1/94 D. Nimmo — Compiled EQMOD, Version 1.1? ,HYDROFLOW (Version 1.1) and HYDROGEOCHEM (Version 5.1) for the IBM 486 PC using the Lahey F77L-EM/32 (Version 5.10) Fortran compilers.

All three codes compiled without fatal error except for HYDROFLOW where the variable TMAX was set on line #460 at 1E50. This exceeds the upper limit of 3.40E38 for real numbers in the Lahey compiler. Resetting TMAX to 1E38 allowed the code to compile and link

These three codes are as distributed in November (1992) by George Yeh, the code author, at Department of Civil Engineering, Penn State Univ, University Park, PA 16802.

(1) EQMOD is a geochemical speciation code, similar in operation to MINTEQA2, only without the nice preprocessing of MINTEQA2/PRODEFA2. EQMOD also does not come with the internal databases like MINTEQA2. The geochemical data and for both the mass balance and mass action must be included in each input file submitted to the system. The format of the input file is discussed in the EQMOD users manual provided with the code + prepared by Dr. Yeh. The code is written in FORTRAN 77
EQMOD forms the basis for the geochemical module in the

coupled hydrogeochemical reactive transport code HYDROGEOCHEM (see below). Running compiled version reproduced EQMOD.OT1 + EQMOD.OT5 sample problems distributed w/ code.

② HYDROFLOW is a finite-element model for groundwater flow through Saturated/Unsaturated Porous Media. HYDROFLOW is a simplified version of the code FEMWATER and provides the hydrologic flow variables required by HYDROGEOCHEM. The code is written in FORTRAN 77. According to the user's manual, HYDROFLOW can account for: 1) treat heterogeneous, anisotropic media, 2) spatially + temporally distributed source/sinks; 3) determine variable BC's of evaporation, infiltration or seepage; 4) check mass balance over entire region @ each time step, and employs a number of different BC's (Cauchy, Neumann, Dirichlet) using a variety of numerical techniques. The formatted input is described by the user's manuals provided by Dr. G. Yeh of Penn State Univ.

2/4/94 DRVerma

③ HYDROGEOCHEM is a reactive transport code developed by George Yeh at Penn State University. The geochemical module is based on EQMOD as described above. The flow module is HYDROFLOW, a simplified version of FEMWATER, also described above

DRVerma

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 4.1: Program structure...) is from the following reference.

HYDROGEOCHEM Users' Manual. Issued November 1992).

DRVerma

EQMOD Description from User's Manual (Issued November, 1992)

HYDROFLOW Description + flow diagram from Users manual (Issued November 1992)

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 2.1: Program structure...) is from the following reference.

HYDROGEOCHEM Users' Manual. Issued November 1992).

Must run first to get flow field for HYDROGEOCHEM

HYDROGEOCHEM - Two-step coupled reactive transport code. Brief description and flow diagram (from November 1992 issue for Version 1.1)

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 4.1: Program structure...) is from the following reference.

HYDROGEOCHEM Users' Manual. Issued November 1992).

02/16/94 D.R. Jenney

Completed modifications to EQMOD.FOR to include an option to read a data file containing the names of the input and output files. To check EQMOD, constructed a set of input files to predict uranium speciation as a function of pH. Compared to EQ3 & MINTEQA2 predictions

$U(VI)_T = 2 \times 10^{-5}$ m
No CO_2
0.1 m $NaNO_3$
pH = 2 to 10

Thermodynamic Data for Uranium from NEA database (Grenthe et al., 1992)

Input example

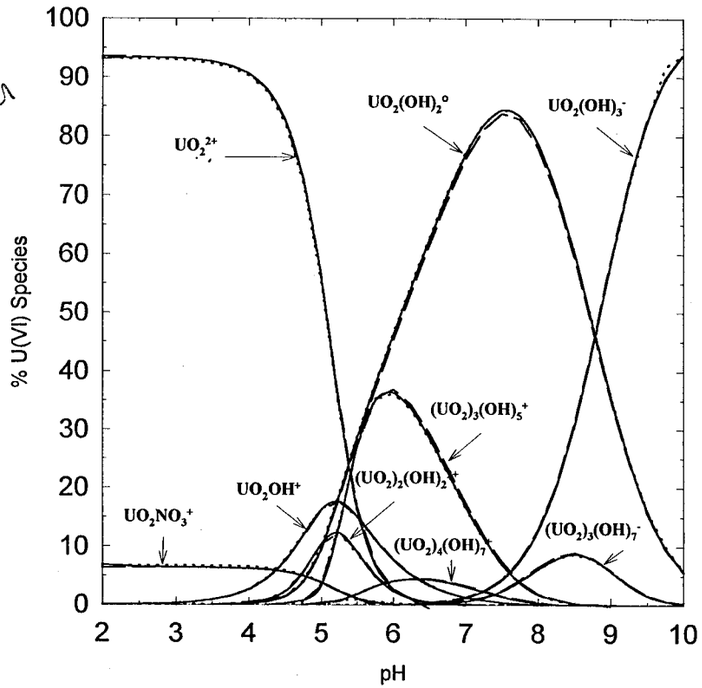
```
   21 Uranium speciation using NEA database: U(total)=2.0 x 10-5 M; pH=7.00    00
C ******* DATA SET 2:  NUMBER OF COMPONENTS, SPECIES, AND TIME INCREMENTS
 4 0 12 0 0 0   NONA NONS NOMX NOMY NOMZ NOMP
C ******* DATA SET 3:  H+, E-, IONIC STRENGTH, AND SORPTION INFORMATION
 0.1 2 3 0 SICOR ICOR LNH LNE
 0.0 0.0 0.0 0.0 298.2 1.0 0 0 0 0  CEC CAP1 CAP2 SREA TEMP PRESU IADS LNO
 -20.0 20.0 0.0 20.0 PEMN PEMX PHMN PHMX
C ******* DATA SET 4:  BASIC AND INTEGER REAL PARAMETERS
 1.0 1.0D-6 4 1 50 10 OMEGA EPS KPR KAU NITER NPCYL
C ******* DATA SET 5:  TOTAL ANALYTICAL CONCENTRATION OF ALL COMPONENTS
Na+                    1.00D-1
UO2+2                  2.00D-5
H+                     0.00D00
NO3-                  1.0004D-1
C ******* DATA SET 6:  COMPONENT SPECIES AND THEIR ION-EXCHANGED SPECIES
FREE NA+                   0
 7.94D-7  1 0 CP(I) VJ(I) IONEX
FREE UO2++                 0
 6.03D-7  2 0 CP(I) VJ(I) IONEX
FREE H+                    3
 1.00D-7  1 0 CP(I) VJ(I) IONEX
FREE NO3-                  0
 3.98D-5 -1 0 CP(I) VJ(I) IONEX
C ******* DATA SET 7:  COMPLEXED SPECIES AND THEIR ION-EXCHANGED SPECIES
OH-                        0
 1.00D-12 -14.00  0  0 -1  0    0    0  0 -1  0  CP(II) PKIPD  AXYZP(I,J) IONEX
UO2NO3+                    0
 1.00D-7    0.28  0  1  0  1    0    0  1  0  1
UO2OH+                     0
 1.00D-7   -5.21  0  1 -1  0    0    0  1 -1  0
UO2(OH)2(aq)               0
 1.00D-9  -10.32  0  1 -2  0    0    0  1 -2  0
UO2(OH)3-                  0
 7.00D-9  -19.22  0  1 -3  0    0    0  1 -3  0
UO2(OH)4--                 0
 3.20D-9  -33.03  0  1 -4  0    0    0  1 -4  0
(UO2)2OH+++                0
 1.00D-9   -2.71  0  2 -1  0    0    0  2 -1  0
(UO2)2(OH)2++              0
 7.00D-9   -5.64  0  2 -2  0    0    0  2 -2  0
(UO2)3(OH)4++              0
 3.20D-9  -11.93  0  3 -4  0    0    0  3 -4  0
(UO2)3(OH)5+               0
 6.80D-8  -15.59  0  3 -5  0    0    0  3 -5  0
(UO2)3(OH)7-               0
 1.00D-7  -31.05  0  3 -7  0    0    0  3 -7  0
(UO2)4(OH)7+               0
 1.00D-7  -21.95  0  4 -7  0    0    0  4 -7  0
                  END OF JOB
```

↑ Log K

D.R. Jenney

Uranium Speciation:

2E-5 M $UO_2(NO_3)_2$; No CO_2; 0.1 M $NaNO_3$



EQMOD ····
MINTEQA2 — — —
EQ3 ——

All speciations calculated using NEA thermodynamic databases for uranium (Grenthe et al 1992)

Agreement is very good considering the complexity of this system, so it seems that EQMOD is installed, compiled, linked, and running properly

3/1/94
D. Turner

Modifications to FIT2DIM to create FIT3DIM.EXE

1) Increased convergence criteria for chemical equilibrium problem
   EPS from 5E-5 to 5E-4
2) Increased convergence criteria for fitting routine
   DEL from 1E-4 to 5E-4
3) Increased ITMAX (number of iterations for convergence of chem equilibrium problem)
   from 30 to 50

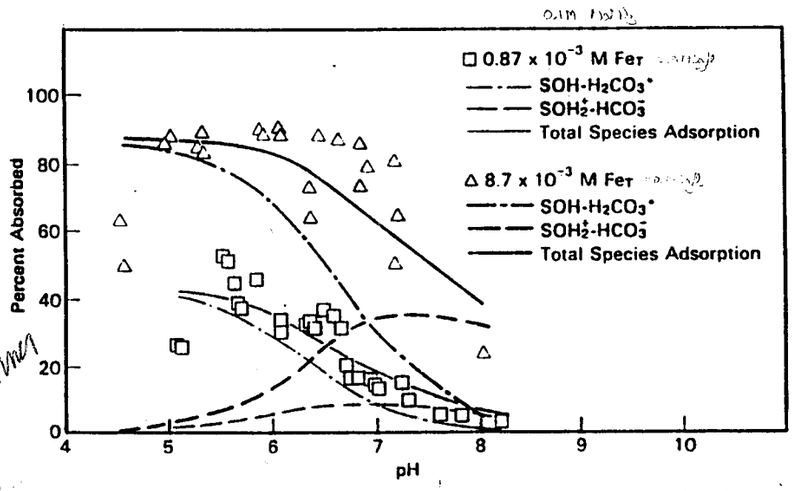
Recompiled using Lahey F77L3-EM32, Version 5.10 for DOS 32 bit. FIT3DIM.EXE. Changes noted in source code. Test files for original FIT2 reproduced.

3/18/94
D. K. Kramer

Carbon sorption on Ferrihydrite

The data come from Zachara et al. (1987) - "Chromate adsorption on Amorphous Iron Oxyhydroxides in the Presence of Major Groundwater Ions" Environ. Science and Technology, Vol. 21, pg. 589-594.

Figure 2 $I = 0.1$ M $NaNO_3$
$A_{SP} = 600$ m²/g (from Davis et al, 1978)
$C(T) = 4.6$ μmol/l $= 4.6 \times 10^{-6}$ M



D. K. Kramer

Figure 2. Closed-system adsorption of carbonate species ($[C_T] = 4.6$

Values digitized from Figure 2 using the Numonics 2200 Digitizing Tablet described on pg. 42 of this notebook. Results are:

Zachara et al.(1987)(Fig. 2)						
C(T)=4.6e-6 mol/l						
Fe(T)=0.87e-3 M = .0773 g/l = 46.4 m2/l						
1st digitiz		2nd digitiz		Avg digitiz		
pH	%C sorbed	pH	%C sorbed	pH	%C sorbed	C srbed (mol/l)
8.23	3.44	8.23	3.39	8.23	3.42	1.5716e-07
7.84	5.20	7.85	5.18	7.84	5.19	2.3870e-07
7.64	5.42	7.64	5.40	7.64	5.41	2.4876e-07
7.33	9.75	7.33	9.85	7.33	9.80	4.5092e-07
7.27	15.09	7.27	15.02	7.27	15.05	6.9242e-07
7.04	13.24	7.04	13.21	7.04	13.22	6.0834e-07
7.01	14.33	7.01	14.31	7.01	14.32	6.5879e-07
6.96	16.00	6.96	15.95	6.96	15.98	7.3505e-07
6.85	16.48	6.84	16.45	6.85	16.46	7.5728e-07
6.77	16.35	6.77	16.32	6.77	16.34	7.5144e-07
6.73	20.14	6.73	20.26	6.73	20.20	9.2928e-07
6.68	31.04	6.68	31.07	6.68	31.05	1.4285e-06
6.61	34.76	6.61	34.73	6.61	34.74	1.5982e-06
6.51	36.45	6.51	36.48	6.51	36.46	1.6773e-06
6.42	30.98	6.42	31.01	6.42	31.00	1.4258e-06
6.38	32.93	6.38	33.05	6.38	32.99	1.5176e-06
6.34	32.10	6.34	32.10	6.34	32.10	1.4768e-06
6.10	29.80	6.10	29.78	6.10	29.79	1.3703e-06
6.09	33.42	6.10	33.42	6.09	33.42	1.5373e-06
5.86	45.54	5.86	45.54	5.86	45.54	2.0948e-06
5.71	36.85	5.71	36.88	5.71	36.86	1.6957e-06
5.68	38.35	5.68	38.32	5.68	38.33	1.7634e-06
5.65	44.36	5.65	44.38	5.65	44.37	2.0411e-06
5.59	50.99	5.58	50.99	5.58	50.99	2.3457e-06
5.54	52.51	5.53	52.54	5.54	52.53	2.4163e-06
5.13	25.33	5.13	25.31	5.13	25.32	1.1647e-06
5.08	25.88	5.08	25.90	5.08	25.89	1.1910e-06
Zachara et al.(1987)(Fig. 2)						
C(T)=4.6e-6 mol/l						
Fe(T)=8.7e-3 M = .773 g/l = 464 m2/l						
pH	%C sorbed	C srbed (mol/l)				
8.05	23.75	3.7043e-07				
7.21	50.29	3.3151e-07				
7.24	64.47	3.3290e-07				
7.21	80.56	3.3154e-07				
6.88	73.01	3.1633e-07				
6.95	78.85	3.1949e-07				
6.88	85.74	3.1639e-07				
6.39	63.77	2.9362e-07				
6.38	72.67	2.9351e-07				
6.66	86.80	3.0657e-07				
6.48	88.02	2.9796e-07				
6.10	87.96	2.8082e-07				
6.09	90.34	2.7993e-07				
5.94	89.16	2.7307e-07				
5.90	89.73	2.7127e-07				
5.35	82.82	2.4616e-07				
5.34	88.84	2.4577e-07				
5.29	84.34	2.4353e-07				
5.03	87.80	2.3146e-07				
4.98	85.46	2.2904e-07				
4.54	62.74	2.0886e-07				
4.58	49.37	2.1056e-07				

Corrected Table on page 68 (next page)

D. K. Kramer

Incorrect formula in spread sheet
(Col A/100)*4.6x10⁻⁶ m/l
should be
(Col B/100)*4.6x10⁻⁶ m

These results will be used together with FITEQL Version 2.0 (Modification FIT3DIM described on pg 66 of this notebook) to determine log K values for $XOH_2 \cdot CO_3^-$; $XOH_2 \cdot HCO_3^0$; $XOH \cdot H_2CO_3^0$.

3/18/94
Central

Correct table digitized results

Zachara et al.(1987)(Fig. 2)						
C(T)=4.6e-6 mol/l						
Fe(T)=0.87e-3 M = .0773 g/l = 46.4 m2/l						
1st digitiz		2nd digitiz		Avg digitiz		
pH	%C sorbed	pH	%C sorbed	pH	%C sorbed	C srbed (mol/l)
8.23	3.44	8.23	3.39	8.23	3.42	1.5716e-07
7.84	5.20	7.85	5.18	7.84	5.19	2.3870e-07
7.64	5.42	7.64	5.40	7.64	5.41	2.4876e-07
7.33	9.75	7.33	9.85	7.33	9.80	4.5092e-07
7.27	15.09	7.27	15.02	7.27	15.05	6.9242e-07
7.04	13.24	7.04	13.21	7.04	13.22	6.0834e-07
7.01	14.33	7.01	14.31	7.01	14.32	6.5879e-07
6.96	16.00	6.96	15.95	6.96	15.98	7.3505e-07
6.85	16.48	6.84	16.45	6.85	16.46	7.5728e-07
6.77	16.35	6.77	16.32	6.77	16.34	7.5144e-07
6.73	20.14	6.73	20.26	6.73	20.20	9.2928e-07
6.68	31.04	6.68	31.07	6.68	31.05	1.4285e-06
6.61	34.76	6.61	34.73	6.61	34.74	1.5982e-06
6.51	36.45	6.51	36.48	6.51	36.46	1.6773e-06
6.42	30.98	6.42	31.01	6.42	31.00	1.4258e-06
6.38	32.93	6.38	33.05	6.38	32.99	1.5176e-06
6.34	32.10	6.34	32.10	6.34	32.10	1.4768e-06
6.10	29.80	6.10	29.78	6.10	29.79	1.3703e-06
6.09	33.42	6.10	33.42	6.09	33.42	1.5373e-06
5.86	45.54	5.86	45.54	5.86	45.54	2.0948e-06
5.71	36.85	5.71	36.88	5.71	36.86	1.6957e-06
5.68	38.35	5.68	38.32	5.68	38.33	1.7634e-06
5.65	44.36	5.65	44.38	5.65	44.37	2.0411e-06
5.59	50.99	5.58	50.99	5.58	50.99	2.3457e-06
5.54	52.51	5.53	52.54	5.54	52.53	2.4163e-06
5.13	25.33	5.13	25.31	5.13	25.32	1.1647e-06
5.08	25.88	5.08	25.90	5.08	25.89	1.1910e-06
Zachara et al.(1987)(Fig. 2)						
C(T)=4.6e-6 mol/l						
Fe(T)=8.7e-3 M = .773 g/l = 464 m2/l						
pH	%C sorbed	C srbed (mol/l)				
8.05	23.75	1.0923e-06				
7.21	50.29	2.3135e-06				
7.24	64.47	2.9654e-06				
7.21	80.56	3.7056e-06				
6.88	73.01	3.3586e-06				
6.95	78.85	3.6272e-06				
6.88	85.74	3.9439e-06				
6.39	63.77	2.9333e-06				
6.38	72.67	3.3430e-06				
6.66	86.80	3.9930e-06				
6.48	88.02	4.0490e-06				
6.10	87.96	4.0462e-06				
6.09	90.31	4.1540e-06				
5.94	88.16	4.0551e-06				
5.90	89.73	4.1274e-06				
5.35	82.82	3.8099e-06				
5.34	88.84	4.0865e-06				
5.29	84.34	3.8798e-06				
5.03	87.80	4.0390e-06				
4.98	85.46	3.9311e-06				
4.54	62.74	2.8861e-06				
4.58	49.37	2.2709e-06				

Calculated values for C srbed (mol/l) for Fe(T)=8.7e-3 M were incorrect.

3/30/94
D.R.Kinn

Modified COMP.DBS to include ClO_4^- and modified THERMO.DBS & REDOX.DBS to include the redox reaction: (For MINTEQA2)

$$Cl^- + 4H_2O = ClO_4^- + 8e^- + 8H^+ \qquad \log k\ (I=0) = -144.7343$$

Data from EQ3/6, Data0.com.R16

CO_3 SORPTION

Result from FITEQL:

DLM (DPJ 3/30)

$$XOH + CO_3^{2-} + H^+ = XOH_2^+ \cdot CO_3^-$$

$$XOH + CO_3^{2-} + 2H^+ = XOH_2 \cdot HCO_3^0$$

	.077 g/l			.773 g/l		
	Log k	V_y	σ	Log k	V_y	σ
$XOH_2CO_3^-$	13.27	203.4	.0066	13.00	63.9	.0083
$XOH_2HCO_3^0$	21.04	749.8	.0057	20.89	627	.0084

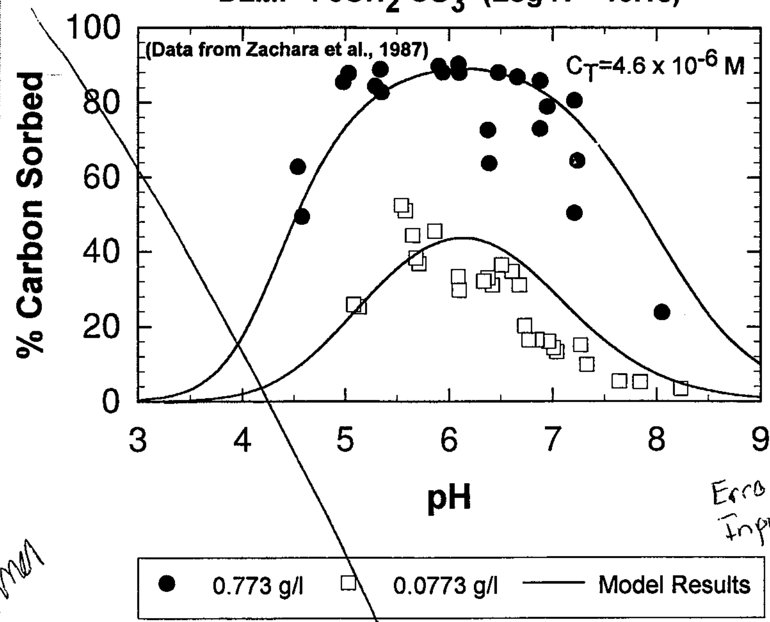
Weighted: (Log k)

$XOH_2CO_3^-$ 13.15

XOH_2HCO_3 20.98

Results

DLM: $>FeOH_2\text{-}CO_3^-$ (Log K = 13.15)

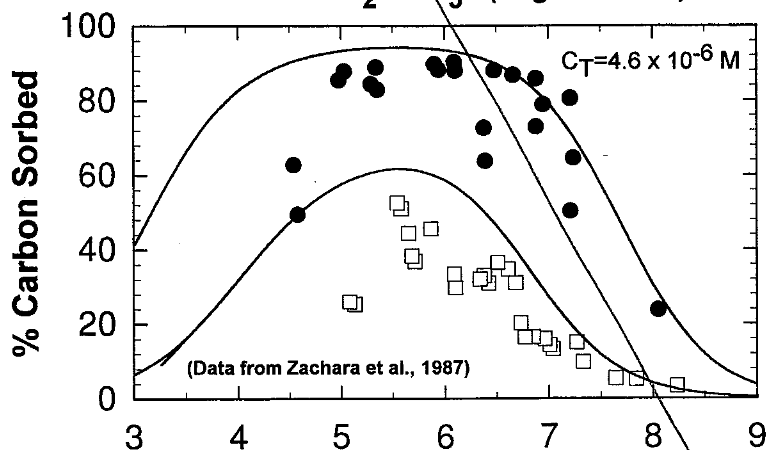


Error in FITEQL Input files. See next page 4/15/44 DBJ

DRJenny

Carbon-Ferrihydrite Sorption

DLM: $>FeOH_2\text{-}HCO_3^o$ (Log K = 20.98)



4/15/94 DRJenny

CO_3 Sorption:

Mistake in FITEQL Input file. Error in stoichiometry for H^+. After correction and application to DLM, CCM, and TLM Models - Following Results:

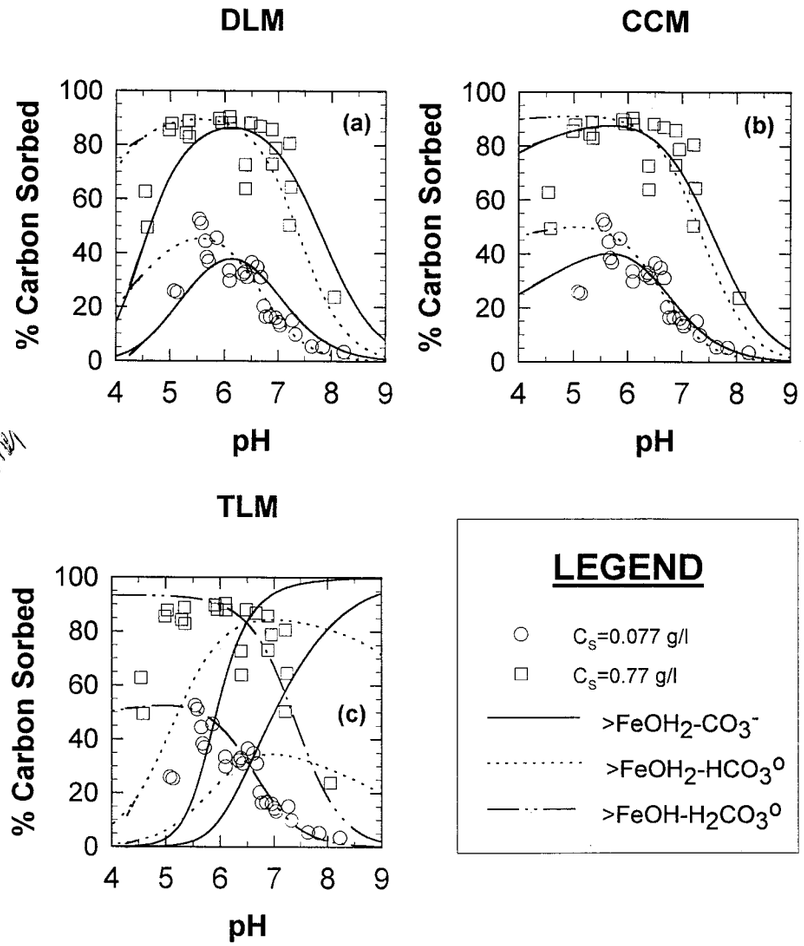
I=0

	DLM			CCM			TLM		
	Log k	V(Y)	σ	Log k	V(Y)	σ	Log k	V(Y)	σ
0.773 g/l									
$XOH_2\text{-}CO_3^-$	13.06	29.3	.0098	13.08	54.7	.0101	17.72	333.2	.0274
$XOH_2\text{-}HCO_3^0$	20.75	66.6	.0112	20.85	84.7	.0119	22.28	239.0	.0112
$XOH\text{-}H_2CO_3^0$	20.75	66.6	.0112	20.85	84.7	.0119	20.84	86.2	.0120
0.0773 g/l									
$XOH_2\text{-}CO_3^-$	13.02	28.1	.0061	13.09	20.3	.0062	13.85	473.3	.0203
$XOH_2\text{-}HCO_3^0$	20.66	26.8	.0064	20.68	38.7	.0065	21.88	200.0	.0065
$XOH\text{-}H_2CO_3^0$	20.66	26.8	.0064	20.68	38.7	.0065	20.66	40.3	.0065
Wtd									
$XOH_2\text{-}CO_3^-$	13.04			13.09			15.48		
$XOH_2\text{-}HCO_3^0$	20.69			20.74			22.03		
$XOH\text{-}H_2CO_3^0$	20.69			20.74			20.72		

The model results are illustrated on the following page.

Carbon-Ferrihydrite Sorption

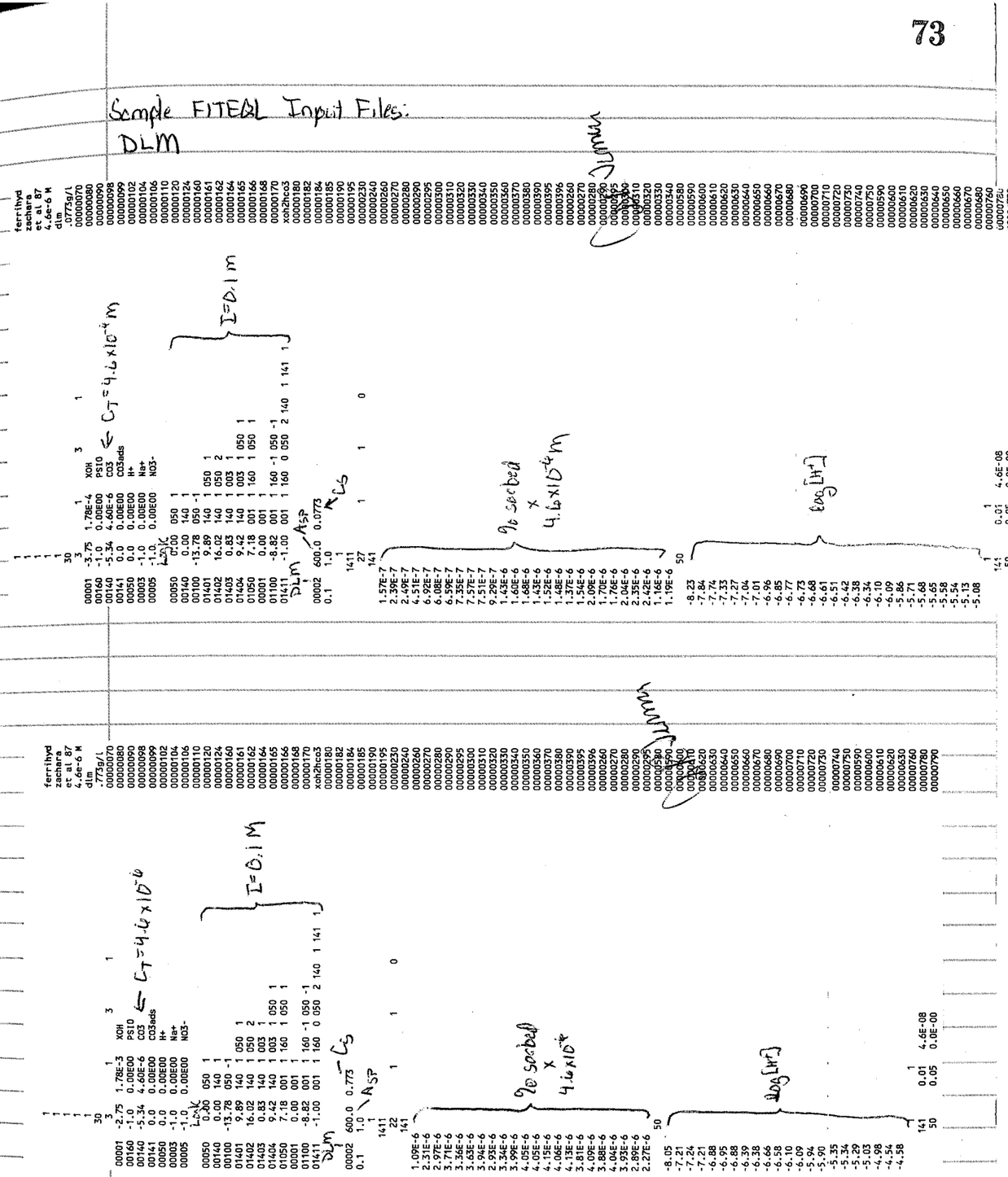
[Data from Zachara et al (1987) - T=25 °C; C_T=4.6x10^{-6} M]



DLM yields best results in terms of picking up low pH data.

Sample FITEQL Input Files:

DLM



Equilibrium constants are from MINTEQA2 database.

4/25/94
D.R. Jenny

Pu - Goethite Sorption

Data are from Sanchez et al. (1985).
Assuming $N_s = 2.31$ sites/nm^2

Equilibrium Constants for Pu^{4+} + PuO_2^+ reactions are taken from MINTEQA2 data base as modified at CNWRA.
Ultimate source of data is EQ3/6, Data0.com.r16

Example FITEQL Input Files

```
-pH
-3.76
-4.04
-5.34
-5.56
-5.87
-6.24
-6.39
-6.68
-7.48
-8.05
-9.08
50

No Surface
x
1E-11
7.29E-14
1.05E-13
8.61E-13
1.06E-12
1.56E-12
2.65E-12
3.51E-12
5.21E-12
8.83E-12
9.72E-12
9.84E-12
50

Corrected from 25°C to 20°C using Van Hoff
00001 -3.98 1.06E-4 XOH
00160 -2.00 0.00E00 PS10
00032 -11.0 1.0E-11 PuO2+ ← Pu(IV)T = 10^-11 M
00033 0.0 0.00E00 PuO2ads
00050 0.0 0.00E00 H+
00003 -1.0 0.00E00 Na+
00005 -1.0 0.00E00 NO3-
00050 0.00 050 1
00032 0.00 032 1
03201 -9.95 032 -1
01050 7.24 001 1 160 1 050 1
01100 -9.06 001 1 160 -1 050 -1
03504 5.60 001 1 160 1 050 0 032 1
DLM
00002 050.0 0.550
0.1 1.0
3304 1
11 1
33 1
1 1 0
0 1 033 1
No error assumed to pH. Helps convergence in extremely dilute solutions.
1
32
0.10 1.0E-16

Goethite Sanchez 2.3s/nm2
00001 -3.98 1.06E-4 XOH
00160 -2.0 0.00E00 PS10
00041 -10. 1.0E-10 Pu+4
00042 0.0 0.00E00 Puads
00050 0.0 0.00E00 H+
00003 -1.0 0.00E00 Na+
00005 -1.0 0.00E00 NO3-
00050 0.00 050 1
00041 0.00 041 1
04101 -1.50 041 1 050 -1
04102 -3.64 041 1 050 -2
04103 -6.89 041 1 050 -3
04104 -11.17 041 1 050 -4
04105 -16.96 041 1 050 -5
01050 -17.24 001 1 160 1 050 1
01100 -9.06 001 1 160 -1 050 -1
00001 0.00 001 1
04207 1.60 001 1 160 2 050 -2 041 1 042 1
00002 50.0 0.550
0.1 1.0
1
4207
9
42 1 0
1
42
0.10 1.0E-13
```

DLM
$XOH\text{-}Pu(OH)_2^{2+}$
A.R. Jenny

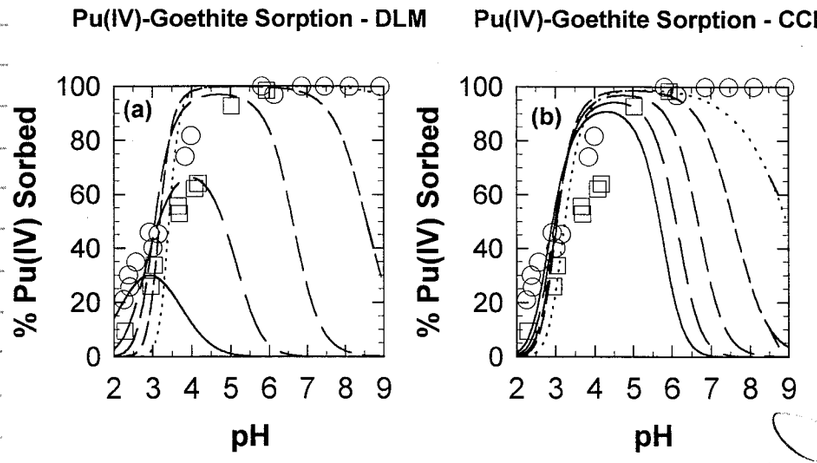
DLM
$XOH_2\text{-}PuO(OH)_3^0$
A.R. Jenny

$Pu(IV)_T = 10^{-11}$ M

```
Goethite Sanchez 2.3s/nm2
00000020
00000030
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
20 deg C
00000140
00000145
00000148
00000150
00000160
00000168
00000170
00000174
00000175
00000180
00000185
00000190
00000195
00000200
00000220
00000230
00000240
00000260
00000280
00000290
00000300
00000310
00000320
00000330
00000340
00000350
00000360
00000400
00000420
00000440
00000460
00000480
00000500
00000520
00000540
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000760
00000880
10%error
```


No error is assigned to pH in FITEQL input files. This is because the concentration is so dilute (10^{-10} + 10^{-11} m) that including pH error on the order of 10^{-4} to 10^{-9} ($\log[H^+]$) leads to a large SOS/DF relative to Pu concentration and the problem will not converge. Removing pH error leads to rapid convergence on the binding constant.

Results (presented) for PuO_2^+ are given on next page. Graphs of predictions as calculated using MINTEQA2 are shown below for Pu^{4+}



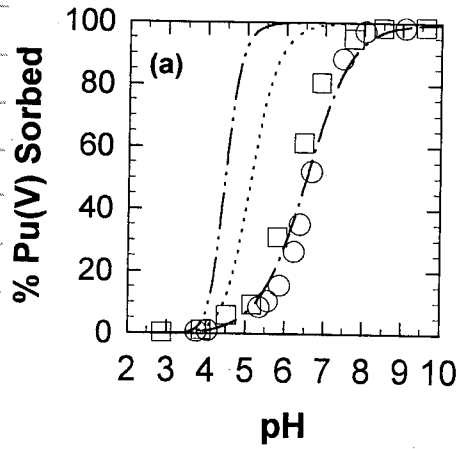
A.R. Jenny

Using weighted values (pg. 77) 10^{-10} + 10^{-11} do not differ significantly

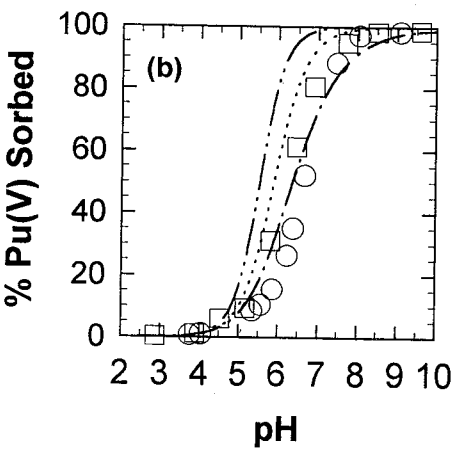
Tend to be overly steep sorption edges

Using weighted binding constants from (77)

Pu(V)-Goethite Sorption - DLM

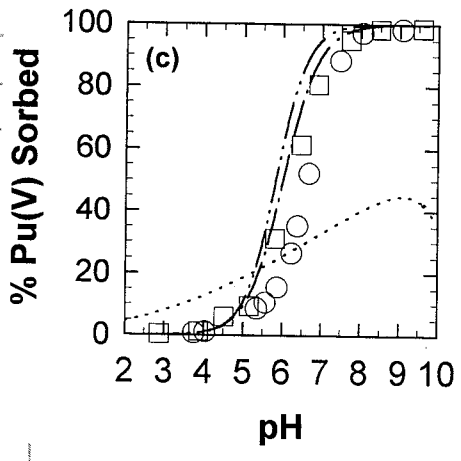


Pu(V)-Goethite Sorption - CCM



Using weighted values for binding constants. 10^{-11} & 10^{-10} Model predictions do not vary significantly

Pu(V)-Goethite Sorption - TLM



LEGEND

- ○ $Pu(V)_T=1x10^{-11}$ M
- □ $Pu(V)_T=1x10^{-10}$ M
- ····· XO-PuO_2^o
- —·—·— XO-PuO_2OH^-
- —··—··— XOH_2-PuO_2OH^+

XOH_2-PuO_2OH^+ gives best results in all cases

Plutonium (IV) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Goethite A_{sp}: 50 m²/g Data Source: Kohler et al (1996) Concentration: Weighted (10^{-5} + 10^{-11})	Rel Error (pH): 2 bc exp. error assumed Abs Error (pH): 5 due to loss [Pu] Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1E-13, 1E-14	Ionic Strength (electrolyte): 0.1 m NaNO₃ N_s = 2.31 sites/nm² 0.550 g/L

No CO_2

	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -4.17 I=0 only 1 deg. freedom ↓			Log K_+ = 6.47 Log K_- = -9.03 I=0			Log K_+ = 6.0 Log K_- = -10.0 Log K_{Cat} = -7.64 Log K_{An} = 8.78 I=0		
	Log K	V_Y	95% $\sigma_{Log K}$	Log K	V_Y	95% $\sigma_{Log K}$	Log K	V_Y	95% $\sigma_{Log K}$
XO-Pu^{3+}	14.26		1.57	15.77		2.87	6.31		2.66
XO-$PuOH^{2+}$	8.92		1.62	9.28		3.46	2.29		2.24
XO-$Pu(OH)_2^+$	3.36		4.66	2.80		4.31	-5.00		1.35
XOH-$Pu(OH)_2^{2+}$	8.92		1.62	9.28		3.46	2.65		1.43
XO-$Pu(OH)_3^o$	-2.62		2.33	-3.64		5.45	-8.10		2.11
XOH-$Pu(OH)_3^+$	3.36		4.66	2.80		4.31	-0.40		1.80
XO-$Pu(OH)_4^-$	-9.19		8.74	-10.46		3.32	-11.28		5.66
XOH-$Pu(OH)_4^o$	-2.62		2.33	-3.64		5.45	-3.58		5.32
XOH_2-$Pu(OH)_4^+$	3.36		4.66	2.80		4.31	4.12		4.92
XOH-$Pu(OH)_5^-$	-9.19		8.74	-10.46		3.32	-8.54 *		3.0648
XOH_2-$Pu(OH)_5^o$	-2.62		2.33	-3.64		5.45	-0.71 *		0.0656
OTHER SPECIES:									

Plutonium (IV) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Goethite A_{SP}: 50 m²/g Data Source: Sanchez et al (1985) Concentration: 10^{-10} M	Rel Error (pH): } No experimental error Abs Error (pH): } specified due to low [Pu] Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1E-13	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm² C_S = 0.555 g/l

No CO_2 / D.R. Turner	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -4.17 I=0.1 (I=0)			Log K_+ = 6.47 Log K_- = -4.03			Log K_+ = 6.0 Log K_- = -10.0 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-Pu^{3+}$	12.42 (14.07)	66.6	.0291	13.79 (15.14)	19.0	.0334	-1.72 (-0.07)	94.5	.0402
$XO-PuOH^{2+}$	7.20 (8.74)	20.4	.0281	7.34 (8.88)	17.5	.0363	-4.14 (-2.60)	87.5	.0396
$XO-Pu(OH)_2^+$	1.37 (2.80)	17.9	.0410	0.86 (2.29)	16.4	.0401	-6.59 (-5.16)	55.5	.0271
$XOH-Pu(OH)_2^{2+}$	7.20 (8.74)	20.4	.0281	7.34 (8.88)	17.5	.0363	0.94 (2.48)	61.3	.0281
$XO-Pu(OH)_3^0$	-4.21 (-2.89)	30.2	.0498	-5.64 (-4.32)	18.7	.0461	-9.66 (-8.34)	20.3	.0306
$XOH-Pu(OH)_3^+$	1.37 (2.80)	17.9	.0410	0.86 (2.29)	16.4	.0401	-2.03 (-0.60)	21.1	.0294
$XO-Pu(OH)_4^-$	-11.50 (-10.29)	38.0	.0660	-12.07 (-10.86)	22.6	.0508	-13.20 (-11.99)	20.6	.0479
$XOH-Pu(OH)_4^0$	-4.21 (-2.89)	30.2	.0498	-5.64 (-4.32)	18.7	.0461	-5.55 (-4.23)	20.4	.0440
$XOH_2-Pu(OH)_4^+$	1.37 (2.80)	17.9	.0410	0.86 (2.29)	16.4	.0401	2.09 (3.52)	16.7	.0428
$XOH-Pu(OH)_5^-$	-11.50 (-10.29)	38.0	.0660	-12.07 (-10.86)	22.6	.0508	-9.75 (-8.54)	34.1	.0418
$XOH_2-Pu(OH)_5^0$	-4.21 (-2.89)	30.2	.0498	-5.64 (-4.32)	18.7	.0461	-2.03 (-0.71)	33.1	.0650
OTHER SPECIES:									

Plutonium (IV) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Goethite A_{SP}: 50m²/g Data Source: Sonnenta et al. (1982) Concentration: 10^{-11} M	Rel Error (pH): } No experimental error specified due to low [Pu] Abs Error (pH): } Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0 E -14	Ionic Strength (electrolyte): 0.1 M NaNO₃ N_S = 2.31 sites/nm² L_S = 0.550 g/L

$NaCO_2$	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -9.17 I=0.1 (I=0)			Log K_+ = 6.47 Log K_- = -9.03			Log K_+ = 6.0 Log K_- = -10.0 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
DR Turner	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-Pu^{3+}	12.77 (14.42)	52.9	.0241	14.43 (16.08)	46.5	.0313	-1.11 (0.54)	76.7	.0303
XO-$PuOH^{2+}$	7.56 (9.10)	44.3	.0277	8.11 (9.65)	43.2	.0333	-3.63 (-2.09)	65.6	.0263
XO-$Pu(OH)_2^+$	2.41 (3.84)	39.9	.0356	1.82 (3.25)	39.2	.0355	-6.39 (-4.86)	49.1	.0241
XOH-$Pu(OH)_2^{2+}$	7.56 (9.10)	44.3	.0277	8.11 (9.65)	43.2	.0333	1.26 (2.80)	50.9	.0241
XO-$Pu(OH)_3^0$	-3.69 (-2.37)	30.6	.0455	-4.42 (-3.10)	30.6	.0365	-9.19 (-7.87)	46.9	.0301
XOH-$Pu(OH)_3^+$	2.41 (3.84)	39.9	.0356	1.82 (3.25)	39.2	.0355	-1.63 (-0.20)	46.2	.0291
XO-$Pu(OH)_4^-$	-9.54 (-8.33)	30.4	.0515	-11.33 (-10.12)	23.7	.0435	-11.93 (-10.72)	29.2	.0334
XOH-$Pu(OH)_4^0$	-3.69 (-2.37)	30.6	.0455	-4.42 (-3.10)	30.6	.0365	-4.36 (-3.04)	31.0	.0361
XOH_2-$Pu(OH)_4^+$	2.41 (3.84)	39.9	.0356	1.82 (3.25)	39.2	.0355	3.19 (4.62)	33.0	.0351
XOH-$Pu(OH)_5^-$	-9.54 (-8.33)	30.4	.0515	-11.33 (-10.12)	23.7	.0435	n.c.		
XOH_2-$Pu(OH)_5^0$	-3.69 (-2.37)	30.6	.0455	-4.42 (-3.10)	30.6	.0365	n.c.		
OTHER SPECIES:									

Plutonium (V) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Goethite
A_{SP}: 50m²/g
Data Source: Sanchez et al. (1985)
Concentration: Weighted

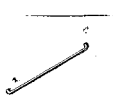
Rel Error (pH): No rep error assigned
Abs Error (pH): 3 due
Rel Error (radionuclide): 0.10
Abs Error (radionuclide): 1×10^{-15} 1×10^{-16}

Ionic Strength (electrolyte): 0.1 m NaNO₃
N_S = 2.31 sites/nm²
C_S = 0.555 mol/L

No CO_2

	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -9.17 I=0		DLW 95% conf.	Log K_+ = 6.47 Log K_- = -9.03 I=0		DLW 95% conf.	Log K_+ = 6.0 Log K_- = -10.0 Log K_{Cat} = 7.04 Log K_{An} = 8.78 I=0		DLW 95% conf.
	Log K	V_Y	~~$\sigma_{Log K}$~~	Log K	V_Y	~~$\sigma_{Log K}$~~	Log K	V_Y	~~$\sigma_{Log K}$~~
XO-PuO_2^+	-0.67		5.52	-1.71		2.56	-4.06		0.19
XOH-PuO_2^+	5.51		1.75	5.02		1.79	4.07		0.63
XO-PuO_2OH^-	-6.58		9.50	-8.38		3.19	-9.44		2.78
XOH-PuO_2OH^0	-0.67		5.52	-1.71		2.56	-1.59		2.47
XOH_2-PuO_2OH^+	5.51		1.75	5.02		1.79	6.28		2.20
OTHER SPECIES:									

Oklahoma



Plutonium (V) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Goethite A_{sp}: 50m²/g Data Source: Sanchez et al (1985) Concentration: 10^{-10} M	Rel Error (pH): } No experimental error assumed for log [H+] Abs Error (pH): } Rel Error (radionuclide): .10 Abs Error (radionuclide): 1×10^{-15}	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm² C_S = 0.550 g/L

No CO_2 D.R Turner	DLM Log K_+ = 7.35 Log K_- = -9.17 I=0.1 (I=0)			CCM Log K_+ = 6.47 Log K_- = -9.63			TLM Log K_+ = 6.0 Log K_- = -10.0 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-PuO_2^o	-0.02 (-0.02)	53.7	.0394	-1.41 (-1.41)	28.7	.0235	-4.00 (-4.00)	83.6	.0201
XOH-PuO_2^+	5.61 (5.72)	7.7	.0213	5.12 (5.23)	6.5	.0214	4.03 (4.14)	87.9	.0218
XO-PuO_2OH^-	-5.28 (-5.39)	39.4	.0396	-7.83 (-7.94)	46.0	.0256	-9.01 (-9.12)	35.0	.0240
XOH-PuO_2OH^o	-0.02 (-0.02)	53.7	.0394	-1.41 (-1.41)	28.7	.0235	-1.30 (-1.30)	55.8	.0233
XOH_2-PuO_2OH^+	5.61 (5.72)	7.7	.0213	5.12 (5.23)	6.5	.0214	6.43 (6.54)	16.0	.0226
OTHER SPECIES:									

Plutonium (V) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Goethite A_{sp}: 50 m²/g Data Source: Sanchez et al. (1985) - Fig 1-b (1 hr) Concentration: 10^{-11} M	Rel Error (pH): } No experimental error Abs Error (pH): } assumed due to ... [Pu] Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0×10^{-16}	Ionic Strength (electrolyte): 0.1 M NaNO₃ N_S = 2.31 sites/nm² C_s = 0.550 g/l

No CO₂ D.R. Turner	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -9.17 I=0.1 (I=0)			Log K_+ = 6.47 Log K_- = -9.03			Log K_+ = 6.0 Log K_- = -10.0 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-PuO$_2^o$	-1.25 (-1.25)	43.1	.0069	-1.98 (-1.98)	30.0	.0219	-4.11 (-4.11)	82.7	.0182
XOH-PuO$_2^+$	5.22 (5.33)	3.3	.0188	4.72 (4.83)	5.5	.0190	3.89 (4.00)	92.5	.0192
XO-PuO$_2$OH$^-$	-7.41 (-7.52)	42.1	.0310	-8.54 (-8.65)	34.6	.0255	-9.63 (-9.74)	33.6	.0225
XOH-PuO$_2$OH^o	-1.25 (-1.25)	43.1	.0069	-1.98 (-1.98)	30.0	.0219	-1.85 (-1.85)	27.7	.0216
XOH$_2$-PuO$_2$OH$^+$	5.22 (5.33)	3.3	.0188	4.72 (4.83)	5.5	.0190	5.94 (6.05)	20.3	.0207
OTHER SPECIES:									

5/3/94
D.R. Turner

Np(V)-SiO_2 Sorption

Data are from Righetto et al. (1991)
"Competitive Actinide Interactions in Colloidal Humic Acid-Mineral Oxide Systems" Environ. Sci. + Technol., V.25: 1913-1919

Equilibrium constants for NpO_2^+ are taken from MINTEQA2 database as modified at CNWRA. Ultimate source of Data is EQ3/6 (data0.com.r16) database with data sources listed on attachment to pg. 58 - this volume.
Example FITEQL Input File:

```
         0                                                           Neptunum
         1                                                              on
         0                                                           silica
         0                                                           2.3s\nm2
         1                                                           00000050
        90                                                           00000060
         3          1          3          1                          00000070
00001   -3.09   8.06E-4    XOH                                       00000080
00160   -2.0    0.00E00    PSIO                                      00000090
00031  -14.0    1.0E-14    NpO2+                                     00000098
00032    0.0    0.00E00    NpO2(ads)                                 00000100
00050    0.0    0.00E00    H+                                        00000102
00003   -1.0    0.10E00    Na+                                       00000104
00005   -1.0    0.10E00    ClO4-                                     00000106
                                                                     00000110
00050     0.00  050  1                                               00000120
00031     0.00  031  1                                               00000124
03100    -8.79  031  1 050 -1                                        00000126
00100   -13.78  050 -1                                               00000139
01100    -7.09  001  1 160 -1 050 -1                                 00000145
00001     0.00  001  1                                               00000150
03201    -5.00  001  1 160  0 050 -1 031  1 032  1                   xonpo2
                                                                     00000174
                                                                     00000175
00002    175.0 1.202                                                 00000180
0.1      1.0                                                         00000185
         1                                                           00000190
      3201                                                           00000195
        15          1          1          0                          00000230
        32                                                           00000240
4.5489E-16                                                           00000260
5.5698E-16                                                           00000280
6.1346E-16                                                           00000300
8.0280E-16                                                           00000320
1.6107E-15                                                           00000660
2.2342E-15                                                           00000680
2.8760E-15                                                           00000700
3.5406E-15                                                           00000710
4.2281E-15                                                           00000660
5.0530E-15                                                           00000680
5.9557E-15                                                           00000700
6.3178E-15                                                           00000710
7.2208E-15                                                           00000660
7.0425E-15                                                           00000680
6.5255E-15                                                           00000700
        50                                                           00000560
-6.21                                                                00000580
-6.64                                                                00000600
-7.11                                                                00000620
-7.62                                                                00000640
-8.24                                                                00000660
-8.49                                                                00000680
-8.74                                                                00000700
-8.96                                                                00000710
-9.18                                                                00000660
-9.38                                                                00000680
-9.61                                                                00000700
-9.74                                                                00000710
-10.04                                                               00000680
-10.13                                                               00000700
-10.24                                                               00000710
         1                                                           00000880
        32      0.10    1.0E-18                                      10%error
```

XO-NpO_2^0 DLM

} Corrected to I=0.1 (lines 00050 through 01100)

- Using FITEQL, Version 2.0 (Modified to FIT3DIM)
- Thermodynamic data from EQ3/6, Version Data0.COM.R16

Neptunium (V) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: SiO_2; A_{SP}: 175 m²/g; Data Source: Righetto et al. (1991); Concentration: 10^{-14} Np	Rel Error (pH): } Set at 0 due to extremely dilute Np concentrations; Abs Error (pH): }; Rel Error (radionuclide): .10; Abs Error (radionuclide): 1.0×10^{-18} M	Ionic Strength (electrolyte): 0.1 M $NaClO_4$; N_S = 2.31 sites/nm²; C_S = 1.2 g/l

Modeled assuming no CO_2 D.R. Turner	DLM			CCM			TLM		
	Log K₊ = n.a.; Log K₋ = -7.20 (-7.04 @ I=0.1m); I=0.1 (I=0)			Log K₊ = n.a.; Log K₋ = -7.04 (-6.93 @ I=0.1 m)			Log K₊ = 0.90, Log K₋ = -4.90 } ΔpK = 4; Log K_{Cat} = -6.22; Log K_{An} = n.a.		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-NpO_2^o	-5.39 (-5.39)	24.9	0.0179	-5.49 (-5.49)	16.9	.0188	-3.89 (-3.89)	50.3	.0174
XOH-NpO_2^+	1.19 (1.30)	41.1	0.0168	1.07 (1.18)	17.4	.0161	-0.25 (-0.14)	55.4	.0179
XO-NpO_2OH^-	-11.78 (-11.89)	22.1	0.0215	-12.16 (-12.27)	21.1	.0221	-9.32 (-9.43)	17.8	.0202
XOH-NpO_2OH^o	-5.39 (-5.39)	24.9	0.0179	-5.49 (-5.49)	16.9	.0188	-5.52 (-5.52)	16.8	.0191
XOH_2-NpO_2OH^+	1.19 (1.30)	41.1	0.0168	1.07 (1.18)	17.4	.0161	-1.74 (-1.63)	16.5	.0181
XOH_2-$NpO_2CO_3^o$									
XOH_2-$NpO_2(CO_3)_2^{2-}$									
XOH_2-$NpO_2(CO_3)_3^{4-}$									
OTHER SPECIES:									
$(XO)_2-NpO_2^-$	-12.42 (-12.53)	23.3	0.0235	-12.16 (-12.27)	21.11	.0221	-12.14	22.0	.0225
Simult { XO-NpO_2^o	-5.65 (-5.65)	18.29	0.0506	-5.57 (-5.57)	19.3		-4.17 (-4.17)	7.8	.0372
Simult { XO-NpO_2OH^-	-12.68 (-12.79)	↓	0.0637	-12.84 (-12.95)			-9.46 (-9.57)		.0286
XOHNpO_2OH^o							n.c. } used single surface complex values in MINTEQA2 (k)		
XO-NpO_2OH^-							n.c.		

Binding constants for NpO_2-SiO_2 sorption given above. In general, >SiO-NpO_2OH^- provided best fit (CCM + TLM). For DLM, >SiO-NpO_2^0 + >SiO-NpO_2OH^- provided the best results.

See next page for results

5/18/94 U(VI)-Montmorillonite Sorption.
D. PALMAN

The Sorption data are from CNLWRA analyses. The Thermodynamic data are from the MINTEQA2 database developed at CNLWRA from EQ3/6 (Data0.com.r16) database. Ultimately, Uranium data are from the NAS NEA database.

For montmorillonite, first need to determine the Si:Al ratio From microprobe analyses provided by R. Pabalan. These were inserted into a QUATTRO Spreadsheet to calculate cation ratios

#Cations=12.7

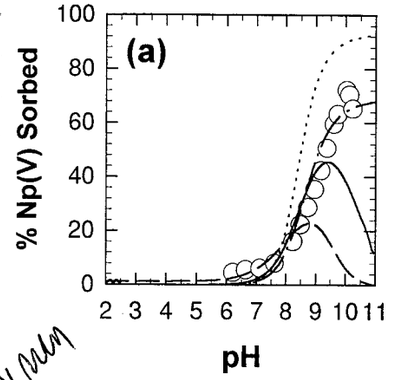
Montmorillonite	Wt%			GFW	Cation Wt			Cation Proportion			Proportions			FINAL CATIONS			
	Sample 1	Sample 2	Sample 3		Sample 1	Sample 2	Sample 3	Sample 1	Sample 2	Sample 3	Sample 1	Sample 2	Sample 3				
SiO2	62.26	62.05	62.13	60.0843	1.036211	1.032716	1.034047	0.6145	0.6153	0.6163	7.8042	7.8145	7.8271	8.0152	8.0238	8.0345	
Al2O3	17.65	17.57	17.5	101.9613	0.346210	0.344641	0.343267	0.2053	0.2053	0.2046	2.6075	2.6079	2.5983	2.6780	2.6777	2.6672	
TiO2	0.29	0.22	0.22	79.8788	0.003631	0.002754	0.002754	0.0022	0.0016	0.0016	0.0273	0.0208	0.0208	0.0281	0.0214	0.0214	
Fe2O3	1.56	1.57	1.58	159.6922	0.019538	0.019663	0.019788	0.0116	0.0117	0.0118	0.1471	0.1488	0.1498	0.1511	0.1528	0.1538	
MnO	0.04	0.02	0.06	70.8375	0.000565	0.000282	0.000847	0.0003	0.0002	0.0005	0.0043	0.0021	0.0064	0.0044	0.0022	0.0066	
MgO	5.98	5.98	5.88	40.3044	0.148371	0.148371	0.145890	0.0880	0.0884	0.0870	1.1175	1.1227	1.1043	1.1477	1.1528	1.1336	
CaO	0.06	0.03	0.05	56.0774	0.001070	0.000535	0.000892	0.0006	0.0003	0.0005	0.0081	0.0040	0.0067	0.0083	0.0042	0.0069	
Na2O	3.99	3.97	3.96	61.9789	0.128753	0.128108	0.127785	0.0764	0.0763	0.0762	0.9697	0.9694	0.9673	0.9959	0.9954	0.9929	
K2O	0.09	0.06	0.12	94.196	0.001911	0.001274	0.002548	0.0011	0.0008	0.0015	0.0144	0.0096	0.0193	0.0148	0.0099	0.0198	
Sum					1.686259	1.678344	1.677819	0.385497	0.384682	0.3837	42.8416	42.8525	42.8641	13.0434	13.0401	13.0365	

Clinoptilolite	Wt%			GFW	Cation Wt			Cation Proportion			Proportions			FINAL CATIONS			
	Untreated	Purified	Na-form		Untreated	Purified	Na-form	Untreated	Purified	Na-form	Untreated	Purified	Na-form				
SiO2	67.26	69.13	68.28	60.0843	1.119427	1.150550	1.136403	0.7188	0.7176	0.7162	10.0631	10.0461	10.0266	9.9544	9.9979	10.0008	Si
Al2O3	11.10	11.38	11.28	101.9613	0.217730	0.223222	0.221260	0.1398	0.1392	0.1394	1.9573	1.9491	1.9522	1.9361	1.9397	1.9472	Al
TiO2	0.10	0.06	0.04	79.8788	0.001252	0.000751	0.000501	0.0008	0.0005	0.0003	0.0113	0.0066	0.0044	0.0111	0.0065	0.0044	Ti
Fe2O3	0.84	0.47	0.40	159.6922	0.010520	0.005886	0.005010	0.0068	0.0037	0.0032	0.0946	0.0514	0.0442	0.0936	0.0512	0.0441	Fe
MgO	0.36	0.27	0.16	40.3044	0.008932	0.006699	0.003970	0.0057	0.0042	0.0025	0.0803	0.0585	0.0350	0.0794	0.0582	0.0349	Mg
CaO	0.73	0.09	0.02	56.0774	0.013018	0.001605	0.000357	0.0084	0.0010	0.0002	0.1170	0.0140	0.0031	0.1158	0.0139	0.0031	Ca
Na2O	3.47	4.83	6.36	61.9789	0.111974	0.155859	0.205231	0.0719	0.0972	0.1293	1.0066	1.3609	1.8108	0.9957	1.3544	1.8061	Na
K2O	3.51	2.77	0.66	94.196	0.074525	0.058814	0.014013	0.0479	0.0367	0.0088	0.6699	0.5135	0.1236	0.6627	0.5111	0.1233	K
Sum	87.37	89.00	87.20		1.557378	1.603387	1.586745	1.000000	1.000000	1.0000	48.5239	48.2313	48.1240	13.8488	13.9329	13.9639	

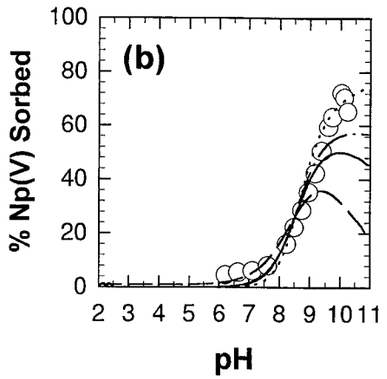
for Montmorillonite - Average Si:Al = 3.00:1.00
For Clinoptilolite - Average Si:Al = 5.15:1.00

For example SiO_2-Montmorillonite Sample 1 $\frac{62.26\ wt\%}{GFW} = 1.036211$, $\frac{1.036211}{Sum} = .6145$, $(.6145)(\#Cations) = 7.8042$

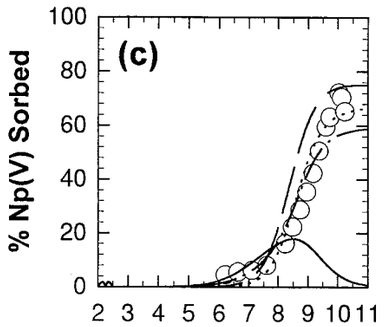
Np(V)-SiO_2 Sorption - DLM



Np(V)-SiO_2 Sorption - CCM

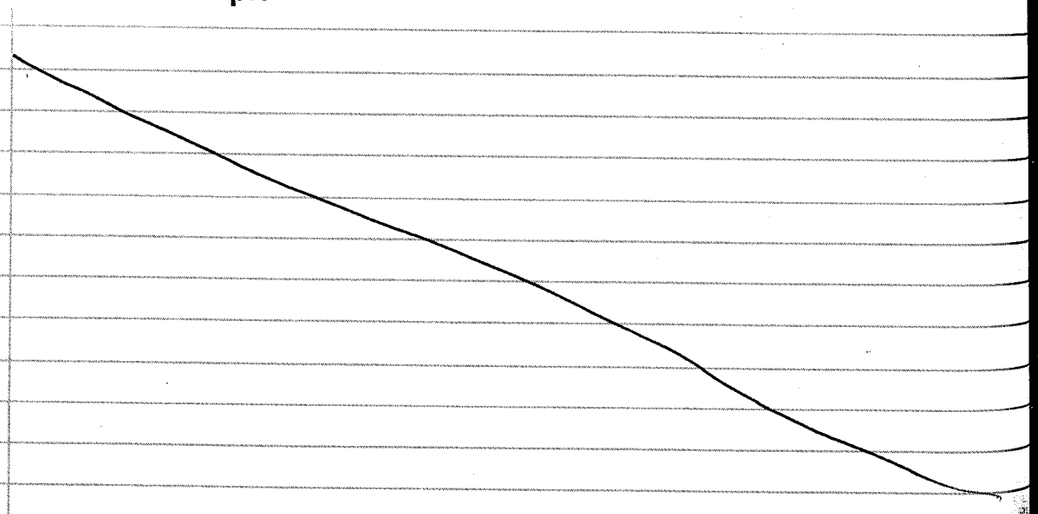


Np(V)-SiO_2 Sorption - TLM



LEGEND

- ——— $>SiO\text{-}NpO_2^o$
- — — — $>SiOH\text{-}NpO_2^+$
- ····· $>SiO\text{-}NpO_2OH^-$
- —·—·— $>SiO\text{-}NpO_2^o$ & $>SiO\text{-}NpO_2OH^-$
- — — $>SiO\text{-}NpO_2OH^-$ & $>SiOH\text{-}NpO_2OH^o$



5/20/94 U(VI)-montmorillonite sorption
DRJenn

Only DLM has been considered

For Mont.: $A_{sp} = 78\ m^2/g$ (Triay et al., 1993 - Int. HLW Management Proceedings)

$N_s = 2.31$ sites/nm^2 (Dzombak + Morel, 1990)

$p(CO_2) = 10^{-3.5}$ atm

Example FITEQL Input Files

For conversion purposes, left out species $(UO_2)_3(CO_3)_6^{6-}$ + $(UO_2)_{11}(CO_3)_6(OH)_{12}^{2-}$.

These are very minor species and have no effect on binding constants.

DLM

~~XO-SiO~~ DRJ 5/20

SiO-UO$_2^+$

```
montmori
CNWRA
1.91e-7M
dlm
3
1
0
0
:
30
5       1       3       1
00001 -4.73  1.87E-5  AlOH
00002 -4.25  5.61E-5  SiOH
00160 -1.0   0.00E00  PSIO
00032 -6.72  1.91E-7  UO2+2
00140 -3.48  3.31E-4  CO2g
00033  0.0   0.00E00  UO2ads
00050  0.0   0.00E00  H+
00003 -1.0   0.00E00  Na+
00005 -1.0   0.00E00  NO3-

00050   0.00 050  1
00032   0.00 032  1
03201  -5.43 032  1 050 -1
03202 -10.54 032  1 050 -2
03203 -19.22 032  1 050 -3
03204 -32.59 032  1 050 -4
03205  -2.49 032  2 050 -1
03206  -5.42 032  2 050 -2
03207 -12.37 032  3 050 -4
03208 -16.25 032  3 050 -5
03209 -31.49 032  3 050 -7
03210 -22.83 032  4 050 -7
03211  -8.77 032  1 140  1 050 -2
03212 -19.35 032  1 140  2 050 -4
03213 -30.81 032  1 140  3 050 -6
03216 -19.28 032  2 140  1 050 -5
03217 -18.11 032  3 140  1 050 -5
03218  -0.05 032  1 005  1
01401 -17.50 140  1 050 -2
01402  -7.61 140  1 050 -1
01403  -1.48 140  1
01404 -16.67 140  1 003  1 050 -2
01405  -8.08 140  1 003  1 050 -1
00100 -13.78 050 -1
00001   0.00 001  1
01050   8.22 001  1 160  1 050  1
01100  -9.62 001  1 160 -1 050 -1
00002   0.00 002  1
02100  -7.09 002  1 160 -1 050 -1
03306  10.00 002  1 160  1 050 -1 032  1 033  1
siouo2

00002  78.00 0.25
0.1    1.0
   1
3306
  29        1        1        0
  33
0.000E-09
4.591E-09
0.000E-09
2.927E-09
2.449E-09
8.973E-09
7.825E-09
1.754E-08
3.468E-08
1.298E-07
1.577E-07
1.537E-07
1.580E-07
1.586E-07
1.581E-07
1.634E-07
1.638E-07
1.616E-07
1.655E-07
1.651E-07
1.496E-07
1.158E-07
1.344E-07
9.749E-08
4.031E-08
1.192E-08
0.000E-09
0.000E-09
0.000E-09
   50
-1.91
-2.18
-2.50
-2.76
-2.99
-3.31
-3.63
-3.97
-4.23
-5.28
-5.55
-6.03
-5.79
-5.94
-5.82
-6.07
-6.17
-6.27
-6.42
-6.64
-6.88
-7.09
-7.16
-7.47
-7.63
-7.90
-8.25
-8.64
-8.88
   1        1
  33     0.01   2.3E-10
  50     0.05   0.0E-00
```

0.25 g/l

DRJenn

DLM

AlOH-UO$_2$(OH)$_2^0$

or

AlO-UO$_2$OH^0

```
montmori
CNWRA
2.30e-7M
dlm
3
1
0
0
:
30
5       1       3       1
00001 -3.73  1.87E-4  AlOH
00002 -3.25  5.61E-4  SiOH
00160 -1.0   0.00E00  PSIO
00032 -6.64  2.30E-7  UO2+2
00140 -3.48  3.31E-4  CO2g
00033  0.0   0.00E00  UO2ads
00050  0.0   0.00E00  H+
00003 -1.0   0.00E00  Na+
00005 -1.0   0.00E00  NO3-

00050   0.00 050  1
00032   0.00 032  1
00140   0.00 140  1
03201  -5.43 032  1 050 -1
03202 -10.54 032  1 050 -2
03203 -19.22 032  1 050 -3
03204 -32.59 032  1 050 -4
03205  -2.49 032  2 050 -1
03206  -5.42 032  2 050 -2
03207 -12.37 032  3 050 -4
03208 -16.25 032  3 050 -5
03209 -31.49 032  3 050 -7
03210 -22.83 032  4 050 -7
03211  -8.77 032  1 140  1 050 -2
03212 -19.35 032  1 140  2 050 -4
03213 -30.81 032  1 140  3 050 -6
03216 -19.28 032  2 140  1 050 -5
03217 -18.11 032  3 140  1 050 -5
03218  -0.05 032  1 005  1
01401 -17.50 140  1 050 -2
01402  -7.61 140  1 050 -1
01403  -1.48 140  1
01404 -16.67 140  1 003  1 050 -2
01405  -8.08 140  1 003  1 050 -1
00100 -13.78 050 -1
01050   8.22 001  1 160  1 050  1
01100  -9.62 001  1 160 -1 050 -1
00001   0.00 001  1
02100  -7.09 002  1 160 -1 050 -1
00002   0.00 002  1
03306 -10.00 001  1 160  0 050 -2 032  1 033  1
alohuoh2

00002  78.00 2.50
0.1    1.0
   1
3306
  29        1        1        0
  33
2.215E-08
2.741E-08
3.054E-08
4.813E-08
6.304E-08
9.576E-08
1.508E-07
1.972E-07
2.208E-07
2.265E-07
2.261E-07
2.238E-07
2.253E-07
2.261E-07
2.238E-07
2.259E-07
2.228E-07
2.226E-07
2.233E-07
2.225E-07
2.151E-07
2.127E-07
2.054E-07
1.781E-07
1.394E-07
6.322E-08
1.860E-08
5.473E-09
2.323E-09
   50
-1.86
-2.18
-2.47
-2.90
-3.23
-3.68
-4.27
-4.68
-5.19
-5.84
-6.14
-6.43
-6.40
-6.24
-6.45
-6.45
-6.58
-6.50
-6.56
-6.83
-6.96
-7.26
-7.48
-7.63
-7.95
-8.21
-8.46
-8.74
-8.96
   1        1
  33     0.01   2.3E-10
  50     0.05   0.0E-00
```

2.5 g/l

DRJenn

5/26/94
DRJenn

Uranium Sorption Binding Constants
Monodentate, mononuclear compounds (SiOH°)

Solid: Montmorillonite
A_{sp}: 78 m²/g (Triay et al., IHLWM '93
Data Source: CNWRA
Concentration: 54.8 ppb (2.30×10^{-7} M)

Rel Error (pH): 0.05
Abs Error (pH): 0.00
Rel Error (radionuclide): 0.01
Abs Error (radionuclide): 2.3×10^{-10}

Ionic Strength (electrolyte):
N_s = 2.31 sites/nm²
2.5 g/l

Atm CO_2	DLM			CCM			TLM		
	Log K_+ = — Log K_- = -7.09 For AlOH° log K_+ = 8.22 ? I=0.1m (I=0) log K_- = -9.62			Log K_+ = Log K_- =			Log K_+ = Log K_- = Log K_{Cat} = Log K_{An} =		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	0.81 (1.14)	275.8	.0076						
$XOH\text{-}UO_2^{2+}$	5.67 (6.11)	3869	.0063						
$XO\text{-}UO_2OH^o$	-6.35 (-6.12)	1258	.0062						
$XOH\text{-}UO_2OH^+$	0.81 (1.14)	275.7	.0076						
$XO\text{-}UO_2(OH)_2^-$	-13.48 (-13.37)	2272	.0040						
$XOH\text{-}UO_2(OH)_2^o$	-6.35 (-6.13)	1257	.0062						
$XOH_2\text{-}UO_2(OH)_2^+$	0.81 (1.14)	275.8	.0076						
$XOH\text{-}UO_2(OH)_3^-$	-13.48 (-13.37)	2272	.0040						
$XOH_2\text{-}UO_2(OH)_3^o$	-6.35 (-6.13)	1257	.0062						
$XOH\text{-}UO_2(OH)_4^{2-}$									
$XOH_2\text{-}UO_2(OH)_4^-$	-13.48 (-13.37)	2272	.0040						
$XOH\text{-}UO_2CO_3^o$	-2.22 (16.16)	373.3	.0077						
$XOH_2\text{-}UO_2(CO_3)_2^-$	-5.22 (31.21)	736.8	.0123						
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	-15.29 (39.02)	855.0	.0131						
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^o$	-5.55 (13.05)	1130	.0125						
$XO\text{-}(UO_2)_3(OH)_5^o$	-12.86 (-12.09)	1424	.0166						

DRJenn

Binding constants. First analyzed 2.5 g/l data. Then analyzed 0.25 g/l data. Only used SiO-UO$_2^+$ + AlO-UO$_2$(OH)^0 for 0.25 g/l data since these gave best results for 2.5 g/l data. Results on next page:

5/26/94

Uranium Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Montmorillonite A_{sp}: 78 m^2/g (Triay et al. 1993) Data Source: CNWRA Concentration: 54.8 ppb (2.30×10^{-7})	Rel Error (pH): Abs Error (pH): Rel Error (radionuclide): Abs Error (radionuclide):	Ionic Strength (electrolyte): N_s = 2.31 sites/nm^2

Atm CO_2	DLM			CCM			TLM		
	Log K_+ = 8.22 } I=.1 m Log K_- = -9.62 } For SiOH: Log K = -7.09 I=0.1m (I=0)			Log K_+ = Log K_- =			Log K_+ = Log K_- = Log K_{Cat} = Log K_{An} =		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-UO_2^+	2.06 (2.39)	1524	.0051						
XOH-UO_2^{2+}	9.27 (9.71)	438.4	.0032						
XO-UO_2OH°	-5.32 (-5.10)	3423	.0035						
XOH-UO_2OH^+	2.06 (2.39)	1524	.0051						
XO-$UO_2(OH)_2^-$	-13.40 (-13.79)	6208	.0043						
XOH-$UO_2(OH)_2^\circ$	-5.32 (-5.10)	3423	.0035						
XOH_2-$UO_2(OH)_2^+$	2.06 (2.39)	1524	.0051						
XOH-$UO_2(OH)_3^-$	-13.40 (-13.79)	6208	.0043						
XOH_2-$UO_2(OH)_3^\circ$	-5.32 (-5.10)	3423	.0035						
XOH-$UO_2(OH)_4^{2-}$									
XOH_2-$UO_2(OH)_4^-$	-13.40 (-13.79)	6208	.0043						
XOH-$UO_2CO_3^\circ$	-.021 (17.57)	1383	.0259						
XOH_2-$UO_2(CO_3)_2^-$	-3.85 (3958)	980.6	.0089						
XOH_2-$UO_2(CO_3)_3^{3-}$	-18.79 (4058)	976.3	.0100						
XOH_2-$(UO_2)_2CO_3(OH)_3^\circ$	-4.13 (1447)	1441	.0097						
XO-$(UO_2)_3(OH)_5^-$	-11.56 (-10.79)	1782	.0126						

Binding constants. First analyzed 2.5 g/l data. Then analyzed 0.25 g/l data. Only used SiO-UO_2^+ + AlO-$UO_2(OH)^\circ$ for 0.25 g/l data since these gave best results for 2.5 g/l data. Results on next page:

5/26/94
[illegible signature]

Monodentate, mononuclear compounds $SiO^{+/o}$

Solid: Montmorillonite (Si:Al = 3.00:1.00) A_{sp}: [illegible] Data Source: [illegible] Concentration: 46.54 ppb	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.01 Abs Error (radionuclide): 2.3×10^{-10}
Ionic Strength (electrolyte): 0.1 m $NaNO_3$ N_s = 2.31 sites/nm^2 C_s = 0.25 g/l	

Atm CO_2	DLM			CCM			TLM		
	Log K_+ = n.a. Log K_- = -7.09 for AlOH: log K_+ = 8.22, log K_- = -9.62, I = 0.1 m			Log K_+ = Log K_- =			Log K_+ = Log K_- = Log K_{Cat} = Log K_{An} =		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-UO_2^+$	1.07 (1.40)	174.0	.0042						
$XOH-UO_2^{2+}$									
$XO-UO_2OH^o$									
$XOH-UO_2OH^+$	1.07 (1.40)	174.0	.0042						
$XO-UO_2(OH)_2^-$									
$XOH-UO_2(OH)_2^o$									
$XOH_2-UO_2(OH)_2^+$	1.07 (1.40)	174.0	.0042						
$XOH-UO_2(OH)_3^-$									
$XOH_2-UO_2(OH)_3^o$									
$XOH-UO_2(OH)_4^{2-}$									
$XOH_2-UO_2(OH)_4^-$									
$XOH-UO_2CO_3^o$									
$XOH_2-UO_2(CO_3)_2^-$									
$XOH_2-UO_2(CO_3)_3^{3-}$									
$XOH_2-(UO_2)_2CO_3(OH)_3^o$									

Binding constants. First analyzed 2.5 g/l data. Then analyzed 0.25 g/l data. Only used $SiO-UO_2^+$ + $AlO-UO_2(OH)^o$ for 0.25 g/l data since these gave best results for 2.5 g/l data. Results on next page:

5/26/94
[signature]

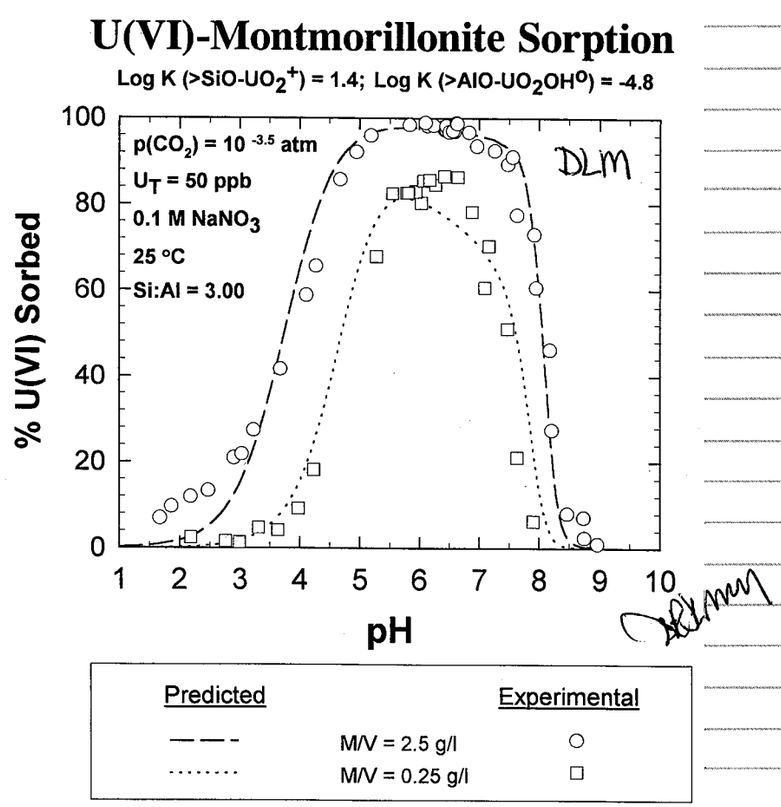
Monodentate, mononuclear compounds AlOH°

Solid: Montmorillonite (Si:Al = 3.00:1.00) A_{sp}: 78 m²/g (Triay et al., IHLWM '93) Data Source: CNWRA Concentration: 45.54 ppb	Rel Error (pH): Abs Error (pH): Rel Error (radionuclide): Abs Error (radionuclide):	Ionic Strength (electrolyte): 0.1 m $NaNO_3$ N_s = 2.31 sites/nm² Cs = 0.25 g/l

Atm CO_2	DLM Log K_+ = 8.22 Log K_- = -9.62 } I = 0.1 m For SiOH° log K_- = -7.04			CCM Log K_+ = Log K_- =			TLM Log K_+ = Log K_- = Log K_{Cat} = Log K_{An} =		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-UO_2^+$									
$XOH-UO_2^{2+}$									
$XO-UO_2OH^\circ$	-5.06 (-4.84)	3772	.0037						
$XOH-UO_2OH^+$									
$XO-UO_2(OH)_2^-$									
$XOH-UO_2(OH)_2^\circ$	-5.06 (-4.84)	3772	.0037						
$XOH_2-UO_2(OH)_2^+$									
$XOH-UO_2(OH)_3^-$									
$XOH_2-UO_2(OH)_3^\circ$	-5.06 (-4.84)	3772	.0037						
$XOH-UO_2(OH)_4^{2-}$									
$XOH_2-UO_2(OH)_4^-$									
$XOH-UO_2CO_3^\circ$									
$XOH_2-UO_2(CO_3)_2^-$									
$XOH_2-UO_2(CO_3)_3^{3-}$									
$XOH_2-(UO_2)_2CO_3(OH)_3^\circ$									

[signature]

Binding constants. First analyzed 2.5 g/l data. Then analyzed 0.25 g/l data. Only used $SiO-UO_2^+$ + $AlO-UO_2(OH)^\circ$ for 0.25 g/l data since these gave best results for 2.5 g/l data. Results on next page:



6/17/94
D.B. Jenner

U(VI)-Sorption on Goethite.
This is being studied for the purposes of providing retardation factors for U-transport through fractures containing Fe-(hydr)oxides at the Peña Blanca Natural Analog site at Chihuahua, Mexico.

The U(VI)-Goethite sorption data is from:
Hsi + Langmuir (1985) Geochimica Cosmochim Acta
Kohler et al. (1992) 7th International Water-Rock Interaction

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 8: Adsorption of uranyl vs. pH...) is from the following reference.

Hsi, C-K.D. and Langmuir. "Adsorption of Uranyl onto Ferric Oxyhydroxides: Application of the Surface Complexation Site-Binding Model." Geochimica et Cosmochimica Acta. Vol. 49. pp. 1,931-1,941. 1985.

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 4: Adsorption of U(VI)...) is from the following reference.

Kohler, M., E. Wieland, and J.O. Leckie. "Metal-Ligand-Surface Interactions during Sorption of Uranyl and Neptunyl on Oxides and Silicates - WRI-7. Volume 1: Low Temperature Environments" Y.K. Kharaka and A.S. Maest, eds. Proceedings of the 7th International Symposium on Water-Rock Interaction. Rotterdam, Netherlands: Balkema. 1992.

Values were digitized using equipment described on pg 42

Kohler et al. (1992) No CO_2

pH	% Sorbed
3.36385	26.66729
3.54728	27.94154
3.69183	35.64942
3.89416	29.54701
3.99455	30.94251
4.00333	52.50006
4.17735	64.30691
4.23548	77.05400
4.47020	87.05881
4.69028	94.44037
4.74790	95.83499
5.65065	98.06661
6.37263	98.24534
6.55880	98.20817
9.57776	97.69626

Kohler et al. (1992) $p(CO_2) = 2\times10^{-2}$ atm

pH	% sorbed
3.77172	24.83138
4.03584	53.60729
4.38035	82.99959
6.70791	94.35876
7.29891	66.87087
8.36919	3.49117
9.84738	9.50506

Kohler et al. (1992) $p(CO_2) = 3\times10^{-4}$ atm

pH	% sorbed
3.96473	0.24517
5.68058	99.54263
7.49690	99.70280
8.11159	94.87933
8.99989	64.85655
9.31299	1.21543

Hsi + Langmuir (1985) $C_T = 10^{-2}$ M

pH	% sorbed
4.42868	70.38815
4.93066	90.17568
5.21908	96.70442
5.86883	98.10858
6.07799	97.98294
6.23162	94.61685
6.34429	95.48171
6.42475	93.65019
6.66725	87.33918
6.72560	84.83987
6.80411	86.39778
7.05328	83.82248
7.18406	74.79109
7.82705	55.16612
8.10241	31.01711
8.45740	41.05834
8.69173	37.46884

Hsi + Langmuir (1985) $C_T = 10^{-3}$ M

pH	% sorbed
3.91014	21.20939
4.24427	39.09347
4.22575	54.65525
4.66649	73.80010
4.74501	92.10714
4.84593	87.92510
4.83912	91.53724
5.09881	94.00885
5.47279	100.06674
5.59268	100.16459
5.72727	100.41074
5.83619	100.75609
5.92670	100.70577
6.00985	100.48234
6.22390	100.35665
6.27159	100.23251
6.58964	100.30378
6.81837	100.17795
7.02629	99.97810
7.41892	99.75180
8.02321	99.82041
8.23841	99.17517

Example FITEQL Input Files:

For Both, Uranium data from NEA database (Grenthe et al, 1992)
For Hsi + Langmuir CO_3^{2-} is component for carbon. For Kohler et al. (1992) equil. constants converted to rxns written with CO_2 as described on pp. 10-12.

DLM XO·UO_2 $C_T = 10^{-5}$ M Hsi + Langmuir

```
         0
         1
         0
         0
         1
        90
         4         1         3         1
00001  -3.72  1.92E-4   XOH
00160  -1.0   0.00E00   PSIO
00032  -5.00  1.00E-5   UO2+2
00140  -3.00  1.00E-3   CO3-2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050     0.00  050  1
00032     0.00  032  1
00140     0.00  140  1
00100   -13.78  050 -1
01401     9.89  140  1 050  1
01402    16.02  140  1 050  2
01403     0.83  140  1 003  1
01404     9.42  140  1 050  1 003  2
03201    -5.43  032  1 050 -1
03202   -10.54  032  1 050 -2
03203   -19.22  032  1 050 -3
03204   -32.59  032  1 050 -4
03205    -2.49  032  2 050 -1
03206    -5.42  032  2 050 -2
03207   -12.37  032  3 050 -4
03208   -16.25  032  3 050 -5
03209   -31.49  032  3 050 -7
03210   -22.83  032  4 050 -7
03211    -0.05  032  1 005  1
03212     8.73  032  1 140  1
03213    16.09  032  1 140  2
03214    21.58  032  1 140  3
03215    -1.78  032  2 140  1 050 -3
03216    30.51  032 11 140  6 050-12
03218    -0.61  032  3 140  1 050 -3
01050     7.24  001  1 160  1 050  1
01100    -9.06  001  1 160 -1 050 -1
00001     0.00  001  1
03301     1.00  001  1 160  1 050 -1 032  1 033  1

00002  050.0  1.0000
0.1    1.0
         1
      3301
        22         1         1         0
        33
2.1209E-06
3.9093E-06
5.4655E-06
7.3800E-06
9.2107E-06
8.7925E-06
9.1537E-06
9.4009E-06
1.0000E-05
1.0000E-05
1.0000E-05
1.0000E-05
1.0000E-05
1.0000E-05
1.0000E-05
1.0000E-05
1.0000E-05
1.0000E-05
9.9978E-06
9.9752E-06
9.9820E-06
9.9175E-06
        50
-3.91
-4.24
-4.23
-4.67
-4.75
-4.85
-4.84
-5.10
-5.47
-5.59
-5.73
-5.84
-5.93
-6.01
-6.22
-6.27
-6.59
-6.82
-7.03
-7.42
-8.02
-8.24
         1         1
        33      0.10   1.0E-08
        50      0.05   0.0E-00
```

```
Goethite
Hsi(81)
U=10-5M
2.3si/nm
00000050
00000060
00000070
00000080
00000090
00000098
00000107
00000100
00000102
00000103
00000104
00000110
00000120
00000124
00000125
00000139
00000146
00000147
00000146
00000147
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000137
00000139
00000140
00000141
00000144
00000144
00000144
00000140
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000361
00000362
00000363
00000364
00000365
00000366
00000300
00000320
00000340
00000360
00000361
00000362
00000363
00000364
00000365
00000366
00000680
00000681
00000690
00000700
00000710
00000720
00000730
00000740
00000741
00000742
00000743
00000744
00000745
00000700
00000710
00000720
00000730
00000740
00000741
00000742
00000743
00000744
00000745
00001170
00001180
00001190
```

DLM XO·UO_2^+ $p(CO_2) = 3\times10^{-4}$ Kohler et al.

```
         0
         1
         0
         0
         1
        90
         4         1         3         1
00001  -3.72  1.92E-4   XOH
00160  -1.0   0.00E00   PSIO
00032  -6.00  1.00E-6   UO2+2
00140  -3.52  3.00E-4   CO3-2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.10E00   Na+
00005  -1.0   0.10E00   ClO4-

00050     0.00  050  1
00032     0.00  032  1
00140     0.00  140  1
03201    -5.43  032  1 050 -1
03202   -10.54  032  1 050 -2
03203   -19.22  032 -1 050 -3
03204   -32.59  032  1 050 -4
03205    -2.49  032  2 050 -1
03206    -5.42  032  2 050 -2
03207   -12.37  032  3 050 -4
03208   -16.25  032  3 050 -5
03209   -31.49  032  3 050 -7
03210   -22.83  032  4 050 -7
03211    -8.77  032  1 140  1 050 -2
03212   -19.35  032  1 140  2 050 -4
03213   -30.81  032  1 140  3 050 -6
03216   -19.28  032  2 140  1 050 -5
03217   -18.11  032  3 140  1 050 -5
01401   -17.50  140  1 050 -2
01402    -7.61  140  1 050 -1
01403    -1.48  140  1
01404   -16.67  140  1 003  1 050 -2
01405    -8.08  140  1 003  1 050 -1
00100   -13.78  050 -1
01050     7.24  001  1 160  1 050  1
01100    -9.06  001  1 160 -1 050 -1
00001     0.00  001  1
03301    -2.50  001  1 160  1 050 -1 032  1 033  1

00002  50.00  1.0000
0.1    1.0
         1
      3301
         6         1         1         0
        33
2.4517E-09
9.9543E-07
9.9703E-07
9.4879E-07
6.4857E-07
1.2154E-08
        50
-3.96
-5.68
-7.50
-8.11
-9.00
-9.31
         1         1
        33      0.10   1.0E-09
        50      0.05   0.0E-00
```

```
Goethite
Kohler
1.00E-6M
2.3si/nm
00000050
00000060
00000070
00000080
00000090
00000098
00000107
00000100
00000102
00000103
00000104
00000110
00000120
00000122
00000124
00000126
00000128
00000130
00000132
00000134
00000136
00000138
00000140
00000142
00000144
00000146
00000148
00000150
00000156
00000158
00000161
00000162
00000163
00000164
00000165
00000160
00000140
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000363
00000364
00000365
00000366
00000300
00000320
00000680
00000742
00000743
00000744
00000745
00000700
00000710
00001170
00001180
00001190
```

6/20/94
D.R. Lumm

FITEQL Results: Some data points eliminated in Kohler data for purposes of convergence (Indicated by asterisk *

Uranium Sorption Binding Constants
Monodentate, mononuclear compounds

Hsi + Langmuir (1985) No CO_2

Solid: Goethite A_{sp}: 50 m^2/g Data Source: Hsia Langmuir (1985) Concentration: 10^{-5} M	Rel Error (pH): .05 Abs Error (pH): 0.00 Rel Error (radionuclide): .10 Abs Error (radionuclide): 1.0E-8	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_s = 2.31 sites/nm² 1 g/l

No CO_2	DLM Log K_+ = 7.24 Log K_- = -9.06 (I=0)			CCM Log K_+ = 6.47 Log K_- = -9.03 (I=0.1)			TLM Log K_+ = 5.89 Log K_- = -9.89 Log K_{OH} = -7.64 Log K_{Am} = 8.56		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}UO_2^+$	2.80 (3.13)	1.6	.0352	2.36(2.69)	1.9	.0350	-2.84(-2.51)	45.0	.0400
$XOH\text{-}UO_2^{2+}$	9.42 (9.76)	10.8	.0278	9.12 (9.56)	8.3	.0338	6.13(6.57)	43.3	.0428
$XO\text{-}UO_2OH^\circ$	-3.76(-3.54)	3.9	.0432	-4.30 (-4.08)	2.0	.0377	-7.55(-7.33)	14.7	.0395
$XOH\text{-}UO_2OH^+$	2.80 (3.13)	1.6	.0352	2.36(2.69)	1.9	.0350	0.64(0.97)	8.3	.0385
$XO\text{-}UO_2(OH)_2^-$	-10.30(-10.14)	6.0	.0518	-10.88(-10.72)	2.4	.0411	-11.49(-11.38)	0.75	.0459
$XOH\text{-}UO_2(OH)_2^\circ$	-3.76(-3.54)	3.9	.0432	-4.30(-4.08)	2.0	.0377	-4.21(3.99)	2.0	.0375
$XOH_2\text{-}UO_2(OH)_2^+$	2.80 (3.13)	1.6	.0352	2.36(2.69)	1.9	.0350	3.96(4.29)	0.66	.0378
$XOH\text{-}UO_2(OH)_3^-$	-10.30(-10.14)	6.0	.0518	-10.88(-10.72)	2.4	.0411	-8.07(-7.96)	2.5	.0430
$XOH_2\text{-}UO_2(OH)_3^\circ$	-3.76(3.54)	3.9	.0432	-4.30(-4.08)	2.0	.0377	-0.77(-0.55)	4.9	.0461
$XOH\text{-}UO_2(OH)_4^{2-}$	-16.80(16.58)	7.3	.0411	-17.39(-17.17)	2.2	.0357	-11.40(-11.18)	1.7	.0734
$XOH_2\text{-}UO_2(OH)_4^-$	-10.30(-10.14)	6.0	.0518	-10.88(-10.72)	2.0	.0411	-4.61(-4.50)	4.8	.0693
$XOH\text{-}UO_2CO_3^\circ$									
$XOH_2\text{-}UO_2(CO_3)_2^-$									
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$									
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^\circ$									

Uranium Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Goethite A_{sp}: 50 m^2/g Data Source: Kohler et al. (1992) Concentration: 1×10^{-6} M	Rel Error (pH): .05 Abs Error (pH): 0.00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1M $NaClO_4$ N_s = 2.31 sites/nm² 1 g/l

No CO_2	DLM Log K_+ = 7.24 (7.35 @ I=0M) Log K_- = -9.06 (-9.17 @ I=0M)			CCM Log K_+ = 6.47 Log K_- = -9.03 } I=0.1			TLM Log K_+ = 5.89 6.0 Log K_- = -9.89 -10.0 } I=0 Log K_{OH} = -7.64 -7.64 Log K_{Am} = 8.56 8.78		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}UO_2^+$	3.08 (3.41)	9.3	.0346	2.64 (2.97)	10.1	.0341	-3.42 (-3.09)	30.2	.0518
$XOH\text{-}UO_2^{2+}$	9.48 (9.82)	11.6	.0276	9.21 (9.65)	13.9	.0330	4.39 (4.83)	39.4	.0388
$XO\text{-}UO_2OH^\circ$	-3.39 (-3.73)	13.4	.0441	-4.00 (-3.78)	9.7	.0374	-7.49 (-7.27)	12.8	.0284
$XOH\text{-}UO_2OH^+$	3.08 (3.41)	9.3	.0346	2.64 (2.97)	10.1	.0341	0.26 (0.59)	13.2	.0284
$XO\text{-}UO_2(OH)_2^-$	-9.88 (-9.77)	16.8	.0534	-10.60 (-10.49)	11.0	.0398	-11.55 (-11.44)	9.6	.0393
$XOH\text{-}UO_2(OH)_2^\circ$	-3.39 (-3.17)	13.4	.0441	-4.00 (-3.78)	9.7	.0374	-3.91 (-3.69)	9.6	.0371
$XOH_2\text{-}UO_2(OH)_2^+$	3.08 (3.41)	9.3	.0346	2.64 (2.97)	10.1	.0341	3.85 (4.18)	8.5	.0380
$XOH\text{-}UO_2(OH)_3^-$	-9.88 (-9.77)	16.8	.0534	-10.60 (-10.49)	11.0	.0398	-8.00 (-7.89)	14.2	.0484
$XOH_2\text{-}UO_2(OH)_3^\circ$	-3.39 (-3.17)	13.4	.0441	-4.00 (-3.78)	9.7	.0374	-0.35 (-0.13)	14.3	.0467
$XOH\text{-}UO_2(OH)_4^{2-}$	-16.36 (-16.14)	28.5	.0631	-17.19 (-17.19)	13.0	.0425	*-10.02 (-12.02)	17.8	.0615
$XOH_2\text{-}UO_2(OH)_4^-$	-9.88 (-9.77)	16.8	.0534	-10.60 (-10.49)	11.0	.0398	*-4.98 (-4.87)	18.8	.0587
$XOH\text{-}UO_2CO_3^\circ$									
$XOH_2\text{-}UO_2(CO_3)_2^-$									
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$									
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^\circ$									

*Deleted highest pH: pH=9.58
% sorbed=97.7%

FITEQL Results: Some data points eliminated in Kohler data for purposes of convergence (Indicated by asterisk *

…ption Binding Constants
…ate, mononuclear compounds

…id: Goethite
A_{sp}: 50 m^2/g
Data Source: Hsi & Langmuir (1985)
Concentration: 1×10^{-5} M

Rel Error (pH): 0.05
Abs Error (pH): 0.00
Rel Error (radionuclide): 0.18
Abs Error (radionuclide): 1.0E-8

Ionic Strength (electrolyte): 0.1 M NaNO3
N_s = 2.31 sites/nm²
C_s = 1 g/L

$C_T = 10^{-2}$ M

	DLM			CCM			TLM		
	Log K_+ = 7.24 (7.33 @ I=0) Log K_- = -9.06 (-9.17 @ I=0)			Log K_+ = 6.47 } I=0.1 Log K_- = -9.03 } I=0.1			Log K_+ = 5.89 4.00 Log K_- = -9.89 -10.00 @ I=0 Log K_{Cu} = -7.64 -7.64 Log K_{Au} = 8.56 8.78		
	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$
XO-UO_2^+	5.87 (6.20)	5.4	.0457	5.61 (5.94)	6.5	.0492	6.27 (6.60)	10.2	.0398
XOH-UO_2^{2+}	14.14 (14.58)	5.9	.0535	13.72 (14.16)	7.3	.0598	15.17 (15.61)	6.8	.0485
XO-UO_2OH°	-2.33 (-2.11)	4.3	.0411	-2.38 (-2.16)	4.4	.0416	-2.18 (-1.96)	9.2	.0552
XOH-UO_2OH^+	5.87 (6.20)	5.4	.0457	5.61 (5.94)	6.5	.0492	6.21 (6.54)	7.1	.0416
XO-$UO_2(OH)_2^-$	-10.44 (-10.33)	2.0	.0387	-10.22 (-10.11)	2.2	.0371	-9.81 (-9.70)	2.6	.0529
XOH-$UO_2(OH)_2^\circ$	-2.33 (-2.11)	4.3	.0414	-2.38 (-2.16)	4.4	.0416	-2.22 (-2.00)	4.3	.0414
XOH_2-$UO_2(OH)_2^+$	5.87 (6.20)	5.4	.0457	5.61 (5.94)	6.5	.0492	6.14 (6.47)	3.1	.0630
XOH-$UO_2(OH)_3^-$	-10.44 (-10.33)	2.0	.0387	-10.22 (-10.11)	2.2	.0371	-9.47 (-9.36)	15.2	.0910
XOH_2-$UO_2(OH)_3^\circ$	-2.33 (-2.11)	4.3	.0414	-2.38 (-2.16)	4.4	.0416	-2.05 (-1.83)	11.5	.0897
XOH-$UO_2(OH)_4^{2-}$	-22.22 (-22.22)	2.4	.0379	-21.62 (-21.40)	5.8	.0369	-16.03 (-16.03)	53.8	.0691
XOH_2-$UO_2(OH)_4^-$	-10.44 (-10.33)	2.0	.0387	-10.22 (-10.11)	2.2	.0371	-5.04 (-4.93)	63.3	.0257
XOH-$UO_2CO_3^\circ$	17.53 (18.41)	18.5	.0517	17.78 (18.66)	11.8	.0494	17.77 (18.65)	9.9	.0406
XOH_2-$UO_2(CO_3)_2^-$	29.43 (30.96)	12.5	.0519	29.68 (31.11)	11.9	.0496	30.35 (31.78)	3.3	.0391
XOH_2-$UO_2(CO_3)_3^{3-}$	n.c.	—	—	34.59 (36.46)	9.6	.0596	33.98 (35.75)	21.9	.0627
XOH_2-$(UO_2)_2CO_3(OH)_3^\circ$	16.62 (17.72)	10.9	.0594	16.56 (17.66)	11.0	.0596	16.82 (17.92)	7.2	.0475

…m Sorption Binding Constants
…nodentate, mononuclear compounds

Solid: Goethite
A_{sp}: 50 m^2/g
Data Source: Kohler et al (1992)
Concentration: 1×10^{-6} M

Rel Error (pH): .05
Abs Error (pH): 0.00
Rel Error (radionuclide): 0.10
Abs Error (radionuclide): 1E-9

Ionic Strength (electrolyte): 0.1 M $NaClO_4$
N_s = 2.31 sites/nm²
1 g/L

$p(CO_2) = 3 \times 10^{-4}$ atm

	DLM			CCM			TLM		
	Log K_+ = 7.24 (7.35 @ I=0) Log K_- = -9.06 (9.17 @ I=0)			Log K_+ = 6.47 } I=0.1 Log K_- = -9.03 } I=0.1			Log K_+ = 5.89 6.0 Log K_- = -9.89 -10.0 I=0 Log K_{Cu} = -7.64 -7.64 Log K_{Au} = 8.56 8.78		
	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$
XO-UO_2^+	1.03 (1.36)	50.6	.0426	0.72 (1.05)	49.6	.0467	-5.91 (-5.58)	84.2	.2174
XOH-UO_2^{2+}	7.21 (7.65)	82.2	.1200	7.11 (7.55)	75.3	.0783	1.79 (2.23)	84.2	.2188
XO-UO_2OH°	-7.34 (-7.12)	66.9	.0485	-7.36 (-7.14)	65.5	.0472	-9.81 (-9.59)	82.7	.1321
XOH-UO_2OH^+	1.03 (1.36)	50.6	.0426	0.72 (1.05)	49.6	.0467	-2.16 (-1.83)	83.2	.1471
XO-$UO_2(OH)_2^-$	-15.86 (-15.75)	74.5	.0614	-15.84 (-15.73)	75.9	.0657	-15.53 (-15.22)	69.6	.0522
XOH-$UO_2(OH)_2^\circ$	-7.34 (-7.12)	66.9	.0485	-7.36 (-7.14)	65.5	.0472	-7.23 (-7.01)	66.1	.0477
XOH_2-$UO_2(OH)_2^+$	1.03 (1.36)	50.6	.0426	0.72 (1.05)	49.6	.0467	0.85 (1.18)	62.1	.0453
XOH-$UO_2(OH)_3^-$	-15.86 (-15.75)	74.5	.0614	-15.84 (-15.73)	75.9	.0657	-16.55 (-16.44)	78.1	.0759
XOH_2-$UO_2(OH)_3^\circ$	-7.34 (-7.12)	66.9	.0485	-7.36 (-7.14)	65.5	.0472	-8.49 (-8.27)	78.0	.0751
XOH-$UO_2(OH)_4^{2-}$	-24.33 (-24.33)	76.8	.0688	-24.32 (-24.32)	77.7	.0730	-25.67 (-25.67)	78.7	.0844
XOH_2-$UO_2(OH)_4^-$	-15.86 (-15.75)	74.5	.0614	-15.84 (-15.73)	75.9	.0657	-17.62 (-17.51)	78.7	.0833
XOH-$UO_2CO_3^\circ$	-2.03 (14.35)	18.7	.0389	-2.38 (16.00)	87.8	.0380	-2.28 (16.10)	29.2	.0377
XOH_2-$UO_2(CO_3)_2^-$	-5.04 (31.39)	12.7	.0488	-5.60 (30.98)	21.6	.0529	-6.59 (29.99)	61.2	.0572
XOH_2-$UO_2(CO_3)_3^{3-}$	-16.27 (38.10)	8.6	.0547	-16.03 (38.34)	9.1	.0514	-19.59 (34.78)	70.3	.0524
XOH_2-$(UO_2)_2CO_3(OH)_3^\circ$	-5.76 (12.84)	16.0	.0489	-5.78 (12.82)	15.6	.04986	-6.62 (11.98)	45.0	.0355

FITEQL Results: Some data points eliminated in Kohler data for purposes of convergence (Indicated by asterisk *

...rption Binding Constants
...ate, mononuclear compounds

...id: Goethite A_{sp}: 50 m²/g Data Source: Hsi and Langmuir (1985) Concentration: 10^{-5} m	Rel Error (pH): .05 Abs Error (pH): 0.00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-8			Ionic Strength (electrolyte): 0.1 m NaNO₃ N_s = 2.31 sites/nm² C_s = 1 g/l					
$C_T = 10^{-3}$ m	DLM			CCM			TLM		
	Log K_+ = 7.24 Log K_- = -9.06 (7.33, -9.17 @ I=0)			Log K_+ = 6.47 Log K_- = -9.03 } I=0.1			Log K_+ = 5.84 Log K_- = -9.84 Log K_{Cat} = -7.64 Log K_{An} = 8.56 (6.00, -10.00, -7.64, 8.78 @ I=0)		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-UO_2^+$	2.82 (3.15)	6.0	.0402	2.37 (2.70)	7.0	.0409	-2.63 (-2.30)	68.4	.0430
$XOH-UO_2^{2+}$	9.54 (9.98)	29.9	.0315	9.16 (9.60)	18.7	.0387	6.66 (7.10)	60.7	.0707
$XO-UO_2OH^\circ$	-3.94 (-3.72)	1.0	.0560	-4.45 (-4.23)	0.83	.0475	-7.42 (-7.20)	32.7	.0330
$XOH-UO_2OH^+$	2.82 (3.15)	6.0	.0402	2.37 (2.70)	7.0	.0409	0.89 (1.22)	34.9	.0434
$XO-UO_2(OH)_2^-$	-10.48 (-10.37)	1.7	.0680	-11.07 (-10.96)	0.59	.0538	-11.65 (-11.54)	0.90	.0560
$XOH-UO_2(OH)_2^\circ$	-3.94 (-3.72)	1.0	.0560	-4.45 (-4.23)	0.83	.0475	-4.35 (-4.13)	0.90	.0468
$XOH_2-UO_2(OH)_2^+$	2.82 (3.15)	6.0	.0402	2.37 (2.70)	7.0	.0409	3.88 (4.21)	2.1	.0531
$XOH-UO_2(OH)_3^-$	-10.48 (-10.37)	1.7	.0680	-11.07 (-10.96)	0.59	.0538	-8.33 (-8.22)	0.65	.0702
$XOH_2-UO_2(OH)_3^\circ$	-3.94 (-3.72)	1.0	.0560	-4.45 (-4.23)	0.83	.0475	-0.96 (-0.74)	1.37	.0606
$XOH-UO_2(OH)_4^{2-}$	-16.97 (-16.97)	2.2	.0808	-17.61 (-17.61)	0.56	.0597	-11.79 (-11.79)	0.47	.1011
$XOH_2-UO_2(OH)_4^-$	-10.48 (-10.37)	1.7	.0680	-11.07 (-10.96)	0.59	.0538	n.c.	—	—
$XOH-UO_2CO_3^\circ$	15.29 (16.17)	7.68	.0361	14.72 (15.60)	10.5	.0311	14.82 (15.70)	23	.0308
$XOH_2-UO_2(CO_3)_2^-$	26.33 (27.76)	26.7	.0288	26.65 (28.08)	17.9	.0253	28.08 (29.51)	78.5	.0242
$XOH_2-UO_2(CO_3)_3^{3-}$	34.00 (35.87)	5.0	.0589	33.23 (35.10)	10.0	.0434	n.c.	—	—
$XOH_2-(UO_2)_2CO_3(OH)_3^\circ$	12.12 (13.22)	4.2	.0586	11.64 (12.74)	5.7	.0533	14.82 (15.92)	21.7	.0642

[illegible]

...Sorption Binding Constants
...odentate, mononuclear compounds

Solid: Goethite A_{sp}: 50 m²/g Data Source: Kohler et al (1992) Concentration: 1×10^{-6} m	Rel Error (pH): 0.05 Abs Error (pH): 0.00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9			Ionic Strength (electrolyte): 0.1 m NaClO₄ N_s = 2.31 sites/nm² 1 g/l					
$p(CO_2)$ = 2×10^{-2} atm	DLM			CCM			TLM		
	Log K_+ = 7.24 Log K_- = -9.06 (7.35, -9.17 @ I=0) (I=0)			Log K_+ = 6.47 Log K_- = -4.03 } I=0.1 (I=0)			Log K_+ = 5.84 Log K_- = -9.84 Log K_{Cat} = -7.64 Log K_{An} = 8.56 ([illegible] @ I=0)		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-UO_2^+$	3.07 (3.40)	39.2	.0543	2.60 (2.93)	39.0	.0343	-3.52 (-3.19)	64.1	.0466
$XOH-UO_2^{2+}$	9.42 (9.86)	54.8	.0471	9.22 (9.66)	45.5	.0511	4.28 (4.72)	65.1	.0538
$XO-UO_2OH^\circ$	-3.19 (-2.97)	19.4	.0578	-3.89 (-3.67)	27.9	.0541	-7.56 (-7.34)	55.7	.0488
$XOH-UO_2OH^+$	3.07 (3.40)	39.2	.0543	2.60 (2.93)	39.0	.0343	0.16 (0.49)	56.9	.0501
$XO-UO_2(OH)_2^-$	-10.62 (-10.51)	25.9	.0343	-10.60 (-10.49)	6.6	.0377	-11.44 (-11.33)	24.5	.0551
$XOH-UO_2(OH)_2^\circ$	-3.19 (-2.97)	19.4	.0578	-3.89 (-3.67)	27.9	.0541	-3.81 (-3.59)	29.0	.0542
$XOH_2-UO_2(OH)_2^+$	3.07 (3.40)	39.2	.0543	2.60 (2.93)	39.0	.0343	3.91 (4.24)	32.6	.0560
$XOH-UO_2(OH)_3^-$	-10.62 (-10.51)	25.9	.0343	-10.60 (-10.49)	6.6	.0377	-10.89 (-10.78)	53.7	.0412
$XOH_2-UO_2(OH)_3^\circ$	-3.19 (-2.97)	19.4	.0578	-3.89 (-3.67)	27.9	.0541	-2.83 (-2.61)	50.0	.0391
$XOH-UO_2(OH)_4^{2-}$	-18.90 (-18.90)	46.1	.0401	-18.55 (-18.55)	34.8	.0329	-20.66 (-20.66)	29.6	.0785
$XOH_2-UO_2(OH)_4^-$	-10.62 (-10.51)	25.9	.0343	-10.60 (-10.49)	6.6	.0377	-12.58 (-12.47)	89.4	.0750
$XOH-UO_2CO_3^\circ$	-1.55 (16.83)	22.7	.0428	-2.21 (16.17)	28.9	.0393	-2.12 (16.26)	29.8	.0394
$XOH_2-UO_2(CO_3)_2^-$	-6.15 (30.28)	9.4	.0510	-7.14 (29.29)	21.9	.0402	-5.85 (30.58)	56.5	.0393
$XOH_2-UO_2(CO_3)_3^{3-}$	n.c.	n.c.	n.c.	n.c.	n.c.	n.c.	-19.64 (34.73)	80.5	.0344
$XOH_2-(UO_2)_2CO_3(OH)_3^\circ$	-3.22 (15.38)	26.0	.0491	-3.91 (14.69)	31.3	.0664	-0.11 (18.49)	21.6	.0704

[illegible]

Weighted results using methods outlined in Dzombak + Morel (1990)

Uranium Sorption Binding Constants
Monodentate, mononuclear compounds

Combined/Weighted "Best Estimates" for U(VI)-Goethite

Solid: Goethite **A_{sp}:** 50 m²/g **Data Source:** Hsi + Langmuir (85); Kohler et al. (1992) **Concentration:**	**Rel Error (pH):** **Abs Error (pH):** **Rel Error (radionuclide):** **Abs Error (radionuclide):**	**Ionic Strength (electrolyte):** N_s = 2.31 sites/nm²

H+L(85): 10^{-5} m; No CO_2; $C_T = 10^{-2}$ m; $C_T = 10^{-3}$ m — Koh (92): 10^{-6} m; No CO_2; 2×10^{-2} atm; $10^{-3.5}$ atm	DLM (I=0)			CCM (I=0.1)			TLM (I=0)		
	Log K_+ = 7.33 Log K_- = -9.17 Corrected to I=0			Log K_+ = 6.47 Log K_- = -9.03 I=0.0			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Ca} = -7.64 Log K_{An} = 8.78		
	Log K	**V_Y**	95% c.l. $\sigma_{Log K}$	**Log K**	**V_Y**	95% c.l. $\sigma_{Log K}$	**Log K**	**V_Y**	95% c.l. $\sigma_{Log K}$
$XO\text{-}UO_2^+$ (n=6)	3.40		0.64	3.00		0.64	-1.97		1.38
$XOH\text{-}UO_2^{2+}$ n=6	10.37		0.78	9.98		0.79	6.43		1.57
$XO\text{-}UO_2OH^\circ$ n=6	-3.73		0.75	-4.13		0.68	-6.74		0.88
$XOH\text{-}UO_2OH^+$ n=6	3.40		0.64	3.00		0.64	1.37		0.96
$XO\text{-}UO_2(OH)_2^-$ n=6	-11.00		0.89	-11.11		0.78	-11.35		0.76
$XOH\text{-}UO_2(OH)_2^\circ$ n=6	-3.73		0.75	-4.13		0.68	-4.01		0.68
$XOH_2\text{-}UO_2(OH)_2^+$ n=6	3.40		0.64	3.00		0.64	4.03		0.72
$XOH\text{-}UO_2(OH)_3^-$ n=6	-11.00		0.89	-11.11		0.78	-9.84		1.22
$XOH_2\text{-}UO_2(OH)_3^\circ$ n=6	-3.73		0.75	-4.13		0.68	-2.01		1.07
$XOH\text{-}UO_2(OH)_4^{2-}$ n=6	-19.52		1.34	-19.20		1.09	-16.08		2.43
$XOH_2\text{-}UO_2(OH)_4^-$ n=6	-11.00		0.89	-11.11		0.78	-7.14		2.79
$XOH\text{-}UO_2CO_3^\circ$	16.83		0.76 n=4	16.44		1.02 n=4	16.59		1.04 n=1
$XOH_2\text{-}UO_2(CO_3)_2^-$	29.70		1.41 n=4	29.46		1.16 n=4	30.09		0.49 n=4
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	37.03		10.01 n=2	36.55		2.41 n=2	35.99		3.79 n=3
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^\circ$	14.76		1.70 n=4	14.34		1.83 n=4	15.50 ~~15.02~~		2.55 ~~3.14~~ n=4

DRJ 11/22/94

D.R. Jenne

8/12/94
DRJ

Sample hand calculations for spreadsheet calculation of ΔH_r. Sources of ΔH_f° values discussed on pg. 2-4, this volume. Also calculates molecular weight of complex

		Americium																
				M.W.Am+3	M.W.Am+4	M.W.AmO2+1	M.W.AmO2+2	M.W.E-1	M.W.H2O	M.W.H+1	M.W.F-1	M.W.Cl-1	M.W.Br-1	M.W.I-1	M.W.CO3-2	M.W.NO3-1	M.W.PO4-3	M.W.SO4-2
				243	243	274.9988	274.9988	0	18.015	1.008	18.998	35.453	79.904	126.905	60.008	62.004	94.97	96.062
			MINTEQA2 ID #	40	41	42	43	1	2	330	270	180	130	380	140	492	580	732
	M.W.	Americium																
H.Rxn	Product	Product	H.f.prod	H.f.Am+3	H.f.Am+4	H.f.AmO2+1	H.f.AmO2+2	H.f.E-1	H.f.H2O	H.f.H+1	H.f.F-1	H.f.Cl-1	H.f.Br-	H.f.I-1	H.f.CO3-2	H.f.NO3-1	H.f.PO4-3	H.f.SO4-2
(kcal/mol)	Species	Species	(kcal/mol)	-147.424	-103.378	-192.434	-155.849	0	-68.317	0	-80.15	-39.933	-29.04	-13.6	-161.385	-49.429	-305.3	-217.4
		Solids																
147.424	243	Am (c)	0	1				3										
48.355	294.021	Am(OH)3	-304.02	1					3	-3								
352.375	294.021	Am(OH)3(am)	----	1					3	-3								
10.256	320.015	AmOHCO3	-366.87	1					1	-1					1			
		Aqueous																
2.464	363.016	Am(CO3)2-1	-467.73	1											2			
3.599	303.008	AmCO3+1	-305.21	1											1			
631.579	423.024	Am(CO3)3-3	----	1											3			
196.853	305.004	AmNO3+2	----	1												1		
246.282	367.008	Am(NO3)2+1	----	1												2		

Example Calculation:

$$Am^{3+} + 2\,CO_3^{2-} = Am(CO_3)^{2-}$$

Enthalpy of Reaction = Σ H_f (products) - Σ H_f (reactants)

H_f values:

Am^{3+} = -147.424 kcal/mol
CO_3^{2-} = -161.385 kcal/mol
$Am(CO_3)^{2-}$ = -467.73 kcal/mol

Therefore:

Enthalpy of Reaction (H. Rxn) = [-467.73] - [(-147.424) + 2(-161.385)] = 2.464 kcal/mol ✓
Molecular Weight of $Am(CO_3)^{2-}$ = (243) + 2(60.008) = 363.016 g/mol ✓

These numbers agree with those calculated for $Am(CO_3)^{2-}$ in the spreadsheet.

8/12/94
DRJ

Conversion of Surface Charge data ($\mu C/cm^2$) to TotalH^+ (TOTH)

type of solid: HYDROUS FERRIC OXIDE
source of data: YATES (1975)

IONIC STRENGTH (mol/L) = .01

SURFACE AREA (sq.m/g) = 257
SOLID CONC (g/L) = 1.4

pH	SURFACE CHARGE			TOTH	
	uC/sq.cm	ueqv/g	mol/L	mol/L	
4.025	30.644	816.245	1.143E-03	1.237E-03	← Sample Hand Calc. (see next page)
4.308	28.038	746.831	1.046E-03	1.095E-03	
4.621	24.731	658.744	9.222E-04	9.462E-04	
5.041	20.889	556.407	7.790E-04	7.8?1E-04	
5.344	18.412	490.429	6.866E-04	6.911E-04	
5.736	14.903	396.962	5.557E-04	5.576E-04	
6.220	10.815	288.072	4.033E-04	4.039E-04	
6.726	7.465	198.841	2.784E-04	2.785E-04	
7.236	4.497	119.784	1.677E-04	1.675E-04	
7.830	1.165	31.031	4.344E-05	4.263E-05	
8.185	-1.115	-29.700	-4.158E-05	-4.346E-05	
8.419	-2.836	-75.541	-1.058E-04	-1.090E-04	
8.892	-6.168	-164.293	-2.300E-04	-2.396E-04	
9.695	-13.672	-364.172	-5.098E-04	-5.708E-04	

This sample problem is from Dzomback (1986) and will serve as a check for the spreadsheet calculations. See next pg (94)

8/12/94
DRW

25 Deg C; No CO2					Surface Charge		TOTH
Area(m2/g)=	257	Solid(g/l)=	1.4				
		I.S.	pH	(uC/cm2)	ueqiv/g	(mol/liter)	(mol/liter)
		0.01	4.025	30.644	816.244995	1.1427e-03	1.2371e-03
		0.01	4.308	28.038	746.830609	1.0456e-03	1.0948e-03
		0.01	4.621	24.731	658.744125	9.2224e-04	9.4617e-04
		0.01	5.041	20.889	556.407182	7.7897e-04	7.8807e-04
		0.01	5.344	18.412	490.428888	6.8660e-04	6.9113e-04
		0.01	5.736	14.903	396.961857	5.5575e-04	5.5758e-04
		0.01	6.22	10.815	288.072367	4.0330e-04	4.0388e-04
		0.01	6.726	7.465	198.84052	2.7838e-04	2.7850e-04
		0.01	7.236	4.497	119.783767	1.6770e-04	1.6754e-04
		0.01	7.83	1.165	31.0313738	4.3444e-05	4.2627e-05
		0.01	8.185	-1.115	-29.699555	-4.1579e-05	-4.3456e-05
		0.01	8.419	-2.836	-75.540752	-1.0576e-04	-1.0898e-04
		0.01	8.892	-6.168	-164.29314	-2.3001e-04	-2.3960e-04
		0.01	9.695	-13.672	-364.17248	-5.0984e-04	-5.7078e-04

Converting Surface Charge ($\mu C/cm^2$) to Total H+ (TOTH in mol/L):

$\mu C/cm^2$ to $\mu eq/g$:

($30.644\ \mu C/cm^2$)*($257\ m^2/g$)*($10000\ cm^2/m^2$)*(1/F) = 816.245 $\mu eq/g$ ✓

where the Faraday Constant, F = 96484.61 $\mu C/\mu eq$

$\mu eq/g$ to moles charge/L:

(816.245 $\mu eq/g$)*(10^{-6} moles/μeq)*(1.4 g/L) = 0.0011427 moles charge/L ✓

moles charge/L to TOTH (in mol/L):

$0.0011427 + 10^{-4.025} - 10^{-(14 - (4.025 + \log\gamma))} = 0.0012371$ mol H+/L ✓

where log γ is the activity coefficient for the ionic strength (I.S.), calculated using the Davies Equation such that

$\log\gamma = [2(-0.508 *\{[SQRT(0.01)]/[1 + SQRT(0.01)] - 0.24*(0.01)\} = -0.09$

DRWumm

Sample calculation matches spreadsheet and also matches output of Dzombak (1986) from previous pg. 93

8/12/94
DRW

Sample calculations for determining best estimate Log K values and 95% confidence limits. All subsequent spreadsheet calculations are made in this manner

Computation of Average Log K for Goethite Sorption Data No CO2																											
Sanchez et al. (1985)							Computation of "Average" Log K values												Computation of Confidence Limits								
I=0M		DLM		CCM		TLM			DLM				CCM				TLM			DLM			CCM			TLM	
Surf Comp	Log K	sig K	Log K	sig K	Log K	sig K	sum1/sig K	w.f.	w.f.*Log K	Log K	sum1/sig K	w.f.	w.f.*Log K	Log K	sum1/sig K	w.f.	w.f.*Log K	Log K	Sum wf*dif	Sx	conflim	Sum wf*dif	Sx	conflim	Sum wf*dif	Sx	conflim
Pu(V)=10-10 M																											
XOPUO2	-0.02	0.0299	-1.41	0.0235	-4	0.0201	70.61954	0.473592	-0.00947	-0.66748	88.21529	0.482379	-0.68015	-1.70504	104.6963	0.475196	-1.90078	-4.05773	0.198545	0.37717	5.519491	0.041992	0.081124	2.559797	0.001584	0.003018	0.493694
XOHPUO2+	5.72	0.0213	5.23	0.0214	4.14	0.0218	100.1398	0.468828	2.681696	5.512843	99.36055	0.470297	2.459653	5.018119	97.95489	0.468293	1.938732	4.065561	0.020119	0.037877	1.74912	0.021113	0.039859	1.794291	0.002595	0.00488	0.627847
XOPUO2OH-	-5.39	0.0396	-7.94	0.0256	-9.12	0.024	57.51059	0.439093	-2.36671	-6.58473	78.27819	0.499022	-3.96223	-8.29569	86.11111	0.483871	-4.4129	-9.44	0.626754	1.117395	9.500225	0.063136	0.126025	3.190495	0.049548	0.096	2.784621
XOHPUO2OH	-0.02	0.0299	-1.41	0.0235	-1.3	0.0233	70.61954	0.473592	-0.00947	-0.66748	88.21529	0.482379	-0.68015	-1.70504	89.21475	0.481069	-0.62539	-1.58541	0.198545	0.37717	5.519491	0.041992	0.081124	2.559797	0.039188	0.075517	2.469743
XOH2PUO2OH+	5.72	0.0213	5.23	0.0214	6.54	0.0226	100.1398	0.468828	2.681696	5.512843	99.36055	0.470297	2.459653	5.018119	92.55697	0.47806	3.126513	6.284249	0.020119	0.037877	1.74912	0.021113	0.039859	1.794291	0.031269	0.059909	2.199774
Pu(V)=10-11 M																											
XOPUO2	-1.25	0.0269	-1.98	0.0219	-4.11	0.0182		0.526408	-0.65801			0.517621	-1.02489			0.524804	-2.15695		0.178624			0.039133			0.001434		
XOHPUO2+	5.33	0.0188	4.83	0.019	4	0.0192		0.531172	2.831147			0.529703	2.558465			0.531707	2.126829		0.017758			0.018745			0.002285		
XOPUO2OH-	-7.52	0.031	-8.65	0.0255	-9.74	0.0225		0.560907	-4.21802			0.500978	-4.33346			0.516129	-5.0271		0.490641			0.062889			0.046452		
XOHPUO2OH	-1.25	0.0269	-1.98	0.0219	-1.85	0.0216		0.526408	-0.65801			0.517621	-1.02489			0.518931	-0.96002		0.178624			0.039133			0.036329		
XOH2PUO2OH+	5.33	0.0188	4.83	0.019	6.05	0.0207		0.531172	2.831147			0.529703	2.558465			0.52194	3.157737		0.017758			0.018745			0.02864		

The analysis used here is from Dzombak (1986) and Dzombak and Morel (1990)

Calculating Best-Fit LogK - Example

For CCM, $XO\text{-}PuO_2^0$: $\sum_i \frac{1}{\sigma_i} = (\text{sum } 1/\text{sig}K) = \frac{1}{\text{sig}K_1} + \frac{1}{\text{sig}K_2} = \frac{1}{.0235} + \frac{1}{.0219} = \boxed{88.2153}$

weighting factor(w.f.) = $\left(\frac{1}{\sigma_1}\right) / \sum_i \frac{1}{\sigma_i}$ and $\left(\frac{1}{\sigma_2}\right) / \sum_i \frac{1}{\sigma_i}$

for 10^{-10} M: w.f. = $\left(\frac{1}{0.0235}\right)/88.2153 = \boxed{0.4824}$

10^{-11} M: w.f. = $\left(\frac{1}{0.0219}\right)/88.2153 = \boxed{0.5176}$

Best-Fit LogK = $(0.4824)(-1.41) + (0.5176)(-1.98) = \boxed{-1.705}$

Continuing to calculate 95% confidence limit

sample variance $S_x^2 = \sum_i (w.f.)_i (\log K_i - \log K_{Avg})^2 / n-1 = [0.4824(-1.41-(-1.705))^2 + 0.5176(-1.98-(-1.705))^2]/2-1 = \boxed{0.08112}$

Standard average error = $S_{\bar{x}} = \frac{S_x}{\sqrt{n}} = \frac{\sqrt{0.08112}}{\sqrt{2}} = \boxed{0.2014}$

For degrees freedom = n-1 = 2-1 = 1 (since there are 2 values), the 95% confidence limit calculated using the single-tailed Students t-distribution

95% conflim = $(t_{\alpha/2})(S_{\bar{x}}) = (12.71)(0.2014) = \boxed{2.5598}$ ✓

From Dzombak (1986)

DRWumm

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Np(V) sorption on Ferrihydrite

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 2: Percentage adsorption versus final pH...) is from the following reference:

Girvin, D.C., L.L. Ames, A.P. Schwab, and J.E. McGarrah. "Neptunium Adsorption on synthetic Amorphous Iron Oxyhydroxide." Journal of Colloid and Interface Science. Vol. 141. pp. 67-78. 1991.

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Girvin et al. (1991)	Np(V)-Ferrihydrite	
Figure 2 (page 71)		
Aso=600 m2/g	atm CO2	
0.1 M NaNO3	M/V=0.01 M=0.89 g/L	
pH	%sorbed	mol sorbed
4.5E-11 M		
4.00	2.956	1.33E-12
4.92	13.864	6.23E-12
5.44	34.444	1.55E-11
5.83	60.667	2.73E-11
6.83	96.667	4.35E-11
7.60	98.889	4.45E-11
8.65	98.889	4.45E-11
4.7E-12 M		
4.00	5.106	2.40E-13
4.10	1.330	6.25E-14
5.02	11.106	5.22E-13
5.13	23.191	1.09E-12
5.49	39.362	1.85E-12
5.33	41.489	1.95E-12
5.59	70.851	3.33E-12
6.09	75.319	3.54E-12
6.71	94.681	4.45E-12
7.02	97.021	4.56E-12
8.63	99.362	4.67E-12
4.5E-13 M		
3.99	1.611	7.25E-15
5.01	13.711	6.17E-14
5.45	36.889	1.66E-13
5.94	72.889	3.28E-13
6.66	97.111	4.37E-13
7.70	99.333	4.47E-13

Girvin, D.C., L.L. Ames, A.P. Schwab, and J.E. McGarrah. 1991. Neptunium adsorption on synthetic amorphous iron oxyhydroxide. *Journal of Colloid and Interface Science.* 141: 67-78.

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```
Neptunium
on
Ferrihyd
2.3s\nm2

0
1
0
0
1
50
4        1        3        1
00001  -2.69  2.05E-3   XOH
00180  -2.0   0.00000   PSIO
00140  -3.5   3.61E-4   CO2g
00031  -12.3  4.5E-13   NpO2+      <--
00032   0.0   0.00000   NpO2(ads)
00050   0.0   0.00000   H+
00003  -1.0   0.00000   Na+
00005  -1.0   0.00000   NO3-

00050    0.00  050  1
00031    0.00  031  1
00140    0.00  140  1
01401  -17.50  140  1 050 -2
01402   -7.61  140  1 050 -1
01403   -1.48  140  1
01404  -16.67  140  1 003  1 050 -2
01405   -8.05  140  1 003  1 050 -1
03100   -8.90  031  1 050 -1
03101  -13.34  031  1 140  1 050 -2
03102  -28.00  031  1 140  2 050 -4
03103  -42.68  031  1 140  3 050 -6
01050    7.35  001  1 160  1 050  1
01100   -8.45  001  1 160 -1 050 -1
00100  -13.78  050 -1
00001    0.00  001  1
03201   -3.00  001  1 160  0 050 -1 031  1 032  1

00001   600.0 0.890  1.0
     0      0
       1
     3201
       6        1        1        0
      32
7.25E-15
6.17E-14
1.66E-13
3.28E-13
4.37E-13
4.47E-13
      50
-3.99
-5.01
-5.45
-5.94
-6.66
-7.70
       1        0
      32        0.10     4.5E-17
```

CCM

$XOH + NpO_2^+ = XONpO_2^0 + H^+$

FITEQL example input

$Np_T = 4.5 \times 10^{-13}$ M

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```
Neptunium
on
Ferrihyd
(Girvin)
2.3s\nm2

0
1
0
0
1
50
4        1        3        1
00001  -2.69  2.05E-3   XOH
00160  -2.0   0.00000   PSIO
00140  -3.5   3.16E-4   CO2g
00031  -11.3  4.7E-12   Np(V)      <--
00032   0.0   0.00000   Npads
00050   0.0   0.00000   H+
00003  -1.0   0.00000   Na+
00005  -1.0   0.00000   NO3-

00050    0.00  050  1
00031    0.00  031  1
00140    0.00  140  1
01401  -17.50  140  1 050 -2
01402   -7.61  140  1 050 -1
01403   -1.48  140  1
01404  -16.67  140  1 003  1 050 -2
01405   -8.08  140  1 003  1 050 -1
03100   -8.90  031  1 050 -1
03101  -13.34  031  1 140  1 050 -2
03102  -28.00  031  1 140  2 050 -4
03103  -42.68  031  1 140  3 050 -6
01050    7.18  001  1 160  1 050  1
01100   -8.82  001  1 160 -1 050 -1
00100  -13.78  050 -1
00001    0.00  001  1
03201   -3.00  001  1 160  0 050 -1 031  1 032  1

00002   600   0.890
0.1    1.1
       1
     3201
      11        1        1        0
      32
2.40E-13
6.25E-14
5.22E-13
1.09E-12
1.85E-12
1.[illegible]E-12
```

DLM

$XOH + NpO_2^+ = XONpO_2^0 + H^+$

FITEQL example input
4.7×10^{-12} M

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```
        0                                                     Neptunum
        1                                                        on
        0                                                     Ferrihyd
        0                                                     2.3s\nm2
        1                                                     00000050
       90                                                     00000060
        6        1         3         1                        00000070
00001  -2.69  2.05E-3   XOH                                   00000080
00160  -2.0   0.00E00   PSIO                                  00000090
00161  -1.0   0.00E00   PSIB                                  00000092
00162  -0.2   0.00E00   PSID                                  00000094
00140  -3.5   3.16E-4   CO2g                                  00000095
00031  -10.3  4.5E-11   NpO2+  <-                             00000098
00032   0.0   0.00E00   NpO2(ads)                             00000100
00050   0.0   0.00E00   H+                                    00000102
00003  -1.0   0.00E00   NA+                                   00000104
00005  -1.0   0.00E00   NO3-                                  00000106
                                                              00000110
00050    0.00  050  1                                         00000120
00031    0.00  031  1                                         00000124
00140    0.00  140  1                                         00000125
01401  -17.50  140  1 050 -2                                  00000127
01402   -7.61  140  1 050 -1                                  00000128
01403   -1.48  140  1                                         00000129
01404  -16.67  140  1 003  1 050 -2                           00000130
01405   -8.08  140  1 003  1 050 -1                           00000131
03100   -8.90  031  1 050 -1                                  00000126
03101  -13.34  031  1 140  1 050 -2                           00000132
03102  -28.00  031  1 140  2 050 -4                           00000133
03103  -42.68  031  1 140  3 050 -6                           00000133
00100  -13.78  050 -1                                         00000139
01050    5.89  001  1 160  1 050  1                           00000140
01100   -9.89  001  1 160 -1 050 -1                           00000145
01103   -7.66  001  1 160 -1 161  1 050 -1 003  1             00000147
01055    8.21  001  1 160  1 161 -1 050  1 005  1             00000149
00001    0.00  001  1                                         00000150
03201   -5.00  001  1 160 -1 161  1 050 -1 031  1 032  1      xoNpo2
                                                              00000174
                                                              00000175
00004   600.0 0.890  0.8    0.2                               00000180
0.1     1.0                                                   00000185
          1                                                   00000190
       3201                                                   00000195
          7        1         1         0                      00000230
         32                                                   00000240
1.33E-12                                                      00000260
6.23E-12                                                      00000280
1.55E-11                                                      00000300
2.73E-11                                                      00000320
4.35E-11                                                      00000340
4.45E-11                                                      00000360
4.45E-11                                                      00000380
         50                                                   00000560
-4.00                                                         00000580
-4.92                                                         00000600
-5.44                                                         00000620
-5.83                                                         00000640
-6.83                                                         00000660
-7.60                                                         00000680
-8.95                                                         00000700
          1        0                                          00000880
         32      0.10   4.5E-15                               10%error
```

TLM

$XOH + NpO_2 = XO\text{-}NpO_2^0 + H^+$

EXAMPLE FITEQL input

$Np_T = 4.5 \times 10^{-11}$

Table BXX. Neptunium (V)-Ferrihydrite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Ferrihydrite; A_{SP}: 600 m^2/g; Data Source: Girvin et al. (1991); Concentration: [Np(V)] = 4.5E-13 M
Rel Error (pH): (a); Abs Error (pH): (a); Rel Error (radionuclide): 0.10; Abs Error (radionuclide): 4.5E-17 M
Ionic Strength (electrolyte): 0.1 M $NaNO_3$; N_S = 2.31 sites/nm²; M/V = 0.89 g/L

$p(CO_2)$ = 1E-3.5 atm	DLM			CCM			TLM		
	Log K_+ = 7.29 Log K_- = -8.93			Log K_+ = 7.35 Log K_- = -8.45			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}NpO_2^o$	-2.96	1.2	.0289	-2.76	1.0	.0298	-5.96	78.6	.0.24
$XOH\text{-}NpO_2^+$	5.10	1.8	.0284	4.72	3.8	.0277	1.72	84.8	.0350
$XO\text{-}NpO_2OH^-$	-11.02	1.1	.0295	-10.29	3.4	.0327	-10.52	1.5	.0309
$XOH\text{-}NpO_2OH^o$	-2.96	1.2	.0289	-2.76	1.0	.0298	-2.84	1.0	.0296
$XOH_2\text{-}NpO_2OH^+$	5.10	1.8	.0284	4.72	3.8	.0277	4.94	1.8	.0285
OTHER SPECIES:									
$(XO)_2\text{-}NpO_2^-$	-8.22	1.1	.0295	-7.32	5.2	.0339	-10.66	63.8	.0286

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

FITEQL Results

3/24/95

Table BXX. Neptunium (V)-Ferrihydrite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Ferrihydrite; A_{SP}: 600 m^2/g; Data Source: Girvin et al. (1991); Concentration: [Np(V)] = 4.7E-12 M
Rel Error (pH): (a); Abs Error (pH): (a); Rel Error (radionuclide): 0.10; Abs Error (radionuclide): 4.7E-16 M
Ionic Strength (electrolyte): 0.1 M $NaNO_3$; N_S = 2.31 sites/nm²; M/V = 0.89 g/L

$p(CO_2)$ = 1E-3.5 atm	DLM			CCM			TLM		
	Log K_+ = 7.29 Log K_- = -8.93			Log K_+ = 7.35 Log K_- = -8.45			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}NpO_2^o$	-3.02	8.9	.0219	-2.83	7.9	.0225	-5.97	77.0	.0256
$XOH\text{-}NpO_2^+$	5.04	9.8	.0216	4.65	12.2	.0211	1.71	81.9	.0277
$XO\text{-}NpO_2OH^-$	-11.08	8.3	.0222	-10.35	8.1	.0242	-10.68	7.5	.0231
$XOH\text{-}NpO_2OH^o$	-3.02	8.9	.0219	-2.83	7.9	.0225	-2.90	8.1	.0223
$XOH_2\text{-}NpO_2OH^+$	5.04	9.8	.0216	4.65	12.2	.0211	4.87	9.7	.0216
OTHER SPECIES:									
$(XO)_2\text{-}NpO_2^-$	-8.28	8.3	.0222	-7.37	9.0	.0250	-10.69	65.3	.0226

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

Table BXX. Neptunium (V)-Ferrihydrite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Ferrihydrite; A_{SP}: 600 m^2/g; Data Source: Girvin et al. (1991); Concentration: [Np(V)] = 4.5E-11 M
Rel Error (pH): (a); Abs Error (pH): (a); Rel Error (radionuclide): 0.10; Abs Error (radionuclide): 4.5E-15 M
Ionic Strength (electrolyte): 0.1 M $NaNO_3$; N_S = 2.31 sites/nm²; M/V = 0.89 g/L

$p(CO_2)$ = 1E-3.5 atm	DLM			CCM			TLM		
	Log K_+ = 7.29 Log K_- = -8.93			Log K_+ = 7.35 Log K_- = -8.45			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}NpO_2^o$	-2.85	1.6	.0308	-2.68	2.9	.0320	-5.63	64.0	.0270
$XOH\text{-}NpO_2^+$	4.56	1.6	.0278	4.85	0.7	.0291	2.05	74.7	.0295
$XO\text{-}NpO_2OH^-$	-10.02	18.6	.0452	-10.24	7.0	.0352	-10.55	4.4	.0332
$XOH\text{-}NpO_2OH^o$	-2.85	1.6	.0308	-2.68	2.9	.0320	-2.75	2.5	.0316
$XOH_2\text{-}NpO_2OH^+$	4.56	1.6	.0278	4.85	0.7	.0291	5.05	1.2	.0302
OTHER SPECIES:									
$(XO)_2\text{-}NpO_2^-$	-7.08	21.9	.0492	-7.28	8.8	.0366	-10.36	42.4	.0245

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

FITEQL results

3/24/95
DBLumm

From Turner (1995)

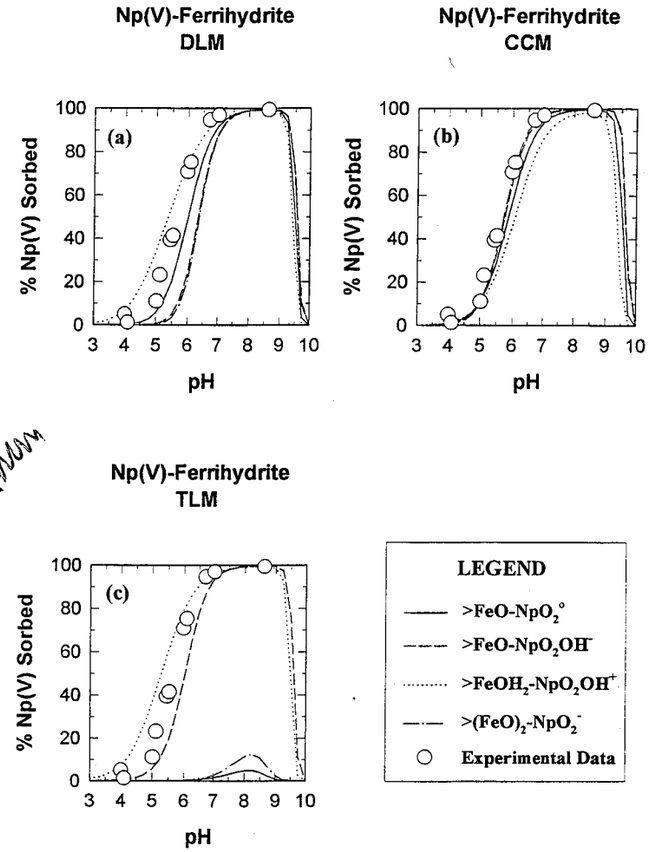

Figure 4-10. Np(V) sorption on ferrihydrite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T=4.7\times10^{-12}$ M, 0.1 M $NaNO_3$, M/V=0.89 g/L. Model parameters from Tables 3-1 and B-10. Data from Girvin et al. (1991).

Plotting results. Calculations made using MINTEQA2 w/ CNWRA modified database (Turner, 1993)

U(VI)-Sorption on Goethite - Hsi (1981) & Hsi & Langmuir (1985)

4/26/95
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Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 8: Adsorption of uranyl vs. pH...) is from the following reference.

Hsi, C-K.D. and Langmuir. "Adsorption of Uranyl onto Ferric Oxyhydroxides: Application of the Surface Complexation Site-Binding Model." Geochimica et Cosmochimica Acta. Vol. 49. pp. 1,931-1,941. 1985.

DBLumm

4/26/95 DRDLmm

Hsi, C-K.D, and D. Langmuir. 1985. Adsorption of uranyl onto ferric oxyhydroxides: Application of the surface complexation site-binding model. *Geochimica et Cosmochimica Acta* 49: 1931-1941.

Also:

Hsi, C-K.D. 1981. *Sorption of Uranium(VI) by Iron Oxides*. Ph.D. Dissertation. Golden, CO: Colorado School of Mines.

Hsi and Langmuir (1985)	U(VI)-Goethite	Hsi (1981)
Figure 8 (page 1939)		Figures 10 and 64
Asp=50 m2/g	M/V=1 g/L	
0.1 M NaNO3	1E-5 M	
pH	%sorbed	mol sorbed
No CO2		
3.70	18.10	1.810E-6
4.09	34.50	3.450E-6
4.08	45.10	4.510E-6
4.04	49.70	4.970E-6
4.26	50.00	5.000E-6
4.40	60.40	6.040E-6
4.25	60.90	6.090E-6
4.56	73.40	7.340E-6
4.51	75.20	7.520E-6
4.74	82.30	8.230E-6
5.00	93.20	9.320E-6
4.97	96.00	9.600E-6
5.33	95.90	9.590E-6
5.74	98.70	9.870E-6
6.10	99.90	9.990E-6
6.62	99.97	9.997E-6
7.32	99.98	9.998E-5
8.11	99.98	9.998E-5
8.91	99.99	9.999E-5
pH	%sorbed	mol sorbed
C(t)=0.001 M		
3.91	21.21	2.12E-06
4.24	39.09	3.91E-06
4.23	54.66	5.47E-06
4.67	73.80	7.38E-06
4.75	92.11	9.21E-06
4.85	87.93	8.79E-06
4.84	91.54	9.15E-06
5.10	94.01	9.40E-06
5.47	99.97	1.00E-05
5.59	99.98	1.00E-05
5.73	99.96	1.00E-05
5.84	99.95	1.00E-05
5.93	99.99	1.00E-05
6.01	99.96	1.00E-05
6.23	99.95	1.00E-05
6.27	99.99	1.00E-05
6.59	99.99	1.00E-05
6.82	99.99	1.00E-05
7.03	99.98	1.00E-05
7.42	99.75	9.98E-06
8.03	99.82	9.98E-06
8.24	99.18	9.92E-06
pH	%sorbed	mol sorbed
C(t)=0.01 M		
4.43	70.39	7.04E-06
4.93	90.18	9.02E-06
5.22	96.70	9.67E-06
5.87	98.11	9.81E-06
6.08	97.98	9.80E-06
6.23	94.62	9.46E-06
6.34	95.48	9.55E-06
6.42	93.65	9.37E-06
6.67	87.34	8.73E-06
6.73	84.84	8.48E-06
6.80	86.40	8.64E-06
7.05	83.82	8.38E-06
7.18	74.79	7.48E-06
7.83	55.17	5.52E-06
8.10	31.02	3.10E-06
8.46	41.06	4.11E-06
8.69	37.47	3.75E-06

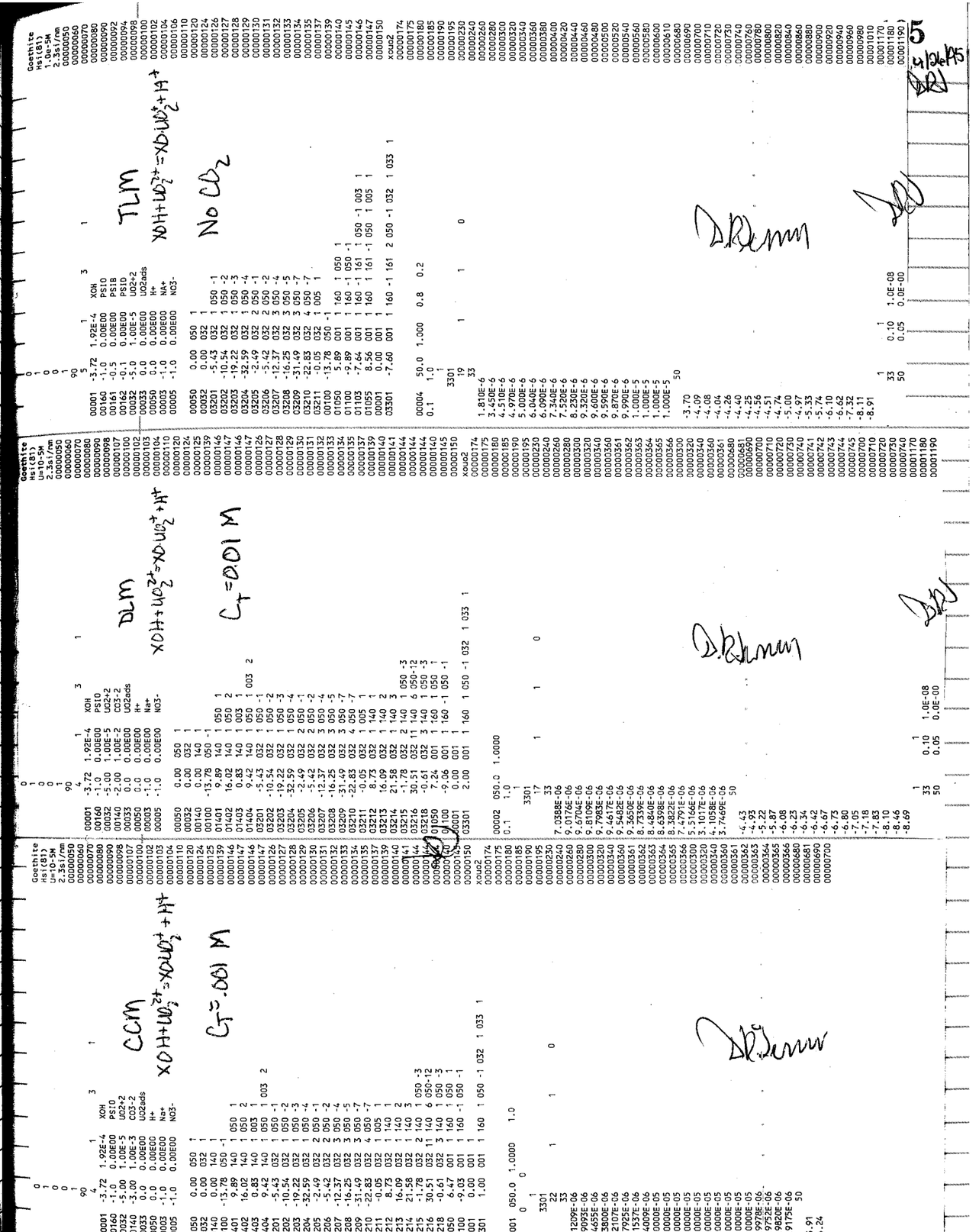
DRDLmm

DRDLmm

DRDLmm

DRDLmm

Example FITEQL Input Files



FITEQL Results

4/26/95 DBLmm

Uranium (VI)-Goethite Sorption Binding Constants; Monodentate, mononuclear compounds

Solid: goethite A_{SP}: 50 m^2/g Data Source: Hsi & Langmuir (1985); Hsi (1981) Concentration: [U(VI)] = 1e-5 M	Rel Error (pH): 0.05 Abs Error (pH):0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0e-8 M	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

Fig. 10, extension .DGO No CO_2	DLM Log K_+ = 7.35 Log K_- = -9.17			CCM Log K_+ = 6.47 Log K_- = -9.03			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$
XO-UO_2^+	3.13	1.6	.0352	2.69	1.9	.0350	-2.51	45.0	.0400
XOH-UO_2^{2+}	9.86	10.8	.0278	9.56	8.3	.0338	6.57	43.3	.0638
XO-UO_2OH^o	-3.54	3.9	.0432	-4.08	2.0	.0377	-7.33	14.7	.0295
XOH-UO_2OH^+	3.13	1.6	.0352	2.69	1.9	.0350	0.97	18.3	.0385
XO-$UO_2(OH)_2^-$	-10.19	6.0	.0518	-10.77	2.4	.0411	-11.38	0.8	.0459
XOH-$UO_2(OH)_2^{-}$	-3.54	3.9	.0432	-4.08	2.0	.0377	-3.99	2.0	.0375
XOH_2-$UO_2(OH)_2^+$	3.13	1.6	.0352	2.69	1.9	.0350	4.29	0.7	.0458
XOH-$UO_2(OH)_3^-$	-10.19	6.0	.0518	-10.77	2.4	.0411	-7.96	2.5	.0530
XOH_2-$UO_2(OH)_3^{-}$	-3.54	3.9	.0432	-4.08	2.0	.0377	-0.55	4.9	.0461
XOH-$UO_2(OH)_4^{2-}$	-16.80	7.3	.0611	-17.39	2.2	.0457	-11.40	1.7	.0734
XOH_2-$UO_2(OH)_4^-$	-10.19	6.0	.0518	-10.77	2.0	.0411	-4.50	4.8.	0623

Results
Calculations made using MINTEQA2 w/NEA/TDB database (Turner, 1993)

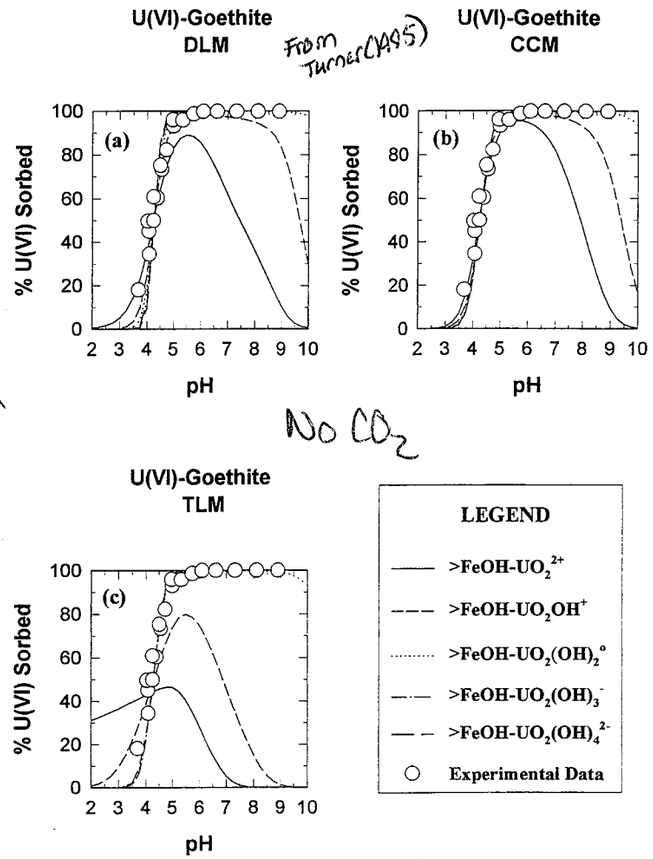


Figure 4-19. U(VI) sorption on goethite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $U(VI)_T = 1 \times 10^{-5}$ M, 0.1 M $NaNO_3$, M/V=1 g/L. Model parameters from Tables 3-1 and B-19. Data from Hsi and Langmuir (1985).

FITEQL Results

4/26/95 DBLmm

Uranium (VI)-Goethite Sorption Binding Constants; Monodentate, mononuclear compounds

Solid: goethite A_{SP}: 50 m^2/g Data Source: Hsi & Langmuir (1985); Hsi (1981) Concentration: [U(VI)] = 1e-5 M	Rel Error (pH): 0.05 Abs Error (pH):0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0e-8 M	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

CO_2: C_T = 0.01 Fig 64 #2 (65)	DLM Log K_+ = 7.35 Log K_- = -9.17			CCM Log K_+ = 6.47 Log K_- = -9.03			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$
XO-UO_2^+	6.20	5.4	.0457	5.94	6.5	.0492	6.60	10.2	.0798
XOH-UO_2^{2+}	14.58	5.9	.0525	14.16	7.3	.0598	15.61	6.8	.0985
XO-UO_2OH^o	-2.11	4.3	.0414	-2.16	4.4	.0416	-1.96	9.2	.0552
XOH-UO_2OH^+	6.20	5.4	.0457	5.94	6.5	.0492	6.54	7.1	.0646
XO-$UO_2(OH)_2^-$	-10.33	2.0	.0387	-10.11	2.2	.0371	-9.70	2.6	.0529
XOH-$UO_2(OH)_2^{o}$	-2.11	4.3	.0414	-2.16	4.4	.0416	-2.00	4.3	.0414
XOH_2-$UO_2(OH)_2^+$	6.20	5.4	.0457	5.94	6.5	.0492	6.47	3.1	.0530
XOH-$UO_2(OH)_3^-$	-10.33	2.0	.0387	-10.11	2.2	.0371	-9.36	15.2	.0410
XOH_2-$UO_2(OH)_3^{o}$	-2.11	4.3	.0414	-2.16	4.4	.0416	-1.83	11.5	.0297
XOH-$UO_2(OH)_4^{2-}$	-22.22	2.4	.0379	-21.60	5.8	.0369	-16.03	53.8	.0691
XOH_2-$UO_2(OH)_4^-$	-10.33	2.0	.0387	-10.11	2.2	.0371	-4.93	63.3	.0207
XOH-$UO_2CO_3^{o}$	18.41	12.5	.0517	18.66	11.8	.0494	18.65	9.9	.0406
XOH_2-$UO_2(CO_3)_2^-$	30.86	12.5	.0519	31.11	11.9	.0496	31.78	3.2	.0391
XOH_2-$UO_2(CO_3)_3^{3-}$	n.c.	n.c.	.n.c.	36.46	9.6	.0596	39.75	21.9	.0627
XOH_2-$(UO_2)_2CO_3(OH)_3^{o}$	17.72	10.9	.0594	17.66	11.0	.0596	17.92	7.2	.0475

Uranium (VI)-Goethite Sorption Binding Constants; Monodentate, mononuclear compounds

Solid: goethite A_{SP}: 50 m^2/g Data Source: Hsi & Langmuir (1985); Hsi (1981) Concentration: [U(VI)] = 1e-5 M	Rel Error (pH): 0.05 Abs Error (pH):0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0e-8 M	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

CO_2: C_T = 0.001 Fig 64 #1	DLM Log K_+ = 7.35 Log K_- = -9.17			CCM Log K_+ = 6.47 Log K_- = -9.03			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$
XO-UO_2^+	3.15	6.0	.0402	2.70	7.0	.0409	-2.30	68.4	.0490
XOH-UO_2^{2+}	9.98	29.9	.0315	9.60	18.7	.0387	7.10	60.7	.0707
XO-UO_2OH^o	-3.72	1.0	.0560	-4.23	0.8	.0475	-7.20	32.7	.0330
XOH-UO_2OH^+	3.15	6.0	.0402	2.70	7.0	.0409	1.22	34.9	.0434
XO-$UO_2(OH)_2^-$	-10.37	1.7	.0680	-10.96	0.6	.0538	-11.54	0.9	.0560
XOH-$UO_2(OH)_2^{o}$	-3.72	1.0	.0560	-4.23	0.8	.0475	-4.13	0.9	.0468
XOH_2-$UO_2(OH)_2^+$	3.15	6.0	.0402	2.70	7.0	.0409	4.21	2.1	.0531
XOH-$UO_2(OH)_3^-$	-10.37	1.7	.0680	-10.96	0.6	.0538	-8.22	0.7	.0702
XOH_2-$UO_2(OH)_3^{o}$	-3.72	1.0	.0560	-4.23	0.8	.0475	-0.74	1.4	.0606
XOH-$UO_2(OH)_4^{2-}$	-16.97	2.2	.0808	-17.61	0.6	.0597	-11.79	0.5	.1011
XOH_2-$UO_2(OH)_4^-$	-10.37	1.7	.0680	-10.96	0.6	.0538	n.c.	n.c.	n.c.
XOH-$UO_2CO_3^{o}$	16.17	7.7	.0361	15.60	10.5	.0311	15.70	10.9	.0308
XOH_2-$UO_2(CO_3)_2$	27.76	26.7	.0288	28.08	17.9	.0253	29.51	78.5	.0242
XOH_2-$UO_2(CO_3)_3^{3-}$	35.87	5.0	.0589	35.10	10.0	.0434	n.c.	n.c.	n.c.
XOH_2-$(UO_2)_2CO_3(OH)_3^{o}$	13.22	4.2	.0586	12.74	5.7	.0533	15.92	21.7	.0692

4/26/95
D.R.Lumm

Same as Before (pg. 106)

Plotted using MINTEQA2/ CALSRA database

D.R.Lumm

U(VI)-Goethite
DLM

Turner(1995)

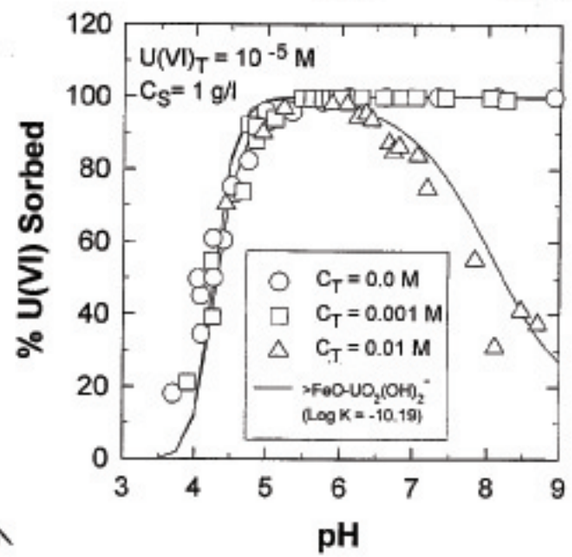


Figure 4-28. DLM predictions of the effects of changing carbon concentration. (a) Model results, U(VI) sorption on goethite. Model parameters from Table B-19. Data from Hsi and Langmuir (1985).

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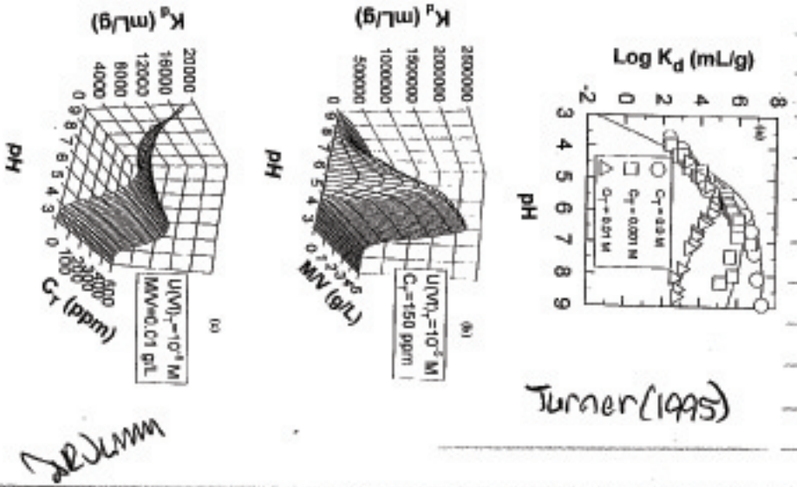
Figure 4-29. DLM predicted K_d for U(VI) sorption on goethite. Values plotted as a function of: (a) pH. Experimental data from Hsi and Langmuir (1985); (b) pH and M/V (in g/L), C_T = 150 ppm; and (c) pH and C_T (in ppm). All model results are calculated for U(VI)$_T$ = 1×10^{-5} M assuming >FeO-UO$_2$(OH)$_2^-$ as a surface complex. Model parameters from Table B-19.



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U(VI)-Goethite Sorption - Kohler et al. (1992)

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 4: Adsorption of U(VI) onto goethite...) is from the following reference:

Kohler, M., E. Wieland, and J.O. Leckie. "Metal-Ligand-Surface Interactions During Sorption of Uranyl and Neptunyl on Oxides and Silicates. Volume 1: Low Temperature Environments." Y.K. Kharaka and A.S. Maest, eds. Proceedings of the 7th International Symposium on Water-Rock Interaction-WRI-7. Rotterdam, Netherlands: A.A. Balkema. 1992.

Kohler, M., E. Wieland, and J.O. Leckie. 1992. Metal-ligand-surface interactions during sorption of uranyl and neptunyl on oxides and silicates. *Proceedings of the 7th International Symposium on Water-Rock Interaction - WRI-7. Volume 1: Low Temperature Environments*. Y.K. Kharaka and A.S. Maest, eds. Rotterdam: A.A. Balkema.

Kohler et al. (1992)	U(VI)-Goethite	
Figure 4 (page 54)		
Asp=50 m2/g	Variable CO2	U(VI)=1E-6 M
0.1 M NaClO4	M/V = 1 g/L	
No CO2		
pH	% sorbed	mol sorbed
3.36	26.67	2.667E-7
3.55	27.94	2.794E-7
3.69	35.65	3.565E-7
3.89	29.55	2.955E-7
3.99	30.94	3.094E-7
4.00	52.50	5.250E-7
4.18	64.31	6.431E-7
4.24	77.05	7.705E-7
4.47	87.06	8.706E-7
4.69	94.44	9.444E-7
4.75	95.83	9.583E-7
4.65	98.07	9.807E-7
6.37	98.25	9.825E-7
6.56	98.21	9.821E-7
9.58	97.70	9.770E-7
p(CO2)=3E-4 atm		
pH	% sorbed	mol sorbed
3.96	0.25	2.500E-9
5.68	99.54	9.954E-7
7.50	99.70	9.970E-7
8.11	94.88	9.488E-7
9.00	64.86	6.486E-7
9.31	1.22	1.220E-8
p(CO2)=2E-2 atm		
pH	% sorbed	mol sorbed
3.71	24.83	2.483E-7
4.04	53.61	5.361E-7
4.38	83.00	8.300E-7
6.71	94.36	8.436E-7
7.30	66.87	6.687E-7
8.37	3.49	3.490E-8
9.85	9.51	9.510E-8

U(VI)-Goethite - Kohler et al. (1992)

4/28/95

D.R. Turner

CCM

No CO_2

$XOH^0 + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

DLM

$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

~~$pCO_2 = 10^{-2.0}$ atm~~ DRT 5/1/95

$pCO_2 = .02$ atm

TLM

$XOH^0 + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

$pCO_2 = 10^{-3.5}$ atm

D.R. Turner

D.R. Turner

4/28/95

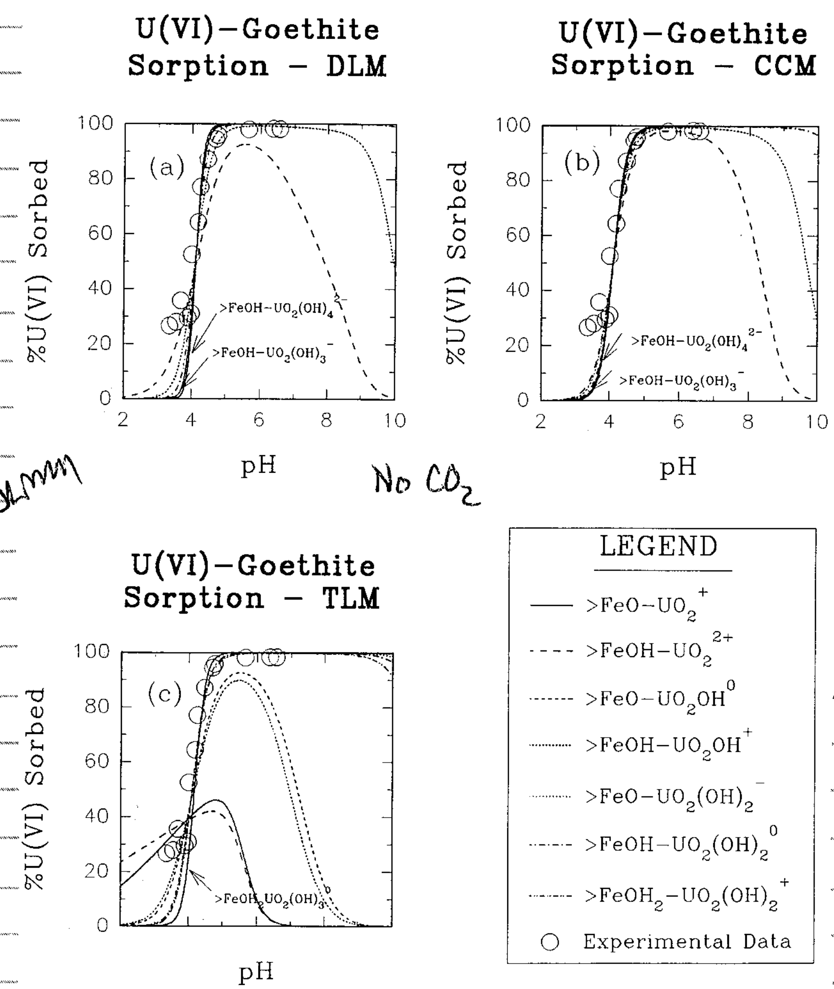
D.R. Turner

Uranium (VI)-Goethite Sorption Binding Constants; Monodentate, mononuclear compounds

Solid: Goethite A_{SP}: 50 m^2/g Data Source: Kohler et al. (1992) Concentration: [U(VI)] = 1E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

No CO_2	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -9.17			Log K_+ = 6.47 Log K_- = -9.03			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-UO_2^+$	3.41	9.3	.0346	2.97	10.1	.0341	-3.09	30.2	.0548
$XOH-UO_2^{2+}$	9.92	11.6	.0276	9.65	13.9	.0330	4.83	32.4	.0288
$XO-UO_2OH^0$	-3.17	13.4	.0441	-3.78	9.7	.0374	-7.27	12.8	.0284
$XOH-UO_2OH^+$	3.41	9.3	.0346	2.97	10.1	.0341	0.59	13.2	.0284
$XO-UO_2(OH)_2^-$	-9.77	16.8	.0534	-10.49	11.0	.0398	-11.44	9.6	.0389
$XOH-UO_2(OH)_2^0$	-3.17	13.4	.0441	-3.78	9.7	.0374	-3.69	9.6	.0371
$XOH_2-UO_2(OH)_2^+$	3.41	9.3	.0346	2.97	10.1	.0341	4.18	8.5	.0370
$XOH-UO_2(OH)_3^-$	-9.77	16.8	.0534	-10.49	11.0	.0398	-7.89	14.2	.0484
$XOH_2-UO_2(OH)_3^0$	-3.17	13.4	.0441	-3.78	9.7	.0374	-0.13	14.3	.0467
$XOH-UO_2(OH)_4^{2-}$	*-16.36	20.5	.0631	-17.19	13.0	.0425	*-12.02	17.8	.0615
$XOH_2-UO_2(OH)_4^-$	-9.77	16.8	.0534	-10.49	11.0	.0398	*-4.37	18.8	.0587

* For convergence, highest pH point not included in optimization (pH=9.58; %sorbed=97.7)



D.R. Turner

4/28/95
DKlemm

Uranium (VI)-Goethite Sorption Binding Constants; Monodentate, mononuclear complexes

Solid: Goethite A_{sp}: 50 m²/g Data Source: Kohler et al. (1992) Concentration: [U(VI)] = 1E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_s = 2.31 sites/nm² M/V = 1 g/L

$p(CO_2)$ = 0.02 atm	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -9.17			Log K_+ = 6.47 Log K_- = -9.03			Log K_1 = 6.00 Log K_2 = -10.00 Log K_{CO_3} = -7.64 Log K_{2m} = 8.78		
	Log K	V_Y	$\sigma_{\log K}$	Log K	V_Y	$\sigma_{\log K}$	Log K	V_Y	$\sigma_{\log K}$
XO-UO_2^+	3.40	39.2	.0543	2.93	39.0	.0543	-3.98	66.1	.0466
XOH-UO_2^{2+}	9.88	54.8	.0471	9.66	43.3	.0511	4.72	65.1	.0838
XO-UO_2OH^0	-2.97	19.4	.0578	-3.67	27.9	.0541	-7.34	55.7	.0488
XOH-$UO_2(OH)^+$	3.40	39.2	.0543	2.93	39.0	.0543	0.49	56.9	.0501
XO-$UO_2(OH)_2^-$	-10.51	25.9	.0393	-10.49	6.6	.0377	-11.33	24.5	.0551
XOH-$UO_2(OH)_2^0$	-2.97	19.4	.0578	-3.67	27.9	.0541	-3.59	29.0	.0542
XOH_2-$UO_2(OH)_3^+$	3.40	39.2	.0543	2.93	39.0	.0543	4.24	32.6	.0560
XOH-$UO_2(OH)_3^-$	-10.51	25.9	.0393	-10.49	6.6	.0377	-10.78	53.7	.0412
XOH_2-$UO_2(OH)_2^0$	-2.97	19.4	.0578	-3.67	27.9	.0541	-2.61	50.0	.0591
XOH-$UO_2(OH)_4^{2-}$	-18.90	46.1	.0401	-18.55	34.8	.0329	-20.66	89.6	.0788
XOH_2-$UO_2(OH)_4^-$	-10.51	25.9	.0393	-10.49	6.6	.0377	-12.47	89.4	.0750
XOH-$UO_2CO_3^0$	16.83	22.7	.0428	16.17	28.9	.0393	14.26	29.8	.0394
XOH_2-$UO_2(CO_3)_2^-$	30.28	9.4	.0510	29.29	21.9	.0402	30.58	56.5	.0593
XOH_2-$UO_2(CO_3)_3^{3-}$	n.c.	n.c.	n.c.	n.c.	n.c.	n.c.	34.73	80.5	.1044
XOH_2-$(UO_2)_3(CO_3)(OH)_3^+$	15.38	26.0	.0661	14.69	31.3	.0664	18.49	21.6	.0704

Uranium (VI)-Goethite Sorption Binding Constants; Monodentate, mononuclear complexes

Solid: Goethite A_{sp}: 50 m²/g Data Source: Kohler et al. (1992) Concentration: [U(VI)] = 1E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_s = 2.31 sites/nm² M/V = 1 g/L

$p(CO_2)$ = 0.0003 atm	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -9.17			Log K_+ = 6.47 Log K_- = -9.03			Log K_1 = 6.00 Log K_2 = -10.00 Log K_{CO_3} = -7.64 Log K_{2m} = 8.78		
	Log K	V_Y	$\sigma_{\log K}$	Log K	V_Y	$\sigma_{\log K}$	Log K	V_Y	$\sigma_{\log K}$
XO-UO_2^+	1.36	50.6	.0426	1.05	49.6	.0407	-5.58	84.2	.2174
XOH-UO_2^{2+}	7.65	82.2	.1200	7.55	75.3	.0783	2.23	84.2	.2188
XO-UO_2OH^0	-7.12	66.9	.0485	-7.14	65.5	.0472	-9.59	82.7	.1321
XOH-UO_2OH^+	1.36	50.6	.0426	1.05	49.6	.0467	-1.83	83.2	.1471
XO-$UO_2(OH)_2^-$	-15.75	74.5	.0614	-15.73	75.9	.0657	-15.22	69.6	.0522
XOH-$UO_2(OH)_2^0$	-7.12	66.9	.0485	-7.14	65.5	.0472	-7.01	66.1	.0477
XOH_2-$UO_2(OH)_3^+$	1.36	50.6	.0426	1.05	49.6	.0467	1.38	62.1	.0453
XOH-$UO_2(OH)_3^-$	-15.75	74.5	.0614	-15.73	75.9	.0657	-16.44	78.1	.0759
XOH_2-$UO_2(OH)_2^0$	-7.12	66.9	.0485	-7.14	65.5	.0472	-8.27	78.0	.0751
XOH-$UO_2(OH)_4^{3-}$	-24.33	76.8	.0688	-24.22	77.7	.0730	-25.67	78.7	.0864
XOH_2-$UO_2(OH)_4^-$	-15.75	74.5	.0614	-15.73	75.9	.0657	-17.51	78.7	.0833
XOH-$UO_2CO_3^+$	16.35	18.7	.0389	16.00	27.8	.0380	16.10	29.2	.0377
XOH_2-$UO_2(CO_3)_2^-$	31.39	12.7	.0498	30.83	21.6	.0529	29.84	61.2	.0372
XOH_2-$UO_2(CO_3)_3^{3-}$	38.80	8.6	.0547	38.36	9.1	.0514	34.78	70.3	.0524
XOH_2-$(UO_2)_3(CO_3)(OH)_3^+$	12.84	16.0	.0489	12.82	15.6	.0486	11.98	45.0	.0355

5/9/95
DKlemm

Np(v)-Kaolinite - Kohler et al. 1992

Kohler, M., E. Wieland, and J.O. Leckie. 1992. Metal-ligand-surface interactions during sorpion of uranyl and neptunyl on oxides and silicates. *Proceedings of the 7th International Symposium on Water-Rock Interaction - WRI-7. Volume 1: Low Temperature Environments*. Y.K. Kharaka and A.S. Maest, eds. Rotterdam: A.A. Balkema.

Kohler et al. (1992)	Np(V)-Kaolinite	
Figure 3 (page 53)	No EDTA	
Asp=11 m2/g	atm CO2	
0.1M NaClO4	M/V= 5 g/L	
Np(V)=1.25E-07	Si:Al = 1:1	
pH	%sorbed	mol sorbed
3.98172	7.04764	8.813E-09
4.98764	3.88953	4.863E-09
6.54432	11.25083	1.406E-08
7.13741	33.86852	4.234E-08
7.27113	40.93505	5.118E-08
7.63603	51.66040	6.459E-08
9.05135	83.14527	1.039E-07
10.01311	89.54764	1.119E-07

Np(V)-Kaolinite - Kohler et al. (1992)

5/9/95

CCM

$SiOH + NpO_2 = SiO{\cdot}NpO_2^0 + H^+$

```
         0
         1
         0
         0
         1
        90
         4         1         3         1
00001  -3.98  1.06E-4   AlOH
00002  -3.98  1.06E-4   SiOH
00160  -1.0   0.00E00   PSIO
00032  -6.9   1.25E-7   NpO2+
00033   0.0   0.00E00   NpO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00032    0.00  032  1
03201   -8.90  032  1 050 -1
00100  -13.78  050 -1
01050    8.12  001  1 160  1 050  1
01100   -9.56  001  1 160 -1 050 -1
00001    0.00  001  1
02100   -7.04  002  1 160 -1 050 -1
00002    0.00  002  1
23301   -2.00  002  1 160  0 050 -1 032  1 033  1

00001  011.0  5.0000     1.0
           0
         1
     23301
         8         1         1         0
        33
8.813E-9
4.863E-9
1.406E-8
4.234E-8
5.118E-8
6.459E-8
1.039E-7
1.119E-7
        50
-3.98
-4.99
-6.54
-7.14
-7.27
-7.64
-9.05
-10.01
         1         1
        33     0.10    1.2E-11
        50     0.05    0.0E-00
```

CCM

$AlOH^0 + NpO_2^+ = AlO{\cdot}NpO_2^0 + H^+$

```
Neptunm            0
   on              1
Kaolinit           0
2.3si/nm           0
00000050           1
00000060          90
00000070           4         1         3         1
00000080  00001  -3.98  1.06E-4   AlOH
00000080  00002  -3.98  1.06E-4   SiOH
00000090  00160  -1.0   0.00E00   PSIO
00000098  00032  -6.9   1.25E-7   NpO2+
00000100  00033   0.0   0.00E00   NpO2ads
00000102  00050   0.0   0.00E00   H+
00000103  00003  -1.0   0.00E00   Na+
00000104  00005  -1.0   0.00E00   ClO4-
00000110
00000120  00050    0.00  050  1
00000124  00032    0.00  032  1
00000126  03201   -8.90  032  1 050 -1
00000139  00100  -13.78  050 -1
00000140  01050    8.12  001  1 160  1 050  1
00000145  01100   -9.56  001  1 160 -1 050 -1
00000150  00001    0.00  001  1
00000145  02100   -7.05  002  1 160 -1 050 -1
00000150  00002    0.00  002  1
xonpo2 -5 13301   -4.00  001  1 160  0 050 -1 032  1 033  1
00000174
00000175
00000180  00001  011.0  5.0000     1.0
00000185      0        0
00000190         1
00000195     13301
00000230         8         1         1         0
00000240        33
00000280  8.813E-9
00000300  4.863E-9
00000320  1.406E-8
00000340  4.234E-8
00000360  5.118E-8
00000370  6.459E-8
00000371  1.039E-7
00000372  1.119E-7
00000680        50
00000700  -3.98
00000710  -4.99
00000720  -6.54
00000730  -7.14
00000740  -7.27
00000750  -7.64
00000751  -9.05
00000752  -10.01
00001170         1         1
00001180        33     0.10    1.2E-11
00001190        50     0.05    0.0E-00
```

DLM

$SiOH^0 + NpO_2^+ = SiO{\cdot}NpO_2^0 + H^+$

```
         0
         1
         0
         0
         1
        90
         4         1         3         1
00001  -3.98  1.06E-4   AlOH
00002  -3.98  1.06E-4   SiOH
00160  -1.0   0.00E00   PSIO
00032  -6.9   1.25E-7   NpO2+
00033   0.0   0.00E00   NpO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00032    0.00  032  1
03201   -8.90  032  1 050 -1
00100  -13.78  050 -1
01050    8.22  001  1 160  1 050  1
01100   -9.62  001  1 160 -1 050 -1
00001    0.00  001  1
02100   -7.09  002  1 160 -1 050 -1
00002    0.00  002  1
23301   -2.05  002  1 160  0 050 -1 032  1 033  1

00002  011.0  5.0000
0.1      1.0
         1
     23301
         8         1         1         0
        33
8.813E-9
4.863E-9
1.406E-8
4.234E-8
5.118E-8
6.459E-8
1.039E-7
1.119E-7
        50
-3.98
-4.99
-6.54
-7.14
-7.27
-7.64
-9.05
-10.01
         1         1
        33     0.10    1.2E-11
        50     0.05    0.0E-00
```

DLM

$AlOH^0 + NpO_2^+ = AlO{\cdot}NpO_2^0 + H^+$

```
Neptunm            0
   on              1
Kaolinit           0
2.3si/nm           0
00000050           1
00000060          90
00000070           4         1         3         1
00000080  00001  -3.98  1.06E-4   AlOH
00000080  00002  -3.98  1.06E-4   SiOH
00000090  00160  -1.0   0.00E00   PSIO
00000098  00032  -6.9   1.25E-7   NpO2+
00000100  00033   0.0   0.00E00   NpO2ads
00000102  00050   0.0   0.00E00   H+
00000103  00003  -1.0   0.00E00   Na+
00000104  00005  -1.0   0.00E00   ClO4-
00000110
00000120  00050    0.00  050  1
00000124  00032    0.00  032  1
00000126  03201   -8.90  032  1 050 -1
00000139  00100  -13.78  050 -1
00000140  01050    8.22  001  1 160  1 050  1
00000145  01100   -9.62  001  1 160 -1 050 -1
00000150  00001    0.00  001  1
00000145  02100   -7.09  002  1 160 -1 050 -1
00000150  00002    0.00  002  1
xonpo2 -5 13301   -3.96  001  1 160  0 050 -1 032  1 033  1
00000174
00000175
00000180  00002  011.0  5.0000
00000185  0.1      1.0
00000190         1
00000195     13301
00000230         8         1         1         0
00000240        33
00000280  8.813E-9
00000300  4.863E-9
00000320  1.406E-8
00000340  4.234E-8
00000360  5.118E-8
00000370  6.459E-8
00000371  1.039E-7
00000372  1.119E-7
00000680        50
00000700  -3.98
00000710  -4.99
00000720  -6.54
00000730  -7.14
00000740  -7.27
00000750  -7.64
00000751  -9.05
00000752  -10.01
00001170         1         1
00001180        33     0.10    1.2E-11
00001190        50     0.05    0.0E-00
```


Np(V)-Kaolinite - Kohler et al. (1992)

5/9/95

TLM

$SiOH^0 + NpO_2^+ = SiO{\cdot}NpO_2^0 + H^+$

```
         0
         1
         0
         0
         1
        90
         6         1         3         1
00001  -3.98  1.06E-4   AlOH
00002  -3.98  1.06E-4   SiOH
00160  -1.0   0.00E00   PSIO
00161  -0.5   0.00E00   PSIB
00162  -0.1   0.00E00   PSID
00032  -6.9   1.25E-7   NpO2+
00033   0.0   0.00E00   NpO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00032    0.00  032  1
03201   -8.90  032  1 050 -1
00100  -13.78  050 -1
01050    6.79  001  1 160  1 050  1
01100  -10.79  001  1 160 -1 050 -1
01055    9.90  001  1 160  1 161 -1 050  1 005  1
01103   -7.73  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
02050    0.79  002  1 160  1 050  1
02100   -4.79  002  1 160 -1 050 -1
02103   -6.22  002  1 160 -1 161  1 050 -1 003  1
00002    0.00  002  1
23301   -3.80  002  1 160 -1 161  1 050 -1 032  1 033  1

00004  011.0  5.0000  0.8   0.2
0.1      1.0
         1
     23301
         8         1         1         0
        33
8.813E-9
4.863E-9
1.406E-8
4.234E-8
5.118E-8
6.459E-8
1.039E-7
1.119E-7
        50
-3.98
-4.99
-6.54
-7.14
-7.27
-7.64
-9.05
-10.01
         1         1
        33     0.10    1.2E-11
        50     0.05    0.0E-00
```

TLM

$AlOH^0 + NpO_2 = AlO{\cdot}NpO_2^0 + H^+$

```
Neptunm            0
   on              1
Kaolinit           0
2.3si/nm           0
00000050           1
00000060          90
00000070           6         1         3         1
00000080  00001  -3.98  1.06E-4   AlOH
00000080  00002  -3.98  1.06E-4   SiOH
00000090  00160  -1.0   0.00E00   PSIO
00000092  00161  -0.5   0.00E00   PSIB
00000094  00162  -0.1   0.00E00   PSID
00000098  00032  -6.9   1.25E-7   NpO2+
00000100  00033   0.0   0.00E00   NpO2ads
00000102  00050   0.0   0.00E00   H+
00000103  00003  -1.0   0.00E00   Na+
00000104  00005  -1.0   0.00E00   ClO4-
00000110
00000120  00050    0.00  050  1
00000124  00032    0.00  032  1
00000126  03201   -8.90  032  1 050 -1
00000139  00100  -13.78  050 -1
00000140  01050    6.79  001  1 160  1 050  1
00000145  01100  -10.79  001  1 160 -1 050 -1
00000140  01055    9.90  001  1 160  1 161 -1 050  1 005  1
00000145  01103   -7.73  001  1 160 -1 161  1 050 -1 003  1
00000150  00001    0.00  001  1
00000140  02050    0.79  002  1 160  1 050  1
00000145  02100   -4.79  002  1 160 -1 050 -1
00000145  02103   -6.22  002  1 160 -1 161  1 050 -1 003  1
00000150  00002    0.00  002  1
xonpo2 -  13301   -2.40  001  1 160 -1 161  1 050 -1 032  1 033  1
00000174
00000175
00000180  00004  011.0  5.0000  0.8   0.2
00000185  0.1      1.0
00000190         1
00000195     13301
00000230         8         1         1         0
00000240        33
00000280  8.813E-9
00000300  4.863E-9
00000320  1.406E-8
00000340  4.234E-8
00000360  5.118E-8
00000370  6.459E-8
00000371  1.039E-7
00000372  1.119E-7
00000680        50
00000700  -3.98
00000710  -4.99
00000720  -6.54
00000730  -7.14
00000740  -7.27
00000750  -7.64
00000751  -9.05
00000752  -10.01
00001170         1         1
00001180        33     0.10    1.2E-11
00001190        50     0.05    0.0E-00
```

FITEQL Results

Table B-XX. Neptunium (V)-Kaolinite Sorption Binding Constants: Monodentate, mononuclear compounds

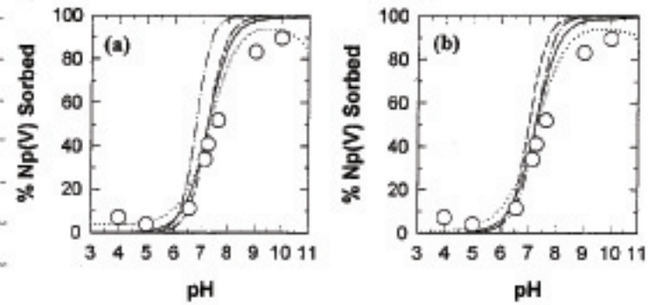
Solid: Kaolinite [$Al_2Si_2O_5(OH)_4$] A_{sp}: 11 m^2/g (Allard et al., 1983) Data Source: Kohler et al. (1992) Concentration: [Np(V)] = 1.25E-7 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.2E-11 M	Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 5 g/L

Si:Al = 1:1 No CO_2		DLM			CCM			TLM		
								(α-Al_2O_3)		(SiO_2)
		Log K_+ = 8.33 (α-Al_2O_3) Log K_- = -9.73 (α-Al_2O_3) Log K_- = -7.20 (SiO_2)			Log K_+ = 9.08 (α-Al_2O_3) Log K_- = -8.32 (α-Al_2O_3) Log K_- = -7.04 (SiO_2)			Log K_+ = 6.90 Log K_+ = 0.90 Log K_- = -10.90 Log K_- = -4.90 Log K_{Cat} = -7.73 Log K_{Cat} = -6.22 Log K_{An} = 10.12		
		Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}NpO_2^0$	SiOH	-2.89	22.1	.0308	-2.80	22.5	.0299	-3.50	53.1	.0235
	AlOH	-2.67	29.3	.0383	-1.97	30.9	.0405	-2.20	21.2	.0307
$XOH\text{-}NpO_2^+$	SiOH	4.65	14.6	.0221	4.83	25.9	.0230	1.37	74.9	.0281
	AlOH	4.95	25.1	.0338	5.75	25.5	.0342	3.26	24.5	.0237
$XO\text{-}NpO_2OH^-$	SiOH	-10.52	27.6	.0360	-10.51	27.3	.0361	-8.12	26.4	.0351
	AlOH	-10.31	32.7	.0427	-9.74	36.4	.0474	-7.36	37.1	.0484
$XOH\text{-}NpO_2OH^0$	SiOH	-2.89	22.1	.0308	-2.80	22.5	.0299	-2.60	22.8	.0290
	AlOH	-2.67	29.3	.0383	-1.97	30.9	.0405	-1.78	31.5	.0413
$XOH_2\text{-}NpO_2OH^+$	SiOH	4.65	14.6	.0221	4.83	25.9	.0230	2.85	33.7	.0238
	AlOH	4.95	25.1	.0338	5.75	25.5	.0342	3.65	26.4	.0351
OTHER SPECIES:										
$(XO)_2\text{-}NpO_2^-$	SiOH	-5.99	25.4	.0329	-5.88	24.7	.0316	-4.10	49.7	.0234
	AlOH	-5.58	35.7	.0465	-4.35	41.3	.0541	2.12	34.8	.0459

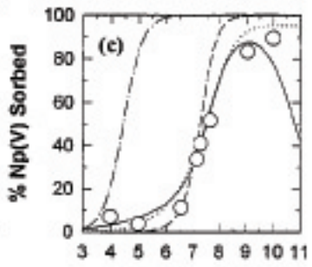
5/9/95

Np(V)-Kaolinite
DLM From Turner (1995)

Np(V)-Kaolinite
CCM



Np(V)-Kaolinite
TLM



LEGEND
- >AlO-NpO_2^+ & SiO-NpO_2^0
- >AlO-NpO_2OH^- & SiO-NpO_2OH^-
- >$AlOH_2$-NpO_2OH^+ & $SiOH_2$-NpO_2OH^+
- >$(AlO)_2$-NpO_2^- & $(SiO)_2$-NpO_2^-
- Experimental Data

Figure 4-24. SCM predictions of Np(V) sorption on kaolinite (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 1.25 \times 10^{-7}$ M, 0.1 M $NaClO_4$, M/V = 5 g/L. Model parameters from Tables 3-1 and B-24. Si:Al ratio of 1:1 assumed. Data from Kohler et al. (1992).

4-26

Sorption results using MINTEQA2 w/ CNWRA radionuclide database

Np(V) Sorption - Lepidocrocite (γFeOOH) - Nakayama & Sakamoto (1991)

5/11/95

Nakayama, S., and Y. Sakamoto. 1991. Sorption of neptunium on naturally-occurring iron-containing minerals. *Radiochimica Acta* 52/53:153-157.

Nakayama and Sakamoto (1991)	Np(V)- Synthetic Lepidocrocite	
Figure 4 (page 156)		
Asp=36 m2/g	No CO2	Np(V)=6E-6 M
0.1 M NaNO3	M/V=1 g/L	
No CO2		
pH	% sorbed	mol sorbed
5.01	22.696	1.362e-06
5.56	10.371	6.223e-07
6.43	36.133	2.168e-06
7.29	56.415	3.385e-06
7.44	65.986	3.959e-06
7.64	77.078	4.625e-06
8.04	72.233	4.334e-06
8.77	92.314	5.539e-06
10.11	95.705	5.742e-06
10.25	97.563	5.854e-06

5/11/95

Example FITEQL Input Files
Nakayama + Sakamoto (1991)

CCM
No CO_2
$>FeOH + NpO_2^+ => FeONpO_2 + H^+$

DLM
$>FeOH + NpO_2^+ => FeONpO_2^0 + H^+$

TLM
$>FeOH + NpO_2^+ = FeONpO_2^0 + H^+$

5/11/95

Table B-8. Neptunium (V)-Lepidocrocite (γ-FeOOH) Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: Lepidocrocite (γ-FeOOH) A_{SP}: 36 m^2/g Data Source: Nakayama and Sakamoto (1991) Concentration: [Np(V)] = 6E-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9			Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L		
No CO_2	DLM (a)			CCM (a)			TLM (a)		
	Log K_+ = 7.35 Log K_- = -9.17			Log K_+ = 6.47 Log K_- = -9.03			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-NpO_2^o$	-3.53	34.8	.0360	-3.59	34.4	.03576	-4.39	40.4	.0217
$XOH-NpO_2^+$	4.51	30.3	.0303	4.05	32.6	.02809	3.71	39.0	.0261
$XO-NpO_2OH^-$	-11.51	38.2	.0407	-11.11	38.7	.04175	-11.25	32.4	.0422
$XOH-NpO_2OH^o$	-3.53	34.8	.0360	-3.59	34.4	.03576	-3.43	34.3	.0356
$XOH_2-NpO_2OH^+$	4.51	30.3	.0303	4.05	32.6	.02809	4.81	30.9	.0395
OTHER SPECIES:									
$(XO)_2-NpO_2^-$	-7.52	38.4	.0420	-7.17	38.8	.04287	-7.82	40.2	.0289

(a) Surface constants for goethite (α-FeOOH).

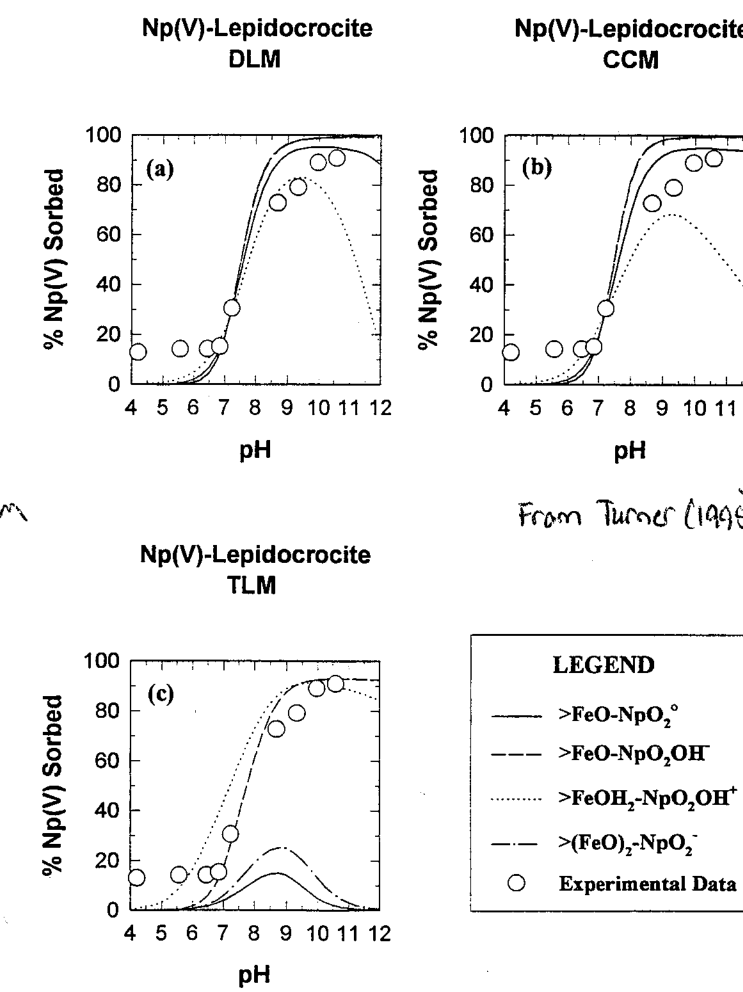


Figure 4-8. Np(V) sorption on lepidocrocite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 6\times10^{-6}$ M, 0.1 M $NaNO_3$, M/V=1 g/L. Model parameters from Tables 3-1 and B-8. Data from Nakayama and Sakamoto (1991).

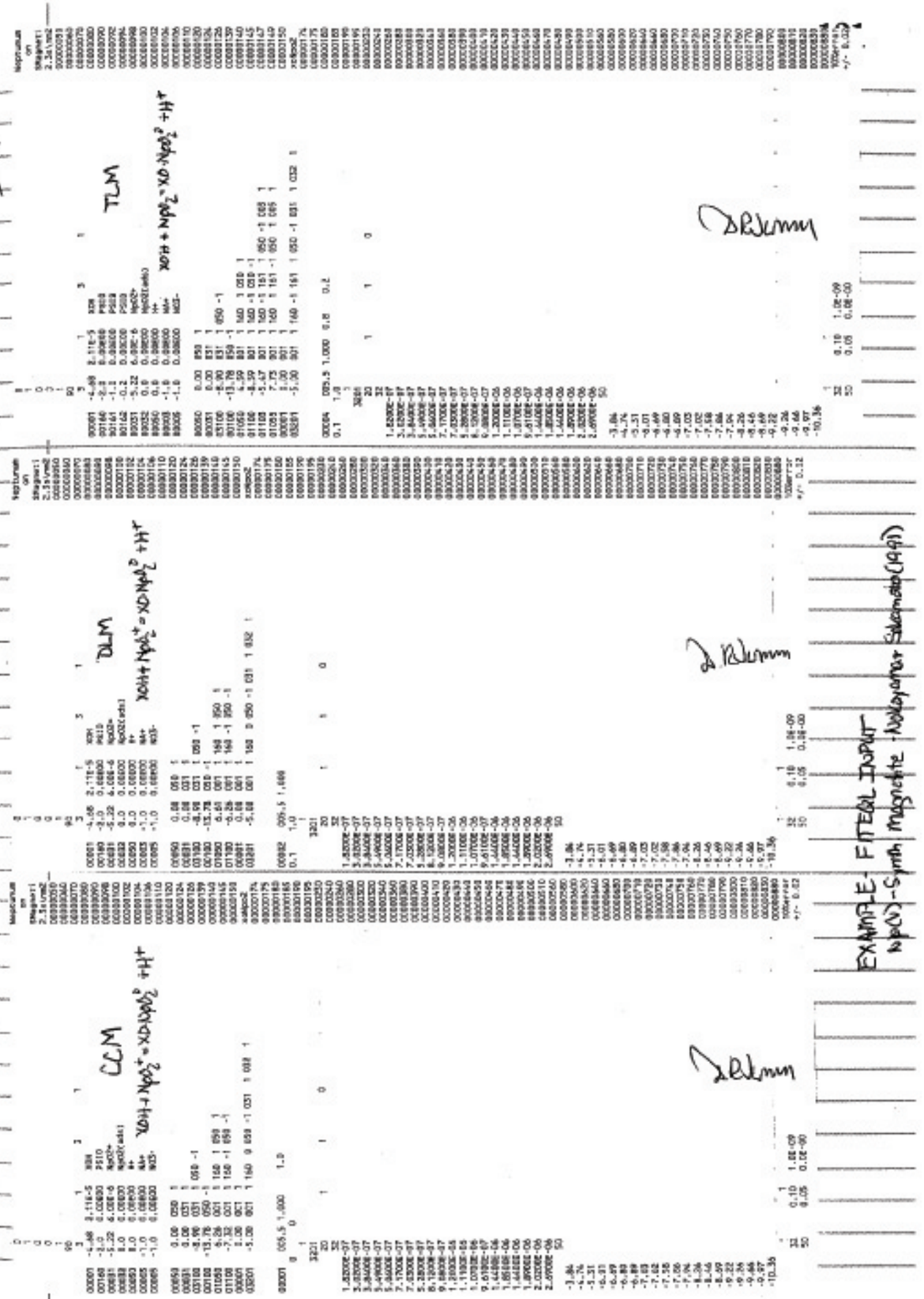
Np(V) Sorption on Synth. Magnetite - Nakayama + Sakamoto (1991)

5/11/95
D.R.Lumm

Nakayama, S., and Y. Sakamoto. 1991. Sorption of neptunium on naturally-occurring iron-containing minerals. Radiochimica Acta 52/53:153-157.

Nakayama and Sakamoto (1991)	Np(V)- Synthetic Magnetite	
Figure 3b (page 156)		
Asp=0.3 mg/g	No CO2	Np(V)=~E-6 M
0.1 M NaNO3	M/V = 1 g/L	
No CO2		
pH	% sorbed	mole sorbed
3.89	1.037	1.822e-07
4.73	1.038	3.023e-07
5.31	6.395	3.837e-07
6.01	9.155	5.493e-07
6.69	8.440	5.864e-07
6.80	11.864	7.366e-07
6.89	11.723	7.852e-07
7.05	6.803	5.282e-07
7.02	15.532	8.119e-07
7.58	15.138	9.084e-07
7.86	20.046	1.203e-06
7.94	18.571	1.114e-06
8.26	17.838	1.070e-06
8.46	16.014	9.608e-07
8.69	23.980	1.438e-06
9.22	20.881	1.812e-06
9.26	24.032	1.442e-06
9.66	31.439	1.698e-06
9.97	31.589	2.083e-06
10.36	44.785	1.687e-06

5/11/95
D.R.Lumm



5/11/95
D.B.Lemm

Table B-6. Neptunium (V)-Synthetic Magnetite Sorption Binding Constants: Monodentate, mononuclear complexes.

Solid: Synthetic Magnetite A_{sp}: 5.5 m²/g Data Source: Nakayama and Sakamoto (1991) Concentration: [Np(V)] = 6E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.03 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_s = 2.31 sites/nm² M/V = 1 g/L

No CO_3	DLM			CCM			TLM		
	Log K_+ = 6.72 Log K_- = -6.37			Log K_o = 6.25 Log K_- = -7.32			Log K_1 = 4.70 Log K_2 = -8.30 Log K_{Cat} = -3.47 Log K_{An} = 7.95		
	Log K	V_T	σ_{fit}	Log K	V_T	σ_{fit}	Log K	V_T	σ_{fit}
XO-NpO_2^+	-3.42	47.8	.0195	-3.97	48.1	.0202	-2.32	33.7	.0139
XOH-NpO_2^+	3.55	44.9	.0198	3.49	35.8	.0203	4.83	42.5	.0276
XO-Np(V)OH	-10.53	56.2	.0229	-11.25	54.7	.0235	-8.95	23.7	.0311
XOH-NpO_2OH^-	-3.42	47.8	.0195	-3.97	48.1	.0202	-3.65	49.1	.0205
XOH_2-NpO_2OH^+	3.55	44.9	.0198	3.49	35.8	.0203	4.55	21.9	.0299
OTHER SPECIES:									
$(XO)_2$-NpO_2^-	-4.82	49.1	.0231	-6.17	50.7	.0249	-3.11	31.1	.0284

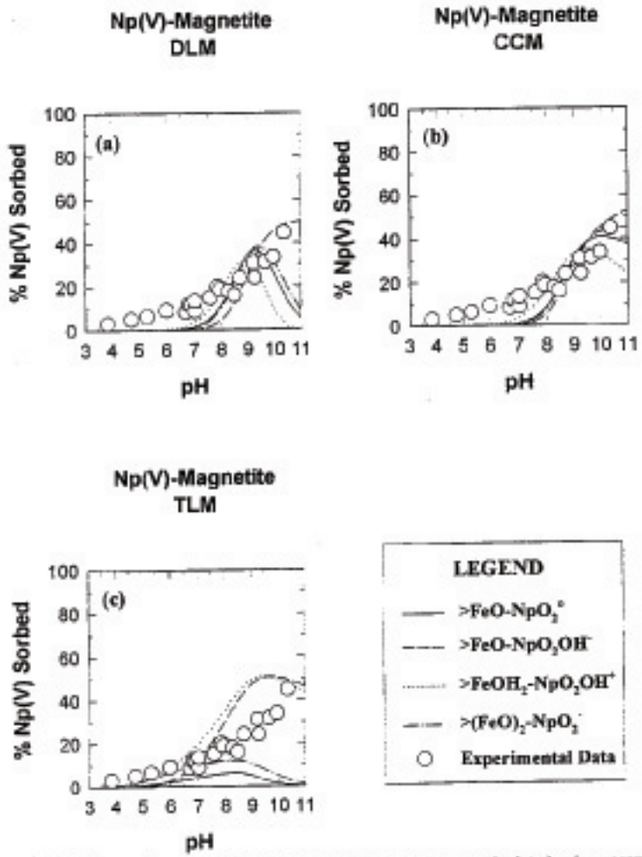


Figure 4-6. Np(V) sorption on synthetic magnetite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM: (b) CCM: and (c) TLM results. $Np(V)_T = 6 \times 10^{-6}$ M, 0.1 M $NaNO_3$, M/V = 1 g/L. Model parameters from Tables 3-1 and B-6. Data from Nakayama and Sakamoto (1991).

Np(V)- Natural Mag.
Nakayama + Sakamoto (91)
D.B.L

5/11/95
D.B.Lemm

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure. 3a: Sorption on naturally-occurring minerals...) is from the following reference:

Nakayama, S. and Y. Sakamoto. "Sorption of Neptunium on Naturally-Occurring Iron-Containing Minerals." Radiochimica Acta. Vols. 52 and 53. pp. 153-157. 1991.

Nakayama, S., and Y. Sakamoto. 1991. Sorption of neptunium on naturally occurring iron-containing minerals. *Radiochimica Acta* 52/53:153-157.

Nakayama and Sakamoto (1991) Figure 3a (page 156)	Np(V)- Natural Magnetite	
A_{sp}=5.5 m²/g 0.1 M $NaNO_3$	No CO_2 M/V = 1 g/L	$[Np(V)] = 6E-6$ M
No CO_2		
pH	% sorbed	mol sorbed
3.35	9.004	5.402e-07
4.31	8.213	4.928e-07
4.86	8.184	4.910e-07
5.30	9.621	5.773e-07
5.80	5.503	3.302e-07
5.86	8.094	4.856e-07
6.05	10.903	6.542e-07
6.09	5.193	3.116e-07
6.57	5.663	3.398e-07
7.48	9.628	5.777e-07
8.07	18.432	1.106e-06
8.41	18.910	1.135e-06
8.88	15.469	9.281e-07
9.08	15.333	1.320e-06
9.24	24.586	1.475e-06
9.43	21.372	1.282e-06
9.55	25.023	1.501e-06
9.81	37.186	2.231e-06
10.15	31.379	1.883e-06
10.66	48.318	2.899e-06

5/12/45
(DRC)

5/12/45
(DRC)

5/11/95
D.R.Lmm

Example FITEQL Inputs
Np(V)-Natural Magnetite - Nakayama + Sakamoto (1991)

CCM
No CO_2
$>FeOH^o + NpO_2^+ = >FeONpO_2^o + H^+$

```
Neptunum
on
NMagneti
2.3s\nm2
    0
    1
    0
    0
    1
   90
    3          1          3          1
00001   -4.65   2.23E-5   XOH
00160   -2.0    0.00E00   PSI0
00031   -5.22   6.00E-6   NpO2+
00032    0.0    0.00E00   NpO2(ads)
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   NO3-

00050     0.00  050  1
00031     0.00  031  1
03100    -8.90  031  1 050 -1
00100   -13.78  050 -1
01050     6.26  001  1 160  1 050  1
01100    -7.32  001  1 160 -1 050 -1
00001     0.00  001  1
03201    -5.00  001  1 160  0 050 -1 031  1 032  1
xoNpo2

00001    005.8 1.000      1.0
     0     0
       1
    3201
      20          1          1          0
      32
5.4300E-07
4.9300E-07
4.9100E-07
5.7700E-07
3.3000E-07
4.8600E-07
6.5400E-07
3.1200E-07
3.4000E-07
5.7800E-07
1.1100E-06
1.1400E-06
9.2800E-07
1.5200E-06
1.4800E-06
1.5200E-06
1.5000E-06
2.2300E-06
1.8900E-06
2.9000E-06
         50
-3.75
-4.31
-4.84
-5.30
-5.80
-5.94
-6.05
-6.40
-6.87
-7.40
-8.17
-8.41
-8.60
-9.08
-9.14
-9.43
-9.57
-9.91
-10.15
-10.64
         1          1
        32       0.10    1.0E-09
        50       0.05    0.0E-00
10%error
+/- 0.02
```

D.R.Lmm

DLM
No CO_2
$>FeOH^o + NpO_2^+ = >FeONpO_2^o + H^+$

```
Neptunum
on
Magnetit
2.3s\nm2
    0
    1
    0
    0
    1
   90
    3          1          3          1
00001   -4.65   2.23E-5   XOH
00160   -2.0    0.00E00   PSI0
00031   -5.22   6.00E-6   NpO2+
00032    0.0    0.00E00   NpO2(ads)
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   NO3-

00050     0.00  050  1
00031     0.00  031  1
03100    -8.90  031  1 050 -1
00100   -13.78  050 -1
01050     6.61  001  1 160  1 050  1
01100    -6.26  001  1 160 -1 050 -1
00001     0.00  001  1
03201     5.00  001  1 160  0 050 -1 031  1 032  1
xoNpo2

00002    005.8 1.000
0.1      1.0
       1
    3201
      20          1          1          0
      32
5.4300E-07
4.9300E-07
4.9100E-07
5.7700E-07
3.3000E-07
4.8600E-07
6.5400E-07
3.1200E-07
3.4000E-07
5.7800E-07
1.1100E-06
1.1400E-06
9.2800E-07
1.5200E-06
1.4800E-06
1.5200E-06
1.5000E-06
2.2300E-06
1.8900E-06
2.9000E-06
         50
-3.75
-4.31
-4.84
-5.30
-5.80
-5.94
-6.05
-6.40
-6.87
-7.40
-8.17
-8.41
-8.60
-9.08
-9.14
-9.43
-9.57
-9.91
-10.15
-10.64
         1          1
        32       0.10    1.0E-09
        50       0.05    0.0E-00
10%error
+/- 0.02
```

D.R.Lmm

TLM
No CO_2
$>FeOH^o + NpO_2^+ = >FeO \cdot NpO_2^o + H^+$

```
Neptunum
on
NMagneti
2.3s\nm2
    0
    1
    0
    0
    1
   90
    5          1          3          1
00001   -4.65   2.23E-5   XOH
00160   -2.0    0.00E00   PSI0
00161   -1.0    0.00E00   PSIB
00162   -0.2    0.00E00   PSID
00031   -5.22   6.00E-6   NpO2+
00032    0.0    0.00E00   NpO2(ads)
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   NO3-

00050     0.00  050  1
00031     0.00  031  1
03100    -8.90  031  1 050 -1
00100   -13.78  050 -1
01050     4.59  001  1 160  1 050  1
01100    -8.59  001  1 160 -1 050 -1
01103    -5.47  001  1 160 -1 161  1 050 -1 003  1
01055     7.73  001  1 160  1 161 -1 050  1 005  1
00001     0.00  001  1
03201    -2.30  001  1 160 -1 161  1 050 -1 031  1 032  1
xoNpo2

00004    005.8 1.000  0.8    0.2
0.1      1.0
       1
    3201
      20          1          1          0
      32
5.4300E-07
4.9300E-07
4.9100E-07
5.7700E-07
3.3000E-07
4.8600E-07
6.5400E-07
3.1200E-07
3.4000E-07
5.7800E-07
1.1100E-06
1.1400E-06
9.2800E-07
1.5200E-06
1.4800E-06
1.5200E-06
1.5000E-06
2.2300E-06
1.8900E-06
2.9000E-06
         50
-3.75
-4.31
-4.84
-5.30
-5.80
-5.94
-6.05
-6.40
-6.87
-7.40
-8.17
-8.41
-8.60
-9.08
-9.14
-9.43
-9.57
-9.91
-10.15
-10.64
         1          1
        32       0.10    1.0E-09
        50       0.05    0.0E-00
10%error
+/- 0.02
```

D.R.Lmm

5/11/95
D.R.Lmm

Table BXX. Neptunium (V)-Natural Magnetite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Natural Magnetite A_{SP}: 5.8 m^2/g Data Source: Nakayama and Sakamoto (1991) Concentration: [Np(V)] = 6E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

No CO_2	DLM			CCM (I = 0.1)			TLM		
	Log K_+ = 6.72 Log K_- = -6.37			Log K_+ = 6.26 Log K_- = -7.32			Log K_+ = 4.70 Log K_- = -8.70 Log K_{Cat} = -5.47 Log K_{An} = 7.95		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-NpO_2^o	-3.58	53.1	.0202	-4.14	49.2	.0200	-2.37	40.3	.0144
XOH-NpO_2^+	3.41	55.8	.0218	3.31	43.6	.0215	4.87	38.0	.0269
XO-NpO_2OH^-	-10.71	53.4	.0214	-11.44	52.5	.0220	-9.21	34.8	.0323
XOH-NpO_2OH^o	-3.58	53.1	.0202	-4.14	49.2	.0200	-3.81	49.6	.0200
XOH_2-NpO_2OH^+	3.41	55.8	.0218	3.31	43.6	.0215	4.31	32.9	.0306
OTHER SPECIES:									
$(XO)_2$-NpO_2^-	-5.05	53.1	.0233	-6.41	50.7	.0240	-3.19	34.8	.0284

D.R.Lmm

No MINTEQA2 Run

Np(V)-Goethite - Nakayama and Sakamoto (1991)

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 3: Sorption of neptunium of...) is from the following reference:

Nakayama, S. and Y. Sakamoto. "Sorption of Neptunium on Naturally-Occurring Iron-Containing Minerals." Radiochimica Acts. Vols. 52 and 53. pp. 153-157. 1991.

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D.R. Lemm

Nakayama, S., and Y. Sakamoto. 1991. Sorption of neptunium on naturally-occurring iron-containing minerals. *Radiochimica Acta* 52/53:153-157.

Nakayama and Sakamoto (1991)	Np(V)-Goethite	
Figure 3a (page 156)		
Asp=15.7 m2/g	No CO2	Np(V)=6E-6 M
0.1 M NaNO3	M/V=1 g/L	
No CO2		
pH	% sorbed	mol sorbed
4.15	0.191	1.148e-08
4.66	2.940	1.764e-07
5.55	10.496	6.297e-07
5.82	11.558	6.935e-07
6.04	15.210	9.126e-07
6.31	20.611	1.237e-06
6.45	29.600	1.776e-06
6.91	40.588	2.435e-06
7.01	40.994	2.460e-06
7.01	44.084	2.645e-06
6.93	44.770	2.686e-06
7.15	50.077	3.005e-06
8.05	58.819	3.529e-06
8.59	65.250	3.915e-06
8.65	66.468	3.988e-06
9.58	70.809	4.249e-06
9.92	79.706	4.782e-06
10.13	79.956	4.797e-06
10.57	81.425	4.885e-06

D.R. Lemm

```
      0
      1
      0
      0
      1
     90
      3         1         3         1
00001  -4.22  6.02E-5   XOH
00160  -2.0   0.00E00   PSIO
00031  -5.22  6.00E-6   NpO2+
00032   0.0   0.00E00   NpO2(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00031    0.00  031  1
03100   -8.90  031  1 050 -1
00100  -13.78  050 -1
01050    6.47  001  1 160  1 050  1
01100   -9.03  001  1 160 -1 050 -1
00001    0.00  001  1
03201   -5.00  001  1 160  0 050 -1 031  1 032  1

00001   015.7 1.000      1.0
    0      0
      1
   3201
     19         1         1         0
     32
1.1500E-08
1.7600E-07
6.3000E-07
6.9300E-07
9.1300E-07
1.2400E-06
1.7800E-06
2.4400E-06
2.4600E-06
2.6500E-06
2.6900E-06
3.0000E-06
3.5300E-06
3.9200E-06
3.9900E-06
4.2500E-06
4.7800E-06
4.8000E-06
4.8900E-06
     50
-4.15
-4.66
-5.55
-5.82
-6.04
-6.31
-6.45
-6.91
-7.01
-7.01
-6.93
-7.15
-8.05
-8.59
-8.65
-9.58
-9.92
-10.13
-10.57
      1      1
     32      0.10   1.0E-09
     50      0.05   0.0E-00
```

```
Neptunum
   on
Goethite
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000139
00000140
00000145
00000150
xoNpo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000390
00000400
00000410
00000420
00000430
00000440
00000450
00000460
00000470
00000480
00000490
00000500
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000710
00000720
00000730
00000740
00000750
00000760
00000770
00000780
00000790
00000800
00000810
00000820
00000880
10%error
+/- 0.02
```

CCM
No CO_2
$>FeOH^0 + NpO_2^+ = >FeO{\cdot}NpO_2^0 + H^+$

D.R. Lemm

Example FITEQL Input
Np-Goethite Sorption: Nakayama + Sakamoto (1991)

5/11/95
D.R. Lemm

```
      0
      1
      0
      0
      1
     90
      3         1         3         1
00001  -4.22  6.02E-5   XOH
00160  -2.0   0.00E00   PSIO
00031  -5.22  6.00E-6   NpO2+
00032   0.0   0.00E00   NpO2(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00031    0.00  031  1
03100   -8.90  031  1 050 -1
00100  -13.78  050 -1
01050    7.24  001  1 160  1 050  1
01100   -9.06  001  1 160 -1 050 -1
00001    0.00  001  1
03201   -5.00  001  1 160  0 050 -1 031  1 032  1

00002  015.7 1.000
0.1    1.0
      1
   3201
     19         1         1         0
     32
1.1500E-08
1.7600E-07
6.3000E-07
6.9300E-07
9.1300E-07
1.2400E-06
1.7800E-06
2.4400E-06
2.4600E-06
2.6500E-06
2.6900E-06
3.0000E-06
3.5300E-06
3.9200E-06
3.9900E-06
4.2500E-06
4.7800E-06
4.8000E-06
4.8900E-06
     50
-4.15
-4.66
-5.55
-5.82
-6.04
-6.31
-6.45
-6.91
-7.01
-7.01
-6.93
-7.15
-8.05
-8.59
-8.65
-9.58
-9.92
-10.13
-10.57
      1      1
     32      0.10   1.0E-09
     50      0.05   0.0E-00
```

D.R. Lemm

DLM
No CO_2
$>FeOH^0 + NpO_2^+ = >FeO{\cdot}NpO_2^0 + H^+$

D.R. Lemm

```
Neptunum           0
   on              1
Goethite           0
2.3s\nm2           0
00000050           1
00000060          90
00000070           5         1         3         1
00000080   00001  -4.22  6.02E-5   XOH
00000090   00160  -2.0   0.00E00   PSIO
00000098   00161  -1.0   0.00E00   PSIB
00000100   00162  -0.2   0.00E00   PSID
00000102   00031  -5.22  6.00E-6   NpO2+
00000104   00032   0.0   0.00E00   NpO2(ads)
00000106   00050   0.0   0.00E00   H+
00000110   00003  -1.0   0.00E00   NA+
00000120   00005  -1.0   0.00E00   NO3-
00000124
00000126   00050    0.00  050  1
00000139   00031    0.00  031  1
00000140   03100   -8.90  031  1 050 -1
00000145   00100  -13.78  050 -1
00000150   01050    5.89  001  1 160  1 050  1
xoNpo2     01100   -9.89  001  1 160 -1 050 -1
00000174   01103   -7.64  001  1 160 -1 161  1 050 -1 003  1
00000175   01055    8.56  001  1 160  1 161 -1 050  1 005  1
00000180   00001    0.00  001  1
00000185   03201   -5.00  001  1 160 -1 161  1 050 -1 031  1 032  1
00000190
00000195
00000230   00004   015.7 1.000  0.8    0.2
00000240   0.1     1.0
00000260           1
00000280        3201
00000300          19         1         1         0
00000320          32
00000340   1.1500E-08
00000360   1.7600E-07
00000380   6.3000E-07
00000390   6.9300E-07
00000400   9.1300E-07
00000410   1.2400E-06
00000420   1.7800E-06
00000430   2.4400E-06
00000440   2.4600E-06
00000450   2.6500E-06
00000460   2.6900E-06
00000470   3.0000E-06
00000480   3.5300E-06
00000490   3.9200E-06
00000500   3.9900E-06
00000560   4.2500E-06
00000580   4.7800E-06
00000600   4.8000E-06
00000620   4.8900E-06
00000640          50
00000660   -4.15
00000680   -4.66
00000700   -5.55
00000710   -5.82
00000720   -6.04
00000730   -6.31
00000740   -6.45
00000750   -6.91
00000760   -7.01
00000770   -7.01
00000780   -6.93
00000790   -7.15
00000800   -8.05
00000810   -8.59
00000820   -8.65
00000880   -9.58
10%error   -9.92
+/- 0.02   -10.13
           -10.57
                1      1
               32      0.10   1.0E-09
               50      0.05   0.0E-00
```

TLM
No CO_2
$>FeOH^0 + NpO_2^+ = >FeO{\cdot}NpO_2^0 + H^+$

D.R. Lemm

Table B-5. Neptunium (V)-Goethite Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: Natural Goethite A_{SP}: 15.7 m^2/g Data Source: Nakayama and Sakamoto (1991) Concentration: [Np(V)] = 6E-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9			Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L		
No CO_2	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -9.17			Log K_+ = 6.47 Log K_- = -9.03			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}NpO_2^o$	-2.54	16.7	.0253	-2.60	14.6	.0242	-5.43	93.4	.0401
$XOH\text{-}NpO_2^+$	5.21	8.4	.0195	4.75	6.3	.0189	2.34	95.1	.0472
$XO\text{-}NpO_2OH^-$	-10.39	23.4	.0312	-9.92	21.5	.0305	-9.98	6.3	.0283
$XOH\text{-}NpO_2OH^o$	-2.54	16.7	.0253	-2.60	14.6	.0242	-2.44	14.1	.0239
$XOH_2\text{-}NpO_2OH^+$	5.21	8.4	.0195	4.75	6.3	.0189	5.86	6.9	.0257
OTHER SPECIES									
$(XO)_2\text{-}NpO_2^-$	-5.96	23.0	.0334	-5.54	20.7	.0320	-8.61	88.8	.0335

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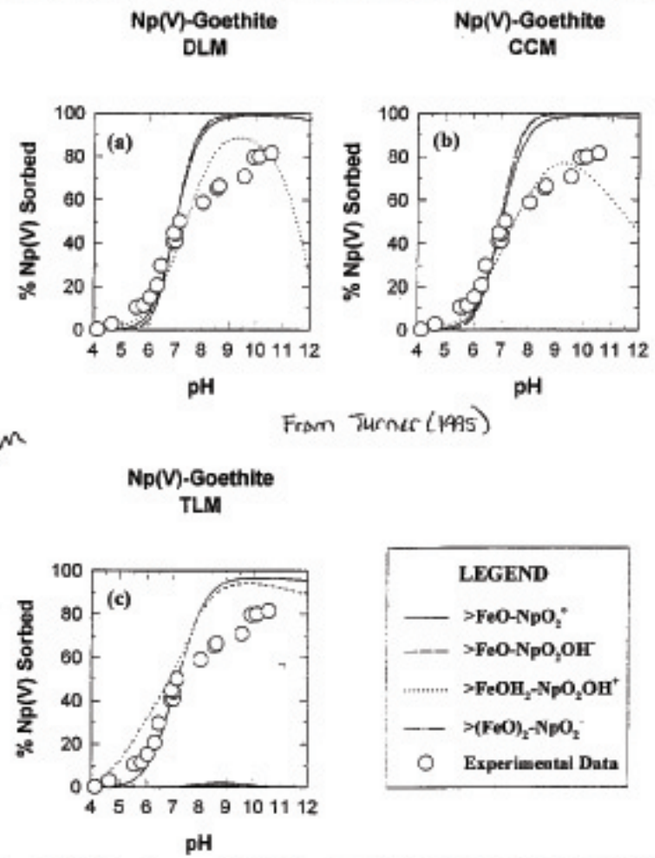


From Turner (1995)

D.R.Kenn

Figure 4-5. Np(V) sorption on goethite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 6 \times 10^{-8}$ M, 0.1 M $NaNO_3$, M/V = 1 g/L. Model parameters from Tables 3-1 and B-5. Data from Nakayama and Sakamoto (1991).

Calculated results using MINTEQA2 with COLDER radionuclide database

Np(V)-Biotite : Nakayama + Sakamoto (1991)

Information potentially subject to copyright protection w as redacted from this location. The redacted material (Figure 3a: Sorption of neptunium on naturally-occurring minerals....) is from the follow ing reference:

Nakayama, s. and Y. Sakamoto. “Sorption of Neptunium on Naturally-Occurring Iron-Containing Minerals.” Radiochimica Acta. Vols. 52 and 53. pp. 153-157. 1991.

D.R.Kenn

Nakayama, S., and Y. Sakamoto. 1991. Sorption of neptunium on naturally-occurring iron-containing minerals. Radiochimica Acta 52/53:153-157.

Nakayama and Sakamoto (1991)	(Np(V)= Natural Biotite	
Figure 3a (page 156)		
Adjust 7.3 ml/g	No CO2	Np(V)=8E-6 M
0.1 M NaNO3	M/V=1 g/L	Si:Al=3:1
No CO2		
pH	% sorbed	not sorbed
4.52	2.845	1.705e-03
4.75	1.597	9.569e-04
4.91	1.786	1.070e-03
5.55	3.378	2.023e-03
6.01	5.225	3.129e-03
6.48	4.643	2.780e-03
6.66	5.287	3.167e-03
7.13	5.820	3.486e-03
7.28	11.806	7.069e-03
7.88	9.644	5.776e-03
8.18	14.562	8.723e-03
8.43	9.383	5.620e-03
9.04	14.628	8.761e-03
9.07	21.276	1.274e-02
9.52	21.682	1.298e-02
9.68	26.356	1.578e-02
9.88	27.502	1.647e-02
9.87	29.643	1.775e-02
10.12	42.035	2.517e-02
10.20	26.364	1.579e-02
10.58	49.594	2.970e-02
10.85	44.126	2.643e-02
11.09	72.802	4.360e-02

Np(V)-Biotite: Nakayama & Sakamoto (1991)

5/11/95
D.R. Turner

```
             0
             1
             0
             0
             1
            90
             4         1          3         1
00001  -4.64  2.30E-5   SiOH
00002  -5.12  7.67E-6   AlOH
00160  -2.0   0.00E00   PSIO
00031  -5.22  6.00E-6   NpO2+
00032   0.0   0.00E00   NpO2(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00031    0.00  031  1
03100   -8.90  031  1 050 -1
00100  -13.78  050 -1
01100   -7.05  001  1 160 -1 050 -1
00001    0.00  001  1
01050    8.12  001  1 160  1 050  1
01100   -9.56  001  1 160 -1 050 -1
00002    0.00  002  1
23201   -3.00  002  1 160  0 050 -1 031  1 032  1

00001   008.0 1.000     1.0
    0       0
            1
        23201
           23         1          1          0
           32
1.7100E-07
9.4000E-08
1.0700E-07
2.6300E-07
3.1300E-07
2.9700E-07
3.1700E-07
3.4900E-07
7.1400E-07
3.3600E-07
8.7400E-07
5.6300E-07
8.7800E-07
1.2800E-06
1.3000E-06
1.5800E-06
1.6700E-06
1.7800E-06
2.5200E-06
1.7300E-06
2.7400E-06
4.1500E-06
4.3700E-06
           50
-4.52
-4.73
-4.91
-5.55
-6.01
-6.48
-6.66
-7.15
-7.28
-7.88
-8.18
-8.43
-9.04
-9.07
-9.52
-9.60
-9.88
-9.87
-10.12
-10.30
-10.58
-10.85
-11.09
        1          1
       32       0.10    1.0E-09
       50       0.05    0.0E-00
```

D.R. Turner

CCM
No CO_2
$>AlOH^0 + NpO_2^+ = >AlONpO_2^0 + H^+$

D.R. Turner

```
Neptunum            0
   on               1
Biotite             0
2.3s\nm2            0
00000050            1
00000060           90
00000070            4         1          3         1
00000080 00001  -4.64  2.30E-5   SiOH
00000080 00002  -5.12  7.67E-6   AlOH
00000090 00160  -2.0   0.00E00   PSIO
00000098 00031  -5.22  6.00E-6   NpO2+
00000100 00032   0.0   0.00E00   NpO2(ads)
00000102 00050   0.0   0.00E00   H+
00000104 00003  -1.0   0.00E00   NA+
00000106 00005  -1.0   0.00E00   NO3-
00000110
00000120 00050    0.00  050  1
00000124 00031    0.00  031  1
00000126 03100   -8.90  031  1 050 -1
00000139 00100  -13.78  050 -1
00000145 01100   -7.05  001  1 160 -1 050 -1
00000150 00001    0.00  001  1
00000140 01050    8.12  001  1 160  1 050  1
00000145 01100   -9.56  001  1 160 -1 050 -1
00000150 00002    0.00  002  1
xonpo2   13201   -3.00  001  1 160  0 050 -1 031  1 032  1
00000174
00000175
00000180 00001   008.0 1.000     1.0
00000185     0       0
00000190             1
00000195         13201
00000230            23         1          1          0
00000240            32
00000260 1.7100E-07
00000280 9.4000E-08
00000300 1.0700E-07
00000320 2.6300E-07
00000340 3.1300E-07
00000360 2.9700E-07
00000380 3.1700E-07
00000390 3.4900E-07
00000400 7.1400E-07
00000410 3.3600E-07
00000420 8.7400E-07
00000430 5.6300E-07
00000440 8.7800E-07
00000450 1.2800E-06
00000460 1.3000E-06
00000470 1.5800E-06
00000480 1.6700E-06
00000490 1.7800E-06
00000500 2.5200E-06
00000501 1.7300E-06
00000502 2.7400E-06
00000503 4.1500E-06
00000504 4.3700E-06
00000560            50
00000580 -4.52
00000600 -4.73
00000620 -4.91
00000640 -5.55
00000660 -6.01
00000680 -6.48
00000700 -6.66
00000710 -7.15
00000720 -7.28
00000730 -7.88
00000740 -8.18
00000750 -8.43
00000760 -9.04
00000770 -9.07
00000780 -9.52
00000790 -9.60
00000800 -9.88
00000810 -9.87
00000820 -10.12
00000830 -10.30
00000840 -10.58
00000850 -10.85
00000860 -11.09
00000880            1          1
10%error           32       0.10    1.0E-09
+/- 0.02           50       0.05    0.0E-00
```

CCM
$>SiOH^0 + NpO_2^+ = >SiO\cdot NpO_2^0 + H^+$


```
Neptunum
on
Biotite
2.3s\nm2
00000050
00000060
00000070
00000080
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000139
00000145
00000150
00000140
00000145
00000150
xonpo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000390
00000400
00000410
00000420
00000430
00000440
00000450
00000460
00000470
00000480
00000490
00000500
00000501
00000502
00000503
00000504
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000710
00000720
00000730
00000740
00000750
00000760
00000770
00000780
00000790
00000800
00000810
00000820
00000830
00000840
00000850
00000860
00000880
10%error
+/- 0.02
```


Example FITEQL Inputs

Np(V)-Biotite: Nakayama + Sakamoto (1991)

5/11/95
D.R. Turner

```
             0
             1
             0
             0
             1
            90
             4         1          3         1
00001  -4.64  2.30E-5   SiOH
00002  -5.12  7.67E-6   AlOH
00160  -2.0   0.00E00   PSIO
00031  -5.22  6.00E-6   NpO2+
00032   0.0   0.00E00   NpO2(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00031    0.00  031  1
03100   -8.90  031  1 050 -1
00100  -13.78  050 -1
01100   -7.10  001  1 160 -1 050 -1
00001    0.00  001  1
02050    8.22  002  1 160  1 050  1
02100   -9.62  002  1 160 -1 050 -1
00002    0.00  002  1
13201   -3.00  001  1 160  0 050 -1 031  1 032  1

00002   008.0 1.000
0.1     1.0
            1
        13201
           23         1          1          0
           32
1.7100E-07
9.4000E-08
1.0700E-07
2.6300E-07
3.1300E-07
2.9700E-07
3.1700E-07
3.4900E-07
7.1400E-07
3.3600E-07
8.7400E-07
5.6300E-07
8.7800E-07
1.2800E-06
1.3000E-06
1.5800E-06
1.6700E-06
1.7800E-06
2.5200E-06
1.7300E-06
2.7400E-06
4.1500E-06
4.3700E-06
           50
-4.52
-4.73
-4.91
-5.55
-6.01
-6.48
-6.66
-7.15
-7.28
-7.88
-8.18
-8.43
-9.04
-9.07
-9.52
-9.60
-9.88
-9.87
-10.12
-10.30
-10.58
-10.85
-11.09
        1          1
       32       0.10    1.0E-09
       50       0.05    0.0E-00
```

D.R. Turner

DLM
No CO_2
$>SiOH^0 + NpO_2^+ = >SiO\cdot NpO_2 + H^+$

D.R. Turner

```
Neptunum            0
   on               1
Biotite             0
2.3s\nm2            0
00000050            1
00000060           90
00000070            4         1          3         1
00000080 00001  -4.64  2.30E-5   SiOH
00000080 00002  -5.12  7.67E-6   AlOH
00000090 00160  -2.0   0.00E00   PSIO
00000098 00031  -5.22  6.00E-6   NpO2+
00000100 00032   0.0   0.00E00   NpO2(ads)
00000102 00050   0.0   0.00E00   H+
00000104 00003  -1.0   0.00E00   NA+
00000106 00005  -1.0   0.00E00   NO3-
00000110
00000120 00050    0.00  050  1
00000124 00031    0.00  031  1
00000126 03100   -8.90  031  1 050 -1
00000139 00100  -13.78  050 -1
00000145 01100   -7.10  001  1 160 -1 050 -1
00000150 00001    0.00  001  1
00000140 02050    8.22  002  1 160  1 050  1
00000145 02100   -9.62  002  1 160 -1 050 -1
00000150 00002    0.00  002  1
xonpo2   23201   -3.00  002  1 160  0 050 -1 031  1 032  1
00000174
00000175
00000180 00002   008.0 1.000
00000185 0.1     1.0
00000190             1
00000195         23201
00000230            23         1          1          0
00000240            32
00000260 1.7100E-07
00000280 9.4000E-08
00000300 1.0700E-07
00000320 2.6300E-07
00000340 3.1300E-07
00000360 2.9700E-07
00000380 3.1700E-07
00000390 3.4900E-07
00000400 7.1400E-07
00000410 3.3600E-07
00000420 8.7400E-07
00000430 5.6300E-07
00000440 8.7800E-07
00000450 1.2800E-06
00000460 1.3000E-06
00000470 1.5800E-06
00000480 1.6700E-06
00000490 1.7800E-06
00000500 2.5200E-06
00000501 1.7300E-06
00000502 2.7400E-06
00000503 4.1500E-06
00000504 4.3700E-06
00000560            50
00000580 -4.52
00000600 -4.73
00000620 -4.91
00000640 -5.55
00000660 -6.01
00000680 -6.48
00000700 -6.66
00000710 -7.15
00000720 -7.28
00000730 -7.88
00000740 -8.18
00000750 -8.43
00000760 -9.04
00000770 -9.07
00000780 -9.52
00000790 -9.60
00000800 -9.88
00000810 -9.87
00000820 -10.12
00000830 -10.30
00000840 -10.58
00000850 -10.85
00000860 -11.09
00000880            1          1
10%error           32       0.10    1.0E-09
+/- 0.02           50       0.05    0.0E-00
```

DLM
No CO_2
$>AlOH^0 + NpO_2^+ = >AlONpO_2^0 + H^+$


```
Neptunum
on
Biotite
2.3s\nm2
00000050
00000060
00000070
00000080
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000139
00000145
00000150
00000140
00000145
00000150
xonpo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000390
00000400
00000410
00000420
00000430
00000440
00000450
00000460
00000470
00000480
00000490
00000500
00000501
00000502
00000503
00000504
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000710
00000720
00000730
00000740
00000750
00000760
00000770
00000780
00000790
00000800
00000810
00000820
00000830
00000840
00000850
00000860
00000880
10%error
+/- 0.02
```


Example FITEQL Input

Np(V)-Biotite Sorption: Nakayama & Sakamoto (1991)

5/11/95
D.R.Kelmm

```
         0
         1
         0
         0
         1
        90
         6         1         3         1
00001   -4.64   2.30E-5   SiOH
00002   -5.12   7.67E-6   AlOH
00160   -2.0    0.00E00   PSI0
00161   -1.0    0.00E00   PSIB
00162   -0.2    0.00E00   PSID
00031   -5.22   6.00E-6   NpO2+
00032    0.0    0.00E00   NpO2(ads)
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   NO3-

00050    0.00   050  1
00031    0.00   031  1
03100   -8.90   031  1 050 -1
00100  -13.78   050 -1
01100   -4.79   001  1 160 -1 050 -1
01103   -6.22   001  1 160 -1 161  1 050 -1 003  1
00001    0.00   001  1
02050    6.69   002  1 160  1 050  1
02100  -10.69   002  1 160 -1 050 -1
02103   -7.73   002  1 160 -1 161  1 050 -1 003  1
02055    9.90   002  1 160  1 161 -1 050  1 005  1
00002    0.00   002  1
13201   -3.00   001  1 160 -1 161  1 050 -1 031  1 032  1

00004   008.0 1.000  0.8    0.2
0.1    1.0
         1
      13201
         23         1         1         0
         32
1.7100E-07
9.4000E-08
1.0700E-07
2.6300E-07
3.1300E-07
2.9700E-07
3.1700E-07
3.4900E-07
7.1400E-07
3.3600E-07
8.7400E-07
5.6300E-07
8.7800E-07
1.2800E-06
1.3000E-06
1.5800E-06
1.6700E-06
1.7800E-06
2.5200E-06
1.7300E-06
2.7400E-06
4.1500E-06
4.3700E-06
        50
-4.52
-4.73
-4.91
-5.55
-6.01
-6.48
-6.66
-7.15
-7.28
-7.88
-8.18
-8.43
-9.04
-9.07
-9.52
-9.60
-9.88
-9.87
-10.12
-10.30
-10.58
-10.85
-11.09
         1         1
        32      0.10   1.0E-09
        50      0.05   0.0E-00
```

TLM
No CO_2

$>SiOH^{\circ} + NpO_2^{+} = >SiO\cdot NpO_2^{\circ} + H^{+}$

```
Neptunum         0
   on            1
Biotite          0
2.3s\nm2         0
00000050         1
00000060        90
00000070         6         1         3         1
00000080 00001   -4.64   2.30E-5   SiOH
00000080 00002   -5.12   7.67E-6   AlOH
00000090 00160   -2.0    0.00E00   PSI0
00000092 00161   -1.0    0.00E00   PSIB
00000094 00162   -0.2    0.00E00   PSID
00000098 00031   -5.22   6.00E-6   NpO2+
00000100 00032    0.0    0.00E00   NpO2(ads)
00000102 00050    0.0    0.00E00   H+
00000104 00003   -1.0    0.00E00   NA+
00000106 00005   -1.0    0.00E00   NO3-
00000110
00000120 00050    0.00   050  1
00000124 00031    0.00   031  1
00000126 03100   -8.90   031  1 050 -1
00000139 00100  -13.78   050 -1
00000145 01100   -4.79   001  1 160 -1 050 -1
00000147 01103   -6.22   001  1 160 -1 161  1 050 -1 003  1
00000150 00001    0.00   001  1
00000140 02050    6.69   002  1 160  1 050  1
00000145 02100  -10.69   002  1 160 -1 050 -1
00000147 02103   -7.73   002  1 160 -1 161  1 050 -1 003  1
00000149 02055    9.90   002  1 160  1 161 -1 050  1 005  1
00000150 00002    0.00   002  1
xonpo2   23201   -3.00   002  1 160 -1 161  1 050 -1 031  1 032  1
00000174
00000175
00000180 00004   008.0 1.000  0.8    0.2
00000185 0.1    1.0
00000190         1
00000195       23201
00000230         23         1         1         0
00000240         32
00000260 1.7100E-07
00000280 9.4000E-08
00000300 1.0700E-07
00000320 2.6300E-07
00000340 3.1300E-07
00000360 2.9700E-07
00000380 3.1700E-07
00000390 3.4900E-07
00000400 7.1400E-07
00000410 3.3600E-07
00000420 8.7400E-07
00000430 5.6300E-07
00000440 8.7800E-07
00000450 1.2800E-06
00000460 1.3000E-06
00000470 1.5800E-06
00000480 1.6700E-06
00000490 1.7800E-06
00000500 2.5200E-06
00000501 1.7300E-06
00000502 2.7400E-06
00000503 4.1500E-06
00000504 4.3700E-06
00000560         50
00000580 -4.52
00000600 -4.73
00000620 -4.91
00000640 -5.55
00000660 -6.01
00000680 -6.48
00000700 -6.66
00000710 -7.15
00000720 -7.28
00000730 -7.88
00000740 -8.18
00000750 -8.43
00000760 -9.04
00000770 -9.07
00000780 -9.52
00000790 -9.60
00000800 -9.88
00000810 -9.87
00000820 -10.12
00000830 -10.30
00000840 -10.58
00000850 -10.85
00000860 -11.09
00000880         1         1
10%error        32      0.10   1.0E-09
+/- 0.02        50      0.05   0.0E-00
```

TLM
No CO_2

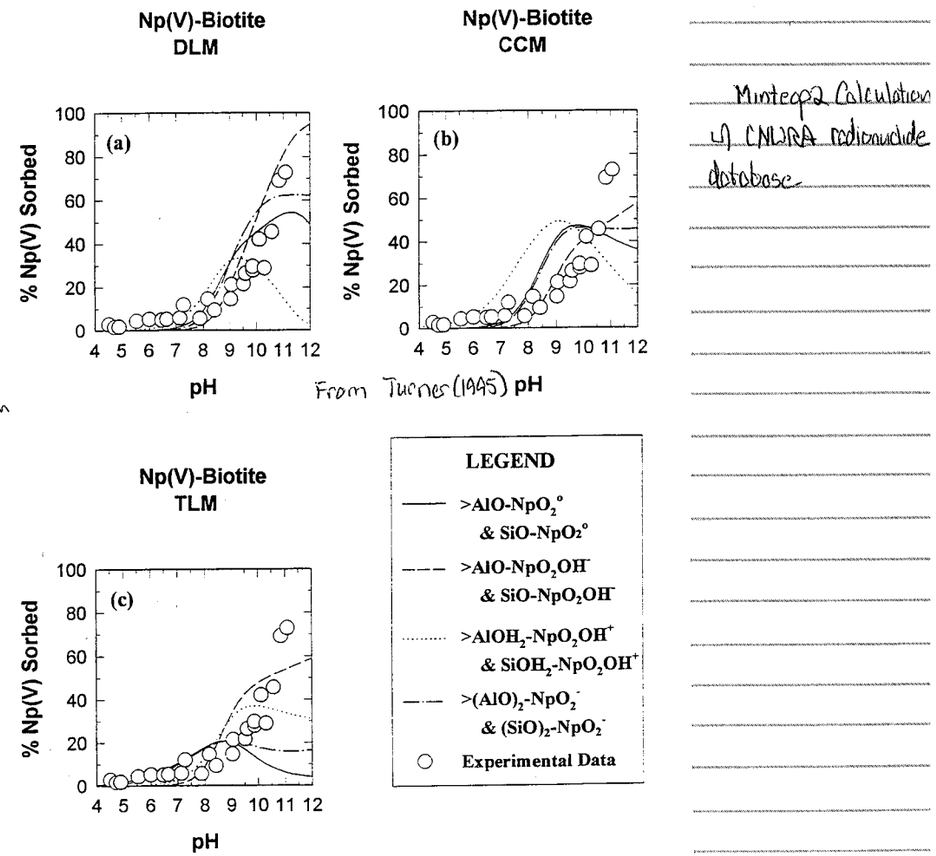
$>AlOH^{\circ} + NpO_2^{+} = >AlO\cdot NpO_2^{\circ} + H^{+}$

Example FITEQL Input

Table B-23. Neptunium (V)-Biotite Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: Natural Biotite $[K(Mg,Fe)_3AlSi_3O_{10}(OH)_2]$ A_{sp}: 8 m^2/g Data Source: Nakayama and Sakamoto (1991) Concentration: [Np(V)] = 6E-6 M		Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_s = 2.31 sites/nm^2 M/V = 1 g/L

Si:Al = 3:1 No CO_2		DLM			CCM			TLM		
								(α-Al_2O_3)	(SiO_2)	
		Log K_+ = 8.33 (α-Al_2O_3) Log K_- = -9.73 (α-Al_2O_3) Log K_- = -7.20 (SiO_2)			Log K_+ = 8.12 (α-Al_2O_3) Log K_- = -9.56 (α-Al_2O_3) Log K_- = -7.04 (SiO_2)			Log K_+ = 6.90 Log K_+ = 0.90 Log K_- = -10.90 Log K_- = -4.90 Log K_{Cat} = -7.73 Log K_{Cat} = -6.22 Log K_{An} = 10.12		
		Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$	Log K	V_Y	$\sigma_{Log\,K}$
XO-NpO_2^+	SiOH	-3.99	51.0	.0171	-3.61	41.6	.0168	-2.83	44.9	.0141
	AlOH	-3.35	45.3	.0229	-4.00	40.2	.0182	0.02	41.7	.0188
XOH-NpO_2^+	SiOH	3.42	56.5	.0184	4.29	42.6	.0175	1.56	52.5	.0152
	AlOH	4.43	44.7	.0181	3.88	40.5	.0180	4.56	44.2	.0163
XO-NpO_2OH^-	SiOH	-11.64	42.8	.0179	-11.41	0.5	.0847	-8.78	0.6	.0907
	AlOH	-11.25	54.2	.0333	11.77	0.5	.1007	-6.26	0.5	.1818
XOH-NpO_2OH^+	SiOH	-3.99	51.0	.0171	-3.61	41.6	.0168	-4.03	43.2	.0171
	AlOH	-3.35	45.3	.0229	-4.00	40.2	.0182	-1.81	41.5	.0224
XOH_2-NpO_2OH^{2+}	SiOH	3.42	56.5	.0184	4.29	42.6	.0175	0.93	45.3	.0199
	AlOH	4.43	44.7	.0181	3.88	40.5	.0180	2.99	40.8	.0189
OTHER SPECIES:										
$(XO)_2$-NpO_2^-	SiOH	-6.31	49.6	.0190	-5.82	41.4	.0193	-2.42	46.0	.0156
	AlOH	-4.61	50.3	.0536	-6.42	39.4	.0263	3.53	36.7	.0351



Minteq2 Calculations w/ CNWRA radionuclide database

Figure 4-23. SCM predictions of Np(V) sorption on biotite (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 6\times10^{-6}$ M, 0.1 M $NaNO_3$, M/V=1 g/L. Model parameters from Tables 3-1 and B-23. Si:Al ratio of 3:1 assumed. Data from Nakayama and Sakamoto (1991).

Np(V)- αAl_2O_3; Nakayama + Sakamoto (1991)

5/11/95 D.R.Lemm

Information potentially subject to copyright protection w as redacted from this location. The redacted material (Figure 4: Sorption of neptunium on synthetic lepidocrocite....) is from the follow ing reference:

Nakayama, S. and Y. Sakamoto. "Sorption of Neptunium on Naturally-Occurring Iron-Containing Minerals." Radiochimica Acta. Vols. 52 and 53. pp. 153-157. 1991.

DIGITIZED DATA:

Nakayama, S., and Y. Sakamoto. 1991. Sorption of neptunium on naturally-occurring iron-containing minerals. *Radiochimica Acta* 52/53:153-157.

D.R.Lemm

Nakayama and Sakamoto (1991)	Np(V)- Alpha Al2O3	
Figure 4 (page 156)		
Asp=2.5 m2/g	No CO2	Np(V)=6E-6 M
0.1 M NaNO3	M/V=1 g/L	
No CO2		
pH	% sorbed	mol sorbed
5.79	8.067	4.840e-07
7.12	11.627	6.976e-07
7.35	8.680	5.208e-07
7.84	8.840	5.304e-07
8.11	9.579	5.748e-07
8.90	10.038	6.023e-07
9.36	13.987	8.392e-07
9.99	14.314	8.588e-07
10.55	19.581	1.175e-06
10.94	25.291	1.517e-06

Np(V)- αAl_2O_3: Nakayama + Sakamoto (1991) 5/11/95 D.R.Lemm

DLM
No CO_2

$>AlOH^0 + NpO_2^+ = >AlO\cdot NpO_2^0 + H^+$

CCM
No CO_2

$>AlOH^0 + NpO_2^+ = >AlO\cdot NpO_2^0 + H^+$

D.R.Lemm

EXAMPLE FITEQL Input

TLM
No CO_2

$>AlOH^0 + NpO_2^{2+} = >AlO\cdot NpO_2^+ + H^+$

5/11/95 - D.R.Kamm

Table B-9. Neptunium (V)-α-Al_2O_3 Sorption Binding Constants: Monodentate, mononuclear complexes.

Solid: α-Al_2O_3 A_{SD}: 2.5 m^2/g Data Source: Nakayama and Sakamoto (1991) Concentration: $[Np(V)]_T$ = 6E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.03 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_s = 2.31 sites/nm^2 M/V = 1 g/L

No CO_2	DLM			CCM			TLM		
	Log K_+ = 8.33 Log K_- = -9.73			Log K_+ = 8.12 Log K_- = -9.56			Log K_+ = 6.90 Log K_- = -10.90 Log K_{Ca} = -7.75 Log K_{Na} = 10.12		
	Log K	V_1	$\sigma_{1,calc}$	Log K	V_1	$\sigma_{1,calc}$	Log K	V_1	$\sigma_{1,calc}$
XO-NpO_2^+	-4.26	42.1	.0231	-4.26	41.9	.0231	-3.97	36.0	.0232
XOH-NpO_2^+	5.07	32.9	.0256	5.00	32.3	.0255	6.03	27.5	.0442
XO-NpO_2OH^-	-13.37	46.9	.0203	-13.31	47.3	.0297	-11.20	21.6	.0440
XOH-NpO_2OH^+	-4.26	42.1	.0231	-4.26	41.9	.0231	-3.88	41.5	.0230
XOH_2-NpO_2OH^+	5.07	32.9	.0256	5.00	32.3	.0255	6.46	20.6	.0424
OTHER SPECIES:									
$(XO)_2$-NpO_2^-	-7.99	43.7	.0352	-7.95	44.5	.0354	-5.74	22.2	.0536

FITEQL Results

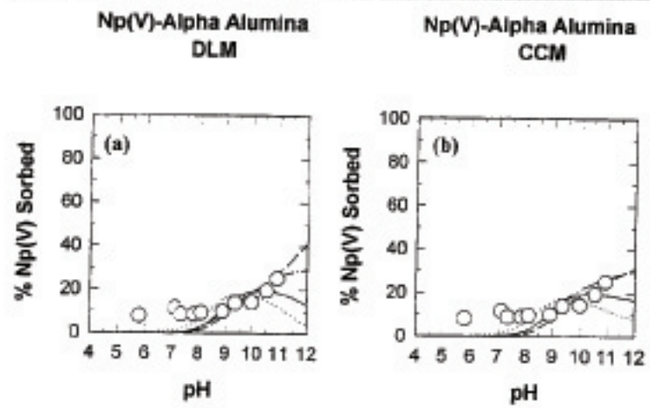


Figure 4-9. Np(V) sorption on α-Al_2O_3. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 6 \times 10^{-6}$ M, 0.1 M $NaNO_3$, M/V = 1 g/L. Model parameters from Tables 3-1 and B-9. Data from Nakayama and Sakamoto (1991).

Np(V)-Boehmite (γAlOOH): Nakayama & Sakamoto (1991) 5/11/95

Information potentially subject to copyright protection w as redacted from this location. The redacted material (Figure 4: Sorption of neptunium on synthetic lepidocrocite...) is from the follow ing reference:

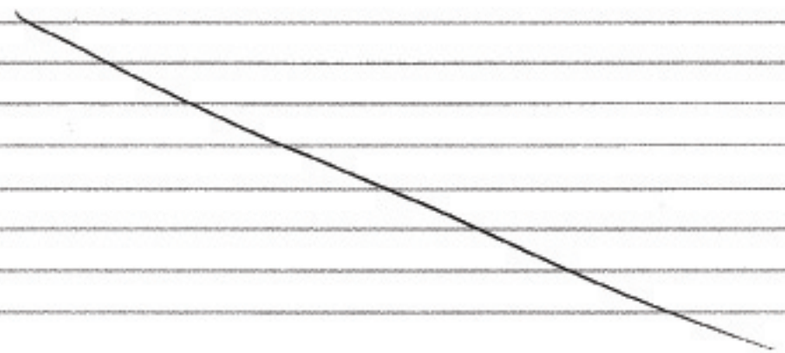
Nakayama, S. and Y. Sakamoto. “Sorption of Neptunium on Naturally-Occurring Iron-Containing Minerals.” Radiochimica Acta. Vols. 52 and 53. pp. 153-157. 1991.

Nakayama, S., and Y. Sakamoto. 1991. Sorption of neptunium on naturally-occurring iron-containing minerals. *Radiochimica Acta* 52/53:153-157.

Nakayama and Sakamoto (1991)	Np(V)- Synthetic Boehmite	
Figure 4 (page 156)		
Asp=175 m2/g	No CO2	Np(V)=6E-6 M
0.1 M NaNO3	M/V=1 g/L	
No CO2		
pH	% sorbed	mol sorbed
3.73	13.450	8.070e-07
4.21	12.968	7.781e-07
5.58	14.194	8.516e-07
6.46	14.177	8.506e-07
6.85	15.252	9.151e-07
7.24	30.502	1.830e-06
8.69	72.604	4.362e-06
9.34	79.110	4.747e-06
9.97	89.145	5.349e-06
10.59	90.994	5.460e-06

D.R.Kamm

Digitized Data



Np(V)-Boehmite (γ-AlOOH) - Nakayama + Sakamoto (1991)

```
Neptunum
   on
gamAlOOH
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000139
00000140
00000145
00000150
xoNpo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000390
00000400
00000410
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000710
00000720
00000730
00000880
10%error
+/- 0.02
```

```
        0
        1
        0
        0
        1
       90
        3         1         3         1
00001  -3.17   6.72E-4   XOH
00160  -2.0    0.00E00   PSI0
00031  -5.22   6.00E-6   Np02+
00032   0.0    0.00E00   Np02(ads)
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   NA+
00005  -1.0    0.00E00   N03-

00050   0.00   050  1
00031   0.00   031  1
03100  -8.90   031  1 050 -1
00100 -13.78   050 -1
01050   6.92   001  1 160  1 050  1
01100  -9.00   001  1 160 -1 050 -1
00001   0.00   001  1
03201  -5.00   001  1 160  0 050 -1 031  1 032  1

00001   175.0 1.000     1.0
        0   0
        1
3201
       10         1         1         0
       32
1.3600E-06
6.2200E-07
2.1700E-06
3.3800E-06
3.9600E-06
4.6200E-06
4.3300E-06
5.5400E-06
5.7400E-06
5.8500E-06
       50
-5.01
-5.56
-6.43
-7.29
-7.44
-7.64
-8.04
-8.77
-10.11
-10.25
       1         1
      32      0.10    1.0E-09
      50      0.05    0.0E-00
```

CCM
No CO_2

$>AlOH^0 + NpO_2^+ = >AlO\cdot NpO_2^0 + H^+$

```
        0
        1
        0
        0
        1
       90
        3         1         3         1
00001  -3.17   6.72E-4   XOH
00160  -2.0    0.00E00   PSI0
00031  -5.22   6.00E-6   Np02+
00032   0.0    0.00E00   Np02(ads)
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   NA+
00005  -1.0    0.00E00   N03-

00050   0.00   050  1
00031   0.00   031  1
03100  -8.94   031  1 050 -1
00100 -13.78   050 -1
01050   6.74   001  1 160  1 050  1
01100  -8.94   001  1 160 -1 050 -1
00001   0.00   001  1
03201  -5.00   001  1 160  0 050 -1 031  1 032  1

00002   175.0 1.000
0.1     1.0
        1
3201
       10         1         1         0
       32
1.3600E-06
6.2200E-07
2.1700E-06
3.3800E-06
3.9600E-06
4.6200E-06
4.3300E-06
5.5400E-06
5.7400E-06
5.8500E-06
       50
-5.01
-5.56
-6.43
-7.29
-7.44
-7.64
-8.04
-8.77
-10.11
-10.25
       1         1
      32      0.10    1.0E-09
      50      0.05    0.0E-00
```

DLM
No CO_2

$>AlOH^0 + NpO_2^+ = >AlO\cdot NpO_2^0 + H^+$

Example FITEQL Inputs

```
        0
        1
        0
        0
        1
       90
        5         1         3         1
00001  -3.17   6.72E-4   XOH
00160  -2.0    0.00E00   PSI0
00161  -1.0    0.00E00   PSIB
00162  -0.2    0.00E00   PSID
00031  -5.22   6.00E-6   Np02+
00032   0.0    0.00E00   Np02(ads)
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   NA+
00005  -1.0    0.00E00   N03-

00050   0.00   050  1
00031   0.00   031  1
03100  -8.90   031  1 050 -1
00100 -13.78   050 -1
01050   6.29   001  1 160  1 050  1
01100 -10.29   001  1 160 -1 050 -1
01103  -7.95   001  1 160 -1 161  1 050 -1 003  1
01055   8.50   001  1 160  1 161 -1 050  1 005  1
00001   0.00   001  1
03201  -5.00   001  1 160 -1 161  1 050 -1 031  1 032  1

00004   175.0 1.000  0.8    0.2
0.1     1.0
        1
3201
       10         1         1         0
       32
1.3600E-06
6.2200E-07
2.1700E-06
3.3800E-06
3.9600E-06
4.6200E-06
4.3300E-06
5.5400E-06
5.7400E-06
5.8500E-06
       50
-5.01
-5.56
-6.43
-7.29
-7.44
-7.64
-8.04
-8.77
-10.11
-10.25
       1         1
      32      0.10    1.0E-09
      50      0.05    0.0E-00
```

TLM
No CO_2

$>AlOH^0 + NpO_2^+ = >AlO\cdot NpO_2^0 + H^+$

Table B-7. Neptunium (V)-Boehmite (γ-AlOOH) Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: Boehmite (γ-AlOOH) A_{SP}: 175 m^2/g Data Source: Nakayama and Sakamoto (1991) Concentration: [Np(V)] = 6E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

No CO_2	DLM (a)			CCM (a)			TLM (a)		
	Log K_+ = 6.85 Log K_- = -9.05			Log K_+ = 6.92 Log K_- = -9.00			Log K_+ = 6.40 Log K_- = -10.40 Log K_{Ca} = -7.95 Log K_{Na} = 8.28		
	Log K	V_Y	$a_{1\sigma Log K}$	Log K	V_Y	$a_{1\sigma Log K}$	Log K	V_Y	$a_{1\sigma Log K}$
XO-NpO_2^+	-3.36	15.7	.0480	-3.34	15.3	.0472	-5.03	43.0	.0241
XOH-NpO_2^+	4.09	8.0	.0351	4.23	9.1	.0376	3.17	52.4	.0259
XO-NpO_2OH^-	-10.84	22.9	.0610	-10.88	20.9	.0551	-11.46	15.4	.0496
XOH-NpO_2OH^0	-3.36	15.7	.0480	-3.34	15.3	.0472	-3.28	15.0	.0466
XOH_2-NpO_2OH^+	4.09	8.0	.0351	4.23	9.1	.0376	4.98	11.8	.0440
OTHER SPECIES:									
$(XO)_2$-NpO_2^-	-7.60	23.8	.0643	-7.58	21.7	.0571	9.79	32.8	.0261

(a) Surface constants for γ-Al_2O_3 used.

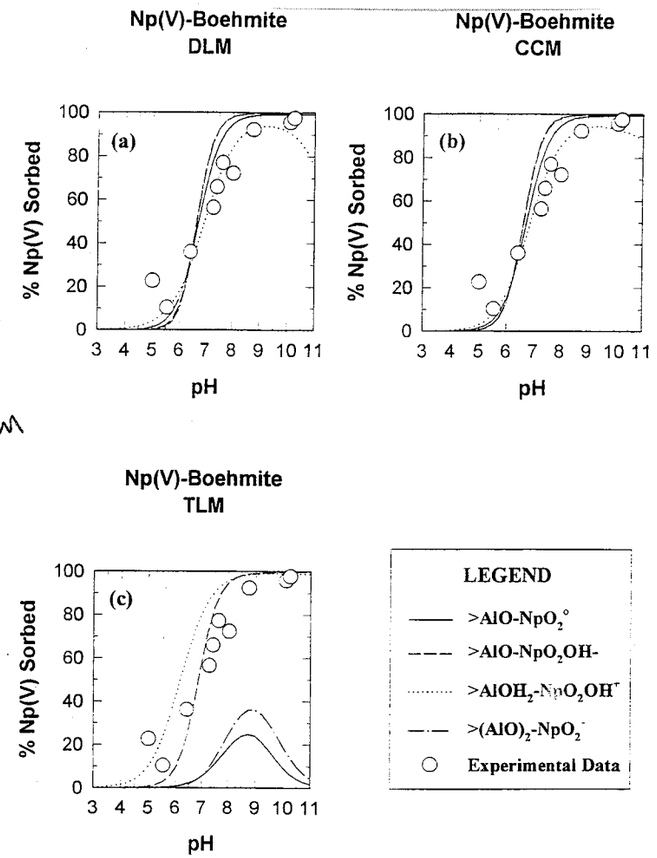


Figure 4-7. Np(V) sorption on boehmite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 6 \times 10^{-6}$ M, 0.1 M $NaNO_3$, M/V = 1 g/L. Model parameters from Tables 3-1 and B-7. Data from Nakayama and Sakamoto (1991).

Np(V)-Hematite - Nakayama + Sakamoto(1991)

5/12/95
D.R.Lamm

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 3: Sorption of neptunium on ... (b) synthetic hematite...) is from the following reference:

Nakayama, S. and Y. Sakamoto. "Sorption of Neptunium on Naturally-Occurring Iron-Containing Minerals." Radiochimica Acta. Vols. 52 and 53. pp. 153-157. 1991.

5/12/95
D.R.Lamm

Nakayama, S., and Y. Sakamoto. 1991. Sorption of neptunium on naturally-occurring iron-containing minerals. *Radiochimica Acta* 52/53:153-157.

Nakayama and Sakamoto (1991)	**Np(V)- Synthetic Hematite**	
Figure 3b (page 156)		
Asp=5.9 m2/g	No CO2	Np(V)=6E-6 M
0.1 M NaNO3	M/V=1 g/L	
No CO2		
pH	% sorbed	mol sorbed
4.32	6.464	3.878e-07
4.80	4.316	2.589e-07
5.57	9.015	5.409e-07
6.44	8.481	5.089e-07
6.56	15.554	9.333e-07
6.64	12.419	7.452e-07
6.90	10.342	6.205e-07
7.22	11.896	7.138e-07
8.06	29.027	1.742e-06
8.68	32.009	1.921e-06
8.68	39.745	2.385e-06
8.85	38.360	2.302e-06
9.21	47.962	2.878e-06
9.42	60.356	3.621e-06
10.16	44.198	2.652e-06
10.34	64.705	3.882e-06
10.51	71.714	4.303e-06
10.57	72.150	4.329e-06
10.62	55.894	3.354e-06
10.86	85.794	5.148e-06

Digitized data.

No FITEQL runs performed due to lack of surface acidity constants for Hematite. No convergence for pot. titration data.

Nakayama, S., and Y. Sakamoto. 1991. Sorption of neptunium on naturally-occurring iron-containing minerals. *Radiochimica Acta* 52/53:153-157.

Nakayama and Sakamoto (1991)	**Np(V)- Natural Hematite**	
Figure 3a (page 156)		
Asp=3.2 m2/g	No CO2	Np(V)=6E-6 M
0.1 M NaNO3	M/V=1 g/L	
No CO2		
pH	% sorbed	mol sorbed
3.50	3.185	1.911e-07
4.15	4.530	2.718e-07
4.44	4.593	2.756e-07
5.15	10.682	6.409e-07
5.36	12.118	7.271e-07
5.94	4.068	2.441e-07
6.18	4.599	2.759e-07
6.75	5.849	3.510e-07
6.94	9.408	5.645e-07
7.05	6.756	4.053e-07
7.19	12.936	7.762e-07
8.36	8.914	5.348e-07
8.79	18.279	1.097e-06
8.93	12.817	7.690e-07
8.95	13.036	7.821e-07
9.16	19.060	1.144e-06
9.51	13.506	8.103e-07
9.93	19.625	1.177e-06
10.35	25.899	1.554e-06
10.72	28.085	1.685e-06

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Np(V)-γAl_2O_3: Righetto et al. (1988)

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 1: Am(III), Th(IV) and Np(V) uptake on 10 ppm...) is from the following reference:

Righetto, L., G. Bidoglio, B. Marcandalli, and I.R. Bellobono. "Surface Interactions of Actinides with Alumina Colloids." Radiochimica Acta. Vols. 44 and 45. pp. 73-75. 1988.

Righetto, L., G. Bidoglio, B. Marcandalli, and I.R. Bellobono. 1988. Surface interactions of actinides with alumina colloids. *Radiochimica Acta* 44/45:73-75.

Righetto et. al. (1988)	Np(V) -γAl_2O_3	
Figure 1(c)		
Asp=130 m^2/g	1E-14 M	
No CO_2		
pH	%sorbed	mol sorbed
0.1 M $NaClO_4$	**M/V = 0.2 g/L**	
1(c)		
5.07	.22	2.2365E-17
5.35	.36	3.5542E-17
5.90	2.15	2.1452E-16
6.44	7.65	7.6531E-16
6.73	14.35	1.4350E-15
6.91	25.23	2.5230E-15
7.08	33.62	3.3616E-15
7.14	42.37	4.2366E-15
7.28	44.19	4.4189E-15
7.39	54.97	5.4971E-15
7.51	59.90	5.9900E-15
7.57	64.88	6.4884E-15
7.60	57.25	5.7246E-15
7.83	75.55	7.5554E-15
8.63	93.92	9.3920E-15
9.69	90.48	9.0479E-15
10.45	97.14	9.7140E-15
10.67	94.27	9.4273E-15
11.06	97.55	9.7552E-15

D.R.Turner

Digitized Data

5/12/95
D.R.Turner

Example FITEQL Input files

CCM
No CO_2
$>AlOH^0 + NpO_2^+ = >AlONpO_2^0 + H^+$

```
       0
       1
       0
       0
       1
      90
       3          1          3          1
00001  -4.00  9.97E-5   XOH
00160  -2.0   0.00E00   PSI0
00031  -14.0  1.0E-14   NpO2+
00032   0.0   0.00E00   NpO2(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.10E00   Na+
00005  -1.0   0.10E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -8.90  031  1 050 -1
00100  -13.78  050 -1
01050    6.92  001  1 160  1 050  1
01100   -9.00  001  1 160 -1 050 -1
00001    0.00  001  1
03201   -2.50  001  1 160  0 050 -1 031  1 032  1

00001   130.0 0.200      1.0
    0        0
       1
    3201
      19          1          1          0
      32
2.2365E-17
3.5542E-17
2.1452E-16
7.6531E-16
1.4350E-15
2.5230E-15
3.3616E-15
4.2366E-15
4.4189E-15
5.4971E-15
5.9900E-15
6.4884E-15
5.7246E-15
7.5554E-15
9.3920E-15
9.0479E-15
9.7140E-15
9.4273E-15
9.7552E-15
      50
-5.07
-5.35
-5.90
-6.44
-6.73
-6.91
-7.08
-7.14
-7.28
-7.39
-7.51
-7.57
-7.60
-7.83
-8.63
-9.69
-10.45
-10.67
-11.06
       1        0
      32     0.10   1.0E-18
```

```
Neptunum
   on
gamAl2O3
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000139
00000140
00000145
00000150
xoNpo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
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00000660
00000680
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00000710
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00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000880
10%error
```

DLM
No CO_2
$>AlOH^0 + NpO_2^+ = >AlO{\cdot}NpO_2^0 + H^+$

```
      90
       3          1          3          1
00001  -4.00  9.97E-5   XOH
00160  -2.0   0.00E00   PSI0
00031  -14.0  1.0E-14   NpO2+
00032   0.0   0.00E00   NpO2(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.10E00   Na+
00005  -1.0   0.10E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -8.90  031  1 050 -1
00100  -13.78  050 -1
01050    6.74  001  1 160  1 050  1
01100   -8.94  001  1 160 -1 050 -1
00001    0.00  001  1
03201   -3.20  001  1 160  0 050 -1 031  1 032  1

00002   130.0 0.200
0.1     1.0
       1
    3201
      19          1          1          0
      32
2.2365E-17
3.5542E-17
2.1452E-16
7.6531E-16
1.4350E-15
2.5230E-15
3.3616E-15
4.2366E-15
4.4189E-15
5.4971E-15
5.9900E-15
6.4884E-15
5.7246E-15
7.5554E-15
9.3920E-15
9.0479E-15
9.7140E-15
9.4273E-15
9.7552E-15
      50
-5.07
-5.35
-5.90
-6.44
-6.73
-6.91
-7.08
-7.14
-7.28
-7.39
-7.51
-7.57
-7.60
-7.83
-8.63
-9.69
-10.45
-10.67
-11.06
       1        0
      32     0.10   1.0E-18
```


```
Neptunum
   on
gamAl2O3
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000139
00000140
00000145
00000150
xoNpo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
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00000660
00000680
00000700
00000710
00000660
00000680
00000700
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000880
10%error
```

5/12/95
DBLeman

```
                  5          1          3          1
00001  -4.00   9.97E-5    XOH
00160  -2.0    0.00E00    PSIO
00161  -1.0    0.00E00    PSIB
00162  -0.2    0.00E00    PSID
00031  -14.0   1.0E-14    NpO2+
00032   0.0    0.00E00    NpO2(ads)
00050   0.0    0.00E00    H+
00003  -1.0    0.10E00    Na+
00005  -1.0    0.10E00    ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -8.90  031  1 050 -1
00100  -13.78  050 -1
01050    6.29  001  1 160  1 050  1
01100  -10.29  001  1 160 -1 050 -1
01103   -7.95  001  1 160 -1 161  1 050 -1 003  1
01055    8.06  001  1 160  1 161 -1 050  1 005  1
00001    0.00  001  1
03202   10.00  001  1 160  0 161  1 050  0 031  1 032  1

00004   130.0 0.200  0.8    0.2
0.1     1.0
          1
       3202
         19          1          1          0
         32
2.2365E-17
3.5542E-17
2.1452E-16
7.6531E-16
1.4350E-15
2.5230E-15
3.3616E-15
4.2366E-15
4.4189E-15
5.4971E-15
5.9900E-15
6.4884E-15
5.7246E-15
7.5554E-15
9.3920E-15
9.0479E-15
9.7140E-15
9.4273E-15
9.7552E-15
         50
-5.07
-5.35
-5.90
-6.44
-6.73
-6.91
-7.08
-7.14
-7.28
-7.39
-7.51
-7.57
-7.60
-7.83
-8.63
-9.69
-10.45
-10.67
-11.06
          1          0
         32       0.10    1.0E-18
```

TLM
No CO_2

DBJ 5/12/95

~~$>AlOH^{\circ} + NpO_2^+ = >AlONpO_2^{\circ} + H^+$~~

$>AlOH^{\circ} + NpO_2^+ = >AlOHNpO_2^+$

```
Neptunum
   on
gamAl2O3
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000139
00000140
00000145
00000147
00000149
00000150
xOHNPO2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000660
00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000660
00000680
00000700
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000880
10%error
```

Table B-4. Neptunium (V)- γ-Al_2O_3 Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: γ-Al_2O_3
A_{SP}: 130 m^2/g
Data Source: Righetto et al. (1988)
Concentration: [Np(V)] = 1E-14 M

Rel Error (pH): (a)
Abs Error (pH): (a)
Rel Error (radionuclide): 0.10
Abs Error (radionuclide): 1.0E-18

Ionic Strength (electrolyte): 0.1 M $NaClO_4$
N_S = 2.31 sites/nm^2
M/V = 0.2 g/L

No CO_2	DLM			CCM			TLM		
	Log K_+ = 6.85 Log K_- = -9.05			Log K_+ = 6.92 Log K_- = -9.00			Log K_+ = 6.40 Log K_- = -10.40 Log K_{Cat} = -7.95 Log K_{An} = 8.28		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-NpO_2°	-3.42	2.7	.0167	-3.42	3.2	.0166	-5.66	87.7	.0300
XOH-NpO_2^+	3.86	42.5	.0159	4.08	28.9	.0153	2.34	89.5	.0324
XO-NpO_2OH^-	-10.98	3.5	.0203	-11.05	1.8	.0195	-11.54	1.2	.0173
XOH-NpO_2OH°	-3.42	2.7	.0167	-3.42	3.2	.0166	-3.41	3.8	.0165
XOH_2-NpO_2OH^+	3.86	42.5	.0159	4.08	28.9	.0153	4.70	9.2	.0161
OTHER SPECIES:									
$(XO)_2$-NpO_2^-	-6.91	4.7	.0209	-6.95	2.6	.0200	-9.47	83.7	.0260

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

5/12/95
DBLeman

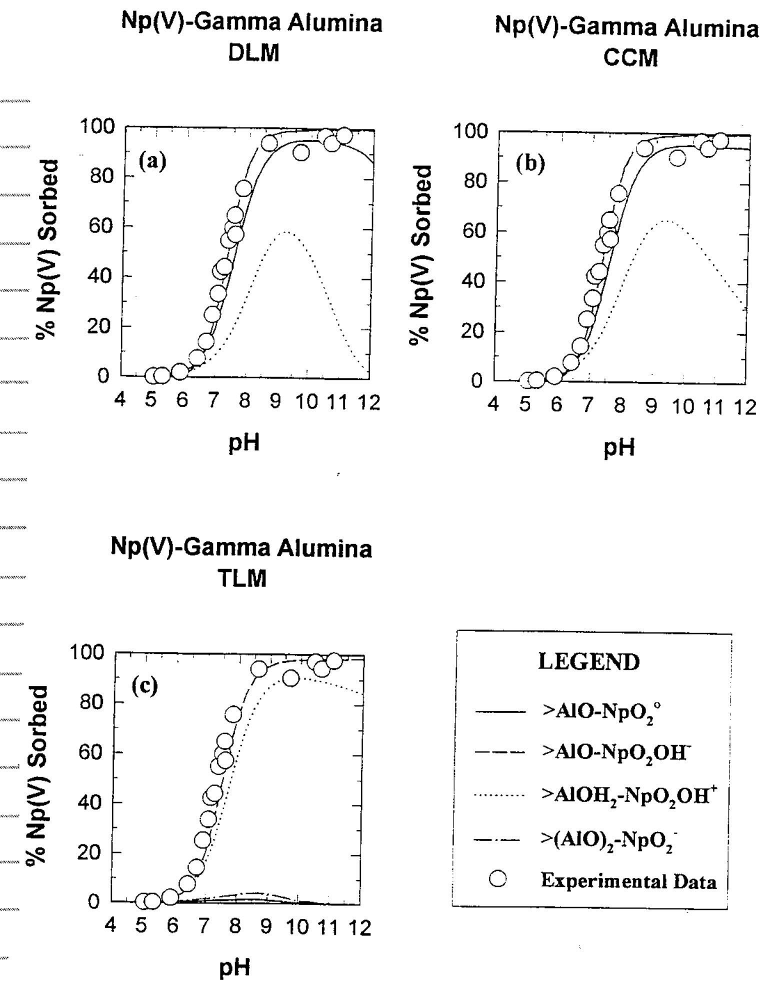


Figure 4-4. Np(V) sorption on γ-Al_2O_3. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 1\times10^{-14}$ M, 0.1 M $NaClO_4$, M/V=0.2 g/L. Model parameters from Tables 3-1 and B-4. Data from Righetto et al. (1988).

4-5

pH	%srb
9.06147	69.17103
9.13503	67.73985
9.22572	66.06696
9.30011	64.46390
9.49867	61.28875
9.63479	59.32063
9.79628	55.16864

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 5: Am(III), Th(IV) and Np(V) uptake on 10 ppm...) is from the following reference:

Righetto, L., G. Bidoglio, B. Marcandalli, and I.R. Bellobono. "Surface Interactions of Actinides with Alumina Colloids." Radiochimica Acta. Vols. 44 and 45. pp. 73-75. 1988.

Np(V) sorption - Digitized
No FITEQL Runs

5/31/95 D.R.Lmm

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 1: Am(III), Th(IV) and Np(V) uptake on 10 ppm...) is from the following reference:

Righetto, L., G. Bidoglio, B. Marcandalli, and I.R. Bellobono. "Surface Interactions of Actinides with Alumina Colloids." Radiochimica Acta. Vols. 44 and 45. pp. 73-75. 1988.

Righetto, L., G. Bidoglio, B. Marcandalli, and I.R. Bellobono. 1988. Surface interactions of actinides with alumina colloids. *Radiochimica Acta* 44/45:73-75.

Righetto et. al. (1988)	**Th(IV) -γAl_2O_3**	
Figure 1(a)		
Asp=130 m^2/g	1E-11 M	
No CO_2		
pH	%sorbed	mol sorbed
0.1 M $NaClO_4$	**M/V = 0.01 g/L**	
1(a)		
.99	9.29	9.2903E-13
1.29	7.64	7.6385E-13
1.54	17.09	1.7088E-12
1.77	8.52	8.5183E-13
2.09	29.87	2.9874E-12
2.31	47.67	4.7673E-12
2.59	46.89	4.6888E-12
2.85	76.55	7.6545E-12
3.10	63.24	6.324E-12
3.62	90.84	9.0841E-12

Digitized Data

5/31/95 D.R.Lmm


```
Thorium on gam-Al2O3 2.3s\nm2
                0
                1
                0
                0
                1
               90
                5          1          3          1
00001   -5.30   4.99E-6   XOH
00160   -1.0    0.00E00   PSI0
00051   -11.0   1.0E-11   Th+4
00052    0.0    0.00E00   Thads
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   ClO4-

00050    0.00   050  1
00051    0.00   051  1
05101   -4.55   051  1 050 -1
05102   -8.21   051  1 050 -2
05103  -13.02   051  1 050 -3
05104  -17.22   051  1 050 -4
05105   -5.80   051  2 050 -2
05106  -20.88   051  4 050 -8
05107  -37.69   051  6 050-15
00100  -13.78   050 -1
01050    6.74   001  1 160  1 050  1
01100   -8.94   001  1 160 -1 050 -1
00001    0.00   001  1
05201   14.00   001  1 160  3 050 -1 051  1 052  1

00002  130.0  0.010
0.1    1.0
          1
       5201
         10          1          1          0
         52
 9.2903E-13
 7.6385E-13
 1.7088E-12
 8.5183E-13
 2.9874E-12
 4.7673E-12
 4.6888E-12
 7.6545E-12
 6.3240E-12
 9.0841E-12
         50
-0.994
-1.294
-1.543
-1.771
-2.085
-2.314
-2.593
-2.847
-3.100
-3.617
          1          0
         52       0.10   8.0E-15
```

DLM
No CO_2
$XOH^0 + Th^{4+} = XO\text{-}Th^{3+} + H^+$

```
Thorium on gam-Al2O3 2.3s\nm2
                0
                1
                0
                0
                1
               90
                5          1          3          1
00001   -5.30   4.99E-6   XOH
00160   -1.0    0.00E00   PSI0
00051   -11.0   1.0E-11   Th+4
00052    0.0    0.00E00   Thads
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   ClO4-

00050    0.00   050  1
00051    0.00   051  1
05101   -4.55   051  1 050 -1
05102   -8.21   051  1 050 -2
05103  -13.02   051  1 050 -3
05104  -17.22   051  1 050 -4
05105   -5.80   051  2 050 -2
05106  -20.88   051  4 050 -8
05107  -37.69   051  6 050-15
00100  -13.78   050 -1
01050    6.92   001  1 160  1 050  1
01100   -9.00   001  1 160 -1 050 -1
00001    0.00   001  1
05201   14.00   001  1 160  3 050 -1 051  1 052  1

00001  130.0  0.010      1.0
          0          0
          1
       5201
         10          1          1          0
         52
 9.2903E-13
 7.6385E-13
 1.7088E-12
 8.5183E-13
 2.9874E-12
 4.7673E-12
 4.6888E-12
 7.6545E-12
 6.3240E-12
 9.0841E-12
         50
-0.994
-1.294
-1.543
-1.771
-2.085
-2.314
-2.593
-2.847
-3.100
-3.617
          1          0
         52       0.10   8.0E-15
10%error
```

CCM
No CO_2
$XOH^0 + Th^{4+} = XO\text{-}Th^{3+} + H^+$

Example FITEQL Input Files

```
Thorium on gam-Al2O3 2.3s\nm2
                0
                1
                0
                0
                1
               90
                5          1          3          1
00001   -5.30   4.99E-6   XOH
00160   -1.0    0.00E00   PSI0
00161   -0.5    0.00E00   PSIB
00162   -0.1    0.00E00   PSID
00051   -11.0   1.0E-11   Th+4
00052    0.0    0.00E00   Thads
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   ClO4-

00050    0.00   050  1
00051    0.00   051  1
05101   -4.55   051  1 050 -1
05102   -8.21   051  1 050 -2
05103  -13.02   051  1 050 -3
05104  -17.22   051  1 050 -4
05105   -5.80   051  2 050 -2
05106  -20.88   051  4 050 -8
05107  -37.69   051  6 050-15
00100  -13.78   050 -1
01050    6.29   001  1 160  1 050  1
01100  -10.29   001  1 160 -1 050 -1
01103   -7.95   001  1 160 -1 161  1 050 -1 003  1
01055    8.06   001  1 160  1 161 -1 050  1 005  1
00001    0.00   001  1
05201    8.00   001  1 160 -1 161  4 050 -1 051  1 052  1

00004  130.0  0.010  0.8    0.2
0.1    1.0
          1
       5201
         10          1          1          0
         52
 9.2903E-13
 7.6385E-13
 1.7088E-12
 8.5183E-13
 2.9874E-12
 4.7673E-12
 4.6888E-12
 7.6545E-12
 6.3240E-12
 9.0841E-12
         50
-0.994
-1.294
-1.543
-1.771
-2.085
-2.314
-2.593
-2.847
-3.100
-3.617
          1          0
         52       0.10   8.0E-15
```

TLM
$XOH^0 + Th^{4+} = XO\text{-}Th^{3+} + H^+$
No CO_2

```
Thorium on gam-Al2O3 2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000091
00000092
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000139
00000140
00000145
00000147
00000149
00000150
xoth+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000380
00000400
00000420
00000421
00000422
00000423
00000424
00000425
00000426
00000427
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000741
00000880
10%error
```

5/31/95
D.R.Turner

Table B-15. Thorium (IV)-γ-Al_2O_3 Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: γ-Al_2O_3
A_{SA}: 130 m^2/g
Data Source: Righetto et al. (1988)
Concentration: [Th(IV)] = 1E-11 M

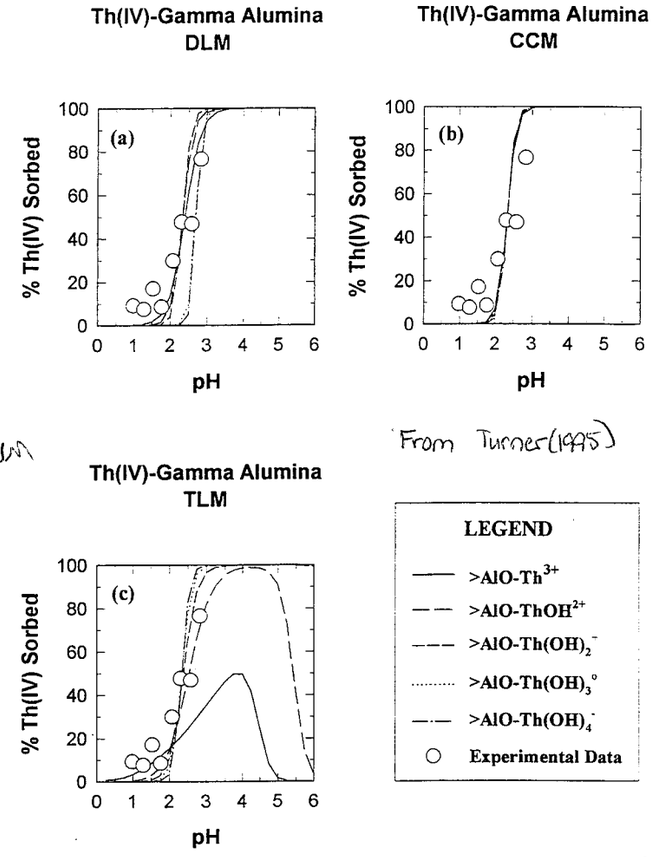
Rel Error (pH): (a)
Abs Error (pH): (a)
Rel Error (radionuclide): 0.10
Abs Error (radionuclide): 8.0E-15

Ionic Strength (electrolyte): 0.1 M $NaClO_4$
N_S = 2.31 sites/nm^2
M/V = 0.01 g/L

No CO_2	DLM			CCM			TLM		
	$Log K_+$ = 6.85 $Log K_-$ = -9.05			$Log K_+$ = 6.92 $Log K_-$ = -9.00			$Log K_+$ = 6.40 $Log K_-$ = -10.40 $Log K_{Cat}$ = -7.95 $Log K_{An}$ = 8.28		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-Th^{3+}	14.30	32.4	.0356	18.29	50.2	.0519	2.08	19.6	.0201
XO-$ThOH^{2+}$	9.51	46.1	.0470	11.62	52.3	.0550	-0.69	20.8	.0286
XO-$Th(OH)_2^+$	4.61	54.5	.0588	4.94	54.1	.0580	-3.57	37.6	.0395
XOH-$Th(OH)_2^{2+}$	9.51	46.1	.0470	11.62	52.3	.0550	4.13	35.5	.0379
XO-$Th(OH)_3^0$	-2.10	61.6	.0816	-1.74	55.7	.0610	-6.52	49.0	.0506
XOH-$Th(OH)_3^+$	4.61	54.5	.0588	4.94	54.1	.0580	1.19	47.7	.0490
XO-$Th(OH)_4^-$	-7.45	62.7	.0823	-8.42	57.1	.0641	-9.57	56.1	.0618
XOH-$Th(OH)_4^0$	-2.10	61.6	.0816	-1.74	55.7	.0610	-1.84	55.3	.0602
XOH$_2$-$Th(OH)_4^+$	4.61	54.5	.0588	4.94	54.1	.0580	5.88	54.5	.0586

FITEQL Results

MINTEQA2 w/ CNWRA radionuclide database



From Turner (1995)

Figure 4-15. Th(IV) sorption on γ-Al_2O_3. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Th(IV)_T = 1 \times 10^{-11}$ M, 0.1 M $NaClO_4$, M/V=0.01 g/L. Model parameters from Tables 3-1 and B-15. Data from Righetto et al. (1988).

Fig. 1 [illegible]

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 1: Am(III), Th(IV) and Np(V) uptake on 10 ppm...) is from the following reference:

Righetto, L., G. Bidoglio, B. Marcandalli, and I.R. Bellobono. "Surface Interactions of Actinides with Alumina Colloids." Radiochimica Acta. Vols. 44 and 45. pp. 73-75. 1988.

6/1/95
D.R.Turner

6/1/95
D.R. Jenny

Righetto. L., G. Bidoglio, B. Marcandalli, and I.R. Bellobono. 1988. Surface interactions of actinides with alumina colloids. *Radiochimica Acta* 44/45:73-75.

Righetto et. al. (1988)	**Am(III) -γAl_2O_3**	
Figures 1(b), 2(a,b)		
Asp=130 m^2/g	5E-10 M	
No CO_2		
pH	%sorbed	mol sorbed
0.1 M $NaClO_4$	**M/V = 0.01 g/L**	
1(b)		
4.54	1.23	6.1552E-12
5.20	11.21	5.6046E-11
5.56	30.07	1.5033E-10
5.90	54.37	2.7186E-10
6.16	74.00	3.7001E-10
6.82	96.30	4.8149E-10
7.09	98.36	4.9182E-10
pH	%sorbed	mol sorbed
0.01 M $NaClO_4$	**M/V = 0.2 g/L**	
2(a)		
3.72	2.97	1.4835E-11
4.22	6.40	3.1995E-11
4.55	1.64	8.2092E-12
4.64	2.88	1.4402E-11
4.75	3.42	1.7095E-11
4.81	32.98	1.6490E-10
4.91	48.48	2.4238E-10
5.05	63.66	3.1830E-10
5.35	77.28	3.8640E-10
5.75	92.02	4.6011E-10
6.17	97.83	4.8914E-10
6.60	97.11	4.8554E-10
6.82	97.87	4.8936E-10
7.28	100	5.0000E-10
7.49	100	5.0000E-10
7.67	100	5.0000E-10
7.92	100	5.0000E-10
8.12	100	5.0000E-10
8.39	100	5.0000E-10
8.60	100	5.0000E-10
pH	%sorbed	mol sorbed
0.1 M $NaClO_4$	**M/V = 0.2 g/L**	
2(b)		
3.47	1.00	4.9923E-12
3.86	5.21	2.6065E-11
4.74	7.15	3.5744E-11
4.83	8.04	4.0188E-11
5.15	20.22	1.0110E-10
5.48	60.88	3.0439E-10
6.17	93.01	4.6506E-10
6.34	95.92	4.7958E-10
6.76	99.47	4.9734E-10
7.01	100	5.0330E-10
7.10	99.61	4.9803E-10
7.23	100	5.0000E-10

D.R. Jenny

Righetto et al. (1988) Digitized Data

6/1/95
D.R. Jenny

CCM
No CO_2
$XOH^0 + Am^{3+} = XO{\cdot}Am^{2+} + H^+$

```
90
 3          1          3          1
00001  -5.30  4.99E-6   XOH
00160  -2.0   0.00E00   PSI0
00031  -9.3   5.0E-10   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -7.03  031  1 050 -1
03101  -16.65  031  1 050 -2
03102  -24.45  031  1 050 -3
00100  -13.78  050 -1
01050    6.92  001  1 160  1 050  1
01100   -9.00  001  1 160 -1 050 -1
00001    0.00  001  1
03201    3.19  001  1 160  2 050 -1 031  1 032  1

00001   130.0 0.010      1.0
   0        0
       1
    3201
       7          1          1          0
      32
6.1552E-12
5.6046E-11
1.5033E-10
2.7186E-10
3.7001E-10
4.8149E-10
4.9182E-10
      50
-4.54
-5.20
-5.56
-5.90
-6.16
-6.82
-7.09
       1          0
      32       0.10    5.0E-14
```

```
Americum
   on
ga-Al2O3
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000126
00000139
00000140
00000145
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000330
00000340
00000350
00000560
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000880
10%error
```

D.R. Jenny

DLM
No CO_2
$XOH^0 + Am^{3+} = XO{\cdot}Am^{2+} + H^+$

```
0
90
 3          1          3          1
00001  -5.30  4.99E-6   XOH
00160  -2.0   0.00E00   PSI0
00031  -9.3   5.0E-10   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -7.03  031  1 050 -1
03101  -16.65  031  1 050 -2
03102  -24.45  031  1 050 -3
00100  -13.78  050 -1
01050    6.74  001  1 160  1 050  1
01100   -8.94  001  1 160 -1 050 -1
00001    0.00  001  1
03201    3.02  001  1 160  2 050 -1 031  1 032  1

00002   130.0 0.010
0.1      1.0
       1
    3201
       7          1          1          0
      32
6.1552E-12
5.6046E-11
1.5033E-10
2.7186E-10
3.7001E-10
4.8149E-10
4.9182E-10
      50
-4.54
-5.20
-5.56
-5.90
-6.16
-6.82
-7.09
       1          0
      32       0.10    5.0E-14
```

```
Americum
   on
ga-Al2O3
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000126
00000139
00000140
00000145
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000330
00000340
00000350
00000560
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000880
10%error
```

D.R. Jenny

TLM
No CO_2
$XOH^0 + Am^{3+} = XO{\cdot}Am^{2+} + H^+$

```
90
 5          1          3          1
00001  -5.30  4.99E-6   XOH
00160  -2.0   0.00E00   PSI0
00161  -1.0   0.00E00   PSIB
00162  -0.2   0.00E00   PSID
00031  -9.3   5.0E-10   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -7.03  031  1 050 -1
03101  -16.65  031  1 050 -2
03102  -24.45  031  1 050 -3
00100  -13.78  050 -1
01050    6.29  001  1 160  1 050  1
01100  -10.29  001  1 160 -1 050 -1
01103   -7.95  001  1 160 -1 161  1 050 -1 003  1
01055    6.06  001  1 160  1 161 -1 050  1 005  1
00001    0.00  001  1
03201   -4.22  001  1 160 -1 161  3 050 -1 031  1 032  1

00004   130.0 0.010  0.8    0.2
0.1      1.0
       1
    3201
       7          1          1          0
      32
6.1552E-12
5.6046E-11
1.5033E-10
2.7186E-10
3.7001E-10
4.8149E-10
4.9182E-10
      50
-4.54
-5.20
-5.56
-5.90
-6.16
-6.82
-7.09
       1          0
      32       0.10    5.0E-14
```

```
Americum
   on
ga-Al2O3
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000126
00000139
00000140
00000145
00000147
00000149
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000330
00000340
00000350
00000560
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000880
10%error
```

D.R. Jenny

Example FITEQL input files.

```
     0
     1
     0
     0
     1
    90
     3         1         3         1
00001  -4.00  9.97E-5   XOH
00160  -2.0   0.00E00   PSI0
00031  -9.3   5.0E-10   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -2.0   0.00E00   NA+
00005  -2.0   0.00E00   C1O4-

00050    0.00  050  1
00031    0.00  031  1
03100   -6.76  031  1 050 -1
03101  -16.24  031  1 050 -2
03102  -24.04  031  1 050 -3
00100  -13.90  050 -1
01050    6.98  001  1 160  1 050  1
01100   -9.06  001  1 160 -1 050 -1
00001    0.00  001  1
03201    3.00  001  1 160  2 050 -1 031  1 032  1

00001   130.0 0.200     1.0
    0      0
      1
   3201
     20         1         1         0
     32
1.4835E-11
3.1995E-11
8.2092E-12
1.4402E-11
1.7095E-11
1.6490E-10
2.4238E-10
3.1830E-10
3.8640E-10
4.6011E-10
4.8914E-10
4.8554E-10
4.8936E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
     50
-3.72
-4.22
-4.55
-4.64
-4.75
-4.81
-4.91
-5.05
-5.35
-5.75
-6.17
-6.60
-6.82
-7.28
-7.49
-7.67
-7.92
-8.12
-8.39
-8.60
     1        0
    32     0.10   5.0E-14
```

CCM
No CO_2
$XOH^0 + Am^{3+} = XOAm^{2+} + H^+$

6/1/95

Example FITEQL Input

```
Americum
  on
ga-Al203
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000126
00000139
00000140
00000145
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000330
00000340
00000350
00000360
00000370
00000380
00000390
00000400
00000410
00000420
00000420
00000420
00000420
00000420
00000420
00000420
00000560
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000680
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000680
00000650
00000660
00000670
00000680
00000880
10%error
```

```
     0
     1
    90
     3         1         3         1
00001  -4.00  9.97E-5   XOH
00160  -2.0   0.00E00   PSI0
00031  -9.3   5.0E-10   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -2.0   0.00E00   NA+
00005  -2.0   0.00E00   C1O4-

00050    0.00  050  1
00031    0.00  031  1
03100   -6.76  031  1 050 -1
03101  -16.24  031  1 050 -2
03102  -24.04  031  1 050 -3
00100  -13.90  050 -1
01050    6.80  001  1 160  1 050  1
01100   -9.00  001  1 160 -1 050 -1
00001    0.00  001  1
03201   -3.33  001  1 160  2 050 -1 031  1 032  1

00002   130.0 0.200
0.01   1.0
      1
   3201
     20         1         1         0
     32
1.4835E-11
3.1995E-11
8.2092E-12
1.4402E-11
1.7095E-11
1.6490E-10
2.4238E-10
3.1830E-10
3.8640E-10
4.6011E-10
4.8914E-10
4.8554E-10
4.8936E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
     50
-3.72
-4.22
-4.55
-4.64
-4.75
-4.81
-4.91
-5.05
-5.35
-5.75
-6.17
-6.60
-6.82
-7.28
-7.49
-7.67
-7.92
-8.12
-8.39
-8.60
     1        0
    32     0.10   5.0E-14
```

DLM
No CO_2
$XOH^0 + Am^{3+} = XOAm^{2+} + H^+$


```
Americum
  on
ga-Al203
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000139
00000140
00000145
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000330
00000340
00000350
00000360
00000370
00000380
00000390
00000400
00000410
00000420
00000420
00000420
00000420
00000420
00000420
00000420
00000560
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000680
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000680
00000650
00000660
00000670
00000680
00000880
10%error
```


6/1/95

```
     0
     1
    90
     5         1         3         1
00001  -4.00  9.97E-5   XOH
00160  -2.0   0.00E00   PSI0
00161  -1.0   0.00E00   PSIB
00162  -0.2   0.00E00   PSID
00031  -9.3   5.0E-10   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -2.0   0.00E00   NA+
00005  -2.0   0.00E00   C1O4-

00050    0.00  050  1
00031    0.00  031  1
03100   -6.76  031  1 050 -1
03101  -16.24  031  1 050 -2
03102  -24.04  031  1 050 -3
00100  -13.90  050 -1
01050    6.35  001  1 160  1 050  1
01100  -10.35  001  1 160 -1 050 -1
01103   -7.95  001  1 160 -1 161  1 050 -1 003  1
01055    8.18  001  1 160  1 161 -1 050  1 005  1
00001    0.00  001  1
03201   -4.55  001  1 160 -1 161  3 050 -1 031  1 032  1

00004   130.0 0.200  0.8    0.2
0.01   1.0
      1
   3201
     20         1         1         0
     32
1.4835E-11
3.1995E-11
8.2092E-12
1.4402E-11
1.7095E-11
1.6490E-10
2.4238E-10
3.1830E-10
3.8640E-10
4.6011E-10
4.8914E-10
4.8554E-10
4.8936E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
5.0000E-10
     50
-3.72
-4.22
-4.55
-4.64
-4.75
-4.81
-4.91
-5.05
-5.35
-5.75
-6.17
-6.60
-6.82
-7.28
-7.49
-7.67
-7.92
-8.12
-8.39
-8.60
     1        0
    32     0.10   5.0E-14
```

TLM
No CO_2
$XOH^0 + Am^{3+} = XOAm^{2+} + H^+$


```
Americum
  on
ga-Al203
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000126
00000139
00000140
00000145
00000147
00000149
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000330
00000340
00000350
00000360
00000370
00000380
00000390
00000400
00000410
00000420
00000420
00000420
00000420
00000420
00000420
00000420
00000560
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000680
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000680
00000650
00000660
00000670
00000680
00000880
10%error
```


Table B-1. Americium (III)-γ-Al_2O_3 Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: γ-Al_2O_3 A_{SP}: 130 m^2/g Data Source: Righetto et al. (1988) Concentration: [Am(III)] = 5E-10 M				Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 5.0E-14			Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 0.01 g/L		
No CO_2	DLM			CCM			TLM		
	Log K_+ = 6.85 Log K_- = -9.05			Log K_+ = 6.92 Log K_- = -9.00			Log K_+ = 6.40 Log K_- = -10.40 Log K_{Cat} = -7.95 Log K_{An} = 8.28		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-Am^{2+}	3.65	14.6	.0399	4.02	20.7	.0449	-1.50	75.7	.0299
XO-$AmOH^+$	-3.59	22.5	.0464	-3.41	24.2	.0481	-6.81	1.7	.0267
XO-$Am(OH)_2^o$	-10.84	28.0	.0519	-10.83	27.2	.0510	-12.71	13.5	.0391
XOH-$Am(OH)_2^+$	-3.59	22.5	.0464	-3.41	24.2	.0481	-4.65	11.4	.0376
XO-$Am(OH)_3^-$	-18.09	32.0	.0561	-18.26	29.8	.0535	-18.91	28.1	.0518
XOH-$Am(OH)_3^o$	-10.84	28.0	.0519	-10.83	27.2	.0510	-10.83	27.0	.0507
XOH_2-$Am(OH)_3^+$	-3.59	22.5	.0464	-3.41	24.2	.0481	-2.76	25.8	.0496

(a)No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

6/1/95
DRLnnm

Table BXX. Americium (III)-γ-Al_2O_3 Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: γ-Al_2O_3 A_{SP}: 130 m^2/g Data Source: Righetto et al. (1988) Concentration: [Am(III)] = 5E-10 M	Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 5.0E-14	Ionic Strength (electrolyte): 0.01 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 0.2 g/L

No CO_2	DLM			CCM (I = 0.01)			TLM		
	Log K_+ = 6.85 Log K_- = -9.05			Log K_+ = 6.98 Log K_- = -9.06			Log K_1 = 6.40 Log K_2 = -10.40 Log K_{Cat} = -7.95 Log K_{An} = 8.28		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-Am^{2+}	3.38	19.7	.0222	3.39	19.1	.0225	-1.27	36.5	.0181
XO-$AmOH^+$	-3.86	18.9	.0226	-3.82	18.7	.0228	-7.19	23.8	.0212
XO-$Am(OH)_2^\circ$	-11106	18.5	.0230	-11.02	18.5	.0230	-13.10	19.9	.0221
XOH-$Am(OH)_2^+$	-3.86	18.9	.0226	-3.82	18.7	.0228	-5.19	20.2	.0220
XO-$Am(OH)_3^-$	-18341	18.3	.0235	-18.23	18.3	.0233	-19.03	18.4	.0231
XOH-$Am(OH)_3^\circ$	-11.10	18.5	.0230	-11.02	18.5	.0230	-11.12	18.5	.0230
XOH_2-$Am(OH)_3^+$	-3.86	18.9	.0226	-3.83	18.7	.0228	-3.21	18.6	.0229

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

Table BXX. Americium (III)-γ-Al_2O_3 Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: γ-Al_2O_3 A_{SP}: 130 m^2/g Data Source: Righetto et al. (1988) Concentration: [Am(III)] = 5E-10 M	Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 5.0E-14	Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 0.2 g/L

No CO_2	DLM			CCM (I = 0.1)			TLM		
	Log K_+ = 6.85 Log K_- = -9.05			Log K_+ = 6.92 Log K_- = -9.00			Log K_1 = 6.40 Log K_2 = -10.40 Log K_{Cat} = -7.95 Log K_{An} = 8.28		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-Am^{2+}	3.09	19.0	.0310	3.62	21.8	.0339	-2.34	49.3	.0192
XO-$AmOH^+$	-3.94	22.6	.0348	-3.70	23.5	.0359	-7.65	13.5	.0250
XO-$Am(OH)_2^\circ$	-11.00	26.2	.0391	-11.02	25.3	.0380	-13.30	18.8	.0308
XOH-$Am(OH)_2^+$	-3.94	22.6	.0348	-3.70	23.5	.0359	-5.28	18.2	.0301
XO-$Am(OH)_3^-$	-18.08	29.2	.0433	-18.35	26.9	.0400	-19.06	25.8	.0386
XOH-$Am(OH)_3^\circ$	-11.00	26.2	.0391	-11.02	25.3	.0380	-11.03	25.1	.0378
XOH_2-$Am(OH)_3^+$	-3.94	22.6	.0348	-3.70	23.5	.0359	-3.21	24.4	.0369

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

FITEQL Results

6/1/95
DRLnnm

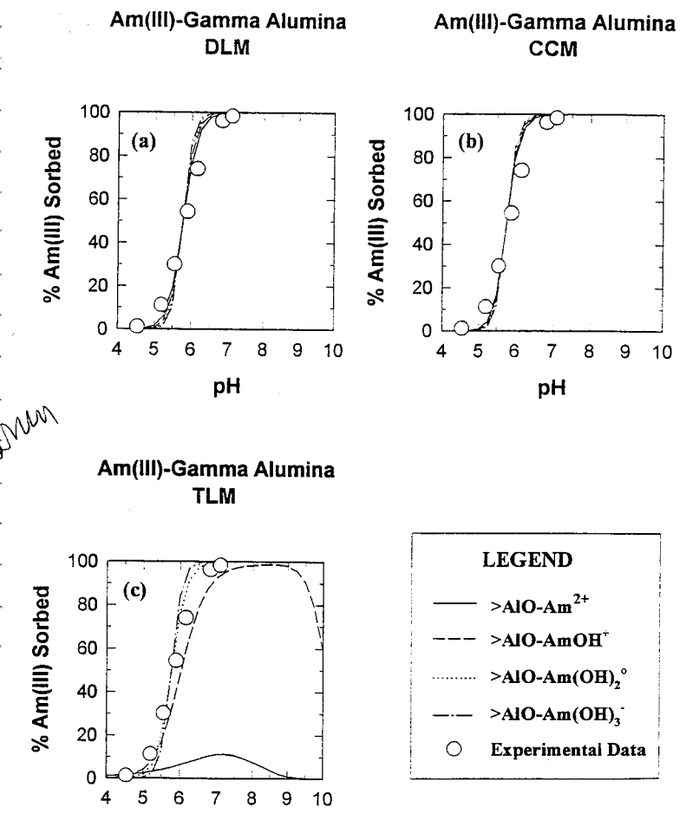


Figure 4-1. Am(III) sorption on γ-Al_2O_3. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Am(III)_T = 5\times10^{-10}$ M, 0.1 M $NaClO_4$, M/V=0.01 g/L. Model parameters from Tables 3-1 and B-1. Data from Righetto et al. (1988).

FITEQL Model Results

6/1/95

```
      0
      1
      0
      0
      1
     90
      5         1         3         1
00001  -4.00  9.97E-5   XOH
00160  -2.0   0.00E00   PSI0
00161  -1.0   0.00E00   PSIB
00162  -0.2   0.00E00   PSID
00031  -9.3   5.0E-10   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -7.03  031  1 050 -1
03101  -16.65  031  1 050 -2
03102  -24.45  031  1 050 -3
00100  -13.78  050 -1
01050    6.29  001  1 160  1 050  1
01100  -10.29  001  1 160 -1 050 -1
01103   -7.95  001  1 160 -1 161  1 050 -1 003  1
01055    8.06  001  1 160  1 161 -1 050  1 005  1
00001    0.00  001  1
03201   -5.23  001  1 160 -1 161  3 050 -1 031  1 032  1

00004   130.0 0.200  0.8    0.2
0.1     1.0
          1
       3201
         12         1         1         0
         32
4.9923E-12
2.6065E-11
3.5744E-11
4.0188E-11
1.0110E-10
3.0439E-10
4.6506E-10
4.7958E-10
4.9734E-10
5.0330E-10
4.9803E-10
5.0000E-10
         50
-3.47
-3.86
-4.74
-4.83
-5.15
-5.48
-6.17
-6.34
-6.76
-7.01
-7.10
-7.23
          1        0
         32     0.10  5.0E-14
```

TLM
No CO_2
$XOH^0 + Am^{3+} = XO{\cdot}Am^{2+} + H^+$

```
Americum           0
   on              1
ga-Al2O3           0
2.3s\nm2           0
00000050           1
00000060          90
00000070           3        1        3        1
00000080  00001  -4.00  9.97E-5   XOH
00000090  00160  -2.0   0.00E00   PSI0
00000092  00031  -9.3   5.0E-10   Am+3
00000094  00032   0.0   0.00E00   Am(ads)
00000098  00050   0.0   0.00E00   H+
00000100  00003  -1.0   0.00E00   NA+
00000102  00005  -1.0   0.00E00   ClO4-
00000104
00000106  00050     0.00  050  1
00000110  00031     0.00  031  1
00000120  03100    -7.03  031  1 050 -1
00000124  03101   -16.65  031  1 050 -2
00000126  03102   -24.45  031  1 050 -3
00000126  00100   -13.78  050 -1
00000126  01050     6.74  001  1 160  1 050  1
00000139  01100    -8.94  001  1 160 -1 050 -1
00000140  00001     0.00  001  1
00000145  03201     2.46  001  1 160  2 050 -1 031  1 032  1
00000147
00000149
00000150  00002   130.0 0.200
xoam      0.1     1.0
00000174           1
00000175        3201
00000180          12        1        1        0
00000185          32
00000190  4.9923E-12
00000195  2.6065E-11
00000230  3.5744E-11
00000240  4.0188E-11
00000260  1.0110E-10
00000280  3.0439E-10
00000300  4.6506E-10
00000320  4.7958E-10
00000330  4.9734E-10
00000340  5.0330E-10
00000350  4.9803E-10
00000360  5.0000E-10
00000370          50
00000380  -3.47
00000390  -3.86
00000400  -4.74
00000560  -4.83
00000580  -5.15
00000600  -5.48
00000620  -6.17
00000640  -6.34
00000650  -6.76
00000660  -7.01
00000670  -7.10
00000680  -7.23
00000580           1         0
00000600          32      0.10   5.0E-14
00000620
00000640
00000880
10%error
```

DLM
No CO_2
$XOH^0 + Am^{3+} = XO{\cdot}Am^{2+} + H^+$

```
Americum
   on
ga-Al2O3
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000126
00000139
00000140
00000145
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000330
00000340
00000350
00000360
00000370
00000380
00000390
00000400
00000560
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000680
00000580
00000600
00000620
00000640
00000880
10%error
```

FITEQL Example
Input Files
Righetto et al. (1988)

Results shown on
Pg. 156, this volume

```
      0
      1
      0
      0
      1
     90
      3         1         3         1
00001  -4.00  9.97E-5   XOH
00160  -2.0   0.00E00   PSI0
00031  -9.3   5.0E-10   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -7.03  031  1 050 -1
03101  -16.65  031  1 050 -2
03102  -24.45  031  1 050 -3
00100  -13.78  050 -1
01050    6.92  001  1 160  1 050  1
01100   -9.00  001  1 160 -1 050 -1
00001    0.00  001  1
03201    2.84  001  1 160  2 050 -1 031  1 032  1

00001   130.0 0.200        1.0
     0       0
          1
       3201
         12         1         1         0
         32
4.9923E-12
2.6065E-11
3.5744E-11
4.0188E-11
1.0110E-10
3.0439E-10
4.6506E-10
4.7958E-10
4.9734E-10
5.0330E-10
4.9803E-10
5.0000E-10
         50
-3.47
-3.86
-4.74
-4.83
-5.15
-5.48
-6.17
-6.34
-6.76
-7.01
-7.10
-7.23
          1        0
         32     0.10  5.0E-14
```

CCM
No CO_2
$XOH^0 + Am^{3+} = XO{\cdot}Am^{2+} + H^+$

```
Americum
   on
ga-Al2O3
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000126
00000139
00000140
00000145
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000330
00000340
00000350
00000360
00000370
00000380
00000390
00000400
00000560
00000580
00000600
00000620
00000640
00000650
00000660
00000670
00000680
00000580
00000600
00000620
00000640
00000880
10%error
```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Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 1: Americium sorption onto a alumina...) is from the following reference:

Moulin, V., D. Stammose, and G. Ouzounian. "Actinide sorption at Oxide-Water Interfaces: Application to a Alumina and Amorphous Silica." Applied Geochemistry Supplemental Issue. Vol. 1. pp. 163-166. 1992.

Moulin, V., D. Stammose, and G. Ouzounian. 1992. Actinide sorption at oxide-water interfaces: Application to α alumina and amorphous silica. *Applied Geochemistry Supplemental Issue* 1:163-166.

Moulin et al. (1992)	Am(III)-Alpha Al2O3			
Figure 1 (page 164)				
Asp=0.070 m2/g	Atm CO2			
Am(III)=1E-8 M	M/V=10 g/L			
0.1 M NaClO4				
pH	Log Kd (mL/g)	Kd (mL/g)	% sorbed	mol sorbed
3.13062	0.81637	6.55194	6.149	6.149E-10
4.04264	0.98010	9.55213	8.719	8.719E-10
5.21459	0.97100	9.35406	8.554	8.554E-10
5.99271	1.55997	36.3053	26.64	2.664E-09
6.56467	2.30130	200.124	66.68	6.668E-09
7.74628	4.03411	10817.1	99.08	9.908E-09
8.53062	3.56566	3678.41	97.35	9.735E-09
10.03201	3.01307	1030.55	91.16	9.116E-09
0.01 M NaClO4				
pH	Log Kd (mL/g)	Kd (mL/g)	% sorbed	mol sorbed
3.11945	1.22342	16.7271	14.33	1.433E-09
4.19006	1.19386	15.6264	13.52	1.352E-09
6.25184	2.19897	158.114	61.26	6.126E-09
7.38728	3.21546	1642.33	94.26	9.426E-09
9.19078	3.19499	1566.72	94.00	9.400E-09
8.96205	3.19272	1558.55	93.97	9.397E-09
9.70272	3.09039	1231.37	92.49	9.249E-09

Digitized Data

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Example FITEQL Inputs

```
    1
    0
    0
    1
   90
    4        1        3        1
00001  -5.57  2.69E-6   XOH
00160  -2.0   0.00E00   PSI0
00140  -3.5   3.16E-4   CO2g
00031  -8.0   1.00E-8   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -2.0   0.00E00   NA+
00005  -2.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -6.76  031  1 050 -1
03101  -16.24  031  1 050 -2
03102  -24.04  031  1 050 -3
03300  -10.65  031  1 140  1 050 -2
03301  -24.17  031  1 140  2 050 -4
03302  -40.73  031  1 140  3 050 -6
01401  -18.38  140  1 050 -2
01402   -8.23  140  1 050 -1
01403   -1.98  140  1
01404  -17.29  140  1 003  1 050 -2
01405   -8.58  140  1 003  1 050 -1
00100  -13.90  050 -1
01050    8.18  001  1 160  1 050  1
01100   -9.62  001  1 160 -1 050 -1
00001    0.00  001  1
03201   10.00  001  1 160  2 050 -1 031  1 032  1

00001   0.070 10.00      1.0
   0     0
    1
 3201
    7        1        1        0
   32
1.4330E-09
1.3515E-09
6.1257E-09
9.4261E-09
9.4000E-09
9.3971E-09
9.2489E-09
   50
-3.12
-4.19
-6.25
-7.39
-8.19
-8.96
-9.70
    1        1
   32     0.10    1.0E-11
   50     0.05    0.0E-00
```

I=0.01

CCM
atmospheric CO_2
$XOH^0 + Am^{3+} = XO\cdot Am^{2+} + H^+$

```
Americum
  on
al-Al2O3
2.3s\nm2
    1
    0
    0
    1
   90
    4        1        3        1
00001  -5.57  2.69E-6   XOH
00160  -2.0   0.00E00   PSI0
00140  -3.5   3.16E-4   CO2g
00031  -8.0   1.00E-8   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -7.03  031  1 050 -1
03101  -16.65  031  1 050 -2
03102  -24.45  031  1 050 -3
03300  -11.06  031  1 140  1 050 -2
03301  -24.46  031  1 140  2 050 -4
03302  -40.37  031  1 140  3 050 -6
01401  -18.00  140  1 050 -2
01402   -8.11  140  1 050 -1
01403   -1.98  140  1
01404  -17.17  140  1 003  1 050 -2
01405   -8.58  140  1 003  1 050 -1
00100  -13.78  050 -1
01050    8.12  001  1 160  1 050  1
01100   -9.56  001  1 160 -1 050 -1
00001    0.00  001  1
03201   10.00  001  1 160  2 050 -1 031  1 032  1

00001   0.070 10.00      1.0
   0     0
    1
 3201
    8        1        1        0
   32
6.1491E-10
8.7193E-10
8.5539E-10
2.6635E-09
6.6680E-09
9.9084E-09
9.7353E-09
9.1155E-09
   50
-3.13
-4.04
-5.21
-5.99
-6.56
-7.75
-8.53
-10.03
    1        1
   32     0.10    1.0E-11
   50     0.05    0.0E-00
```

I=0.1

CCM
atmospheric CO_2
$XOH^0 + Am^{3+} = XO\cdot Am^{2+} + H^+$

```
    0
    1
    0
    0
    1
   90
    4        1        3        1
00001  -5.57  2.69E-6   XOH
00160  -2.0   0.00E00   PSI0
00140  -3.5   3.16E-4   CO2g
00031  -8.0   1.00E-8   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -2.0   0.00E00   NA+
00005  -2.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -6.76  031  1 050 -1
03101  -16.24  031  1 050 -2
03102  -24.04  031  1 050 -3
03300  -10.65  031  1 140  1 050 -2
03301  -24.17  031  1 140  2 050 -4
03302  -40.73  031  1 140  3 050 -6
01401  -18.38  140  1 050 -2
01402   -8.23  140  1 050 -1
01403   -1.98  140  1
01404  -17.29  140  1 003  1 050 -2
01405   -8.58  140  1 003  1 050 -1
00100  -13.90  050 -1
01050    8.28  001  1 160  1 050  1
01100   -9.68  001  1 160 -1 050 -1
00001    0.00  001  1
03201   10.00  001  1 160  2 050 -1 031  1 032  1

00002   0.070 10.00
0.01    1.0
    1
 3201
    7        1        1        0
   32
1.4330E-09
1.3515E-09
6.1257E-09
9.4261E-09
9.4000E-09
9.3971E-09
9.2489E-09
   50
-3.12
-4.19
-6.25
-7.39
-8.19
-8.96
-9.70
    1        1
   32     0.10    1.0E-11
   50     0.05    0.0E-00
```

I=0.01

DLM
atmospheric CO_2
$XOH^0 + Am^{3+} = XOAm^{2+} + H^+$

```
Americum
  on
al-Al2O3
2.3s\nm2
    0
    1
    0
    0
    1
   90
    6        1        3        1
00001  -5.57  2.69E-6   XOH
00160  -2.0   0.00E00   PSI0
00161  -1.0   0.00E00   PSIb
00162  -0.2   0.00E00   PSId
00140  -3.5   3.16E-4   CO2g
00031  -8.0   1.00E-8   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -7.03  031  1 050 -1
03101  -16.65  031  1 050 -2
03102  -24.45  031  1 050 -3
03300  -11.06  031  1 140  1 050 -2
03301  -24.46  031  1 140  2 050 -4
03302  -40.37  031  1 140  3 050 -6
01401  -18.00  140  1 050 -2
01402   -8.11  140  1 050 -1
01403   -1.98  140  1
01404  -17.17  140  1 003  1 050 -2
01405   -8.58  140  1 003  1 050 -1
00100  -13.78  050 -1
01050    6.79  001  1 160  1 050  1
01100  -10.79  001  1 160 -1 050 -1
01055    9.90  001  1 160  1 161 -1 050  1 005  1
01103   -7.73  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
03201   -5.00  001  1 160 -1 161  3 050 -1 031  1 032  1

00004   0.070 10.00  0.80   0.20
0.1     1.0
    1
 3201
    8        1        1        0
   32
6.1491E-10
8.7193E-10
8.5539E-10
2.6635E-09
6.6680E-09
9.9084E-09
9.7353E-09
```

I=0.1

TLM
atmospheric CO_2

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Example FITEQL Input Files:

```
    0
    1
    0
    0
    1
   90
    6        1        3        1
00001  -5.57  2.69E-6   XOH
00160  -2.0   0.00E00   PSI0
00161  -1.0   0.00E00   PSIB
00162  -0.2   0.00E00   PSID
00140  -3.5   3.16E-4   CO2g
00031  -8.0   1.00E-8   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -2.0   0.00E00   NA+
00005  -2.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -6.76  031  1 050 -1
03101  -16.24  031  1 050 -2
03102  -24.04  031  1 050 -3
03300  -10.65  031  1 140  1 050 -2
03301  -24.17  031  1 140  2 050 -4
03302  -40.73  031  1 140  3 050 -6
01401  -18.38  140  1 050 -2
01402   -8.23  140  1 050 -1
01403   -1.98  140  1
01404  -17.29  140  1 003  1 050 -2
01405   -8.58  140  1 003  1 050 -1
00100  -13.90  050 -1
01050    6.85  001  1 160  1 050  1
01100  -10.85  001  1 160 -1 050 -1
01103   -7.73  001  1 160 -1 161  1 050 -1 003  1
01055   10.02  001  1 160  1 161 -1 050  1 005  1
00001    0.00  001  1
03201   -5.39  001  1 160 -1 161  3 050 -1 031  1 032  1

00004   0.070 10.00  0.8    0.2
0.01    1.0
    1
 3201
    7        1        1        0
   32
1.4330E-09
1.3515E-09
6.1257E-09
9.4261E-09
9.4000E-09
9.3971E-09
9.2489E-09
   50
-3.12
-4.19
-6.25
-7.39
-8.19
-8.96
-9.70
    1        1
   32     0.10    1.0E-11
   50     0.05    0.0E-00
```

I=0.01

TLM
atmospheric CO_2
$XOH^0 + Am^{3+} = XOAm^{2+} + H^+$

```
    0
    1
    0
    0
    1
   90
    4        1        3        1
00001  -5.57  2.69E-6   XOH
00160  -2.0   0.00E00   PSI0
00140  -3.5   3.16E-4   CO2g
00031  -8.0   1.00E-8   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00031    0.00  031  1
03100   -7.03  031  1 050 -1
03101  -16.65  031  1 050 -2
03102  -24.45  031  1 050 -3
03300  -11.06  031  1 140  1 050 -2
03301  -24.46  031  1 140  2 050 -4
03302  -40.37  031  1 140  3 050 -6
01401  -18.00  140  1 050 -2
01402   -8.11  140  1 050 -1
01403   -1.98  140  1
01404  -17.17  140  1 003  1 050 -2
01405   -8.58  140  1 003  1 050 -1
00100  -13.78  050 -1
01050    8.22  001  1 160  1 050  1
01100   -9.62  001  1 160 -1 050 -1
00001    0.00  001  1
03201   -1.75  001  1 160  2 050 -1 031  1 032  1

00002   0.070 10.00
0.1     1.0
    1
 3201
    8        1        1        0
   32
6.1491E-10
8.7193E-10
8.5539E-10
2.6635E-09
6.6680E-09
9.9084E-09
9.7353E-09
9.1155E-09
   50
-3.13
-4.04
-5.21
-5.99
-6.56
-7.75
-8.53
-10.03
    1        1
   32     0.10    1.0E-11
   50     0.05    0.0E-00
```

I=0.1

DLM
atmospheric CO_2
$XOH^0 + Am^{3+} = XOAm^{2+} + H^+$

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DRL [signature]

Table B-2. Americium (III)-α-Al_2O_3 Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: α-Al_2O_3 A_{SP}: 0.07 m^2/g Data Source: Moulin et al. (1992) Concentration: [Am(III)] = 1E-8 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-11	Ionic Strength (electrolyte): 0.01 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 10 g/L

$p(CO_2)$ = 1E-3.5 atm	DLM			CCM			TLM		
	Log K_+ = 8.33 Log K_- = -9.73			Log K_+ = 8.18 Log K_- = -9.62			Log K_+ = 6.90 Log K_- = -10.90 Log K_{Cat} = -7.73 Log K_{An} = 10.12		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log 06036 K}$
XO-Am^{2+}	8.54	21.1	.0707	8.91	21.3	.0797	-1.32	65.1	.0378
XO-$AmOH^+$	0.86	21.3	.0823	0.89	21.3	.0831	-6.32	18.9	.0618
XO-$Am(OH)_2^o$	-6.81	21.3	.0949	-7.13	21.3	.0867	-11.07	21.2	.0727
XOH-$Am(OH)_2^+$	0.86	21.3	.0823	0.89	21.3	.0831	-2.49	21.1	.0722
XO-$Am(OH)_3^-$	-14.47	21.3	.1084	-15.10	21.3	.0905	-15.79	21.3	.0883
XOH-$Am(OH)_3^o$	-6.81	21.3	.0949	-7.13	21.3	.0867	-7.24	21.3	.0859
XOH_2-$Am(OH)_3^+$	0.86	21.3	.0823	0.89	21.3	.0831	1.33	21.3	.0850
XO-$AmCO_3^o$	12.88	19.7	.0670	12.55	19.7	.0612	8.62	19.5	.0513
XOH-$AmCO_3^+$	16.48	27.0	.0830	16.28	27.0	.0834	17.19	19.5	.0509
XOH_2-$Am(CO_3)_2^o$	32.56	12.4	.0765	32.23	12.4	.0709	35.92	12.4	.0803
XOH_2-$Am(CO_3)_3^{2-}$	n.c.	n.c.	n.c.	33.05	23.2	.0949	36.86	15.2	.1417

n.c. FITEQL optimization did not converge.

FITEQL Results

Table BXX. Americium (III)-α-Al_2O_3 Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: α-Al_2O_3 A_{SP}: 0.07 m^2/g Data Source: Moulin et al. (1992) Concentration: [Am(III)] = 1E-8 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-11	Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 10 g/L

$p(CO_2)$ = 1E-3.5 atm	DLM			CCM (I = 0.1)			TLM		
	Log K_+ = 8.33 Log K_- = -9.73			Log K_+ = 8.12 Log K_- = -9.56			Log K_+ = 6.90 Log K_- = -10.90 Log K_{Cat} = -7.73 Log K_{An} = 10.12		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log .06036 K}$
XO-Am^{2+}	4.72	32.0	.0683	4.91	33.9	.0785	-2.11	53.6	.0294
XO-$AmOH^+$	-3.55	16.0	.0803	-3.50	34.6	.0826	-7.73	37.8	.0379
XO-$Am(OH)_2^o$	-11.77	35.5	.0908	-11.90	35.1	.0866	-14.07	31.2	.0646
XOH-$Am(OH)_2^+$	-3.55	16.0	.0803	-3.50	34.6	.0826	-5.24	30.5	.0642
XO-$Am(OH)_3^-$	-19.96	36.2	.0999	-20.29	35.5	.0904	-20.32	34.9	.0882
XOH-$Am(OH)_3^o$	-11.77	35.5	.0908	-11.90	35.1	.0866	-11.56	35.0	.0857
XOH_2-$Am(OH)_3^+$	-3.55	16.0	.0803	-3.50	34.6	.0826	-2.76	34.6	.0858
XO-$AmCO_3^o$	8.15	29.0	.0580	8.04	31.5	.0541	5.99	40.1	.0365
XOH-$AmCO_3^+$	16.32	33.0	.0700	16.45	30.8	.0507	14.83	40.1	.0359
XOH_2-$Am(CO_3)_2^o$	28.16	28.0	.0577	28.06	27.7	.0542	30.87	20.7	.0727
XOH_2-$Am(CO_3)_3^{2-}$	31.75	26.5	.0644	31.39	29.2	.0518	38.57	19.1	.1077

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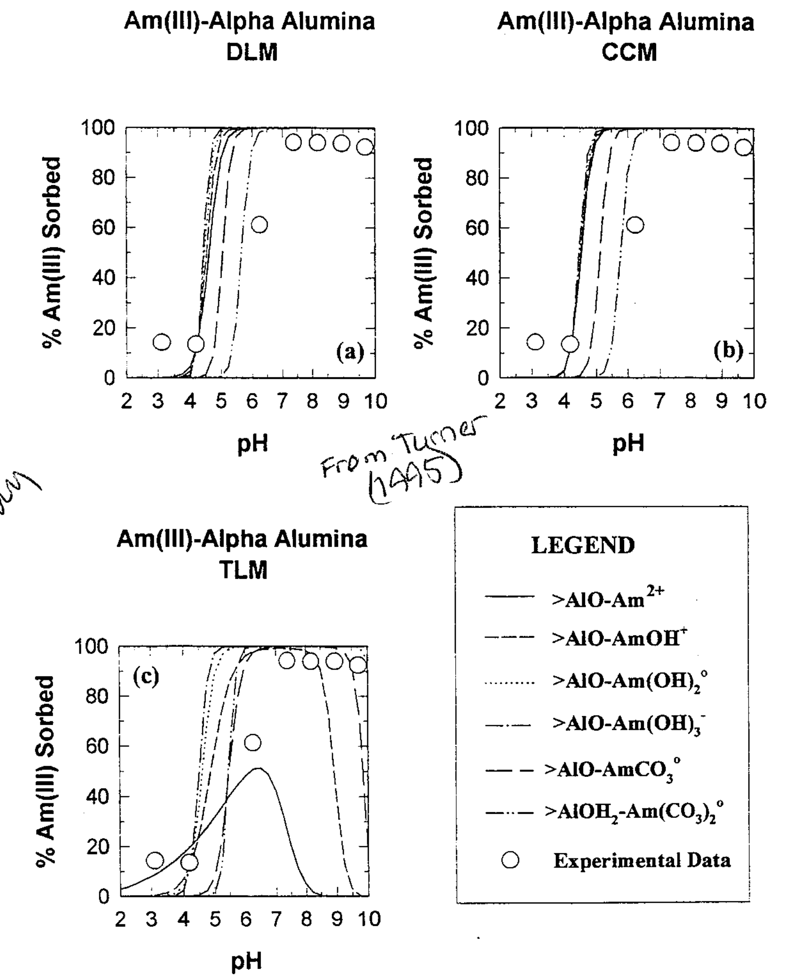
DRL [signature]



From Turner (1995)

Figure 4-2. Am(III) sorption on α-Al_2O_3. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Am(III)_T = 1\times10^{-8}$ M, 00.1 M $NaClO_4$, M/V=10 g/L; $p(CO_2) = 10^{-3.5}$ atm. Model parameters from Tables 3-1 and B-2. Data from Moulin et al. (1992).

4-3

MINTEQA2 results - Calculated using CNWRA radionuclide database.

6/2/95
DRJenne

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 2: Adsorption of thorium on goethite...) is from the following reference:

LaFlamme, B.D. and J.W. Murray. "Solid/Solution Interaction: The Effect of Carbonate Alkalinity on Adsorbed Thorium. Geochimica et Cosmochimica Acta. Vol. 51. pp. 243-250. 1987.

LaFlamme, B.D., and J.W. Murray. 1987. Solid/Solution Interaction: The effect of carbonate alkalinity on adsorbed thorium. *Geochimica et Cosmochimica Acta* 51:243-250.

Digitized Data

LaFlamme and Murray (1987)	Th(IV)-Goethite	
Figure 2b (page 245)		
Asp=50 m2/g	No CO2	Th(IV)=1E-13 M
0.1 M NaNO3	M/V=0.27 m2/L = 0.00522 g/L	
No CO2		
pH	% sorbed	mol sorbed
1.77	0.556	5.56E-16
2.13	9.950	9.95E-15
2.13	23.99	2.40E-14
2.92	58.70	5.87E-14
3.57	58.20	5.82E-14
4.00	59.87	5.99E-14
4.34	87.22	8.72E-14
4.23	87.08	8.71E-14
5.65	88.74	8.87E-14
5.98	88.85	8.89E-14
6.80	90.61	9.06E-14
7.28	88.74	8.87E-14
7.78	88.88	8.89E-14
8.69	87.77	8.78E-14
9.84	88.49	8.85E-14
10.63	90.52	9.05E-14

DRJenne

```
    0
    1
    0
    0
    1
   50
    3        1        3        1
00001 -6.00  9.97E-7   XOH
00160 -1.0   0.00E00   PSIO
00051 -13.0  1.0E-13   Th+4
00052  0.0   0.00E00   Thads
00050  0.0   0.00E00   H+
00003 -1.0   0.00E00   NA+
00005 -1.0   0.00E00   NO3-

00050    0.00  050  1
00051    0.00  051  1
05101   -4.55  051  1 050 -1
05102   -8.21  051  1 050 -2
05103  -13.02  051  1 050 -3
05104  -17.22  051  1 050 -4
05105   -5.80  051  2 050 -2
05106  -20.88  051  4 050 -8
05107  -37.69  051  6 050 -15
00100  -13.78  050 -1
01050    6.47  001  1 160  1 050  1
01100   -9.03  001  1 160 -1 050 -1
00001    0.00  001  1
05201   14.00  001  1 160  3 050 -1 051  1 052  1

00001   50.0  0.00520   1.0
  0      0
    1
 5201
   10        1        1        0
   52
5.56E-16
9.95E-15
2.40E-14
5.87E-14
5.82E-14
5.99E-14
8.72E-14
8.71E-14
8.87E-14
8.89E-14
   50
-1.77
-2.13
-2.13
-2.92
-3.57
-4.00
-4.34
-5.23
-5.65
-5.98
    1     0
   52     0.10    1.0E-18
```

CCM
No CO_2
$XOH^0 + Th^{4+} = XO{\cdot}Th^{3+} + H^+$

```
    0
    1
    0
    0
    1
   50
    3        1        3        1
00001 -6.00  9.97E-7   XOH
00160 -1.0   0.00E00   PSIO
00051 -13.0  1.0E-13   Th+4
00052  0.0   0.00E00   Thads
00050  0.0   0.00E00   H+
00003 -1.0   0.00E00   NA+
00005 -1.0   0.00E00   NO3-

00050    0.00  050  1
00051    0.00  051  1
05101   -4.55  051  1 050 -1
05102   -8.21  051  1 050 -2
05103  -13.02  051  1 050 -3
05104  -17.22  051  1 050 -4
05105   -5.80  051  2 050 -2
05106  -20.88  051  4 050 -8
05107  -37.69  051  6 050 -15
00100  -13.78  050 -1
01050    7.24  001  1 160  1 050  1
01100   -9.06  001  1 160 -1 050 -1
00001    0.00  001  1
05201   14.00  001  1 160  3 050 -1 051  1 052  1

00002   50.0  0.0052
0.1     1.0
    1
 5201
   10        1        1        0
   52
5.56E-16
9.95E-15
2.40E-14
5.87E-14
5.82E-14
5.99E-14
8.72E-14
8.71E-14
8.87E-14
8.89E-14
   50
-1.77
-2.13
-2.13
-2.92
-3.57
-4.00
-4.34
-5.23
-5.65
-5.98
    1     0
   52     0.10    1.0E-18
```

DLM
No CO_2
$XOH^0 + Th^{4+} = XO{\cdot}Th^{3+} + H^+$

```
Thorium         0
  on            1
Goethite        0
2.3s\nm2        0
00000050        1
00000060       90
00000070        5        1        3        1
00000080  00001  -6.00  9.97E-7   XOH
00000090  00160  -1.0   0.00E00   PSIO
00000098  00161  -0.5   0.00E00   PSIB
00000100  00162  -0.1   0.00E00   PSID
00000102  00051  -13.0  1.0E-13   Th+4
00000104  00052   0.0   0.00E00   Thads
00000106  00050   0.0   0.00E00   H+
00000110  00003  -1.0   0.00E00   NA+
00000120  00005  -1.0   0.00E00   NO3-
00000124
00000126  00050    0.00  050  1
00000127  00051    0.00  051  1
00000128  00001    0.00  001  1
00000129  05101   -4.55  051  1 050 -1
00000130  05102   -8.21  051  1 050 -2
00000131  05103  -13.02  051  1 050 -3
00000132  05104  -17.22  051  1 050 -4
00000139  05105   -5.80  051  2 050 -2
00000140  05106  -20.88  051  4 050 -8
00000145  05107  -37.69  051  6 050-15
00000150  00100  -13.78  050 -1
 xoth+3   01050    5.89  001  1 160  1 050  1
00000174  01100   -9.89  001  1 160 -1 050 -1
00000175  01103   -7.64  001  1 160 -1 161  1 050 -1 003  1
00000180  01055    8.56  001  1 160  1 161 -1 050  1 005  1
00000185  05201   -5.00  001  1 160 -1 161  4 050 -1 051  1 052  1
00000190
00000195
00000230  00004   50.0  0.0052 0.8    0.2
00000240  0.1     1.0
00000260           1
00000280        5201
00000300          10        1        1        0
00000320          52
00000340  5.56E-16
00000360  9.95E-15
00000380  2.40E-14
00000400  5.87E-14
00000420  5.82E-14
00000421  5.99E-14
00000560  8.72E-14
00000580  8.71E-14
00000600  8.87E-14
00000620  8.89E-14
00000640          50
00000660  -1.77
00000680  -2.13
00000700  -2.13
00000720  -2.92
00000740  -3.57
00000741  -4.00
00000880  -4.34
10%error  -5.23
          -5.65
Thorium   -5.98
  on               1      0
Goethite          52      0.10    1.0E-18
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000139
00000140
00000145
00000150
 xoth+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000421
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000741
00000880
10%error
```

TLM
No CO_2
$XOH^0 + Th^{4+} = XO{\cdot}Th^{3+} + H^+$

Example FITEQL Inputs


```
Thorium
  on
Goethite
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000091
00000092
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000150
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000139
00000140
00000145
00000147
00000149
xoth+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000421
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000741
00000880
10%error
```

6/2/95
DRJenne

Table BXX. Thorium (IV)-amorphous SiO_2 Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: amorphous Goethite A_{SP}: 50 m^2/g Data Source: LaFlamme and Murray (1987) Concentration:[Th(IV)] = 1E-13 M				Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1E-18			Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm² M/V = 0.00522 g/L		
No CO_2 For convergence, only data for pH < 6.0 used in optimization (n=10)	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- =-9.17			Log K_+ = 6.47 Log K_- =-9.03			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}Th^{3+}$	14.40	23.5	.0325	17.24	20.6	.0288	-0.33	94.4	.0362
$XO\text{-}ThOH^{2+}$	9.92	22.1	.0298	9.28	43.4	.1145	-2.45	54.5	.0302
$XO\text{-}Th(OH)_2^{+}$	0.59	49.0	.1015	0.11	49.0	.1014	-4.63	22.9	.0324
$XOH\text{-}Th(OH)_2^{2+}$	9.92	22.1	.0298	9.28	43.4	.1145	2.94	23.5	.0313
$XO\text{-}Th(OH)_3^{0}$	-7.23	54.8	.1149	-6.51	49.2	.1020	-10.41	47.8	.0962
$XOH\text{-}Th(OH)_3^{+}$	0.59	49.0	.1015	0.11	49.0	.1014	-2.63	47.5	.0939
$XO\text{-}Th(OH)_4^{-}$	-13.89	55.5	.1100	-13.12	49.3	.1023	-14.20	49.2	.1021
$XOH\text{-}Th(OH)_4^{0}$	-7.23	54.8	.1149	-6.51	49.2	.1020	-6.42	49.1	.1019
$XOH_2\text{-}Th(OH)_4^{+}$	0.59	49.0	.1015	0.11	49.0	.1014	1.35	49.1	.1017

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

6/2/95
D.R. Leimen

FITEQL Results - No MINTEQA2 results

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 5: Percentage adsorption of actinides on precipitated amorphous silica...) is from the following reference:

Righetto, L., G. Bidoglio, G. Azimonti, and I.R. Bellobono. "Competitive Actinide Interactions in Colloidal Humic Acid-Mineral Oxide Systems." Environmental Science and Technology. Vol. 25. pp. 1,913-1,919. 1991.

Righetto, L., G. Bidoglio, G. Azimonti, and I.R. Bellobono. 1991. Competitive actinide interactions in colloidal humic acid-mineral oxide systems. *Environmental Science and Technology* 25: 1913-1919.

6/2/95
D.R. Leimen

Righetto et. al. (1991)	**Am(III) - amorphous silica (SiO_2)**	
Figure 5(b)		
Asp=175 m²/g	5E-10 M	
No CO_2		
pH	%sorbed	mol sorbed
0.1 M $NaClO_4$	**M/V =1.202 g/L**	
5(b)		
3.91	2.87	1.4362E-11
4.51	11.77	5.8873E-11
5.17	22.88	1.1438E-10
5.60	37.27	1.8634E-10
6.17	47.36	2.3679E-10
6.44	56.85	2.8423E-10
6.70	55.85	2.7923E-10
7.08	67.08	3.3540E-10
7.43	68.60	3.4299E-10
7.69	74.10	3.7051E-10
8.25	85.29	4.2646E-10
8.78	91.22	4.5608E-10
9.23	95.31	4.7653E-10
9.65	96.23	4.8117E-10
9.98	93.82	4.6909E-10

Digitized Data

D.R. Leimen

```
      0                                               Americum
      1                                                  on
      0                                               am-Silic
      0                                               2.3s\nm2
      1                                               00000050
     90                                               00000060
      3        1         3         1                  00000070
00001  -3.09  8.05E-4   XOH                           00000080
00160  -2.0   0.00E00   PSIO                          00000090
00031  -9.30  5.0E-10   Am+3                          00000098
00032   0.0   0.00E00   Am(ads)                       00000100
00050   0.0   0.00E00   H+                            00000102
00003  -1.0   0.00E00   NA+                           00000104
00005  -1.0   0.00E00   ClO4                          00000106
                                                      00000110
00050    0.00  050  1                                 00000120
00031    0.00  031  1                                 00000124
03100   -7.03  031  1 050 -1                          00000126
03101  -16.65  031  1 050 -2                          00000126
03102  -24.45  031  1 050 -3                          00000126
00100  -13.78  050 -1                                 00000139
01100   -7.04  001  1 160 -1 050 -1                   00000145
00001    0.00  001  1                                 00000150
03201   -3.00  001  1 160  2 050 -1 031  1 032  1     xoam
                                                      00000174
                                                      00000175
00001   175.0  1.20      1.0                          00000180
    0      0                                          00000185
      1                                               00000190
   3201                                               00000195
     15         1         1         0                 00000230
     32                                               00000240
1.4362E-11                                            00000260
5.8873E-11                                            00000280
1.1438E-10                                            00000300
1.8634E-10                                            00000320
2.3679E-10                                            00000260
2.8423E-10                                            00000280
2.7923E-10                                            00000300
3.3540E-10                                            00000320
3.4299E-10                                            00000260
3.7051E-10                                            00000280
4.2646E-10                                            00000300
4.5608E-10                                            00000320
4.7653E-10                                            00000280
4.8117E-10                                            00000300
4.6909E-10                                            00000320
        50                                            00000560
-3.91                                                 00000580
-4.51                                                 00000600
-5.17                                                 00000620
-5.60                                                 00000640
-6.17                                                 00000580
-6.44                                                 00000600
-6.70                                                 00000620
-7.08                                                 00000640
-7.43                                                 00000580
-7.69                                                 00000600
-8.25                                                 00000620
-8.78                                                 00000640
-9.23                                                 00000600
-9.65                                                 00000620
-9.98                                                 00000640
      1        0                                      00000880
     32     0.10   5.0E-14                            10%error
```

CCM
No CO_2
$>SiOH^0 + Am^{3+} = >SiO\text{-}Am^{2+} + H^+$

D.R. Leimen

Example FITEQL Input

6/2/95
DRLeMay

```
                0
                1
                0
                0
                1
               90
                3         1         3         1
00001  -3.09  8.05E-4   XOH
00160  -2.0   0.00E00   PSIO
00031  -9.30  5.0E-10   Am+3
00032   0.0   0.00E00   Am(ads)
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4

00050    0.00  050  1
00031    0.00  031  1
03100   -7.03  031  1 050 -1
03101  -16.65  031  1 050 -2
03102  -24.45  031  1 050 -3
00100  -13.78  050 -1
01100   -7.09  001  1 160 -1 050 -1
00001    0.00  001  1
03201   -3.01  001  1 160  2 050 -1 031  1 032  1

00002   175.0  1.20
0.1     1.0
            1
         3201
           15         1         1         0
           32
1.4362E-11
5.8873E-11
1.1438E-10
1.8634E-10
2.3679E-10
2.8423E-10
2.7923E-10
3.3540E-10
3.4299E-10
3.7051E-10
4.2646E-10
4.5608E-10
4.7653E-10
4.8117E-10
4.6909E-10
           50
-3.91
-4.51
-5.17
-5.60
-6.17
-6.44
-6.70
-7.08
-7.43
-7.69
-8.25
-8.78
-9.23
-9.65
-9.98
            1        0
           32     0.10   5.0E-14
```

DLM
No CO_2
$>SiOH^{\circ} + Am^{3+} = >SiO{\cdot}Am^{2+} + H^+$

DRLeMay

```
Americum            0
   on               1
am-Silic            0
2.3s\nm2            0
00000050            1
00000060           90
00000070            5         1         3         1
00000080   00001  -3.09  8.05E-4   XOH
00000090   00160  -2.0   0.00E00   PSIO
00000098   00161  -1.0   0.00E00   PSIB
00000100   00162  -0.2   0.00E00   PSID
00000102   00031  -9.30  5.0E-10   Am+3
00000104   00032   0.0   0.00E00   Am(ads)
00000106   00050   0.0   0.00E00   H+
00000110   00003  -1.0   0.00E00   NA+
00000120   00005  -1.0   0.00E00   ClO4
00000124
00000126   00050    0.00  050  1
00000126   00031    0.00  031  1
00000126   03100   -7.03  031  1 050 -1
00000139   03101  -16.65  031  1 050 -2
00000145   03102  -24.45  031  1 050 -3
00000150   00100  -13.78  050 -1
xoam       01050    0.79  001  1 160  1 050  1
00000174   01100   -4.79  001  1 160 -1 050 -1
00000175   01103   -6.22  001  1 160 -1 161  1 050 -1 003  1
00000180   00001    0.00  001  1
00000185   03201   -4.80  001  1 160 -1 161  3 050 -1 031  1 032  1
00000190
00000195
00000230   00004   175.0  1.20  0.8   0.2
00000240   0.1     1.0
00000260             1
00000280          3201
00000300            15         1         1         0
00000320            32
00000260   1.4362E-11
00000280   5.8873E-11
00000300   1.1438E-10
00000320   1.8634E-10
00000260   2.3679E-10
00000280   2.8423E-10
00000300   2.7923E-10
00000320   3.3540E-10
00000280   3.4299E-10
00000300   3.7051E-10
00000320   4.2646E-10
00000560   4.5608E-10
00000580   4.7653E-10
00000600   4.8117E-10
00000620   4.6909E-10
00000640            50
00000580   -3.91
00000600   -4.51
00000620   -5.17
00000640   -5.60
00000580   -6.17
00000600   -6.44
00000620   -6.70
00000640   -7.08
00000600   -7.43
00000620   -7.69
00000640   -8.25
00000880   -8.78
10%error   -9.23
           -9.65
           -9.98
             1        0
            32     0.10   5.0E-14
```

TLM
No CO_2
$>SiOH^{\circ} + Am^{3+} = >SiO{\cdot}Am^{2+} + H^+$

```
Americum
   on
am-Silic
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000126
00000139
00000140
00000145
00000147
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000260
00000280
00000300
00000320
00000260
00000280
00000300
00000320
00000280
00000300
00000320
00000560
00000580
00000600
00000620
00000640
00000580
00000600
00000620
00000640
00000580
00000600
00000620
00000640
00000600
00000620
00000640
00000880
10%error
```

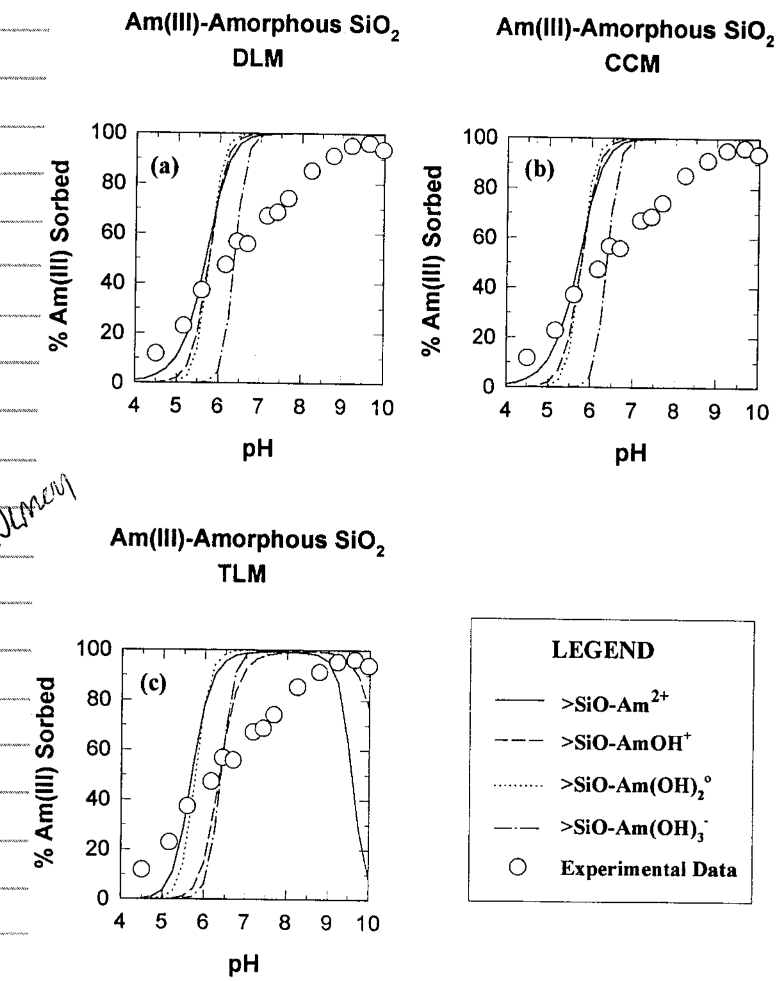
Table BXX. Americium (III)-amorphous SiO_2 Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: amorphous SiO_2 A_{SP}: 175 m^2/g Data Source: Righetto et al. (1991) Concentration: [Am(III)] = 5.0E-10 M			Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 5.0E-14			Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_s = 2.31 sites/nm^2 M/V = 1.2 g/L			
no CO_2	DLM			CCM (I = 0.1)			TLM		
	Log K_+ = (b) Log K_- = -7.20			Log K_+ = (b) Log K_- = -7.04			Log K_+ = 0.90 Log K_- = -4.90 Log K_{Cat} = -6.22 Log K_{An} = (b)		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}Am^{2+}$	-1.93	24.6	.0390	-1.89	23.7	.0381	-4.60	43.2	.0489
$XO\text{-}AmOH^+$	-7.62	35.7	.0589	-7.60	35.6	.0586	-10.02	33.1	.0603
$XO\text{-}Am(OH)_2^{\circ}$	-13.20	39.4	.0656	-13.19	39.4	.0657	-12.80	38.4	.0654
$XOH\text{-}Am(OH)_2^+$	-7.62	35.7	.0589	-7.60	35.6	.0586	-9.22	37.7	.0645
$XO\text{-}Am(OH)_3^-$	-20.90	37.6	.0794	-20.94	37.6	.0794	-18.67	36.6	.0755
$XOH\text{-}Am(OH)_3^{\circ}$	-13.20	39.4	.0656	-13.19	39.4	.0656	-13.18	39.4	.0656
$XOH_2\text{-}Am(OH)_3^+$	-7.62	34.7	.0589	-7.60	35.6	.0586	-11.33	35.9	.0729

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.
(b) Due to low zero-point of charge (pH_{ZPC}=2.1 for SiO_2), XOH_2^+ (DLM, CCM) and XOH_2-An (TLM only) are assumed to be insignficant at slightly acid to basic pH [see discussion in Turner (1993)].

DRLeMay

6/2/95
DRLeMay



DRLeMay

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 5: Percentage adsorption of actinides on precipitated amorphous silica...) is from the following reference:

Righetto, L., G. Bidoglio, G. Azimonti, and I.R. Bellobono. "Competitive Actinide Interactions in Colloidal Humic Acid-Mineral Oxide Systems." Environmental Science and Technology. Vol. 25. pp. 1,913-1,919. 1991.

Np(V)-SiO_2
Adsorption

6/2/95
DRLmm

Righetto, L., G. Bidoglio, G. Azimonti, and I.R. Bellobono. 1991. Competitive actinide interactions in colloidal humic acid-mineral oxide systems. *Environmental Science and Technology* 25: 1913-1919.

Digitized Results

DRLmm

Righetto et. al. (1991)	**Np(V) - amorphous silica (SiO_2)**	
Figure 5(c)		
Asp=175 m^2/g	1E-14 M	
No CO_2		
pH	%sorbed	mol sorbed
0.1 M $NaClO_4$	**M/V =1.202 g/L**	
5(c)		
6.21	4.55	4.5489E-16
6.64	5.57	5.5698E-16
7.11	6.13	6.1346E-16
7.62	8.03	8.0280E-16
8.24	16.11	1.6107E-15
8.49	22.34	2.2342E-15
8.74	28.76	2.8760E-15
8.96	35.41	3.5406E-15
9.18	42.28	4.2281E-15
9.38	50.53	5.0530E-15
9.61	59.56	5.9557E-15
9.74	63.18	6.3178E-15
10.04	72.21	7.2208E-15
10.13	70.43	7.0425E-15
10.24	65.25	6.5255E-15

DRLmm

```
                0
                1
                0
                0
                1
               90
                3          1          3          1
00001   -3.09   8.07E-4    XOH
00160   -2.0    0.00E00    PSI0
00031   -14.0   1.0E-14    NpO2+
00032    0.0    0.00E00    NpO2(ads)
00050    0.0    0.00E00    H+
00003   -1.0    0.10E00    Na+
00005   -1.0    0.10E00    ClO4-

00050     0.00   050  1
00031     0.00   031  1
03100    -8.90   031  1 050 -1
00100   -13.78   050 -1
01050     0.79   001  1 160  1 050  1
01100    -6.93   001  1 160 -1 050 -1
00001     0.00   001  1
03201    -5.69   001  1 160  0 050 -1 031  1 032  1

00001   175.0 1.202      1.0
0.1     1.0
           1
        3201
          15          1          1          0
          32
4.5489E-16
5.5698E-16
6.1346E-16
8.0280E-16
1.6107E-15
2.2342E-15
2.8760E-15
3.5406E-15
4.2281E-15
5.0530E-15
5.9557E-15
6.3178E-15
7.2208E-15
7.0425E-15
6.5255E-15
          50
-6.21
-6.64
-7.11
-7.62
-8.24
-8.49
-8.74
-8.96
-9.18
-9.38
-9.61
-9.74
-10.04
-10.13
-10.24
           1
          32       0.10    1.0E-18
```

CCM
No CO_2
$>SiOH^0 + NpO_2^+ = >SiO\cdot NpO_2^0 + H^+$

```
Neptunum
   on
silica                0
2.3s\nm2              1
00000050              0
00000060              0
00000070              1
00000080             90
00000090              3          1          3          1
00000098    00001   -3.09   8.06E-4    XOH
00000100    00160   -2.0    0.00E00    PSI0
00000102    00031   -14.0   1.0E-14    NpO2+
00000104    00032    0.0    0.00E00    NpO2(ads)
00000106    00050    0.0    0.00E00    H+
00000110    00003   -1.0    0.10E00    Na+
00000120    00005   -1.0    0.10E00    ClO4-
00000124
00000126    00050     0.00   050  1
00000139    00031     0.00   031  1
00000140    03100    -8.79   031  1 050 -1
00000145    00100   -13.78   050 -1
00000146    01100    -7.09   001  1 160 -1 050 -1
00000147    00001     0.00   001  1
xoNpo2      03201    -5.00   001  1 160  0 050 -1 031  1 032  1
00000174
00000175    00002   175.0 1.202
00000180    0.1     1.0
00000185               1
00000190            3201
00000195              15          1          1          0
00000230              32
00000240    4.5489E-16
00000260    5.5698E-16
00000280    6.1346E-16
00000300    8.0280E-16
00000320    1.6107E-15
00000660    2.2342E-15
00000680    2.8760E-15
00000700    3.5406E-15
00000710    4.2281E-15
00000660    5.0530E-15
00000680    5.9557E-15
00000700    6.3178E-15
00000710    7.2208E-15
00000660    7.0425E-15
00000680    6.5255E-15
00000700              50
00000560    -6.21
00000580    -6.64
00000600    -7.11
00000620    -7.62
00000640    -8.24
00000660    -8.49
00000680    -8.74
00000700    -8.96
00000710    -9.18
00000660    -9.38
00000680    -9.61
00000700    -9.74
00000710    -10.04
00000680    -10.13
00000700    -10.24
00000710               1
00000880              32       0.10    1.0E-18
10%error
```

DLM
No CO_2
$>SiOH^0 + NpO_2 = >SiO\cdot NpO_2^0 + H^+$

DRLmm

6/2/95
DRLmm

```
                0
                1
                0
                0
                1
               90
                5          1          3          1
00001   -3.09   8.07E-4    XOH
00160   -2.0    0.00E00    PSI0
00161   -1.0    0.00E00    PSIB
00162   -0.2    0.00E00    PSID
00031   -14.0   1.0E-14    NpO2+
00032    0.0    0.00E00    NpO2(ads)
00050    0.0    0.00E00    H+
00003   -1.0    0.10E00    Na+
00005   -1.0    0.10E00    ClO4-

00050     0.00   050  1
00031     0.00   031  1
03100    -8.90   031  1 050 -1
00100   -13.78   050 -1
00001     0.00   001  1
01100    -4.79   001  1 160 -1 050 -1
01050     0.79   001  1 160  1 050  1
01103    -6.11   001  1 160 -1 161  1 050 -1 003  1
03202     1.90   001  1 160  0 161  1 050  0 031  1 032  1

00004   175.0 1.202  0.8     0.2
0.1     1.0
           1
        3202
          15          1          1          0
          32
4.5489E-16
5.5698E-16
6.1346E-16
8.0280E-16
1.6107E-15
2.2342E-15
2.8760E-15
3.5406E-15
4.2281E-15
5.0530E-15
5.9557E-15
6.3178E-15
7.2208E-15
7.0425E-15
6.5255E-15
          50
-6.21
-6.64
-7.11
-7.62
-8.24
-8.49
-8.74
-8.96
-9.18
-9.38
-9.61
-9.74
-10.04
-10.13
-10.24
           1
          32       0.10    1.0E-18
```

```
Neptunum
   on
silica
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000139
00000145
00000146
00000147
xoHNPO2
00000174
00000175
00000184
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000660
00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000660
00000680
00000700
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000710
00000660
00000680
00000700
00000710
00000880
10%error
```

Example FITEQL Inputs

Table B-11. Neptunium (V)-Amorphous SiO_2 Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: Amorphous SiO_2 A_{sp}: 175 m^2/g Data Source: Righetto et al. (1991) Concentration:[Np(V)] = 1E-14 M	Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-18	Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_s = 2.31 sites/nm^2 M/V = 1.2 g/L

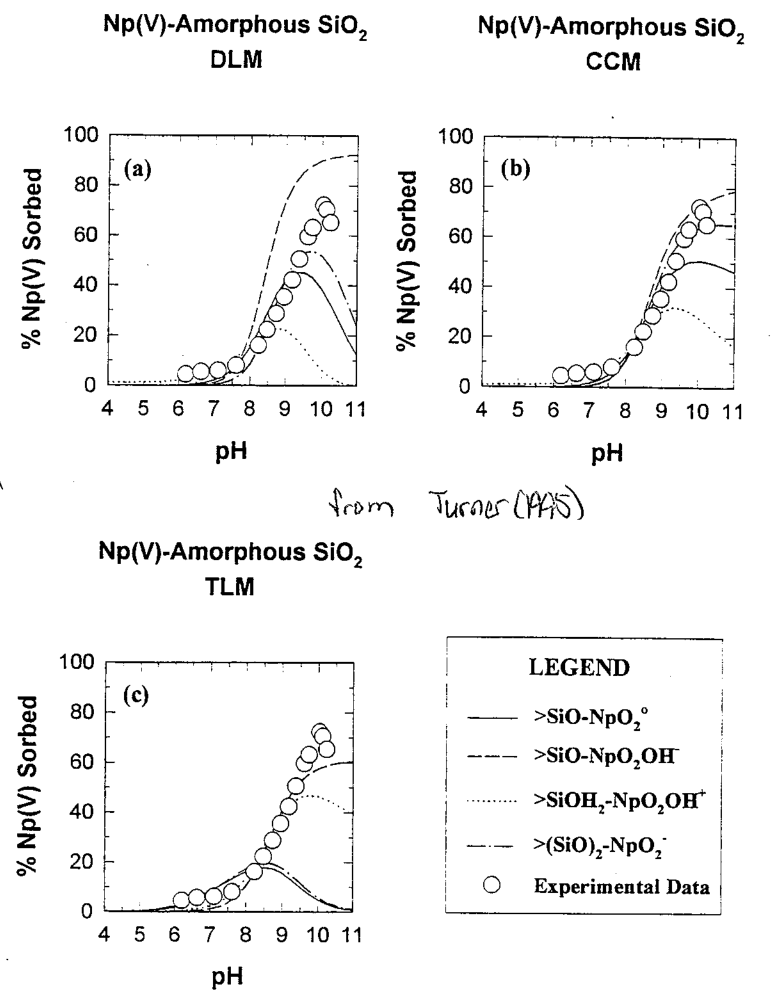
No CO_2	DLM Log K_1 = (b) Log K_{-1} =-7.20			CCM Log K_1 = (b) Log K_{-1} = -7.04			TLM Log K_1 = 0.90 Log K_{-1} = -4.90 Log K_{Cat} = -6.22 Log K_{An} = (b)		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}NpO_2^+$	-5.39	24.9	.0179	-5.49	16.9	.0188	-3.89	50.3	.0174
$XOH\text{-}NpO_2^+$	1.30	41.1	.0168	1.18	17.4	.0161	-0.14	55.4	.0179
$XO\text{-}NpO_2OH^-$	-11.89	22.1	.0215	-12.27	21.1	.0221	-9.43	17.8	.0202
$XOH\text{-}NpO_2OH^0$	-5.39	24.9	.0179	-5.49	16.9	.0188	-5.52	16.8	.0191
$XOH_2\text{-}NpO_2OH^+$	1.30	41.1	.0168	1.18	17.4	.0161	-1.63	16.5	.0181
OTHER SPECIES:									
$(XO)_2\text{-}NpO_2^-$	-12.53	23.3	.0235	-12.27	21.1	.0221	-12.25	22.0	.0225

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.
(b) Due to low zero-point of charge (pH_{zpc}=2.1 for SiO_2), XOH_2^+ (DLM, CCM) and XOH_2-An (TLM only) are assumed to be insignficant at slightly acid to basic pH [see discussion in Turner (1993)].

FITEQL Results

6/2/95
DR Jenn

MINTEQA2
Model Results



from Turner (1995)

DR Jenn

Figure 4-11. Np(V) sorption on amorphous SiO_2. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 1\times10^{-14}$ M, 0.1 M $NaClO_4$, M/V=1.2 g/L. Model parameters from Tables 3-1 and B-11. Data from Righetto et al. (1991).

4-12

Th(IV)-SiO_2
sorption

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 5: Percentage adsorption of actinides on precipitated amorphous silica...) is from the following reference:

Righetto, L., G. Bidoglio, G. Azimonti, and I.R. Bellobono. "Competitive Actinide Interactions in Colloidal Humic Acid-Mineral Oxide Systems." Environmental Science and Technology. Vol. 25. pp. 1,913-1,919. 1991.

Righetto, L., G. Bidoglio, G. Azimonti, and I.R. Bellobono. 1991. Competitive actinide interactions in colloidal humic acid-mineral oxide systems. *Environmental Science and Technology* 25: 1913-1919.

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Digitized Data

DR Jenn

Righetto et. al. (1991)	**Th(IV) - amorphous silica (SiO_2)**	
Figure 5(a)		
Asp=175 m²/g	1E-11 M	
No CO_2		
pH	%sorbed	mol sorbed
0.1 M $NaClO_4$	**M/V = 0.06 g/L**	
5(a)		
.063	.14	1.3936E-14
.285	12.88	1.2875E-12
.610	52.17	5.2172E-12
.871	62.48	6.2482E-12
1.144	69.08	6.9084E-12
1.430	74.91	7.4908E-12
1.935	76.34	7.6344E-12
2.245	76.31	7.6308E-12
2.512	74.90	7.4897E-12
2.760	76.28	7.6279E-12
3.308	74.69	7.4694E-12

D.R. Jenn

```
          0
          1
          0
          0
          1
         90
          3          1          3          1
00001  -4.40  4.03E-5   XOH
00160  -1.0   0.00E00   PSI0
00051  -11.0  1.0E-11   Th+4
00052   0.0   0.00E00   Thads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00051    0.00  051  1
05101   -4.55  051  1 050 -1
05102   -8.21  051  1 050 -2
05103  -13.02  051  1 050 -3
05104  -17.22  051  1 050 -4
05105   -5.80  051  2 050 -2
05106  -20.88  051  4 050 -8
05107  -37.69  051  6 050-15
00100  -13.78  050 -1
01100   -7.09  001  1 160 -1 050 -1
00001    0.00  001  1
05201   14.00  001  1 160  3 050 -1 051  1 052  1

00002  175.0  0.060
0.1    1.0
          1
       5201
         11          1          1          0
         52
1.3936E-14
1.2875E-12
5.2172E-12
6.2482E-12
6.9084E-12
7.4908E-12
7.6344E-12
7.6308E-12
7.4897E-12
7.6279E-12
7.4694E-12
         50
-0.063
-0.285
-0.610
-0.871
-1.144
-1.430
-1.935
-2.245
-2.512
-2.760
-3.308
          1          0
         52     0.10   1.0E-15
```

DLM
No CO_2
$>SiOH^0 + Th^{4+} = >SiO\text{-}Th^{3+} + H^+$

DR Jenn

```
Thorium          0
 on              1
am SiO2          0
2.3s\nm2         0
00000050         1
00000060        90
00000070         3          1          3          1
00000080  00001  -4.40  4.03E-5   XOH
00000090  00160  -1.0   0.00E00   PSI0
00000098  00051  -11.0  1.0E-11   Th+4
00000100  00052   0.0   0.00E00   Thads
00000102  00050   0.0   0.00E00   H+
00000104  00003  -1.0   0.00E00   NA+
00000106  00005  -1.0   0.00E00   ClO4-
00000110
00000120  00050    0.00  050  1
00000124  00051    0.00  051  1
00000126  05101   -4.55  051  1 050 -1
00000127  05102   -8.21  051  1 050 -2
00000128  05103  -13.02  051  1 050 -3
00000129  05104  -17.22  051  1 050 -4
00000130  05105   -5.80  051  2 050 -2
00000131  05106  -20.88  051  4 050 -8
00000132  05107  -37.69  051  6 050-15
00000139  00100  -13.78  050 -1
00000145  01100   -7.04  001  1 160 -1 050 -1
00000150  00001    0.00  001  1
xoth+3    05201    4.00  001  1 160  3 050 -1 051  1 052  1
00000174
00000175
00000180  00001  175.0  0.060     1.0
00000185      0        0
00000190         1
00000195      5201
00000230        11          1          1          0
00000240        52
00000380  1.3936E-14
00000400  1.2875E-12
00000420  5.2172E-12
00000421  6.2482E-12
00000422  6.9084E-12
00000423  7.4908E-12
00000424  7.6344E-12
00000425  7.6308E-12
00000426  7.4897E-12
00000427  7.6279E-12
00000427  7.4694E-12
00000560        50
00000580  -0.063
00000600  -0.285
00000620  -0.610
00000640  -0.871
00000660  -1.144
00000680  -1.430
00000700  -1.935
00000720  -2.245
00000740  -2.512
00000741  -2.760
00000741  -3.308
00000880         1          0
10%error        52     0.10   1.0E-15
```

CCM
No CO_2
$>SiOH^0 + Th^{4+} = >SiO\text{-}Th^{3+} + H^+$

```
Thorium
 on
am SiO2
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000139
00000145
00000150
xoth+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000380
00000400
00000420
00000421
00000422
00000423
00000424
00000425
00000426
00000427
00000427
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000741
00000741
00000880
10%error
```

No pH uncertainty specified to allow convergence

6/2/95
DRLemm

DRLemm

```
        0
        1
        0
        0
        1
       90
        5         1         3         1
00001  -4.40  4.03E-5   XOH
00160  -1.0   0.00E00   PSI0
00161  -0.5   0.00E00   PSIB
00162  -0.1   0.00E00   PSID
00051  -11.0  1.0E-11   Th+4
00052   0.0   0.00E00   Thads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00051    0.00  051  1
05101   -4.55  051  1 050 -1
05102   -8.21  051  1 050 -2
05103  -13.02  051  1 050 -3
05104  -17.22  051  1 050 -4
05105   -5.80  051  2 050 -2
05106  -20.88  051  4 050 -8
05107  -37.69  051  6 050-15
00100  -13.78  050 -1
01050    0.79  001  1 160  1 050  1
01100   -4.79  001  1 160 -1 050 -1
01103   -6.22  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
05201    8.00  001  1 160 -1 161  4 050 -1 051  1 052  1

00004  175.0  0.060  0.8    0.2
0.1    1.0
         1
      5201
        11        1         1         0
        52
1.3936E-14
1.2875E-12
5.2172E-12
6.2482E-12
6.9084E-12
7.4908E-12
7.6344E-12
7.6308E-12
7.4897E-12
7.6279E-12
7.4694E-12
        50
-0.063
-0.285
-0.610
-0.871
-1.144
-1.430
-1.935
-2.245
-2.512
-2.760
-3.308
         1        0
        52      0.10   1.0E-15
```

```
Thorium
  on
am SiO2
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000091
00000092
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000139
00000140
00000145
00000147
00000150
xoth+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000380
00000400
00000420
00000421
00000422
00000423
00000424
00000425
00000426
00000427
00000427
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000741
00000741
00000880
10%error
```

pH uncertainty left blank to allow for convergence

TLM
No CO_2
$>SiOH^0 + Th^{4+} = >SiO\text{-}Th^{3+} + H^+$

Table B-16. Thorium (IV)-Amorphous SiO_2 Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: Amorphous SiO_2
A_{SP}: 175 m^2/g
Data Source: Righetto et al. (1991)
Concentration: [Th(IV)] = 1E-11 M

Rel Error (pH): (a)
Abs Error (pH): (a)
Rel Error (radionuclide): 0.10
Abs Error (radionuclide): 1.0E-15

Ionic Strength (electrolyte): 0.1 M $NaClO_4$
N_S = 2.31 sites/nm^2
M/V = 0.06 g/L

DRLemm

No CO_2	DLM			CCM			TLM		
	Log K_+ = (b) Log K_- = -7.20			Log K_+ = (b) Log K_- = -7.04			Log K_+ = 0.90 Log K_- = -4.90 Log K_{Cat} = -6.22 Log K_{An} = (b)		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}Th^{3+}$	3.43	61.1	.0329	3.43	61.1	.0329	8.15	34.8	.0418
$XO\text{-}ThOH^{2+}$	3.20	35.8	.0390	3.20	35.8	.0390	6.25	22.7	.0429
$XO\text{-}Th(OH)_2^+$	2.98	24.2	.0423	2.98	24.2	.0423	4.35	21.2	.0443
$XOH\text{-}Th(OH)_2^{2+}$	3.20	35.8	.0390	3.20	35.8	.0390	6.58	22.0	.0434
$XO\text{-}Th(OH)_3^o$	2.76	19.8	.0457	2.76	19.8	.0457	2.45	20.2	.0455
$XOH\text{-}Th(OH)_3^+$	2.98	24.2	.0423	2.98	24.2	.0423	4.68	20.7	.0448
$XO\text{-}Th(OH)_4^-$	2.54	18.0	.0479	2.54	18.0	.0479	0.56	19.4	.0458
$XOH\text{-}Th(OH)_4^o$	2.76	19.8	.0457	2.76	19.8	.0457	2.78	19.8	.0457
$XOH_2\text{-}Th(OH)_4^+$	2.98	24.2	.0423	2.98	24.2	.0423	5.01	20.3	.0453

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.
(b) Due to low zero-point of charge (pH_{ZPC}=2.1 for SiO_2), XOH_2^+ (DLM, CCM) and XOH_2-An (TLM only) are assumed to be insignficant at slightly acid to basic pH [see discussion in Turner (1993)].

FITEQL Results

6/2/95
DRLemm

DRLemm

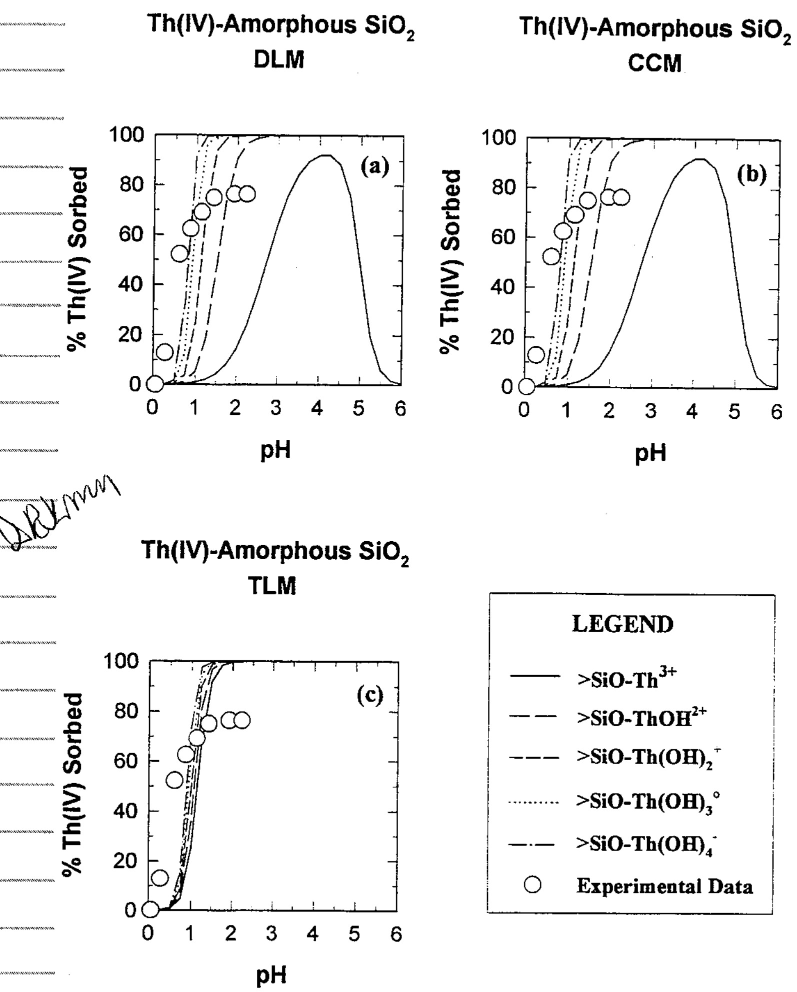

Figure 4-16. Th(IV) sorption on amorphous SiO_2. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Th(IV)_T = 1\times10^{-11}$ M, 0.1 M $NaClO_4$, M/V=0.06 g/L. Model parameters from Tables 3-1 and B-16. Data from Righetto et al. (1991).

4-17

$Pu(V) - \gamma Al_2O_3$

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 8: Adsorption behavior of AM...) is from the following reference:

Righetto, L., G. Bidoglio, G. Azimonti, and I.R. Bellobono. "Competitive Actinide Interactions in Colloidal Humic Acid-Mineral Oxide Systems." Environmental Science and Technology. Vol. 25. pp. 1,913-1,919. 1991.

6/2/95
DRLmm

Righetto, L., G. Bidoglio, G. Azimonti, and I.R. Bellobono. 1991. Competitive actinide interactions in colloidal humic acid-mineral oxide systems. *Environmental Science and Technology* 25: 1913-1919.

Righetto et. al. (1991)	**Pu(V) - γAl_2O_3**	
Figure 8, HA conc. = 0		
Asp=130 m^2/g	2E-10 M	
No CO_2		
pH	%sorbed	mol sorbed
0.1 M $NaClO_4$	**M/V =0.2 g/L**	
Fig. 8		
7.25	51.0	1.02E-10
7.70	71.0	1.42E-10
9.35	96.0	1.92E-10
9.75	97.0	1.94E-10
9.80	97.0	1.94E-10
10.20	99.0	1.98E-10
10.48	100	2.00E-10

Digtized Data

DRLmm

```
          0
          1
          0
          0
          1
         90
          3          1          3          1
00001   -4.00   9.97E-5   XOH
00160   -1.00   0.00E00   PSI0
00032   -9.70   2.0E-10   PuO2+
00033    0.0    0.00E00   PuO2ads
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   Na+
00005   -1.0    0.00E00   ClO4-

00050     0.00   050  1
00032     0.00   032  1
03201    -9.74   032  1 050 -1
00100   -13.78   050 -1
01050     6.74   001  1 160  1 050  1
01100    -8.94   001  1 160 -1 050 -1
00001     0.00   001  1
03302     5.60   001  1 160  1 050  0 032  1 033  1


00002  130.0  0.200
0.1    1.0
          1
       3302
          7          1          1          0
         33
1.02E-10
1.42E-10
1.92E-10
1.94E-10
1.94E-10
1.98E-10
2.00E-10
         50
-7.25
-7.70
-9.35
-9.75
-9.80
-10.20
-10.48
          1          0
         32       0.10    1.0E-13
```

DLM
No CO_2
$>AlOH^o + PuO_2^+ = >AlO{\cdot}PuO_2^o + H^+$

Example FITEQL Inputs

```
GamA1203
Righetto
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000160
00000166
00000170
00000168
xohpuo2+
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001480
00001490
```

DRLmm

```
          0
          1
          0
          0
          1
         90
          3          1          3          1
00001   -4.00   9.97E-5   XOH
00160   -2.00   0.00E00   PSI0
00032   -9.70   2.0E-10   PuO2+
00033    0.0    0.00E00   PuO2ads
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   Na+
00005   -1.0    0.00E00   ClO4-

00050     0.00   050  1
00032     0.00   032  1
03201    -9.74   032  1 050 -1
00100   -13.78   050 -1
01050     6.92   001  1 160  1 050  1
01100    -9.00   001  1 160 -1 050 -1
00001     0.00   001  1
03301    -3.00   001  1 160  0 050 -1 032  1 033  1


00001  130.0  0.200      1.0
    0      0
          1
       3301
          7          1          1          0
         33
1.02E-10
1.42E-10
1.92E-10
1.94E-10
1.98E-10
2.00E-10
         50
-7.25
-7.70
-9.35
-9.75
-9.80
-10.20
-10.48
          1          0
         32       0.10    1.0E-13
```

CCM
No CO_2
$>AlOH^o + PuO_2^+ = >AlO{\cdot}PuO_2^o + H^+$

```
GamA1203
Righetto
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000160
00000140
00000145
00000147
00000149
00000168
xopuo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001480
00001490
```


DRLmm

```
          0
          1
          0
          0
          1
         90
          5          1          3          1
00001   -4.00   9.97E-5   XOH
00160   -2.00   0.00E00   PSI0
00161   -1.00   0.00E00   PSIB
00162   -0.20   0.00E00   PSID
00032   -9.70   2.0E-10   PuO2+
00033    0.0    0.00E00   PuO2ads
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   Na+
00005   -1.0    0.00E00   ClO4-

00050     0.00   050  1
00032     0.00   032  1
03201    -9.74   032  1 050 -1
00100   -13.78   050 -1
01050     6.29   001  1 160  1 050  1
01100   -10.29   001  1 160 -1 050 -1
01103    -7.95   001  1 160 -1 161  1 050 -1 003  1
01055     8.06   001  1 160  1 161 -1 050  1 005  1
00001     0.00   001  1
03301    -3.00   001  1 160 -1 161  1 050 -1 032  1 033  1


00004  130.0  0.200  0.8    0.2
0.1    1.0
          1
       3301
          7          1          1          0
         33
1.02E-10
1.42E-10
1.92E-10
1.94E-10
1.94E-10
1.98E-10
2.00E-10
         50
-7.25
-7.70
-9.35
-9.75
-9.80
-10.20
-10.48
          1          0
         32       0.10    1.0E-13
```

TLM
No CO_2
$>AlOH^o + PuO_2^+ = >AlO{\cdot}PuO_2^o + H^+$

```
GamA1203
Righetto
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000160
00000140
00000145
00000147
00000149
00000168
xopuo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
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00000270
00000280
00000290
00000300
00000310
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001480
00001490
```

6/2/95
DRLmm

Example FITEQL Input

Table B-14. Plutonium (V)-γ-Al_2O_3 Sorption Binding Constants: Monodentate, mononuclear compounds..

Solid: γ-Al_2O_3 A_{sp}: 130 m^2/g Data Source: Righetto et al. (1991) Concentration: [Pu(V)] = 2E-10 M				Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-13			Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_s = 2.31 sites/nm^2 M/V = 0.2 g/L		
No CO_2	DLM $Log K_+$ = 6.85 $Log K_-$ = -9.05			CCM $Log K_+$ = 6.92 $Log K_-$ = -9.00			TLM $Log K_+$ = 6.40 $Log K_-$ = -10.40 $Log K_{Cat}$ = -7.95 $Log K_{An}$ = 8.28		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-PuO_2^o	-3.18	0.1	.0772	-3.17	0.1	.0773	-2.94	4.8	.1337
XOH-PuO_2^+	4.65	0.1	.0760	4.72	0.04	.0760	5.71	5.2	.2049
XO-PuO_2OH^-	-10.98	0.2	.0788	-11.04	0.2	.0790	-11.37	0.1	.0777
XOH-PuO_2OH^o	-3.18	0.1	.0772	-3.17	0.1	.0773	-3.15	0.1	.0772
XOH_2-PuO_2OH^+	4.65	0.1	.0760	4.72	0.04	.0760	5.08	0.03	.0768

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

FITEQL Results

6/2/95
DKLmm

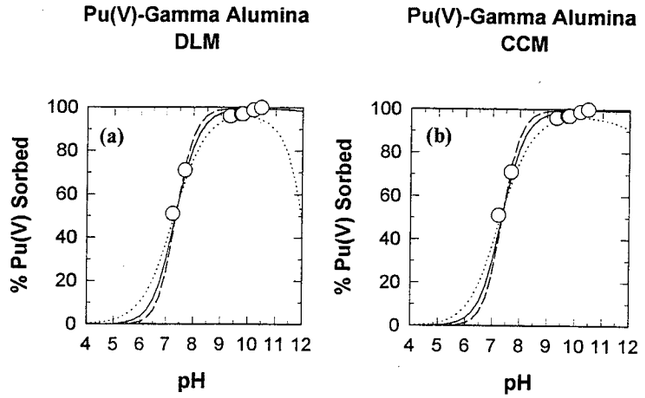

Figure 4-14. Pu(V) sorption on γ-Al_2O_3. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Pu(V)_T = 2\times10^{-10}$ M, 0.1 M $NaClO_4$, M/V=0.2 g/L. Model parameters from Tables 3-1 and B-14. Data from Righetto et al. (1991).

Fig 8a, Pu(V), no F

Results using MINTEQA2 with CNWRA database

6/9/95
DKLmm

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 1: Adsorption of Pu(IV) on a goethite as a function of pH...) is from the following reference:

Sanchez, A.L. J.W. Murray, and T.H. Sibley. "the Adsorption of Plutonium IV and V on Goethite. Geochimica et Cosmochimica Acta. Vol. 49. pp. 2,297-2,307. 1985.

Sanchez et al 1985
Σ Pu(V) = 1e-10 M
C_s = 0.55 g/L
I = 0.10 M $NaNO_3$

DKLmm

Fig 1a, 1 hr data

No plot of unadjusted data

DKLmm

Authors state equilibrium in ~1 hr. longer times lead to reduction to Pu(IV)

Sanchez, A.L., J.W. Murray, and T.H. Sibley. 1985. The adsorption of plutonium IV and V on goethite. *Geochimica et Cosmochimica Acta* 49:2297-2307.

DKLmm

Sanchez et. al. (1985)	Pu(V) - goethite (αFeOOH)	
Figure 1(c), **1 hr** data		
Asp=50 m^2/g	**1E-10 M**	
No CO_2		
0.1 M $NaNO_3$	M/V = 0.55 g/L	
pH	%sorbed	mol sorbed
2.877611	0.305694	3.06E-13
3.884123	1.182018	1.18E-12
4.524815	5.971229	5.97E-12
5.159443	9.395005	9.40E-12
5.806198	31.14006	3.11E-11
6.473164	61.3019	6.13E-11
6.913766	80.64216	8.06E-11
7.744442	94.88751	9.49E-11
8.502358	98.37243	9.84E-11
9.59982	98.73926	9.87E-11

Digitized Data

```
          1
          1
          1
          1
          1
         90
          3          1          3          1
  00001  -3.98  1.06E-4   XOH
  00160  -2.00  0.00E00   PSI0
  00032  -10.0  1.0E-10   PuO2+
  00033   0.0   0.00E00   PuO2ads
  00050   0.0   0.00E00   H+
  00003  -1.0   0.00E00   Na+
  00005  -1.0   0.00E00   NO3-

  00050    0.00  050  1
  00032    0.00  032  1
  03201   -9.95  032  1 050 -1
  00100  -13.95  050 -1
  01050    7.24  001  1 160  1 050  1
  01100   -9.06  001  1 160 -1 050 -1
  00001    0.00  001  1
  03301   -0.10  001  1 160  0 050 -1 032  1 033  1

  00002  050.0  0.550
  0.1    1.0
           1
        3301
          10          1          1          0
          33
  3.06E-13
  1.18E-12
  5.97E-12
  9.40E-12
  3.11E-11
  6.13E-11
  8.06E-11
  9.49E-11
  9.84E-11
  9.87E-11
         50
  -2.88
  -3.88
  -4.52
  -5.16
  -5.81
  -6.47
  -6.91
  -7.74
  -8.50
  -9.60
           1
          32       0.10   1.0E-13
```

```
Goethite
Sanchez
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
20 deg C
20 deg C
00000140
00000145
00000168
xopuo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000320
00000320
00000320
00001070
00001080
00001080
00001080
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001480
00001490
```

Fig 1c, 1Pu data
Σ Pu(V) = 1e-10
DLM

DRLmm

6/9/95
DRLmm

```
          1
          1
          1
          1
          1
         90
          3          1          3          1
  00001  -3.98  1.06E-4   XOH
  00160  -2.00  0.00E00   PSI0
  00032  -10.0  1.0E-10   PuO2+
  00033   0.0   0.00E00   PuO2ads
  00050   0.0   0.00E00   H+
  00003  -1.0   0.00E00   Na+
  00005  -1.0   0.00E00   NO3-

  00050    0.00  050  1
  00032    0.00  032  1
  03201   -9.95  032  1 050 -1
  00100  -13.95  050 -1
  01050    6.47  001  1 160  1 050  1
  01100   -9.03  001  1 160 -1 050 -1
  00001    0.00  001  1
  03301   -1.40  001  1 160  0 050 -1 032  1 033  1

  00001  050.0  0.550      1.0
       0      0
           1
        3301
          10          1          1          0
          33
  3.06E-13
  1.18E-12
  5.97E-12
  9.40E-12
  3.11E-11
  6.13E-11
  8.06E-11
  9.49E-11
  9.84E-11
  9.87E-11
         50
  -2.88
  -3.88
  -4.52
  -5.16
  -5.81
  -6.47
  -6.91
  -7.74
  -8.50
  -9.60
           1
          32       0.10   1.0E-13
```

```
Goethite
Sanchez
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
20 deg C
20 deg C
00000140
00000145
00000168
xopuo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000320
00000320
00000320
00001070
00001080
00001080
00001080
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001480
00001490
```

Fig 1c, 1Pu dal
Σ Pu(V) = 1e-10.
CCM

$XOH + PuO_2^+ \rightleftharpoons XOHPuO_2^\circ + H^+$

Example FITEQL Input Files

No pH error estimate to allow convergence at low ΣPu(V)


```
          0
          1
          0
          0
          1
         90
          5          1          3          1
  00001  -3.98  1.06E-4   XOH
  00160  -2.00  0.00E00   PSI0
  00161  -1.00  0.00E00   PSIB
  00162  -0.20  0.00E00   PSID
  00032  -10.0  1.0E-10   PuO2+)
  00033   0.0   0.00E00   PuO2ads
  00050   0.0   0.00E00   H+
  00003  -1.0   0.00E00   Na+
  00005  -1.0   0.00E00   NO3-

  00050    0.00  050  1
  00032    0.00  032  1
  03201   -9.95  032  1 050 -1
  00100  -13.95  050 -1
  01050    5.89  001  1 160  1 050  1
  01100   -9.89  001  1 160 -1 050 -1
  01103   -7.64  001  1 160 -1 161  1 050 -1 003  1
  01055    8.56  001  1 160  1 161 -1 050  1 005  1
  00001    0.00  001  1
  03301   -3.00  001  1 160 -1 161  1 050 -1 032  1 033  1

  00004  050.0  0.550  0.8    0.2
  0.1    1.0
           1
        3301
          10          1          1          0
          33
  3.06E-13
  1.18E-12
  5.97E-12
  9.40E-12
  3.11E-11
  6.13E-11
  8.06E-11
  9.49E-11
  9.84E-11
  9.87E-11
         50
  -2.88
  -3.88
  -4.52
  -5.16
  -5.81
  -6.47
  -6.91
  -7.74
  -8.50
  -9.60
           1          1
          32       0.10   1.0E-13
```

```
Goethite
Sanchez
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
20 deg C
20 deg C
00000140
00000145
00000147
00000149
00000168
xopuo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000320
00000320
00000320
00001070
00001080
00001080
00001080
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001480
00001490
```

Fig 1c, 1Pu data
Σ Pu(V) = 1e-10.
TLM

6/9/95
DRLmm

Table BXX. Plutonium (V)-Goethite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: goethite A_{SP}: 50 m^2/g Data Source: Sanchez et al. (1985) Concentration: [Pu(V)] = 1E-10 M	Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-15	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 0.55 g/L

No CO_2	DLM			CCM (I = 0.1)			TLM		
	Log K_+ = 7.35 Log K_- = -9.17			Log K_+ = 6.47 Log K_- = -9.03			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}PuO_2^\circ$	-0.02	53.7	.0299	-1.41	28.7	.0235	-4.00	83.6	.0201
$XOH\text{-}PuO_2^+$	5.72	7.7	.0213	5.23	6.5	.0214	4.14	87.9	.0218
$XO\text{-}PuO_2OH^-$	-5.39	39.4	.0396	-7.94	46.0	.0256	-9.12	35.0	.0240
$XOH\text{-}PuO_2OH^\circ$	-0.02	53.7	.0299	-1.41	28.7	.0235	-1.30	25.8	.0233
$XOH_2\text{-}PuO_2OH^+$	5.72	7.7	.0213	5.23	6.5	.0214	6.54	16.6	.0226

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

FITEQL Results - No plot available for model results

6/9/95

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Sanchez, A.L. J.W. Murray, and T.H. Sibley. "the Adsorption of Plutonium IV and V on Goethite. Geochimica et Cosmochimica Acta. Vol. 49. pp. 2,297-2,307. 1985.

Sanchez, A.L., J.W. Murray, and T.H. Sibley. 1985. The adsorption of plutonium IV and V on goethite. *Geochimica et Cosmochimica Acta* 49:2297-2307.

Sanchez et. al. (1985)	**Pu(V) - goethite (αFeOOH)**	
Figure 1(b), 1 hr data		
Asp=50 m^2/g	**1E-11 M**	
No CO_2		
0.1 M $NaNO_3$	M/V = 0.55 g/L	
pH	%sorbed	mol sorbed
3.756502	0.729335	7.29E-14
4.036996	1.053485	1.05E-13
5.344619	8.610211	8.61E-13
5.562556	10.55511	1.06E-12
5.867265	15.55916	1.56E-12
6.238565	26.47893	2.65E-12
6.385874	35.17018	3.51E-12
6.678475	52.12723	5.21E-12
7.477578	88.31037	8.83E-12
8.046637	97.26499	9.73E-12
9.075785	98.37925	9.84E-12

Digitized Data

6/9/95

Example FITEQL Input

```
         1
         1
         1
         1
         1
        90
         3          1          3          1
00001  -3.98  1.06E-4   XOH
00160  -2.00  0.00E00   PSI0
00032  -11.0  1.0E-11   PuO2+
00033   0.0   0.00E00   PuO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -9.95  032  1 050 -1
00100  -13.95  050 -1
01050    7.24  001  1 160  1 050  1
01100   -9.06  001  1 160 -1 050 -1
00001    0.00  001  1
03301   -0.10  001  1 160  0 050 -1 032  1 033  1


00002  050.0  0.550
0.1    1.0
         1
      3301
        11          1          1          0
        33
7.29E-14
1.05E-13
8.61E-13
1.06E-12
1.56E-12
2.65E-12
3.51E-12
5.21E-12
8.83E-12
9.73E-12
9.84E-12
        50
-3.76
-4.04
-5.34
-5.56
-5.87
-6.24
-6.39
-6.68
-7.48
-8.05
-9.08
         1
        32       0.10    1.0E-16
```

```
Goethite
Sanchez
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
20 deg C
20 deg C
00000140
00000145
00000168
xopuo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000320
00000320
00000320
00000320
00001070
00001080
00001080
00001080
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001140
00001480
00001490
```

Σ Pu(V) = 1e-11 M

DLM

```
         1
         1
         1
         1
         1
        90
         3          1          3          1
00001  -3.98  1.06E-4   XOH
00160  -2.00  0.00E00   PSI0
00032  -11.0  1.0E-11   PuO2+
00033   0.0   0.00E00   PuO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -9.95  032  1 050 -1
00100  -13.95  050 -1
01050    6.47  001  1 160  1 050  1
01100   -9.03  001  1 160 -1 050 -1
00001    0.00  001  1
03301   -1.40  001  1 160  0 050 -1 032  1 033  1


00001  050.0  0.550      1.0
    0         0
         1
      3301
        11          1          1          0
        33
7.29E-14
1.05E-13
8.61E-13
1.06E-12
1.56E-12
2.65E-12
3.51E-12
5.21E-12
8.83E-12
9.73E-12
9.84E-12
        50
-3.76
-4.04
-5.34
-5.56
-5.87
-6.24
-6.39
-6.68
-7.48
-8.05
-9.08
         1
        32       0.10    1.0E-16
```

```
Goethite
Sanchez
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
20 deg C
20 deg C
00000140
00000145
00000168
xopuo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000320
00000320
00000320
00000320
00001070
00001080
00001080
00001080
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001140
00001480
00001490
```

Σ Pu(V) = 1e-11 M

6/9/95

```
          1
          1
          1
          1
          1
         90
          5         1         3         1
00001  -3.98  1.06E-4   XOH
00160  -2.00  0.00E00   PSI0
00161  -1.00  0.00E00   PSIB
00162  -0.20  0.00E00   PSID
00032  -11.0  1.0E-11   PuO2+
00033   0.0   0.00E00   PuO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -9.95  032  1 050 -1
00100  -13.95  050 -1
01050    5.89  001  1 160  1 050  1
01100   -9.89  001  1 160 -1 050 -1
01103   -7.64  001  1 160 -1 161  1 050 -1 003  1
01055    8.78  001  1 160  1 161 -1 050  1 005  1
00001    0.00  001  1
03301   -3.00  001  1 160 -1 161  1 050 -1 032  1 033  1


00004  050.0  0.550  0.8    0.2
0.1    1.0
          1
       3301
         11         1         1         0
         33
7.29E-14
1.05E-13
8.61E-13
1.06E-12
1.56E-12
2.65E-12
3.51E-12
5.21E-12
8.83E-12
9.73E-12
9.84E-12
         50
-3.76
-4.04
-5.34
-5.56
-5.87
-6.24
-6.39
-6.68
-7.48
-8.05
-9.08
          1
         32       0.10   1.0E-16
```

```
Goethite
Sanchez
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
20 deg C
20 deg C
00000140
00000145
00000147
00000149
00000168
xopuo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000320
00000320
00000320
00000320
00001070
00001080
00001080
00001080
00001080
00001090
00001100
00001110
00001120
00001130
00001140
00001140
00001480
00001490
```

Fig. 13, for data
ΣPu(V) 1e-11M
TLM

Table B-13. Plutonium (V)-Goethite Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: goethite
A_{sp}: 50 m²/g
Data Source: Sanchez et al. (1985)
Concentration: [Pu(V)] = 1E-11 M

Rel Error (pH): (a)
Abs Error (pH): (a)
Rel Error (radionuclide): 0.10
Abs Error (radionuclide): 1.0E-16

Ionic Strength (electrolyte): 0.1 M $NaNO_3$
N_S = 2.31 sites/nm²
M/V = 0.55 g/L

No CO_2	DLM			CCM			TLM		
	Log K_+ = 7.35 Log K_- = -9.17			Log K_+ = 6.47 Log K_- = -9.03			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}PuO_2^o$	-1.25	43.1	.0269	-1.98	30.0	.0219	-4.11	82.7	.0182
$XOH\text{-}PuO_2^+$	5.33	3.3	.0188	4.83	5.5	.0190	4.00	92.5	.0192
$XO\text{-}PuO_2OH^-$	-7.52	42.1	.0310	-8.65	39.6	.0255	-9.74	33.6	.0225
$XOH\text{-}PuO_2OH^o$	-1.25	43.1	.0269	-1.98	30.0	.0219	-1.85	27.7	.0216
$XOH_2\text{-}PuO_2OH^+$	5.33	3.3	.0188	4.83	5.5	.0190	6.05	20.3	.0207

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

Fig. 16, for data

FITEQL Results

Model Results from Turner (1995)

6/9/95

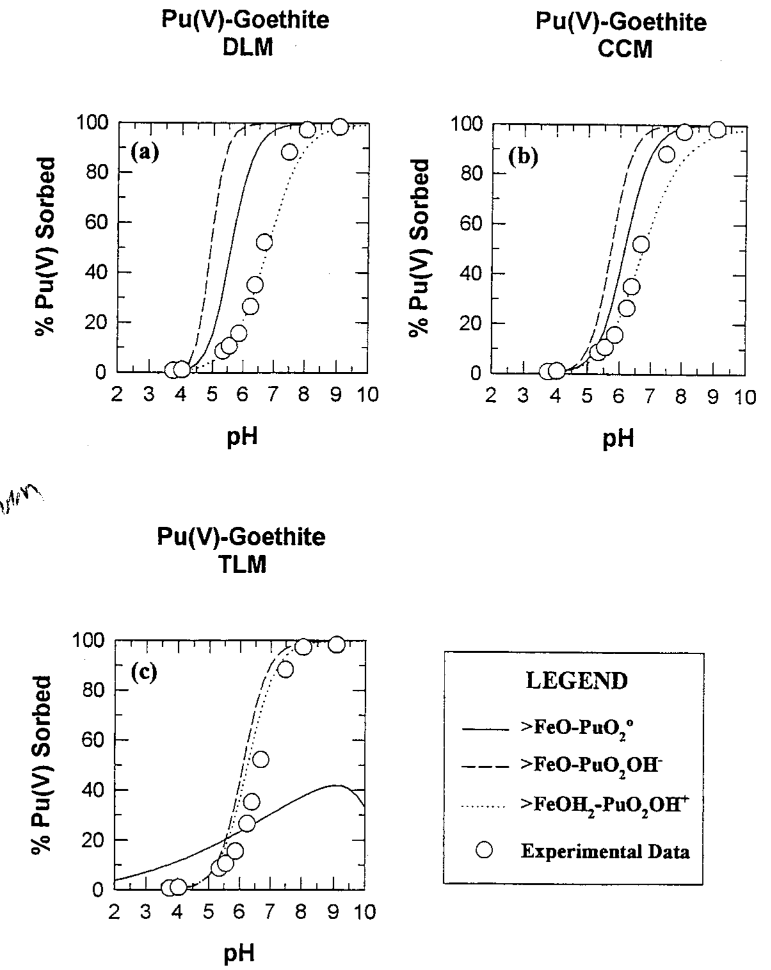

Figure 4-13. Pu(V) sorption on goethite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Pu(V)_T = 1\times10^{-11}$ M, 0.1 M $NaNO_3$, M/V=0.55 g/L. Model parameters from Tables 3-1 and B-13. Data from Sanchez et al. (1985).

Fig. 16, for data

6/12/45
DBLmm

DBLmm

Sanchez et al (1985)
Σ Pu(IV) = $1e^{-10}$ M
C_s = 0.55 g/L
I = 0.1M $NaNO_3$
Fig 1a, 24 hrs data

No plot of modeled data

Experimental Data

Sanchez, A.L., J.W. Murray, and T.H. Sibley. 1985. The adsorption of plutonium IV and V on goethite. *Geochimica et Cosmochimica Acta* 49:2297-2307.

Sanchez et. al. (1985)	**Pu(IV) - goethite (αFeOOH)**	
Figure 1(a), **24 hrs** data		
Asp=50 m^2/g	**1E-10 M**	
No CO_2		
0.1 M $NaNO_3$	M/V = 0.55 g/L	
pH	%sorbed	mol sorbed
2.28	9.394946	9.39E-12
2.95	25.93333	2.59E-11
3.04	33.64987	3.36E-11
3.69	52.91054	5.29E-11
3.65	55.63282	5.56E-11
4.08	62.18267	6.22E-11
4.17	64.04529	6.40E-11
5.02	92.7009	9.27E-11
5.93	98.39108	9.84E-11

Digitized Experimental Results

```
1
1
1
1
1
90
3          1          3          1
00001  -3.98  1.06E-4   XOH
00160  -2.0   0.00E00   PSI0
00041  -10.   1.0E-10   Pu+4
00042   0.0   0.00E00   Puads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050   0.00  050  1
00041   0.00  041  1
04101  -1.30  041  1 050 -1
04102  -3.64  041  1 050 -2
04103  -6.89  041  1 050 -3
04104 -11.17  041  1 050 -4
04105 -16.46  041  1 050 -5
00100 -13.95  050 -1
01050   7.24  001  1 160  1 050  1
01100  -9.06  001  1 160 -1 050 -1
00001   0.00  001  1
04201  14.50  001  1 160  3 050 -1 041  1 042  1

00002  50.0  0.550
0.1    1.0
          1
       4201
          9          1          1          0
         42
9.39E-12
2.59E-11
3.36E-11
5.29E-11
5.56E-11
6.22E-11
6.40E-11
9.27E-11
9.84E-11
         50
-2.28
-2.95
-3.04
-3.69
-3.65
-4.08
-4.17
-5.02
-5.93
          1
         42       0.10   1.0E-13
```


6/12/45
DBLmm

```
00000020 Fig. 1a, 24 hrs data
00000030
00000040
00000050
00000060 DLM
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
00000140
00000145
00000150
xopu+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000880
10%error
```

Example FITEQL Input

DBLmm

DBLmm

```
          1
          1
          1
          1
          1
         90
          3          1          3          1
00001  -3.98  1.06E-4   XOH
00160  -2.0   0.00E00   PSI0
00041  -10.   1.0E-10   Pu+4
00042   0.0   0.00E00   Puads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050   0.00  050  1
00041   0.00  041  1
04101  -1.30  041  1 050 -1
04102  -3.64  041  1 050 -2
04103  -6.89  041  1 050 -3
04104 -11.17  041  1 050 -4
04105 -16.46  041  1 050 -5
00100 -13.95  050 -1
01050   6.47  001  1 160  1 050  1
01100  -9.03  001  1 160 -1 050 -1
00001   0.00  001  1
04201  14.50  001  1 160  3 050 -1 041  1 042  1

00001   50.0  0.550      1.0
    0       0
          1
       4201
          9          1          1          0
         42
9.39E-12
2.59E-11
3.36E-11
5.29E-11
5.56E-11
6.22E-11
6.40E-11
9.27E-11
9.84E-11
         50
-2.28
-2.95
-3.04
-3.69
-3.65
-4.08
-4.17
-5.02
-5.93
          1
         42       0.10   1.0E-13
```

```
00000020
00000030
00000040
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
00000140
00000145
00000150
xopu+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000880
10%error
```

Fig. 1a, 24hr data
$\Sigma Pu(IV) = 1e^{-10}$ M

CCM

$XOH + Pu^{4+} \rightleftharpoons XOPu^{3+} + H^{+}$

6/12/95 DRMurray

Example FITEQL Input

```
                0
                1
                0
                0
                1
               90
                5          1          3          1
00001   -3.98   1.06E-4   XOH
00160   -2.0    0.00E00   PSI0
00161   -1.0    0.00E00   PSI0
00162   -0.5    0.00E00   PSI0
00041   -10.    1.0E-10   Pu+4
00042    0.0    0.00E00   Puads
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   NO3-

00050    0.00   050  1
00041    0.00   041  1
04101   -1.30   041  1 050 -1
04102   -3.64   041  1 050 -2
04103   -6.89   041  1 050 -3
04104  -11.17   041  1 050 -4
04105  -16.46   041  1 050 -5
00100  -13.95   050 -1
01050    5.89   001  1 160  1 050  1
01100   -9.89   001  1 160 -1 050 -1
01055    8.56   001  1 160  1 161 -1 050  1 005  1
01103   -7.64   001  1 160 -1 161  1 050 -1 003  1
00001    0.00   001  1
04201    2.00   001  1 160 -1 161  4 050 -1 041  1 042  1


00004   50.0  0.550  0.8    0.2
0.1    1.0
          1
       4201
          9          1          1          0
         42
9.39E-12
2.59E-11
3.36E-11
5.29E-11
5.56E-11
6.22E-11
6.40E-11
9.27E-11
9.84E-11
         50
-2.28
-2.95
-3.04
-3.69
-3.65
-4.08
-4.17
-5.02
-5.93
          1
         42       0.10    1.0E-13
```

Fig. 1a, 24 hrs data TLM

```
00000020
00000030
00000040
00000050
00000060
00000070
00000080
00000090
00000090
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
00000140
00000145
00000140
00000145
00000150
xopu+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000880
10%error
```

Table BXX. Plutonium (IV)-Goethite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Goethite A_{SP}: 50 m^2/L Data Source: Sanchez et al. (1985) Concentration: [Pu(IV)] = 1E-10 M			Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-13			Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 0.55 g/L		
No CO_2	DLM Log K_+ = 7.35 Log K_- = -9.17			CCM (I = 0.1) Log K_+ = 6.47 Log K_- = -9.03			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Ca} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-Pu^{3+}	14.07	66.6	.0291	15.44	19.0	.0334	-0.07	94.5	.0492
XO-$PuOH^{2+}$	8.74	20.4	.0281	8.88	17.5	.0363	-2.60	87.5	.0396
XO-$Pu(OH)_2^+$	2.80	17.9	.0410	2.29	16.4	.0401	-5.16	55.5	.0271
XOH-$Pu(OH)_2^{2+}$	8.74	20.4	.0281	8.88	17.5	.0363	2.48	61.3	.0281
XO-$Pu(OH)_3^o$	-2.89	30.2	.0498	-4.32	18.7	.0461	-8.34	20.3	.0306
XOH-$Pu(OH)_3^+$	2.80	17.9	.0410	2.29	15.5	.0401	-0.60	21.1	.0294
XO-$Pu(OH)_4^-$	-10.29	38.0	.0656	-10.86	22.6	.0508	-11.99	20.0	.0479
XOH-$Pu(OH)_4^o$	-2.89	30.2	.0498	-4.32	18.7	.0461	-4.23	18.3	.0440
XOH_2-$Pu(OH)_4^+$	2.80	17.9	.0410	2.29	16.4	.0401	3.52	16.7	.0428
XOH-$Pu(OH)_5^-$	-10.29	38.0	.0656	-10.86	22.6	.0508	-8.54	34.1	.0648
XOH_2-$Pu(OH)_5^o$	-2.89	30.2	.0498	-4.32	18.7	.0461	-0.71	33.1	.0650

(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

Fig. 1a 24 hrs data

FITEQL Results. No plot available for model results

6/12/95 DRMurray

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Fig. 1a, 24 & 96 hrs dat

Information potentially subject to copyright protection was redacted from this location. The redacted material (a line drawing on p. 2,299) is from the following reference:

Sanchez, A.L. J.W. Murray, and T.H. Sibley. "the Adsorption of Plutonium IV and V on Goethite. Geochimica et Cosmochimica Acta. Vol. 49. pp. 2,297-2,307. 1985.

Experimental Results

DRMurray

Sanchez, A.L., J.W. Murray, and T.H. Sibley. 1985. The adsorption of plutonium IV and V on goethite. *Geochimica et Cosmochimica Acta* 49:2297-2307.

Sanchez et. al. (1985)	**Pu(IV) - goethite (αFeOOH)**	
Figure 1(a), **24 + 96 hrs** data		
Asp=50 m^2/g	**1E-11 M**	
No CO_2		
0.1 M $NaNO_3$	M/V = 0.55 g/L	
pH	%sorbed	mol sorbed
2.26	21.0414	2.10E-12
2.38	29.96558	3.00E-12
2.41	25.5649	2.56E-12
2.57	34.87797	3.49E-12
2.92	45.88991	4.59E-12
3.01	40.15879	4.02E-12
3.15	45.19399	4.52E-12
3.84	73.97241	7.40E-12
3.99	81.58661	8.16E-12
5.81	100.7449	9.99E-12
6.13	96.93783	9.69E-12
6.86	101.011	9.99E-12
7.46	100.4174	9.99E-12
8.11	100.9292	9.99E-12
8.91	101.1543	9.99E-12

Digitized Experimental Results

DRMurray

6/12/95
DLMmm

```
        1
        1
        1
        1
        1
       90
        3          1          3          1
00001  -3.98  1.06E-4   XOH
00160  -2.0   0.00E00   PSIO
00041  -11.   1.0E-11   Pu+4
00042   0.0   0.00E00   Puads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00041    0.00  041  1
04101   -1.30  041  1 050 -1
04102   -3.64  041  1 050 -2
04103   -6.89  041  1 050 -3
04104  -11.17  041  1 050 -4
04105  -16.46  041  1 050 -5
00100  -13.95  050 -1
01050    7.24  001  1 160  1 050  1
01100   -9.06  001  1 160 -1 050 -1
00001    0.00  001  1
04201   14.50  001  1 160  3 050 -1 041  1 042  1


00002   50.0  0.550
0.1    1.0
          1
       4201
         15          1          1          0
         42
2.10E-12
3.00E-12
2.56E-12
3.49E-12
4.59E-12
4.02E-12
4.52E-12
7.40E-12
8.16E-12
9.99E-12
9.69E-12
9.99E-12
9.99E-12
9.99E-12
9.99E-12
         50
-2.26
-2.38
-2.41
-2.57
-2.92
-3.01
-3.15
-3.84
-3.99
-5.81
-6.13
-6.86
-7.46
-8.11
-8.91
        1
       42       0.10    1.0E-14
```

Example FITEQL Input Files

```
        1
        1
        1
        1
        1
       90
        3          1          3          1
00001  -3.98  1.06E-4   XOH
00160  -2.0   0.00E00   PSIO
00041  -11.   1.0E-11   Pu+4
00042   0.0   0.00E00   Puads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00041    0.00  041  1
04101   -1.30  041  1 050 -1
04102   -3.64  041  1 050 -2
04103   -6.89  041  1 050 -3
04104  -11.17  041  1 050 -4
04105  -16.46  041  1 050 -5
00100  -13.95  050 -1
01050    6.47  001  1 160  1 050  1
01100   -9.03  001  1 160 -1 050 -1
00001    0.00  001  1
04201   14.50  001  1 160  3 050 -1 041  1 042  1


00001   50.0  0.550      1.0
          0          0
        1
       4201
         15          1          1          0
         42
2.10E-12
3.00E-12
2.56E-12
3.49E-12
4.59E-12
4.02E-12
4.52E-12
7.40E-12
8.16E-12
9.99E-12
9.69E-12
9.99E-12
9.99E-12
9.99E-12
9.99E-12
         50
-2.26
-2.38
-2.41
-2.57
-2.92
-3.01
-3.15
-3.84
-3.99
-5.81
-6.13
-6.86
-7.46
-8.11
-8.91
        1
       42       0.10    1.0E-14
```

```
00000020 Fig. 1a, 24 Hours
00000030 Σ Pu(IV) = 1e-11M
00000040 DLM
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
00000140
00000145
00000150
xopu+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000320
00000340
00000360
00000380
00000400
00000420
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000640
00000660
00000680
00000700
00000720
00000740
00000880
10%error
```

DLMmm

```
        1
        1
        1
        1
        1
       90
        5          1          3          1
00001  -3.98  1.06E-4   XOH
00160  -2.0   0.00E00   PSIO
00161  -1.0   0.00E00   PSIO
00162  -0.5   0.00E00   PSIO
00041  -11.   1.0E-11   Pu+4
00042   0.0   0.00E00   Puads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00041    0.00  041  1
04101   -1.30  041  1 050 -1
04102   -3.64  041  1 050 -2
04103   -6.89  041  1 050 -3
04104  -11.17  041  1 050 -4
04105  -16.46  041  1 050 -5
00100  -13.95  050 -1
01050    5.89  001  1 160  1 050  1
01100   -9.89  001  1 160 -1 050 -1
01055    8.56  001  1 160  1 161 -1 050  1 005  1
01103   -7.64  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
04201    1.00  001  1 160 -1 161  4 050 -1 041  1 042  1


00004   50.0  0.550  0.8    0.2
0.1    1.0
          1
       4201
         15          1          1          0
         42
2.10E-12
3.00E-12
2.56E-12
3.49E-12
4.59E-12
4.02E-12
4.52E-12
7.40E-12
8.16E-12
9.99E-12
9.69E-12
9.99E-12
9.99E-12
9.99E-12
9.99E-12
         50
-2.26
-2.38
-2.41
-2.57
-2.92
-3.01
-3.15
-3.84
-3.99
-5.81
-6.13
-6.86
-7.46
-8.11
-8.91
        1
       42       0.10    1.0E-14
```

```
00000020 Fig. 1a, 24 & 96 Hours
00000030 Σ Pu(IV) = 1e-11M
00000040 TLM
00000050
00000060
00000070
00000080
00000090
00000090
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
20 deg C
00000140
00000145
00000140
00000145
00000150
xopu+3
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000320
00000340
00000360
00000380
00000400
00000420
00000560
00000580
00000600
00000620
00000640
00000660
00000680
00000700
00000720
00000740
00000640
00000660
00000680
00000700
00000720
00000740
00000880
10%error
```


6/12/95
DLMmm

Example FITEQL Input

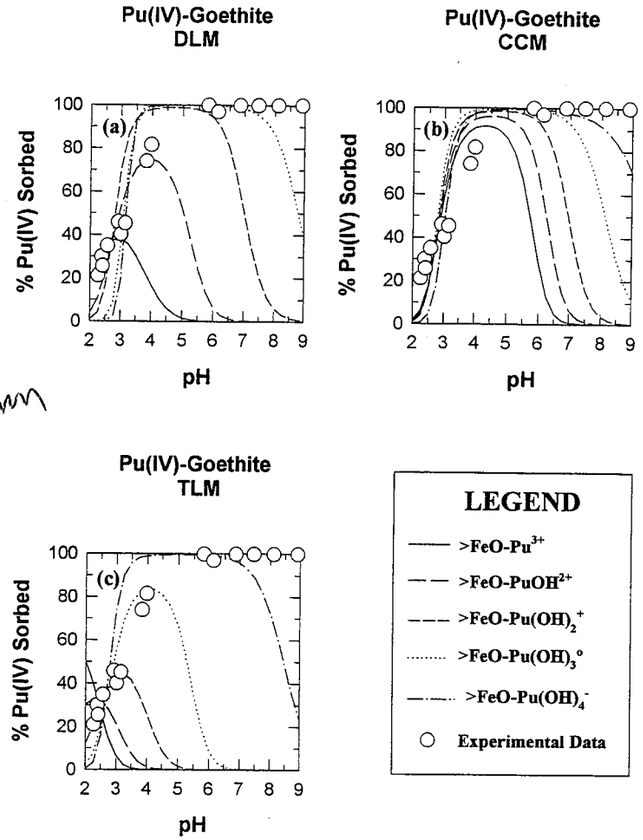
Table B-12. Plutonium (IV)-Goethite Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: Goethite A_{sp}: 50 m^2/L Data Source: Sanchez et al. (1985) Concentration: [Pu(IV)] = 1E-11 M				Rel Error (pH): (a) Abs Error (pH): (a) Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-14			Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 0.55 g/L		
No CO_2	DLM Log K_+ = 7.35 Log K_- = -9.17			CCM Log K_+ = 6.47 Log K_- = -9.03			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.64 Log K_{An} = 8.78		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-Pu^{3+}	14.42	52.9	.0241	16.08	46.5	.0313	0.54	76.7	.0303
XO-$PuOH^{2+}$	9.10	44.3	.0277	9.65	43.2	.0333	-2.09	65.6	.0263
XO-$Pu(OH)_2^+$	3.84	39.9	.0356	3.25	39.2	.0355	-4.86	49.1	.0241
XOH-$Pu(OH)_2^{2+}$	9.10	44.3	.0277	9.65	43.2	.0333	2.80	50.9	.0241
XO-$Pu(OH)_3^\circ$	-2.37	30.6	.0455	-3.10	30.6	.0365	-7.87	46.9	.0301
XOH-$Pu(OH)_3^+$	3.84	39.9	.0356	3.25	39.2	.0355	-0.20	46.2	.0291
XO-$Pu(OH)_4^-$	-8.33	30.4	.0515	-10.12	23.7	.0435	-10.72	29.2	.0374
XOH-$Pu(OH)_4^\circ$	-2.37	30.6	.0455	-3.10	30.6	.0365	-3.04	31.0	.0361
XOH_2-$Pu(OH)_4^+$	3.84	39.9	.0356	3.25	39.2	.0355	4.62	33.0	.0351
XOH-$Pu(OH)_5^-$	-8.33	30.4	.0515	-10.12	23.7	.0435	n.c	n.c	n.c.
XOH_2-$Pu(OH)_5^\circ$	-2.37	30.6	.0455	-3.10	30.6	.0365	n.c.	n.c.	n.c.

n.c. FITEQL did not converge
(a) No error assigned to pH to allow convergence for extremely low radionuclide concentrations.

Fig 1a, 24 & 96 Hours

6/2/95 DPLamm



DPLamm

Model results using MINTEQA2 of CNWRA radionuclide database

Figure 4-12. Pu(IV) sorption on goethite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Pu(IV)_T = 1 \times 10^{-11}$ M, 0.1 M $NaNO_3$, M/V=0.55 g/L. Model parameters from Tables 3-1 and B-12. Data from Sanchez et al. (1985).

Fig 1a, 2/5 pg

Am(III)- am SiO_2 (Moulin et al., 1992)

6/26/95 DPLamm

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 2: Americium sorption onto amorphous silica...) is from the following reference:

Moulin, V., D. Stammose, and G. Ouzounian. "Actinide Sorption at Oxide-Water Interfaces: Application to a Alumina and Amorphous Silica." Applied Geochemistry supplemental Isue. Vol. 1. pp. 163-166. 1992.

Moulin, V., D. Stammose, and G. Ouzounian. 1992. Actinide sorption at oxide-water interfaces: Application to α alumina and amorphous silica. *Applied Geochemistry Supplemental Issue* 1:163-166.

DPLamm

Moulin et al. (1992)	Am(III)-SiO2			
Figure 2 (page 164)				
Asp=0.075 m2/g	Atm CO2			
Am(III)=1E-8 M	M/V=10 g/L			
0.1 M NaClO4				
pH	Log Kd (mL/g)	Kd (mL/g)	% sorbed	mol sorbed
2.66515	0.27335	1.87651	1.842	1.842E-10
4.13703	0.68725	4.86687	4.641	6.641E-10
5.91044	2.06165	115.252	53.54	5.354E-09
6.88318	2.86485	732.571	87.99	8.799E-09
0.01 M NaClO4				
pH	Log Kd (mL/g)	Kd (mL/g)	% sorbed	mol sorbed
3.07530	0.39874	2.50461	2.443	2.443E-10
4.47244	1.29325	19.6449	16.42	1.642E-09
6.43667	2.33715	217.345	68.49	6.849E-09
7.78816	2.66229	459.505	82.13	8.213E-09

Digitized Data

6/26/95 DBLamm

TLM

$>SiOH^0 + Am^{3+} = >SiO\cdot Am^{2+} + H^+$

```
                0
                1
                0
                0
                1
               90
                6         1         3         1
00001   -5.54   2.88E-6   XOH
00160   -2.0    0.00E00   PSIO
00161   -1.0    0.00E00   PSIB
00162   -0.2    0.00E00   PSID
00140   -3.5    3.16E-4   CO2g
00031   -8.0    1.00E-8   Am+3
00032    0.0    0.00E00   Am(ads)
00050    0.0    0.00E00   H+
00003   -2.0    0.00E00   NA+
00005   -2.0    0.00E00   ClO4-

00050    0.00   050   1
00031    0.00   031   1
03100   -6.76   031   1  050 -1
03101  -16.24   031   1  050 -2
03102  -24.04   031   1  050 -3
03300  -10.65   031   1  140   1  050 -2
03301  -24.17   031   1  140   2  050 -4
03302  -40.73   031   1  140   3  050 -6
01401  -18.38   140   1  050 -2
01402   -8.23   140   1  050 -1
01403   -1.98   140   1
01404  -17.29   140   1  003   1  050 -2
01405   -8.58   140   1  003   1  050 -1
00100  -13.90   050  -1
01050    0.85   001   1  160   1  050   1
01100   -4.85   001   1  160  -1  050  -1
01103   -6.22   001   1  160  -1  161   1  050  -1  003   1
00001    0.00   001   1
03201   -1.00   001   1  160  -1  161   3  050  -1  031   1  032   1

00004   0.075  10.00   0.8     0.2
0.01    1.0
          1
       3201
          4         1         1         0
         32
2.4434E-10
1.6419E-09
6.8489E-09
8.2127E-09
         50
-3.08
-4.47
-6.44
-7.79

          1         1
         32       0.10    1.0E-11
         50       0.05    0.0E-00
```

I=0.01

```
Americum
    on
am-Silic
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000095
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000147
00000147
00000147
00000146
00000147
00000147
00000147
00000147
00000139
00000140
00000145
00000147
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000560
00000580
00000600
00000620
00000640
00000880
10%error
+/- 0.02
```

```
                0
                1
                0
                0
                1
               90
                6         1         3         1
00001   -5.54   2.88E-6   XOH
00160   -2.0    0.00E00   PSIO
00161   -1.0    0.00E00   PSIB
00162   -0.2    0.00E00   PSID
00140   -3.5    3.16E-4   CO2g
00031   -8.0    1.00E-8   Am+3
00032    0.0    0.00E00   Am(ads)
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   ClO4-

00050    0.00   050   1
00031    0.00   031   1
03100   -7.03   031   1  050 -1
03101  -16.65   031   1  050 -2
03102  -24.45   031   1  050 -3
03300  -11.06   031   1  140   1  050 -2
03301  -24.46   031   1  140   2  050 -4
03302  -40.37   031   1  140   3  050 -6
01401  -18.00   140   1  050 -2
01402   -8.11   140   1  050 -1
01403   -1.98   140   1
01404  -17.17   140   1  003   1  050 -2
01405   -8.58   140   1  003   1  050 -1
00100  -13.78   050  -1
01050    0.79   001   1  160   1  050   1
01100   -4.79   001   1  160  -1  050  -1
01103   -6.22   001   1  160  -1  161   1  050  -1  003   1
00001    0.00   001   1
03201   -1.00   001   1  160  -1  161   3  050  -1  031   1  032   1

00004   0.075  10.00   0.8     0.2
0.1     1.0
          1
       3201
          4         1         1         0
         32
1.8419E-10
4.6410E-10
5.3543E-09
8.7989E-09
         50
-2.67
-4.14
-5.91
-6.88

          1         1
         32       0.10    1.0E-11
         50       0.05    0.0E-00
```

I=0.1

```
Americum
    on
am-Silic
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000095
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000126
00000147
00000147
00000147
00000146
00000147
00000147
00000147
00000147
00000139
00000140
00000145
00000147
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000560
00000580
00000600
00000620
00000640
00000880
10%error
+/- 0.02
```

DLM

$>SiOH^0 + Am^{3+} = >SiO\cdot Am^{2+} + H^+$

```
                0
                1
                0
                0
                1
               90
                4         1         3         1
00001   -5.54   2.88E-6   XOH
00160   -2.0    0.00E00   PSIO
00140   -3.5    3.16E-4   CO2g
00031   -8.0    1.00E-8   Am+3
00032    0.0    0.00E00   Am(ads)
00050    0.0    0.00E00   H+
00003   -2.0    0.00E00   NA+
00005   -2.0    0.00E00   ClO4-

00050    0.00   050   1
00031    0.00   031   1
03100   -6.76   031   1  050 -1
03101  -16.24   031   1  050 -2
03102  -24.04   031   1  050 -3
03300  -10.65   031   1  140   1  050 -2
03301  -24.17   031   1  140   2  050 -4
03302  -40.73   031   1  140   3  050 -6
01401  -18.38   140   1  050 -2
01402   -8.23   140   1  050 -1
01403   -1.98   140   1
01404  -17.29   140   1  003   1  050 -2
01405   -8.58   140   1  003   1  050 -1
00100  -13.90   050  -1
01100   -7.15   001   1  160  -1  050  -1
00001    0.00   001   1
03201   -3.01   001   1  160   2  050  -1  031   1  032   1

00002   0.075  10.00
0.01    1.0
          1
       3201
          4         1         1         0
         32
2.4434E-10
1.6419E-09
6.8489E-09
8.2127E-09
         50
-3.08
-4.47
-6.44
-7.79

          1         1
         32       0.10    1.0E-11
         50       0.05    0.0E-00
```

I=0.01

6/26/95 DBLamm

DLM

$>SiOH^0 + Am^{3+} = >SiO\cdot Am^{2+} + H^+$

```
                0
                1
                0
                0
                1
               90
                4         1         3         1
00001   -5.54   2.88E-6   XOH
00160   -2.0    0.00E00   PSIO
00140   -3.5    3.16E-4   CO2g
00031   -8.0    1.00E-8   Am+3
00032    0.0    0.00E00   Am(ads)
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   ClO4-

00050    0.00   050   1
00031    0.00   031   1
03100   -7.03   031   1  050 -1
03101  -16.65   031   1  050 -2
03102  -24.45   031   1  050 -3
03300  -11.06   031   1  140   1  050 -2
03301  -24.46   031   1  140   2  050 -4
03302  -40.37   031   1  140   3  050 -6
01401  -18.00   140   1  050 -2
01402   -8.11   140   1  050 -1
01403   -1.98   140   1
01404  -17.17   140   1  003   1  050 -2
01405   -8.58   140   1  003   1  050 -1
00100  -13.78   050  -1
01100   -7.09   001   1  160  -1  050  -1
00001    0.00   001   1
03201   -3.00   001   1  160   2  050  -1  031   1  032   1

00002   0.075  10.00
0.1     1.0
          1
       3201
          4         1         1         0
         32
2.4434E-10
1.6419E-09
6.8489E-09
8.2127E-09
         50
-3.08
-4.47
-6.44
-7.79

          1         1
         32       0.10    1.0E-11
         50       0.05    0.0E-00
```

I=0.1

```
Americum
    on
am-Silic
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000095
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
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00000147
00000147
00000147
00000147
00000139
00000140
00000145
00000147
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000560
00000580
00000600
00000620
00000640
00000880
10%error
+/- 0.02
```

Example FITEQL Inputs

CCM

$>SiOH^0 + Am^{3+} = >SiO\cdot Am^{2+} + H^+$

```
                0
                1
                0
                0
                1
               90
                4         1         3         1
00001   -5.54   2.88E-6   XOH
00160   -2.0    0.00E00   PSIO
00140   -3.5    3.16E-4   CO2g
00031   -8.0    1.00E-8   Am+3
00032    0.0    0.00E00   Am(ads)
00050    0.0    0.00E00   H+
00003   -2.0    0.00E00   NA+
00005   -2.0    0.00E00   ClO4-

00050    0.00   050   1
00031    0.00   031   1
03100   -6.76   031   1  050 -1
03101  -16.24   031   1  050 -2
03102  -24.04   031   1  050 -3
03300  -10.65   031   1  140   1  050 -2
03301  -24.17   031   1  140   2  050 -4
03302  -40.73   031   1  140   3  050 -6
01401  -18.38   140   1  050 -2
01402   -8.23   140   1  050 -1
01403   -1.98   140   1
01404  -17.29   140   1  003   1  050 -2
01405   -8.58   140   1  003   1  050 -1
00100  -13.90   050  -1
01100   -7.10   001   1  160  -1  050  -1
00001    0.00   001   1
03201   -3.00   001   1  160   2  050  -1  031   1  032   1

00001   0.075  10.00      1.0
0       0
          1
       3201
          4         1         1         0
         32
2.4434E-10
1.6419E-09
6.8489E-09
8.2127E-09
         50
-3.08
-4.47
-6.44
-7.79

          1         1
         32       0.10    1.0E-11
         50       0.05    0.0E-00
```

I=0.01

```
Americum
    on
am-Silic
2.3s\nm2
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00000070
00000080
00000090
00000092
00000094
00000095
00000098
00000100
00000102
00000104
00000106
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00000120
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00000147
00000139
00000140
00000145
00000147
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000560
00000580
00000600
00000620
00000640
00000880
10%error
+/- 0.02
```

```
                0
                1
                0
                0
                1
               90
                4         1         3         1
00001   -5.54   2.88E-6   XOH
00160   -2.0    0.00E00   PSIO
00140   -3.5    3.16E-4   CO2g
00031   -8.0    1.00E-8   Am+3
00032    0.0    0.00E00   Am(ads)
00050    0.0    0.00E00   H+
00003   -1.0    0.00E00   NA+
00005   -1.0    0.00E00   ClO4-

00050    0.00   050   1
00031    0.00   031   1
03100   -7.03   031   1  050 -1
03101  -16.65   031   1  050 -2
03102  -24.45   031   1  050 -3
03300  -11.06   031   1  140   1  050 -2
03301  -24.46   031   1  140   2  050 -4
03302  -40.37   031   1  140   3  050 -6
01401  -18.00   140   1  050 -2
01402   -8.11   140   1  050 -1
01403   -1.98   140   1
01404  -17.17   140   1  003   1  050 -2
01405   -8.58   140   1  003   1  050 -1
00100  -13.78   050  -1
01100   -7.04   001   1  160  -1  050  -1
00001    0.00   001   1
03201   -3.00   001   1  160   2  050  -1  031   1  032   1

00001   0.075  10.00      1.0
0       0
          1
       3201
          4         1         1         0
         32
1.8419E-10
4.6410E-10
5.3543E-09
8.7989E-09
         50
-2.67
-4.14
-5.91
-6.88

          1         1
         32       0.10    1.0E-11
         50       0.05    0.0E-00
```

I=0.1

```
Americum
    on
am-Silic
2.3s\nm2
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000095
00000098
00000100
00000102
00000104
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00000140
00000145
00000147
00000150
xoam
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000560
00000580
00000600
00000620
00000640
00000880
10%error
+/- 0.02
```

Table BXX. Americium (III)-Amorphous SiO_2 Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: amorphous SiO_2 A_{SP}: 0.075 m^2/g Data Source: Moulin et al. (1992) Concentration: [Am(III)] = 1E-8 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-11			Ionic Strength (electrolyte): 0.01 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 10 g/L		
$p(CO_2)$ = 1E-3.5 atm	DLM Log K_+ = (a) Log K_- = -7.20			CCM (I = 0.01) Log K_+ = (a) Log K_- = -7.10			TLM Log K_+ = 0.90 Log K_- = -4.90 Log K_{Cat} = -6.22 Log K_{An} = (a)		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-Am^{2+}	0.77	15.5	.0570	0.78	14.3	.0528	-1.25	24.9	.0783
XO-$AmOH^+$	-3.83	24.7	.0722	-3.81	24.7	.0703	-4.71	25.1	.0801
XO-$Am(OH)_2^0$	-8.32	25.2	.0852	-8.32	25.2	.0852	-8.16	25.2	.0838
XOH-$Am(OH)_2^+$	-3.83	24.7	.0722	-3.81	24.7	.0703	-5.04	25.1	.0813
XO-$Am(OH)_3^-$	-12.78	25.2	.1017	-12.82	25.2	.1024	-11.58	25.2	.0891
XOH-$Am(OH)_3^0$	-8.32	25.2	.0852	-8.32	25.2	.0852	-8.31	25.2	.0852
XOH_2-$Am(OH)_3^+$	-3.83	24.7	.0722	-3.81	24.7	.0703	-5.03	25.1	.0824
XO-$AmCO_3^0$	11.36	21.6	.0601	11.36	21.6	.0601	11.53	21.6	.0591
XOH-$AmCO_3^+$	15.85	21.2	05109	15.88	21.2	.0496	14.81	21.5	.0570
XOH_2-$Am(CO_3)_2^0$	31.05	14.2	.0701	31.05	14.2	.0701	30.92	14.2	.0715
XOH_2-$Am(CO_3)_3^{2-}$	36.29	22.7	.1204	35.64	22.7	.1171	39.31	22.9	.1405

(a) Due to low zero-point of charge (pH_{ZPC}=2.1 for SiO_2), XOH_2^+ (DLM, CCM) and XOH_2-An (TLM only) are assumed to be insignficant at slightly acid to basic pH [see discussion in Turner (1993)].

FITEQL Results I=0.01 M

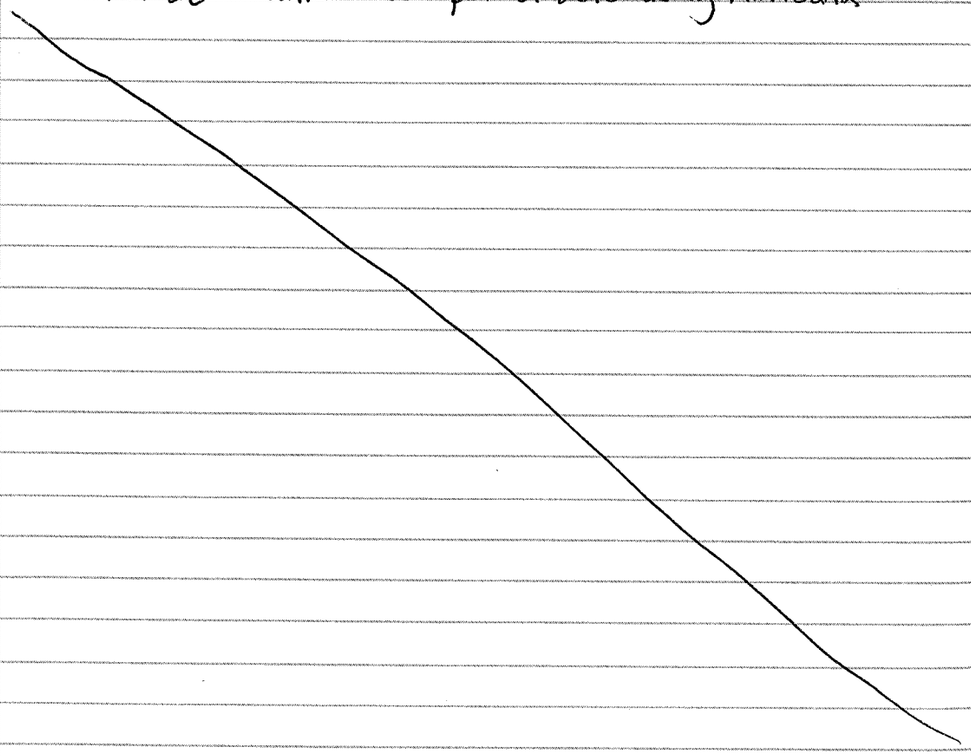
6/26/95 DRDunn

Table BXX. Americium (III)-Amorphous SiO_2 Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: amorphous SiO_2 A_{SP}: 0.075 m^2/g Data Source: Moulin et al. (1992) Concentration: [Am(III)] = 1E-8 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-11			Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 10 g/L		
$p(CO_2)$ = 1E-3.5 atm	DLM Log K_+ = (a) Log K_- = -7.20			CCM (I = 0.1) Log K_+ = (a) Log K_- = -7.04			TLM Log K_+ = 0.90 Log K_- = -4.90 Log K_{Cat} = -6.22 Log K_{An} = (a)		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-Am^{2+}	0.83	24.3	.0697	0.83	23.2	.0693	-0.46	37.7	.0746
XO-$AmOH^+$	-3.30	38.3	.0713	-3.31	38.3	.0712	-3.90	38.6	.0780
XO-$Am(OH)_2^0$	-7.53	38.8	.0855	-7.53	38.8	.0855	-7.36	38.8	.0834
XOH-$Am(OH)_2^+$	-3.30	38.3	.0713	-3.31	38.3	.0712	-4.07	38.7	.0796
XO-$Am(OH)_3^-$	-11.77	38.8	.1027	-11.77	38.8	.1027	-10.81	38.8	.0897
XOH-$Am(OH)_3^0$	-7.53	38.8	.0855	-7.53	38.3	.0855	-7.52	38.8	.0854
XOH_2-$Am(OH)_3^+$	-3.30	38.3	.0713	-3.31	38.3	.0712	-5.23	38.8	.0816
XO-$AmCO_3^0$	12.15	31.7	.0766	12.15	33.2	.0603	12.33	33.2	.0589
XOH-$AmCO_3^+$	16.38	32.6	.0506	16.39	32.6	.0506	15.62	33.2	.0562
XOH_2-$Am(CO_3)_2^0$	31.84	21.5	.0694	31.84	21.5	.0694	31.69	21.5	.0709
XOH_2-$Am(CO_3)_3^{2-}$	36.85	18.4	.1087	36.78	18.4	.1083	39.70	18.4	.1156

(a) Due to low zero-point of charge (pH_{ZPC}=2.1 for SiO_2), XOH_2^+ (DLM, CCM) and XOH_2-An (TLM only) are assumed to be insignficant at slightly acid to basic pH [see discussion in Turner (1993)].

FITEQL Results - No plot of data using MINTEQA2



U(VI) - Kaolinite Sorption (Payne et al, 1992)

7/6/95 DRDunn

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 7: Effect of solid/liquid ratio on U(VI) adsorption to KGa-1 kaolinite...) is from the following reference:

Payne, T.E., K. Sekine, J.A. Davis, and T.D. Waite. "Modeling of Radionuclide sorption Processes in the Weathered Zone of the Koongarra Ore Body." Alligator Rivers Analogue Project Annual Report, 1990-1991. P. Duerden, ed. Australian Nuclear Science and Technology Organization. pp. 57-85. 1992.

DRDunn

Payne et al. (1992)	U(VI)-Kaolinite	
Figure 7 (page 75)		
Asp=11 m2/g (assumed)	No CO2	U(VI)=1E-06
0.1M NaNO3	Si:Al = 1:1	
M/V = 1 g/L		
pH	%sorbed	mol sorbed
2.99511	0.24102	2.410E-09
3.98533	8.75121	8.751E-08
4.88398	23.93280	2.393E-07
5.42983	39.10222	3.910E-07
5.89250	52.05378	5.205E-07
6.52955	76.70657	7.671E-07
6.91263	85.16631	8.517E-07
7.12724	80.33023	8.033E-07
7.58807	72.04723	7.205E-07
M/V = 4 g/L		
pH	%sorbed	mol sorbed
2.97867	1.33318	1.333E-08
3.48851	2.44349	2.443E-08
3.98533	8.81028	8.810E-08
4.47388	18.04152	1.804E-07
4.94350	35.18706	3.519E-07
5.47024	65.32925	6.533E-07
6.10257	90.80881	9.081E-07
6.62757	95.43410	9.543E-07
7.13625	95.74696	9.575E-07
M/V = 16 g/L		
pH	%sorbed	mol sorbed
2.99510	0.30008	3.001E-09
3.57160	7.76236	7.762E-08
3.98397	16.81378	1.681E-07
4.42887	38.35893	3.836E-07
4.88566	52.31443	5.231E-07
5.43677	92.79413	9.279E-07
5.80361	94.22438	9.422E-07
7.01900	97.51492	9.751E-07
7.33777	99.32744	9.933E-07

Digitized data

Payne, T.E., K. Sekine, J.A. Davis, and T.D. Waite. 1992. Modeling of radionuclide sorption processes in the weathered zone of the Koongarra ore body. P. Duerden, ed. *Alligator Rivers Analogue Project Annual Report, 1990-1991*. Australian Nuclear Science and Technology Organization (ANSTO):57-85.

```
Uranium
  on
Kaolinit
2.3si/nm
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00000060
00000070
00000080
00000080
00000090
00000092
00000094
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00000100
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00000690
00000700
00000710
00000720
00000730
00000740
00000750
00000751
00000752
00001170
00001180
00001190
```

```
        0
        1
        0
        0
        1
       90
        6         1         3         1
00001  -4.07  8.44E-5   AlOH
00002  -4.07  8.44E-5   SiOH
00160  -1.0   0.00E00   PSIO
00161  -0.5   0.00E00   PSIB
00162  -0.1   0.00E00   PSID
00032  -6.0   1.00E-6   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
00100  -13.78  050 -1
01050    6.79  001  1 160  1 050  1
01100  -10.79  001  1 160 -1 050 -1
01055    9.90  001  1 160  1 161 -1 050  1 005  1
01103   -7.73  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
02050    0.79  002  1 160  1 050  1
02100   -4.79  002  1 160 -1 050 -1
02103   -6.22  002  1 160 -1 161  1 050 -1 003  1
00002    0.00  002  1
23301   -2.71  002  1 160 -1 161  2 050 -1 032  1 033  1


00004  011.0  4.0000  0.8   0.2
0.1    1.0
         1
     23301
         9         1         1         0
        33
1.333E-8
2.444E-8
8.810E-8
1.804E-7
3.519E-7
6.533E-7
9.081E-7
9.543E-7
9.575E-7
        50
-2.98
-3.49
-3.99
-4.47
-4.94
-5.47
-6.10
-6.63
-7.14
         1         1
        33      0.10    1.0E-10
        50      0.05    0.0E-00
```

TLM

$>SiOH^0 + UO_2^{2+} = >SiOUO_2^+ + H^+$

```
Uranium
  on
Kaolinit
2.3si/nm
00000050
00000060
00000070
00000080
00000080
00000090
00000092
00000094
00000098
00000100
00000102
00000103
00000104
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00000120
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00000690
00000700
00000710
00000720
00000730
00000740
00000750
00000751
00000752
00001170
00001180
00001190
```

```
        0
        1
        0
        0
        1
       90
        6         1         3         1
00001  -4.07  8.44E-5   AlOH
00002  -4.07  8.44E-5   SiOH
00160  -1.0   0.00E00   PSIO
00161  -0.5   0.00E00   PSIB
00162  -0.1   0.00E00   PSID
00032  -6.0   1.00E-6   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
00100  -13.78  050 -1
01050    6.79  001  1 160  1 050  1
01100  -10.79  001  1 160 -1 050 -1
01055    9.90  001  1 160  1 161 -1 050  1 005  1
01103   -7.73  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
02050    0.79  002  1 160  1 050  1
02100   -4.79  002  1 160 -1 050 -1
02103   -6.22  002  1 160 -1 161  1 050 -1 003  1
00002    0.00  002  1
23301   -2.71  001  1 160 -1 161  2 050 -1 032  1 033  1


00004  011.0  4.0000  0.8   0.2
0.1    1.0
         1
     23301
         9         1         1         0
        33
1.333E-8
2.444E-8
8.810E-8
1.804E-7
3.519E-7
6.533E-7
9.081E-7
9.543E-7
9.575E-7
        50
-2.98
-3.49
-3.99
-4.47
-4.94
-5.47
-6.10
-6.63
-7.14
         1         1
        33      0.10    1.0E-10
        50      0.05    0.0E-00
```

TLM

$>AlOH^0 + UO_2^{2+} = >AlOUO_2^+ + H^+$

```
Uranium
  on
Kaolinit
2.3si/nm
00000050
00000060
00000070
00000080
00000080
00000090
00000092
00000094
00000098
00000100
00000102
00000103
00000104
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00000340
00000360
00000370
00000371
00000372
00000680
00000690
00000700
00000710
00000720
00000730
00000740
00000750
00000751
00000752
00001170
00001180
00001190
```

```
        0
        1
        0
        0
        1
       90
        4         1         3         1
00001  -4.07  8.44E-5   SiOH
00002  -4.07  8.44E-5   SiOH
00160  -1.0   0.00E00   PSIO
00032  -6.0   1.00E-6   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
00100  -13.78  050 -1
01050    8.12  001  1 160  1 050  1
01100   -9.56  001  1 160 -1 050 -1
00001    0.00  001  1
02100   -7.04  002  1 160 -1 050 -1
00002    0.00  002  1
23301    2.00  002  1 160  1 050 -1 032  1 033  1


00001  011.0  4.0000     1.0
         0         0
         1
     23301
         9         1         1         0
        33
1.333E-8
2.444E-8
8.810E-8
1.804E-7
3.519E-7
6.533E-7
9.081E-7
9.543E-7
9.575E-7
        50
-2.98
-3.49
-3.99
-4.47
-4.94
-5.47
-6.10
-6.63
-7.14
         1         1
        33      0.10    1.0E-10
        50      0.05    0.0E-00
```

CCM

$>SiOH^0 + UO_2^{2+} = >SiOUO_2^+ + H^+$

```
Uraniu
  on
Kaolini
2.3si/n
0000005
0000006
0000007
0000008
0000008
0000009
0000009
0000010
0000010
0000010
0000011
0000012
0000012
0000012
0000012
0000012
0000012
0000013
0000013
0000013
0000013
0000013
0000013
0000014
0000014
0000015
0000014
0000015
xouo2
0000017
0000017
0000018
0000018
0000019
0000019
0000023
0000024
0000026
0000028
0000030
0000032
0000034
0000036
0000037
0000037
0000037
0000068
0000069
0000070
0000071
0000072
0000073
0000074
0000075
0000075
0000117
0000118
0000119
```

Example FITEQL Inputs

```
Uranium on Kaolinit 2.3si/nm
        0
        1
        0
        0
        1
       90
        4        1        3        1
00001  -4.07  8.44E-5   AlOH
00002  -4.07  8.44E-5   SiOH
00160  -1.0   0.00E00   PSIO
00032  -6.0   1.00E-6   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
00100  -13.78  050 -1
01050    8.12  001  1 160  1 050  1
01100   -9.56  001  1 160 -1 050 -1
00001    0.00  001  1
02100   -7.04  002  1 160 -1 050 -1
00002    0.00  002  1
13301    2.00  001  1 160  1 050 -1 032  1 033  1


00001  011.0  4.0000     1.0
     0      0
     1
    13301
       9         1         1         0
      33
1.333E-8
2.444E-8
8.810E-8
1.804E-7
3.519E-7
6.533E-7
9.081E-7
9.543E-7
9.575E-7
      50
-2.98
-3.49
-3.99
-4.47
-4.94
-5.47
-6.10
-6.63
-7.14
       1        1
      33     0.10   1.0E-10
      50     0.05   0.0E-00
```

CCM

$>AlOH^0 + UO_2^{2+} = >AlO{\cdot}UO_2^+ + H^+$

```
Uranium on Kaolinit 2.3si/nm
        0
        1
        0
        0
        1
       90
        4        1        3        1
00001  -4.07  8.44E-5   AlOH
00002  -4.07  8.44E-5   SiOH
00160  -1.0   0.00E00   PSIO
00032  -6.0   1.00E-6   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
00100  -13.78  050 -1
01050    8.22  001  1 160  1 050  1
01100   -9.62  001  1 160 -1 050 -1
00001    0.00  001  1
02100   -7.09  002  1 160 -1 050 -1
00002    0.00  002  1
xouo2   23301    3.00  002  1 160  1 050 -1 032  1 033  1


00002  011.0  4.0000
0.1    1.0
         1
     23301
        9         1         1         0
       33
1.333E-8
2.444E-8
8.810E-8
1.804E-7
3.519E-7
6.533E-7
9.081E-7
9.543E-7
9.575E-7
      50
-2.98
-3.49
-3.99
-4.47
-4.94
-5.47
-6.10
-6.63
-7.14
       1        1
      33     0.10   1.0E-10
      50     0.05   0.0E-00
```

DLM

$>SiOH^0 + UO_2^{2+} = >SiO{\cdot}UO_2^+ + H^+$

```
Uranium on Kaolinit 2.3si/nm
        0
        1
        0
        0
        1
       90
        4        1        3        1
00000080 00001  -4.07  8.44E-5   AlOH
00000080 00002  -4.07  8.44E-5   SiOH
00000090 00160  -1.0   0.00E00   PSIO
00000098 00032  -6.0   1.00E-6   UO2+2
00000100 00033   0.0   0.00E00   UO2ads
00000102 00050   0.0   0.00E00   H+
00000103 00003  -1.0   0.00E00   Na+
00000104 00005  -1.0   0.00E00   NO3-
00000110
00000120 00050    0.00  050  1
00000124 00032    0.00  032  1
00000126 03201   -5.43  032  1 050 -1
00000127 03202  -10.54  032  1 050 -2
00000128 03203  -19.22  032  1 050 -3
00000129 03204  -32.59  032  1 050 -4
00000130 03205   -2.49  032  2 050 -1
00000131 03206   -5.42  032  2 050 -2
00000132 03207  -12.37  032  3 050 -4
00000133 03208  -16.25  032  3 050 -5
00000134 03209  -31.49  032  3 050 -7
00000135 03210  -22.83  032  4 050 -7
00000139 00100  -13.78  050 -1
00000140 01050    8.22  001  1 160  1 050  1
00000145 01100   -9.62  001  1 160 -1 050 -1
00000150 00001    0.00  001  1
00000145 02100   -7.09  002  1 160 -1 050 -1
00000150 00002    0.00  002  1
xouo2    13301    3.00  001  1 160  1 050 -1 032  1 033  1
00000174
00000175
00000180 00002  011.0  4.0000
00000185 0.1    1.0
00000190          1
00000195       13301
00000230          9         1         1         0
00000240         33
00000260 1.333E-8
00000280 2.444E-8
00000300 8.810E-8
00000320 1.804E-7
00000340 3.519E-7
00000360 6.533E-7
00000370 9.081E-7
00000371 9.543E-7
00000372 9.575E-7
00000680        50
00000690 -2.98
00000700 -3.49
00000710 -3.99
00000720 -4.47
00000730 -4.94
00000740 -5.47
00000750 -6.10
00000751 -6.63
00000752 -7.14
00001170          1        1
00001180         33     0.10   1.0E-10
00001190         50     0.05   0.0E-00
```

DLM

$>AlOH^0 + UO_2^{2+} = >AlO{\cdot}UO_2^+ + H^+$

```
Uranium on Kaolinit 2.3si/nm
00000050
00000060
00000070
00000080
00000080
00000090
00000098
00000100
00000102
00000103
00000104
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000139
00000140
00000145
00000150
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000370
00000371
00000372
00000680
00000690
00000700
00000710
00000720
00000730
00000740
00000750
00000751
00000752
00001170
00001180
00001190
```

Example FITEQL Input

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FITEQL Results

Table B-XX. Uranium (V)-Kaolinite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Kaolinite $[Al_2Si_2O_5(OH)_4]$ A_{sp}: 11 m^2/g (Allard et al., 1983) Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.2E-11			Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 4 g/L			
Si:Al = 1:1 No CO_2		DLM			CCM			TLM		
								(α-Al_2O_3)	(SiO_2)	
		Log K_+ = 8.33 (α-Al_2O_3) Log K_- = -9.73 (α-Al_2O_3) Log K_- = -7.20 (SiO_2)			Log K_+ = 9.08 (α-Al_2O_3) Log K_- = -8.32 (α-Al_2O_3) Log K_- = -7.04 (SiO_2)			Log K_+ = 6.90 Log K_- = -10.90 Log K_{Cat} = -7.73 Log K_{An} = 10.12	Log K_+ = 0.90 Log K_- = -4.90 Log K_{Cat} = -6.22	
		Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	SiOH	1.41	20.1	.0228	1.91	22.5	.0288	-4.46	60.1	.0239
	AlOH	3.02	30.1	.0453	3.87	30.3	.0457	-1.69	37.8	.0238
$XOH\text{-}UO_2^{2+}$	SiOH	6.82	76.9	.0276	8.53	29.6	.0222	0.02	70.9	.0261
	AlOH	9.68	12.2	.0238	10.90	20.2	.0321	2.93	47.0	.0231
$XO\text{-}UO_2OH^o$	SiOH	-5.16	28.8	.0409	-5.07	28.6	.0409	-6.72	30.1	.0263
	AlOH	-3.85	40.1	.0647	-3.14	36.7	.0572	-4.51	25.3	.0377
$XOH\text{-}UO_2OH^+$	SiOH	1.41	20.1	.0228	1.91	22.5	.0288	-2.00	35.2	.0240
	AlOH	3.02	30.1	.0453	3.87	30.3	.0457	0.40	25.0	.0306
$XO\text{-}UO_2(OH)_2^-$	SiOH	-12.05	38.9	.0608	-12.11	35.1	.0534	-9.89	32.3	.0488
	AlOH	-10.70	45.3	.0817	-10.10	40.7	.0675	-7.82	38.7	.0627
$XOH\text{-}UO_2(OH)_2^{-o}$	SiOH	-5.16	28.8	.0409	-5.07	28.6	.0409	-4.92	28.4	.0404
	AlOH	-3.85	40.1	.0647	-3.14	36.7	.0572	-2.92	36.1	.0562
$XOH_2\text{-}UO_2(OH)_2^+$	SiOH	1.41	20.1	.0228	1.91	22.5	.0288	0.02	27.3	.0329
	AlOH	3.02	30.1	.0453	3.87	30.3	.0457	2.01	32.5	.0492
$XOH\text{-}UO_2(OH)_3^-$	SiOH	-12.05	38.9	.0608	-12.11	35.1	.0534	-8.24	40.3	.0657
	AlOH	-10.70	45.3	.0817	-10.10	40.7	.0675	-6.20	44.4	.0785
$XOH_2\text{-}UO_2(OH)_3^{-o}$	SiOH	-5.16	28.8	.0409	-5.07	28.6	.0409	-3.31	37.4	.0594
	AlOH	-3.85	40.1	.0647	-3.14	36.7	.0572	-1.28	42.7	.0723
$XOH\text{-}UO_2(OH)_4^{2-}$	SiOH	-18.90	44.5	.0782	-19.09	39.6	.0641	-11.53	46.4	.0878
	AlOH	-17.54	47.9	.0970	-17.05	43.4	.0779	-9.50	48.2	.0988
$XOH_2\text{-}UO_2(OH)_4^-$	SiOH	-12.16	38.9	.0608	-12.11	35.1	.0534	-6.58	45.0	.0820
	AlOH	-10.81	45.3	.0817	-10.10	40.7	.0675	-4.58	47.5	.0931

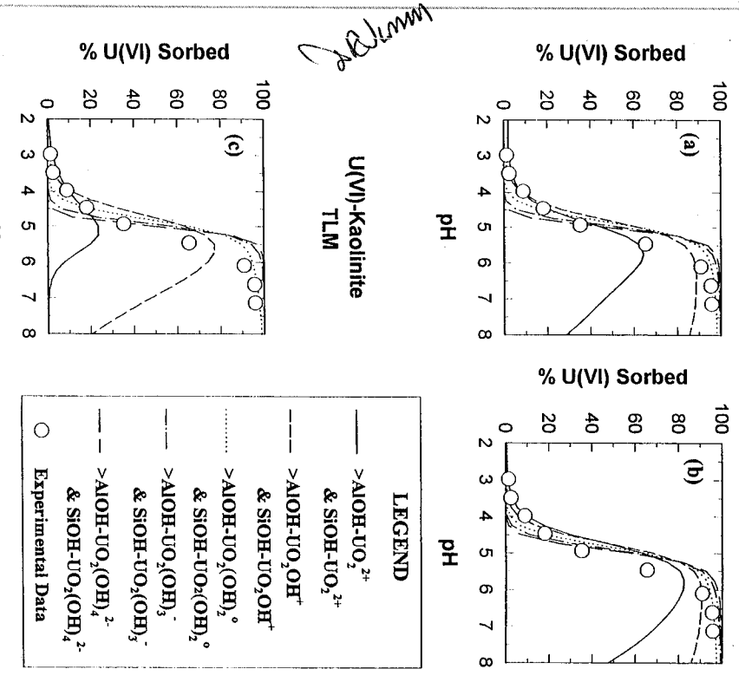

Figure 4-25. SCM predictions of U(VI) sorption on kaolinite (a) DLM; (b) CCM; and (c) TLM results. $U(VI)_T = 1 \times 10^{-6}$ M, 0.1 M $NaNO_3$, M/V = 4 g/L. Model parameters from Tables 3-1 and B-25. Si:Al ratio of 1:1 assumed. Data from Payne et al. (1992).

Modeling Results using MINTEQA2 and CNLRA radionuclide database (NEA database for uranium)

$JO_2^0 + 2H^+ + H_2O$

Waite et al (1993)
$\Sigma U(VI) = 1e^{-6} M$
$C_S = 100\ g/L$
$I = 0.1 M\ KNO_3$

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Waite, T.D., T.E. Payne, J.A. Davis, and K. Sekine. 1993. Uranium Sorption Modeling - A Surface Complexation Approach. *5th CEC Natural Analogue Working Group Meeting and Alligator River Analogue Project (ARAP) Final Workshop.* H. von Maravic and J. Smellie, eds. Pre-print; to be published in the EUR series. Commission of the European Communities: 83-88.

Waite et. al. (1993)	**U(VI) - quartz**	
Figure 2, no fluoride plot		
Asp=0.03 m^2/g	**1E-6 M**	
No CO_2		
0.1 M KNO_3	M/V =100 g/L	
pH	%sorbed	mol sorbed
3.39	0.0544	5.44e-10
4.04	6.23	6.23e-08
4.36	19.1	1.91e-07
4.48	27.2	2.72e-07
4.72	41.2	4.12e-07
4.86	54.9	5.49e-07
5.04	71.8	7.18e-07
5.18	80.1	8.01e-07
5.43	91.4	9.14e-07
5.79	96.4	9.64e-07
6.22	98.2	9.82e-07

Digtized Data

7/21/95
[signature]

[signature]

Example
FITEQL
Input files

Fig 2
CCM
XOH - UO_2^{+2} ⇌ $XOUO_2^+ + H^+$
0.1M KNO_3
M/V = 100 g/L

```
quartz00
waite930
1.0E-600
2.31s/nm
00000050
00000060
00000070
00000080
00000090
00000097
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000124
00000160
00000126
00000128
00000130
00000132
00000134
00000136
00000138
00000140
00000142
00000144
00000146
00000148
00000150
00000152
00000154
00000156
00000158
00000159
00000161
00000162
00000163
00000168
00000170
xouo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000250
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000330
00000340
00000350
00000480
00000490
00000500
00000510
00000520
00000530
00000540
00000550
00000560
00000570
00000580
00000590
00000760
00000770
00000790
```

```
       0
       1
       0
       0
       1
      90
       4        1         3         1
00001  -4.94   1.15E-5   XOH
00160  -1.0    0.00E00   PSIO
00032  -6.0    1.00E-6   UO2+2
00140  -3.5    3.16E-4   CO2g
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   K+
00005  -1.0    0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
00140    0.00  140  1
00100  -13.78  050 -1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -8.77  032  1 140  1 050 -2
03212  -19.35  032  1 140  2 050 -4
03213  -30.81  032  1 140  3 050 -6
03214  -51.09  032  3 140  6 050-12
03215  -70.09  032 11 140  6 050-24
03216  -19.28  032  2 140  1 050 -5
03217  -18.11  032  3 140  1 050 -5
03218   -0.05  032  1 005  1
01401  -17.50  140  1 050 -2
01402   -7.61  140  1 050 -1
01403   -1.48  140  1
00001    0.00  001  1
01100   -7.04  001  1 160 -1 050 -1
03301   -7.60  001  1 160  1 050 -1 032  1 033  1

00001   0.03  100.0  1.0
0.1     1.0
          1
       3301
         11        1         1         0
         33
5.44e-10
6.23e-08
1.91e-07
2.72e-07
4.12e-07
5.49e-07
7.18e-07
8.01e-07
9.14e-07
9.64e-07
9.82e-07
         50
-3.39
-4.04
-4.36
-4.48
-4.72
-4.86
-5.04
-5.18
-5.43
-5.79
-6.22
          1         1
         33      0.10    1.0E-12
         50      0.05    0.0E-00
```

[signature]

Fig 2
DLM

```
quartz00
waite930
1.0E-600
2.31s/nm
00000050
00000060
00000070
00000080
00000090
00000097
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000124
00000160
00000126
00000128
00000130
00000132
00000134
00000136
00000138
00000140
00000142
00000144
00000146
00000148
00000150
00000152
00000154
00000156
00000158
00000159
00000161
00000162
00000163
00000168
00000170
xouo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000250
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000330
00000340
00000350
00000480
00000490
00000500
00000510
00000520
00000530
00000540
00000550
00000560
00000570
00000580
00000590
00000760
00000770
00000790
```

```
       0
       1
       0
       0
       1
      90
       4        1         3         1
00001  -4.94   1.15E-5   XOH
00160  -1.0    0.00E00   PSIO
00032  -6.0    1.00E-6   UO2+2
00140  -3.5    3.16E-4   CO2g
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   K+
00005  -1.0    0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
00140    0.00  140  1
00100  -13.78  050 -1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -8.77  032  1 140  1 050 -2
03212  -19.35  032  1 140  2 050 -4
03213  -30.81  032  1 140  3 050 -6
03214  -51.09  032  3 140  6 050-12
03215  -70.09  032 11 140  6 050-24
03216  -19.28  032  2 140  1 050 -5
03217  -18.11  032  3 140  1 050 -5
03218   -0.05  032  1 005  1
01401  -17.50  140  1 050 -2
01402   -7.61  140  1 050 -1
01403   -1.48  140  1
00001    0.00  001  1
01100   -7.09  001  1 160 -1 050 -1
03301    7.60  001  1 160  1 050 -1 032  1 033  1

00002   0.03  100.0
0.1     1.0
          1
       3301
         11        1         1         0
         33
5.44e-10
6.23e-08
1.91e-07
2.72e-07
4.12e-07
5.49e-07
7.18e-07
8.01e-07
9.14e-07
9.64e-07
9.82e-07
         50
-3.39
-4.04
-4.36
-4.48
-4.72
-4.86
-5.04
-5.18
-5.43
-5.79
-6.22
          1         1
         33      0.10    1.0E-12
         50      0.05    0.0E-00
```


7/21/95
[signature]

Example
FITEQL
Input

[signature]

Fig 2
TLM

```
quartz00
waite930
1.0E-600
2.31s/nm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000097
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000124
00000160
00000126
00000128
00000130
00000132
00000134
00000136
00000138
00000140
00000142
00000144
00000146
00000148
00000150
00000152
00000154
00000156
00000158
00000159
00000161
00000162
00000163
00000166
00000168
00000170
00000171
xouo2
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000250
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000330
00000340
00000350
00000480
00000490
00000500
00000510
00000520
00000530
00000540
00000550
00000560
00000570
00000580
00000590
00000760
00000770
00000790
```

```
       0
       1
       0
       0
       1
      90
       6        1         3         1
00001  -4.94   1.15E-5   XOH
00160  -1.0    0.00E00   PSIO
00161  -0.5    0.00E00   PSIB
00162  -0.1    0.00E00   PSID
00032  -6.0    1.00E-6   UO2+2
00140  -3.5    3.16E-4   CO2g
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   K+
00005  -1.0    0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
00140    0.00  140  1
00100  -13.78  050 -1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -8.77  032  1 140  1 050 -2
03212  -19.35  032  1 140  2 050 -4
03213  -30.81  032  1 140  3 050 -6
03214  -51.09  032  3 140  6 050-12
03215  -70.09  032 11 140  6 050-24
03216  -19.28  032  2 140  1 050 -5
03217  -18.11  032  3 140  1 050 -5
03218   -0.05  032  1 005  1
01401  -17.50  140  1 050 -2
01402   -7.61  140  1 050 -1
01403   -1.48  140  1
01050    0.79  001  1 160  1 050  1
00001    0.00  001  1
01100   -4.79  001  1 160 -1 050 -1
01103   -6.22  001  1 160 -1 161  1 050 -1 003  1
03301   -7.60  001  1 160 -1 161  2 050 -1 032  1 033  1

00004  0.03   100.0   0.8   0.2
0.1    1.0
         1
      3301
        11        1         1         0
        33
5.44e-10
6.23e-08
1.91e-07
2.72e-07
4.12e-07
5.49e-07
7.18e-07
8.01e-07
9.14e-07
9.64e-07
9.82e-07
        50
-3.39
-4.04
-4.36
-4.48
-4.72
-4.86
-5.04
-5.18
-5.43
-5.79
-6.22
         1         1
        33      0.10    1.0E-12
        50      0.05    0.0E-00
```

Table B-21. Uranium (VI)-Quartz Sorption Binding Constants: Monodentate, mononuclear compounds.

Solid: Quartz A_{SP}: 0.03 m^2/g Data Source: Waite et al. (1993) Concentration: [U(VI)] = 1E-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9			Ionic Strength (electrolyte): 0.1 M KNO_3 N_S = 2.31 sites/nm^2 M/V = 100 g/L		
$p(CO_2)$ = 1E-3.5 atm	DLM			CCM			TLM		
	Log K_+ = (a) Log K_- = -7.20			Log K_+ = (a) Log K_- = -7.04			Log K_+ = 0.90 Log K_- = -4.90 Log K_{Cat} = -6.22 Log K_{An} = (a)		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}UO_2^+$	-1.23	94.9	.0402	-1.23	95.0	.0402	-1.24	78.6	.0357
$XOH\text{-}UO_2^{2+}$	2.14	99.7	.0437	2.14	99.7	.0436	1.64	91.6	.0399
$XO\text{-}UO_2OH^o$	-4.34	8.5	.0292	-4.34	8.5	.0291	-4.04	15.6	.0291
$XOH\text{-}UO_2OH^+$	-1.23	94.9	.0402	-1.23	95.0	.0402	-0.89	43.2	.0296
$XO\text{-}UO_2(OH)_2^-$	-8.45	3.7	.0421	-8.50	4.9	.0422	-7.40	7.1	.0347
$XOH\text{-}UO_2(OH)_2^o$	-4.34	8.5	.0292	-4.34	8.5	.0291	-4.33	8.5	.0291
$XOH_2\text{-}UO_2(OH)_2^+$	-1.23	94.9	.0402	-1.23	95.0	.0402	-0.97	24.8	.0289
$XOH\text{-}UO_2(OH)_3^-$	-8.45	3.7	.0421	-8.50	4.9	.0422	-7.53	5.4	.0363
$XOH_2\text{-}UO_2(OH)_3^o$	-4.34	8.5	.0292	-4.34	8.5	.0291	-4.39	7.6	.0319
$XOH\text{-}UO_2(OH)_4^{2-}$	-12.29	4.7	.0595	-12.46	7.6	.0610	-10.55	18.4	.0485
$XOH_2\text{-}UO_2(OH)_4^-$	-8.45	3.7	.0421	-8.45	4.9	.0422	-7.52	8.9	.0403
$XOH\text{-}UO_2CO_3^o$	17.33	8.1	.0206	17.34	8.1	.0206	17.35	8.2	.0206
$XOH_2\text{-}UO_2(CO_3)_2^-$	34.91	2.3	.0360	34.86	3.0	.0361	35.87	5.9	.0289
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	49.10	2.5	.0725	48.81	4.0	.0759	46.77	5.9	.0263
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^o$	14.82	36.1	.0364	14.82	36.1	.0364	14.83	35.9	.0364

(a) Due to low zero-point of charge (pH_{ZPC}=2.1 for SiO_2), XOH_2^+ (DLM, CCM) and XOH_2-An (TLM only) are assumed to be insignficant at slightly acid to basic pH [see discussion in Turner (1993)].

[signature]

FITEQL
Results:

7/21/95 DRJ

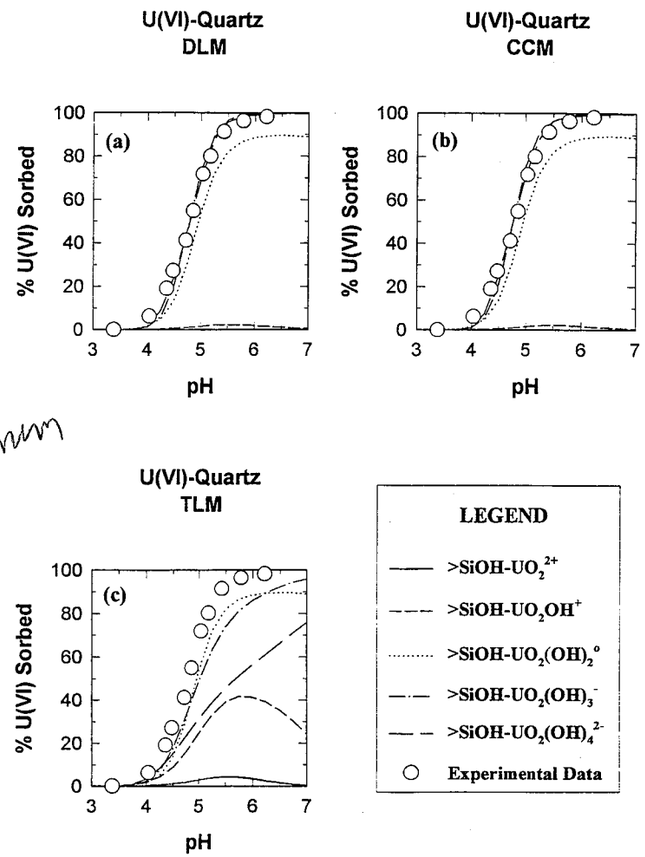
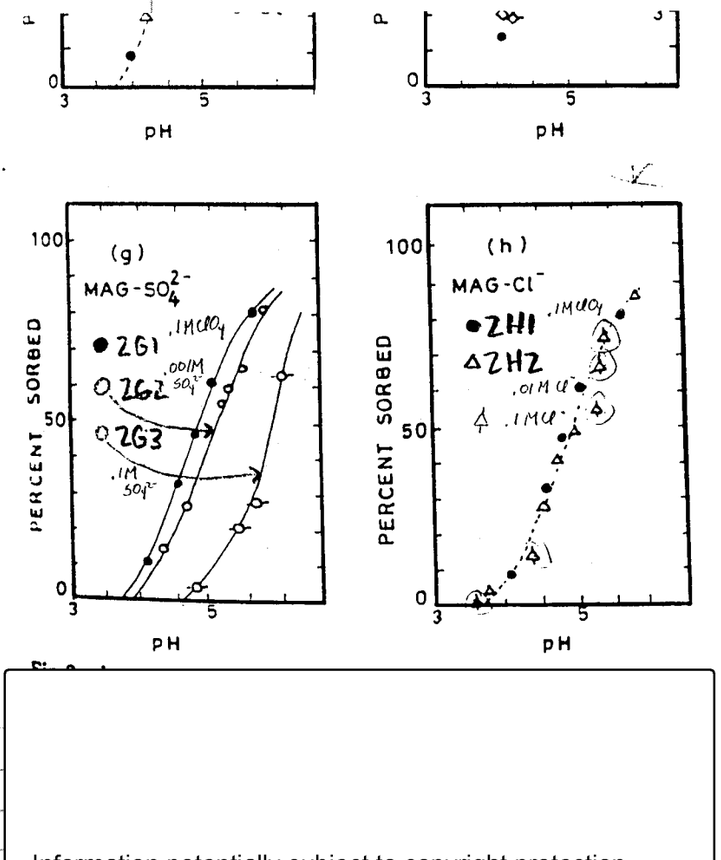


Figure 4-21. U(VI) sorption on quartz. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $U(VI)_T = 1 \times 10^{-6}$ M, 0.1 M ~~KClO4~~ KNO_3, M/V = 100 g/L. Model parameters from Tables 3-1 and B-21. Data from Waite et al. (1993).

DRJ (Version 3.11) 7/24/95

Plotted results using MINTEQA2, w/ CNWRA radionuclide database



Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 2: Uranyl sorption isotherms on hydrous oxides...) is from the following reference:

Venkataramani, B. and A.R. Gupta. "Effect of Anions on the sorption of Uranyl Ions on Hydrous Oxides: Application of the Surface Hydrolysis Model. Colloids and Surfaces. Vol. 53. pp. 1-19. 1991.

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I = 0.1

$U(VI)_T = 10^{-6}$ M

C_s = 8 g/L

Note: "All sorption experiments were done at a total ionic strength of 0.1 mol/dm³ using NaClO4... and varying the anion concentration"

HOWEVER, FITEQL input used the anion being changed (e.g. Cl^-, NO_3^-) and its ionic strength (e.g. 0.01M). This approach seems to be supported by information given in the article's abstract.

7/28/95
DRJ

Venkataramani, B., and A.R. Gupta. 1991. Effect of anions on the sorption of uranyl ions on hydrous oxides: Application of the surface hydrolysis model. *Colloids and Surfaces* 53:1-19.

Venkataramani and Gupta (1991)	**U(VI) - magnetite**	
Asp=5 m^2/g	1E-4 M	
No CO_2	M/V = 8.0 g/L	
Fig. 2(h)2, 0.01 M Cl^-		
pH	%sorbed	mol sorbed
3.73	3.847	3.847E-06
4.52	27.34	2.734E-05
4.72	40.44	4.044E-05
4.97	48.27	4.827E-05
5.84	85.81	8.581E-05
Fig. 2(h)3, 0.1 M Cl^-		
pH	%sorbed	mol sorbed
3.53	0.26	2.6000E-07
4.35	13.674	1.3674E-05
5.28	54.245	5.4245E-05
5.33	66.138	6.6138E-05
5.40	74.343	7.4343E-05
Fig. 2(i)1, 0.1 M ClO_4^-		
pH	%sorbed	mol sorbed
3.55	0.26076	2.6076E-07
4.04	8.6617	8.6617E-06
4.56	32.593	3.2593E-05
4.80	46.836	4.6836E-05
5.06	60.659	6.0659E-05
5.64	80.834	8.0834E-05
Fig. 2(i)2, 0.01 M NO_3^-		
pH	%sorbed	mol sorbed
3.21	0.57072	5.7072E-07
3.53	6.1047	6.1047E-06
4.23	14.236	1.4236E-05
4.98	60.359	6.0359E-05
5.11	64.582	6.4582E-05
5.58	83.176	8.3176E-05
Fig. 2(i)3, 0.1 M NO_3^-		
pH	%sorbed	mol sorbed
4.21	8.7309	8.7309E-06
4.58	20.215	2.0215E-05
4.73	28.166	2.8166E-05
5.41	52.465	5.2465E-05
5.49	61.032	6.1032E-05
6.51	88.793	8.8793E-05

Digitized Data

DRJ/mm

```
Magnetit
Venkat91
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000128
00000130
00000132
00000134
00000126
00000128
00000130
00000132
00000134
00000132
00000160
00000166
00000170
00000168
xouo2+
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000300
00000310
00000320
00000320
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001480
00001490
00001500
```

DRJ/mm

Fig 2(h)
I=0.01 M Cl^-
CCM

$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

```
                0
                1
                0
                0
                1
               90
                3          1          3          1
00001    -3.81  1.54E-4    XOH
00160    -1.00  0.00E00    PSI0
00032    -4.00  1.0E-04    UO2+2
00033     0.0   0.00E00    UO2ads
00050     0.0   0.00E00    H+
00003    -2.0   0.00E00    Na+
00005    -2.0   0.00E00    Cl-

00050     0.00  050  1
00032     0.00  032  1
03201    -5.29  032  1 050 -1
03202   -10.40  032  1 050 -2
03203   -19.20  032  1 050 -3
03204   -32.83  032  1 050 -4
03205    -2.62  032  2 050 -1
03206    -5.72  032  2 050 -2
03207   -12.09  032  3 050 -4
03208   -15.83  032  3 050 -5
03209   -31.19  032  3 050 -7
03210   -22.27  032  4 050 -7
03211    -0.02  032  1 005  1
03212    -1.41  032  1 005  2
00100   -13.90  050 -1
01050     6.32  001  1 160  1 050  1
01100    -7.38  001  1 160 -1 050 -1
00001     0.00  001  1
03301    -1.00  001  1 160  1 050 -1 032  1 033  1


00001  005.0  8.000      1.0
     0      0
          1
       3301
          5          1          1          0
         33
3.847E-06
2.734E-05
4.044E-05
4.827E-05
8.581E-05
         50
-3.73
-4.52
-4.72
-4.97
-5.84
          1          1
         33       0.10    4.0E-08
         50       0.05    0.0E-00
```

DRJ/mm

Fig 2(h)
I=0.01 M Cl^-
DLM

$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

```
                0
                1
                0
                0
                1
               90
                3          1          3          1
00001    -3.81  1.54E-4    XOH
00160    -1.00  0.00E00    PSI0
00032    -4.00  1.0E-04    UO2+2
00033     0.0   0.00E00    UO2ads
00050     0.0   0.00E00    H+
00003    -2.0   0.00E00    Na+
00005    -2.0   0.00E00    Cl-

00050     0.00  050  1
00032     0.00  032  1
03201    -5.29  032  1 050 -1
03202   -10.40  032  1 050 -2
03203   -19.20  032  1 050 -3
03204   -32.83  032  1 050 -4
03205    -2.62  032  2 050 -1
03206    -5.72  032  2 050 -2
03207   -12.09  032  3 050 -4
03208   -15.83  032  3 050 -5
03209   -31.19  032  3 050 -7
03210   -22.27  032  4 050 -7
03211    -0.02  032  1 005  1
03212    -1.41  032  1 005  2
00100   -13.90  050 -1
01050     6.67  001  1 160  1 050  1
01100    -6.32  001  1 160 -1 050 -1
00001     0.00  001  1
03301    -1.00  001  1 160  1 050 -1 032  1 033  1


00002  005.0  8.000
0.01   1.0
          1
       3301
          5          1          1          0
         33
3.847E-06
2.734E-05
4.044E-05
4.827E-05
8.581E-05
         50
-3.73
-4.52
-4.72
-4.97
-5.84
          1          1
         33       0.10    4.0E-08
         50       0.05    0.0E-00
```


Example FITEQL Inputs

7/28/95
DRJ

Fig 2(h)
I=0.01 M Cl^-
TLM

$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

```
                0
                1
                0
                0
                1
               90
                5          1          3          1
00001    -3.81  1.54E-4    XOH
00160    -1.00  0.00E00    PSI0
00161    -0.50  0.00E00    PSIB
00162    -0.10  0.00E00    PSID
00032    -4.00  1.0E-04    UO2+2
00033     0.0   0.00E00    UO2ads
00050     0.0   0.00E00    H+
00003    -2.0   0.00E00    Na+
00005    -2.0   0.00E00    Cl-

00050     0.00  050  1
00032     0.00  032  1
03201    -5.29  032  1 050 -1
03202   -10.40  032  1 050 -2
03203   -19.20  032  1 050 -3
03204   -32.83  032  1 050 -4
03205    -2.62  032  2 050 -1
03206    -5.72  032  2 050 -2
03207   -12.09  032  3 050 -4
03208   -15.83  032  3 050 -5
03209   -31.19  032  3 050 -7
03210   -22.27  032  4 050 -7
03211    -0.02  032  1 005  1
03212    -1.41  032  1 005  2
00100   -13.90  050 -1
01050     4.65  001  1 160  1 050  1
01100    -8.65  001  1 160 -1 050 -1
01055     7.85  001  1 160  1 161 -1 050  1 005  1
01103    -5.47  001  1 160 -1 161  1 050 -1 003  1
00001     0.00  001  1
03301    -1.00  001  1 160 -1 161  2 050 -1 032  1 033  1


00004  005.0  8.000  0.8    0.2
0.01   1.0
          1
       3301
          5          1          1          0
         33
3.847E-06
2.734E-05
4.044E-05
4.827E-05
8.581E-05
         50
-3.73
-4.52
-4.72
-4.97
-5.84
          1          1
         33       0.10    4.0E-08
         50       0.05    0.0E-00
```

DRJ/mm

```
Magnetit
Venkat91
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000128
00000130
00000132
00000134
00000126
00000128
00000130
00000132
00000134
00000132
00000160
00000166
00000170
00000166
00000170
00000168
xouo2+
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000300
00000310
00000320
00000320
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001480
00001490
00001500
```

Fig. 2(h)
I=0.1 M Cl⁻
CCM
$XOH + UO_2^{2+} = XO \cdot UO_2^{+} + H^{+}$

```
       0
       1
       0
       0
       1
      90
       3       1       3       1
00001  -3.81  1.54E-4   XOH
00160  -1.00  0.00E00   PSI0
00032  -4.00  1.0E-04   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   Cl-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.28  032  1 005  1
03212   -1.79  032  1 005  2
00100  -13.78  050 -1
01050    6.26  001  1 160  1 050  1
01100   -7.32  001  1 160 -1 050 -1
00001    0.00  001  1
03301   -1.00  001  1 160  1 050 -1 032  1 033  1

00001  005.0  8.000     1.0
    0       0
       1
    3301
       5       1       1       0
      33
2.6000E-07
1.3674E-05
5.4245E-05
6.6138E-05
7.4343E-05
      50
-3.53
-4.35
-5.28
-5.33
-5.40
       1       1
      33    0.10   2.6E-09
      50    0.05   0.0E-00
```

Fig. 2(h)
I=0.1 M Cl⁻
DLM
$XOH + UO_2^{2+} = XO \cdot UO_2^{+} + H^{+}$

```
Magnetit          0
Venkat91          1
2.3s/nm2          0
00000040          0
00000050          1
00000060         90
00000070          3       1       3       1
00000080  00001  -3.81  1.54E-4   XOH
00000090  00160  -1.00  0.00E00   PSI0
00000097  00032  -4.00  1.0E-04   UO2+2
00000100  00033   0.0   0.00E00   UO2ads
00000102  00050   0.0   0.00E00   H+
00000104  00003  -1.0   0.00E00   Na+
00000106  00005  -1.0   0.00E00   Cl-
00000110
00000120  00050    0.00  050  1
00000122  00032    0.00  032  1
00000126  03201   -5.43  032  1 050 -1
00000128  03202  -10.54  032  1 050 -2
00000130  03203  -19.22  032  1 050 -3
00000132  03204  -32.59  032  1 050 -4
00000134  03205   -2.49  032  2 050 -1
00000126  03206   -5.42  032  2 050 -2
00000128  03207  -12.37  032  3 050 -4
00000130  03208  -16.25  032  3 050 -5
00000132  03209  -31.49  032  3 050 -7
00000134  03210  -22.83  032  4 050 -7
00000132  03211   -0.28  032  1 005  1
00000132  03212   -1.79  032  1 005  2
00000160  00100  -13.78  050 -1
00000166  01050    6.61  001  1 160  1 050  1
00000170  01100   -6.26  001  1 160 -1 050 -1
00000168  00001    0.00  001  1
xouo2+    03301   -1.00  001  1 160  1 050 -1 032  1 033  1
00000180
00000182
00000184  00002  005.0  8.000
00000185  0.1    1.0
00000190          1
00000195       3301
00000230          5       1       1       0
00000240         33
00000300  2.6000E-07
00000310  1.3674E-05
00000320  5.4245E-05
00000320  6.6138E-05
00000320  7.4343E-05
00001070         50
00001080  -3.53
00001090  -4.35
00001130  -5.28
00001110  -5.33
00001120  -5.40
00001480          1       1
00001490         33    0.10   2.6E-09
00001500         50    0.05   0.0E-00
```

Fig. 2(h)
I=0.1 M Cl⁻
TLM
$XOH + UO_2^{2+} = XO \cdot UO_2^{+} + H^{+}$

```
       0
       1
       0
       0
       1
      90
       5       1       3       1
00001  -3.81  1.54E-4   XOH
00160  -1.00  0.00E00   PSI0
00161  -0.50  0.00E00   PSIB
00162  -0.10  0.00E00   PSID
00032  -4.00  1.0E-04   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   Cl-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.28  032  1 005  1
03212   -1.79  032  1 005  2
00100  -13.78  050 -1
01050    4.59  001  1 160  1 050  1
01100   -8.59  001  1 160 -1 050 -1
01055    7.95  001  1 160  1 161 -1 050  1 005  1
01103   -5.47  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
03301   -1.00  001  1 160 -1 161  2 050 -1 032  1 033  1

00004  005.0  8.000  0.8    0.2
0.1    1.0
       1
    3301
       5       1       1       0
      33
2.6000E-07
1.3674E-05
5.4245E-05
6.6138E-05
7.4343E-05
      50
-3.53
-4.35
-5.28
-5.33
-5.40
       1       1
      33    0.10   2.6E-09
      50    0.05   0.0E-00
```

Example FITEQL Inputs
7/28/95
DRJ

```
Magnetit
Venkat91
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000128
00000130
00000132
00000134
00000126
00000128
00000130
00000132
00000134
00000132
00000132
00000160
00000166
00000170
00000166
00000170
00000168
xouo2+
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000300
00000310
00000320
00000320
00000320
00001070
00001080
00001090
00001130
00001110
00001120
00001480
00001490
00001500
```


Fig. 2(i)
I=0.1 M ClO₄⁻
CCM
$XOH + UO_2^{2+} = XO \cdot UO_2^{+} + H^{+}$

```
       0
       1
       0
       0
       1
      90
       3       1       3       1
00001  -3.81  1.54E-4   XOH
00160  -1.00  0.00E00   PSI0
00032  -4.00  1.0E-04   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
00100  -13.78  050 -1
01050    6.26  001  1 160  1 050  1
01100   -7.32  001  1 160 -1 050 -1
00001    0.00  001  1
03301    1.00  001  1 160  1 050 -1 032  1 033  1

00001  005.0  8.000     1.0
    0       0
       1
    3301
       6       1       1       0
      33
2.6076E-07
8.6617E-06
3.2593E-05
4.6836E-05
6.0659E-05
8.0834E-05
      50
-3.55
-4.04
-4.56
-4.80
-5.06
-5.64
       1       1
      33    0.10   3.0E-09
      50    0.05   0.0E-00
```

Fig. 2(i)
I=0.1 M ClO₄⁻
DLM
$XOH + UO_2^{2+} = XO \cdot UO_2^{+} + H^{+}$

```
Magnetit          1
Venkat91          1
2.3s/nm2          1
00000040          1
00000050          1
00000060         90
00000070          3       1       3       1
00000080  00001  -3.81  1.54E-4   XOH
00000090  00160  -1.00  0.00E00   PSI0
00000097  00032  -4.00  1.0E-04   UO2+2
00000100  00033   0.0   0.00E00   UO2ads
00000102  00050   0.0   0.00E00   H+
00000104  00003  -1.0   0.00E00   Na+
00000106  00005  -1.0   0.00E00   ClO4-
00000110
00000120  00050    0.00  050  1
00000122  00032    0.00  032  1
00000126  03201   -5.43  032  1 050 -1
00000128  03202  -10.54  032  1 050 -2
00000130  03203  -19.22  032  1 050 -3
00000132  03204  -32.59  032  1 050 -4
00000134  03205   -2.49  032  2 050 -1
00000126  03206   -5.42  032  2 050 -2
00000128  03207  -12.37  032  3 050 -4
00000130  03208  -16.25  032  3 050 -5
00000132  03209  -31.49  032  3 050 -7
00000134  03210  -22.83  032  4 050 -7
00000160  00100  -13.78  050 -1
00000166  01050    6.61  001  1 160  1 050  1
00000170  01100   -6.26  001  1 160 -1 050 -1
00000168  00001    0.00  001  1
xouo2+    03301    1.00  001  1 160  1 050 -1 032  1 033  1
00000180
00000182
00000184  00002  005.0  8.000
00000185  0.1    1.0
00000190          1
00000195       3301
00000230          6       1       1       0
00000240         33
00000300  2.6076E-07
00000310  8.6617E-06
00000320  3.2593E-05
00000300  4.6836E-05
00000310  6.0659E-05
00000320  8.0834E-05
00001070         50
00001080  -3.55
00001090  -4.04
00001100  -4.56
00001110  -4.80
00001120  -5.06
00001130  -5.64
00001480          1       1
00001490         33    0.10   3.0E-09
00001500         50    0.05   0.0E-00
```

Fig. 2(i)
I=0.1 M ClO₄⁻
TLM
$XOH + UO_2^{2+} = XO \cdot UO_2^{+} + H^{+}$

```
       0
       1
       0
       0
       1
      90
       5       1       3       1
00001  -3.81  1.54E-4   XOH
00160  -1.00  0.00E00   PSI0
00161  -0.50  0.00E00   PSIB
00162  -0.10  0.00E00   PSID
00032  -4.00  1.0E-04   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   ClO4-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
00100  -13.78  050 -1
01050    4.59  001  1 160  1 050  1
01100   -8.59  001  1 160 -1 050 -1
01055    7.73  001  1 160  1 161 -1 050  1 005  1
01103   -5.47  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
03301   -1.00  001  1 160 -1 161  2 050 -1 032  1 033  1

00004  005.0  8.000  0.8    0.2
0.1    1.0
       1
    3301
       6       1       1       0
      33
2.6076E-07
8.6617E-06
3.2593E-05
4.6836E-05
6.0659E-05
8.0834E-05
      50
-3.55
-4.04
-4.56
-4.80
-5.06
-5.64
       1       1
      33    0.10   3.0E-09
      50    0.05   0.0E-00
```

Example FITEQL Inputs
7/28/95
DRJ

```
Magnetit
Venkat91
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000128
00000130
00000132
00000134
00000126
00000128
00000130
00000132
00000134
00000160
00000166
00000170
00000166
00000170
00000168
xouo2+
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000300
00000310
00000320
00000300
00000310
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001130
00001480
00001490
00001500
```

```
0
1
0
0
1
90
3          1          3          1
00001  -3.81   1.54E-4   XOH
00160  -1.00   0.00E00   PSI0
00032  -4.00   1.0E-04   UO2+2
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -2.0    0.00E00   Na+
00005  -2.0    0.00E00   NO3-

00050    0.00   050  1
00032    0.00   032  1
03201   -5.29   032  1 050 -1
03202  -10.40   032  1 050 -2
03203  -19.20   032  1 050 -3
03204  -32.83   032  1 050 -4
03205   -2.62   032  2 050 -1
03206   -5.72   032  2 050 -2
03207  -12.09   032  3 050 -4
03208  -15.83   032  3 050 -5
03209  -31.19   032  3 050 -7
03210  -22.27   032  4 050 -7
03211    0.05   032  1 005  1
00100  -13.90   050 -1
01050    6.32   001  1 160  1 050  1
01100   -7.38   001  1 160 -1 050 -1
00001    0.00   001  1
03301   -1.00   001  1 160  1 050 -1 032  1 033  1


00001  005.0  8.000      1.0
     0      0
       1
    3301
       6          1          1          0
      33
5.7072E-07
6.1047E-06
1.4236E-05
6.0359E-05
6.4582E-05
8.3176E-05
      50
-3.21
-3.53
-4.23
-4.98
-5.11
-5.58
       1          1
      33       0.10    6.0E-09
      50       0.05    0.0E-00
```

Fig 2(i)
I=0.01 M NO_3^-
CCM
$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

```
Magnetit
Venkat91
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000128
00000130
00000132
00000134
00000126
00000128
00000130
00000132
00000160
00000166
00000170
00000168
xouo2+
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000300
00000310
00000320
00000320
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001130
00001480
00001490
00001500
```

Fig 2(i)
I=0.01 M NO_3^-
DLM
$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

```
0
1
0
0
1
90
3          1          3          1
00001  -3.81   1.54E-4   XOH
00160  -1.00   0.00E00   PSI0
00032  -4.00   1.0E-04   UO2+2
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   Na+
00005  -1.0    0.00E00   NO3-

00050    0.00   050  1
00032    0.00   032  1
03201   -5.43   032  1 050 -1
03202  -10.54   032  1 050 -2
03203  -19.22   032  1 050 -3
03204  -32.59   032  1 050 -4
03205   -2.49   032  2 050 -1
03206   -5.42   032  2 050 -2
03207  -12.37   032  3 050 -4
03208  -16.25   032  3 050 -5
03209  -31.49   032  3 050 -7
03210  -22.83   032  4 050 -7
03211   -0.16   032  1 005  1
00100  -13.78   050 -1
01050    6.26   001  1 160. 1 050  1
01100   -7.32   001  1 160 -1 050 -1
00001    0.00   001  1
03301   -1.00   001  1 160  1 050 -1 032  1 033  1


00001  005.0  8.000      1.0
     0      0
       1
    3301
       6          1          1          0
      33
8.7309E-06
2.0215E-05
2.8166E-05
5.2465E-05
6.1032E-05
8.8793E-05
      50
-4.21
-4.58
-4.73
-5.41
-5.49
-6.51
       1          1
      33       0.10    9.0E-08
      50       0.05    0.0E-00
```

Fig 2(i)
I=0.1 M NO_3^-
CCM
$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

```
Magnetit
Venkat91
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000128
00000130
00000132
00000134
00000126
00000128
00000130
00000132
00000160
00000166
00000170
00000168
xouo2+
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000300
00000310
00000320
00000320
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001130
00001480
00001490
00001500
```

Fig 2(i)
I=0.1 M NO_3^-
DLM
$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

Example EITEQL Inputs
7/28/95
DRJ

```
0
1
0
0
1
90
5          1          3          1
00001  -3.81   1.54E-4   XOH
00160  -1.00   0.00E00   PSI0
00161  -0.50   0.00E00   PSIB
00162  -0.10   0.00E00   PSID
00032  -4.00   1.0E-04   UO2+2
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -2.0    0.00E00   Na+
00005  -2.0    0.00E00   NO3-

00050    0.00   050  1
00032    0.00   032  1
03201   -5.29   032  1 050 -1
03202  -10.40   032  1 050 -2
03203  -19.20   032  1 050 -3
03204  -32.83   032  1 050 -4
03205   -2.62   032  2 050 -1
03206   -5.72   032  2 050 -2
03207  -12.09   032  3 050 -4
03208  -15.83   032  3 050 -5
03209  -31.19   032  3 050 -7
03210  -22.27   032  4 050 -7
03211    0.05   032  1 005  1
00100  -13.90   050 -1
01050    4.65   001  1 160  1 050  1
01100   -8.65   001  1 160 -1 050 -1
01055    7.85   001  1 160  1 161 -1 050  1 005  1
01103   -5.47   001  1 160 -1 161  1 050 -1 003  1
00001    0.00   001  1
03301   -1.00   001  1 160 -1 161  2 050 -1 032  1 033  1


00004  005.0  8.000  0.8    0.2
0.01   1.0
         1
      3301
         6          1          1          0
        33
5.7072E-07
6.1047E-06
1.4236E-05
6.0359E-05
6.4582E-05
8.3176E-05
        50
-3.21
-3.53
-4.23
-4.98
-5.11
-5.58
         1          1
        33       0.10    6.0E-09
        50       0.05    0.0E-00
```

Fig 2(i)
I=0.01 M NO_3^-
TLM
$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

```
Magnetit
Venkat91
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000128
00000130
00000132
00000134
00000126
00000128
00000130
00000132
00000160
00000166
00000170
00000168
xouo2+
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000300
00000310
00000320
00000320
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001130
00001480
00001490
00001500
```

Example EITEQL Inputs
7/28/95
DRJ

```
0
1
0
0
1
90
5          1          3          1
00001  -3.81   1.54E-4   XOH
00160  -1.00   0.00E00   PSI0
00161  -0.50   0.00E00   PSIB
00162  -0.10   0.00E00   PSID
00032  -4.00   1.0E-04   UO2+2
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   Na+
00005  -1.0    0.00E00   NO3-

00050    0.00   050  1
00032    0.00   032  1
03201   -5.43   032  1 050 -1
03202  -10.54   032  1 050 -2
03203  -19.22   032  1 050 -3
03204  -32.59   032  1 050 -4
03205   -2.49   032  2 050 -1
03206   -5.42   032  2 050 -2
03207  -12.37   032  3 050 -4
03208  -16.25   032  3 050 -5
03209  -31.49   032  3 050 -7
03210  -22.83   032  4 050 -7
03211   -0.16   032  1 005  1
00100  -13.78   050 -1
01050    4.59   001  1 160  1 050  1
01100   -8.59   001  1 160 -1 050 -1
01055    7.73   001  1 160  1 161 -1 050  1 005  1
01103   -5.47   001  1 160 -1 161  1 050 -1 003  1
00001    0.00   001  1
03301   -1.00   001  1 160 -1 161  2 050 -1 032  1 033  1


00004  005.0  8.000  0.8    0.2
0.1    1.0
         1
      3301
         6          1          1          0
        33
8.7309E-06
2.0215E-05
2.8166E-05
5.2465E-05
6.1032E-05
8.8793E-05
        50
-4.21
-4.58
-4.73
-5.41
-5.49
-6.51
         1          1
        33       0.10    9.0E-08
        50       0.05    0.0E-00
```

Fig 2(i)
I=0.1 M NO_3^-
TLM
$XOH + UO_2^{2+} = XO{\cdot}UO_2^+ + H^+$

```
Magnetit
Venkat91
2.3s/nm2
00000040
00000050
00000060
00000070
00000080
00000090
00000090
00000097
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000126
00000128
00000130
00000132
00000134
00000126
00000128
00000130
00000132
00000160
00000166
00000170
00000168
xouo2+
00000180
00000182
00000184
00000185
00000190
00000195
00000230
00000240
00000300
00000310
00000320
00000320
00000320
00001070
00001080
00001090
00001100
00001110
00001120
00001130
00001480
00001490
00001500
```

Example EITEQL Inputs
7/28/95
DRJ

7/28/95 DRJ

Table BXX. Uranium (VI)-Magnetite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Magnetite A_{SP}: 5 m^2/g Data Source: Venkataramani and Gupta (1991) Concentration: [U(VI)] = 1E-4 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 2.6E-9 M	Ionic Strength (electrolyte): 0.1 M NaCl N_S = 2.31 sites/nm^2 M/V = 8 g/L

No CO_2 Fig. 2(h)	DLM			CCM (I = 0.1 M)			TLM		
	Log K_+ = 6.72 Log K_- = -6.37			Log K_+ = 6.26 Log K_- = -7.32			Log K_+ = 4.70 Log K_- = -8.70 Log K_{Cat} = -5.47 Log K_{An} = 7.95		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-UO_2^+$	1.53	16.2	.0361	1.40	17.6	.0376	-4.11	98.8	.0526
$XOH-UO_2^{2+}$	7.46	59.0	.0377	7.76	51.7	.0423	2.67	98.9	.0687
$XO-UO_2OH^o$	-4.69	1.2	.0394	-5.12	2.8	.0375	-7.72	88.5	.0435
$XOH-UO_2OH^+$	1.53	16.2	.0361	1.40	17.6	.0376	1.11	93.3	.0527
$XO-UO_2(OH)_2^-$	-10.71	2.5	.0522	-11.44	10.1	.0464	-11.24	68.0	.0567
$XOH-UO_2(OH)_2^o$	-4.69	1.2	.0394	-5.12	2.8	.0375	-4.72	3.5	.0366
$XOH_2-UO_2(OH)_2^+$	1.53	16.2	.0361	1.40	17.6	.0376	1.98	71.6	.0560
$XOH-UO_2(OH)_3^-$	-10.71	2.5	.0522	-11.44	10.1	.0464	-8.14	19.6	.0629
$XOH_2-UO_2(OH)_3^o$	-4.69	1.2	.0394	-5.12	2.8	.0375	-2.32	13.1	.0633
$XOH-UO_2(OH)_4^{2-}$	-16.69	11.9	.0674	-17.78	16.3	.0547	-11.60	47.1	.0944
$XOH_2-UO_2(OH)_4^-$	-10.71	2.5	.0522	-11.44	10.1	.0464	-5.41	7.3	.0806

Table BXX. Uranium (VI)-Magnetite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Magnetite A_{SP}: 5 m^2/g Data Source: Venkataramani and Gupta (1991) Concentration: [U(VI)] = 1E-4 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 4.0E-8 M	Ionic Strength (electrolyte): 0.01 M NaCl N_S = 2.31 sites/nm^2 M/V = 8 g/L

No CO_2 Fig. 2(h)	DLM			CCM (I = 0.01 M)			TLM		
	Log K_+ = 6.72 Log K_- = -6.37			Log K_+ = 6.32 Log K_- = -7.38			Log K_+ = 4.70 Log K_- = -8.70 Log K_{Cat} = -5.47 Log K_{An} = 7.95		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-UO_2^+$	1.99	3.5	.0450	1.73	4.0	.0446	-1.99	80.2	.1013
$XOH-UO_2^{2+}$	8.59	12.6	.0487	8.43	19.8	.0511	6.05	79.1	.1591
$XO-UO_2OH^o$	-4.63	5.9	.0423	-4.95	5.9	.0444	-6.82	35.9	.0425
$XOH-UO_2OH^+$	1.99	3.5	.0450	1.73	4.0	.0446	0.40	58.6	.0806
$XO-UO_2(OH)_2^-$	-10.79	4.1	.0556	-10.97	2.4	.0600	-10.43	16.3	.0675
$XOH-UO_2(OH)_2^o$	-4.63	5.9	.0423	-4.95	5.9	.0444	-5.06	5.9	.0435
$XOH_2-UO_2(OH)_2^+$	1.99	3.5	.0450	1.73	4.0	.0446	2.77	20.4	.0692
$XOH-UO_2(OH)_3^-$	-10.79	4.1	.0556	-10.97	2.4	.0600	-8.31	4.1	.0799
$XOH_2-UO_2(OH)_3^o$	-4.63	5.9	.0423	-4.95	5.9	.0444	-3.08	14.4	.0722
$XOH-UO_2(OH)_4^{2-}$	-16.85	8.6	.0668	-17.06	13.5	.0738	-11.06	20.5	.1336
$XOH_2-UO_2(OH)_4^-$	-10.79	4.1	.0556	-10.97	2.4	.0600	-5.81	7.5	.1054

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Table BXX. Uranium (VI)-Magnetite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Magnetite A_{SP}: 5 m^2/g Data Source: Venkataramani and Gupta (1991) Concentration: [U(VI)] = 1E-4 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 3.0E-9 M	Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_S = 2.31 sites/nm^2 M/V = 8 g/L

No CO_2 Fig. 2(i)	DLM			CCM (I = 0.1 M)			TLM		
	Log K_+ = 6.72 Log K_- = -6.37			Log K_+ = 6.26 Log K_- = -7.32			Log K_+ = 4.70 Log K_- = -8.70 Log K_{Cat} = -5.47 Log K_{An} = 7.95		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-UO_2^+$	1.63	21.9	.0335	1.50	22.7	.0349	-4.05	98.1	.0518
$XOH-UO_2^{2+}$	7.46	65.8	.0363	7.79	56.3	.0400	2.65	98.1	.0672
$XO-UO_2OH^o$	-4.54	5.2	.0361	-4.99	9.2	.0346	-7.71	88.2	.0419
$XOH-UO_2OH^+$	1.63	21.9	.0335	1.50	22.7	.0349	1.17	92.7	.0511
$XO-UO_2(OH)_2^-$	-10.56	3.5	.0468	-11.32	15.8	.0425	-11.25	69.9	.0540
$XOH-UO_2(OH)_2^o$	-4.54	5.2	.0361	-4.99	9.2	.0346	-4.68	10.1	.0338
$XOH_2-UO_2(OH)_2^+$	1.63	21.9	.0335	1.50	22.7	.0349	1.80	74.8	.0542
$XOH-UO_2(OH)_3^-$	-10.56	3.5	.0468	-11.32	15.8	.0425	-8.17	25.6	.0593
$XOH_2-UO_2(OH)_3^o$	-4.54	5.2	.0361	-4.99	9.2	.0346	-2.31	7.1	.0511
$XOH-UO_2(OH)_4^{2-}$	-16.52	10.8	.0591	-17.69	31.7	.0503	-11.76	52.8	.0912
$XOH_2-UO_2(OH)_4^-$	-10.56	3.5	.0468	-11.32	15.8	.0425	-5.49	10.8	.0734

Table BXX. Uranium (VI)-Magnetite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Magnetite A_{SP}: 5 m^2/g Data Source: Venkataramani and Gupta (1991) Concentration: [U(VI)] = 1E-4 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 6.0E-9 M	Ionic Strength (electrolyte): 0.01 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 8 g/L

No CO_2 Fig. 2(i)	DLM			CCM (I = 0.01 M)			TLM		
	Log K_+ = 6.72 Log K_- = -6.37			Log K_+ = 6.32 Log K_- = -7.38			Log K_+ = 4.70 Log K_- = -8.70 Log K_{Cat} = -5.47 Log K_{An} = 7.95		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO-UO_2^+$	2.13	13.5	.0394	1.87	14.1	.0393	-3.53	91.5	.0515
$XOH-UO_2^{2+}$	8.57	23.2	.0376	8.43	26.9	.0394	3.22	92.5	.0790
$XO-UO_2OH^o$	-4.42	18.8	.0440	-4.73	18.5	.0451	-7.08	50.4	.0337
$XOH-UO_2OH^+$	2.13	13.5	.0394	1.87	14.1	.0393	-0.61	75.7	.0488
$XO-UO_2(OH)_2^-$	-10.57	18.9	.0510	-10.76	14.7	.0500	-10.59	26.1	.0491
$XOH-UO_2(OH)_2^o$	-4.42	18.8	.0440	-4.73	14.1	.0451	-4.84	18.2	.0443
$XOH_2-UO_2(OH)_2^+$	2.13	13.5	.0394	1.87	14.1	.0393	2.38	35.9	.0492
$XOH-UO_2(OH)_3^-$	-10.57	18.9	.0510	-10.76	14.7	.0500	-8.05	12.4	.0605
$XOH_2-UO_2(OH)_3^o$	-4.42	18.8	.0440	-4.73	14.1	.0451	-2.84	32.1	.0720
$XOH-UO_2(OH)_4^{2-}$	-16.57	21.2	.0560	-16.83	18.8	.0534	-11.12	26.2	.0887
$XOH_2-UO_2(OH)_4^-$	-10.57	18.9	.0510	-10.76	14.7	.0500	-5.30	17.6	.0767

FITEQL Output

DRJ 7/28/95 FITEQL Output DRJ/mm

Table BXX. Uranium (VI)-Magnetite Sorption Binding Constants: Monodentate, mononuclear compounds

Solid: Magnetite A_{SP}: 5 m^2/g Data Source: Venkataramani and Gupta (1991) Concentration: [U(VI)] = 1E-4 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 9.0E-8 M			Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 8 g/L		
No CO_2 Fig. 2(i)	DLM Log K_+ = 6.72 Log K_- = -6.37			CCM (I = 0.1 M) Log K_+ = 6.26 Log K_- = -7.32			TLM Log K_+ = 4.70 Log K_- = -8.70 Log K_{Cat} = -5.47 Log K_{An} = 7.95		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-UO_2^+	1.69	3.8	.0363	1.57	5.6	.0387	-0.40	61.1	.1056
XOH-UO_2^{2+}	8.17	16.8	.0428	8.41	21.5	.0543	n.c.	n.c	n.c.
XO-UO_2OH°	-4.76	1.9	.0368	-5.13	1.5	.0370	-6.55	37.7	.0381
XOH-UO_2OH^+	1.69	3.8	.0363	1.57	5.6	.0387	1.59	42.9	.0790
XO-$UO_2(OH)_2^-$	-10.96	1.7	.0500	-11.33	2.3	.0534	-9.72	13.4	.0693
XOH-$UO_2(OH)_2^\circ$	-4.76	1.9	.0368	-5.13	1.5	.0370	-4.80	1.4	.0360
XOH_2-$UO_2(OH)_2^+$	1.69	3.8	.0363	1.57	5.6	.0387	n.c.	n.c.	n.c.
XOH-$UO_2(OH)_3^-$	-10.86	1.7	.0500	-11.33	2.3	.0534	-7.86	2.9	.0792
XOH_2-$UO_2(OH)_3^\circ$	-4.76	1.9	.0368	-5.13	1.5	.0370	-2.91	10.1	.0541
XOH-$UO_2(OH)_4^{2-}$	-16.81	7.7	.0729	-17.35	11.8	.0833	-10.04	12.4	.1403
XOH_2-$UO_2(OH)_4^-$	-10.86	1.7	.0500	-11.33	2.3	.0534	-5.72	4.9	.1024

FITEQL results plotted using MINTEQA2, version 3.11 and LNLRA radionuclide database

DBL/mm

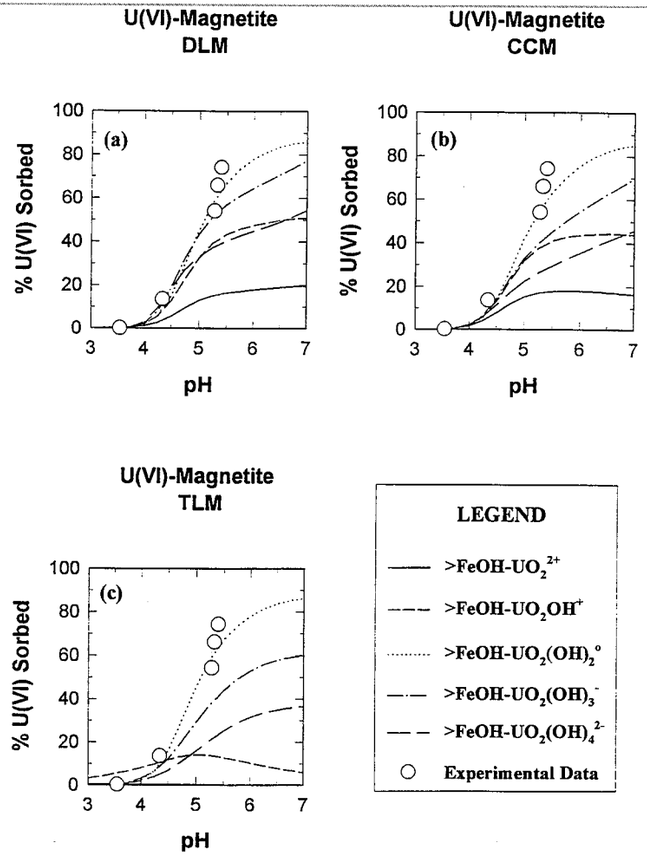

Figure 4-17. U(VI) sorption on magnetite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $U(VI)_T = 1 \times 10^{-4}$ M, 0.1 M NaCl, M/V=8 g/L. Model parameters from Tables 3-1 and B-17. Data from Venkataramani and Gupta (1991).

(Fig 2k, VG '91)

8/3/95 DRJ U(VI) Ferrihydrite sorption

Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 11: Adsorption of uranium (VI) onto Amorphous ferric..... and Figure 28: Effect of carbonate complexing....) is from the following reference:

Hsi, C-K.D. "Sorption of Uranium(VI) by Iron Oxides." Ph.D. dissertation. Colorado School of Mines. Golden, Colorado. 1981.

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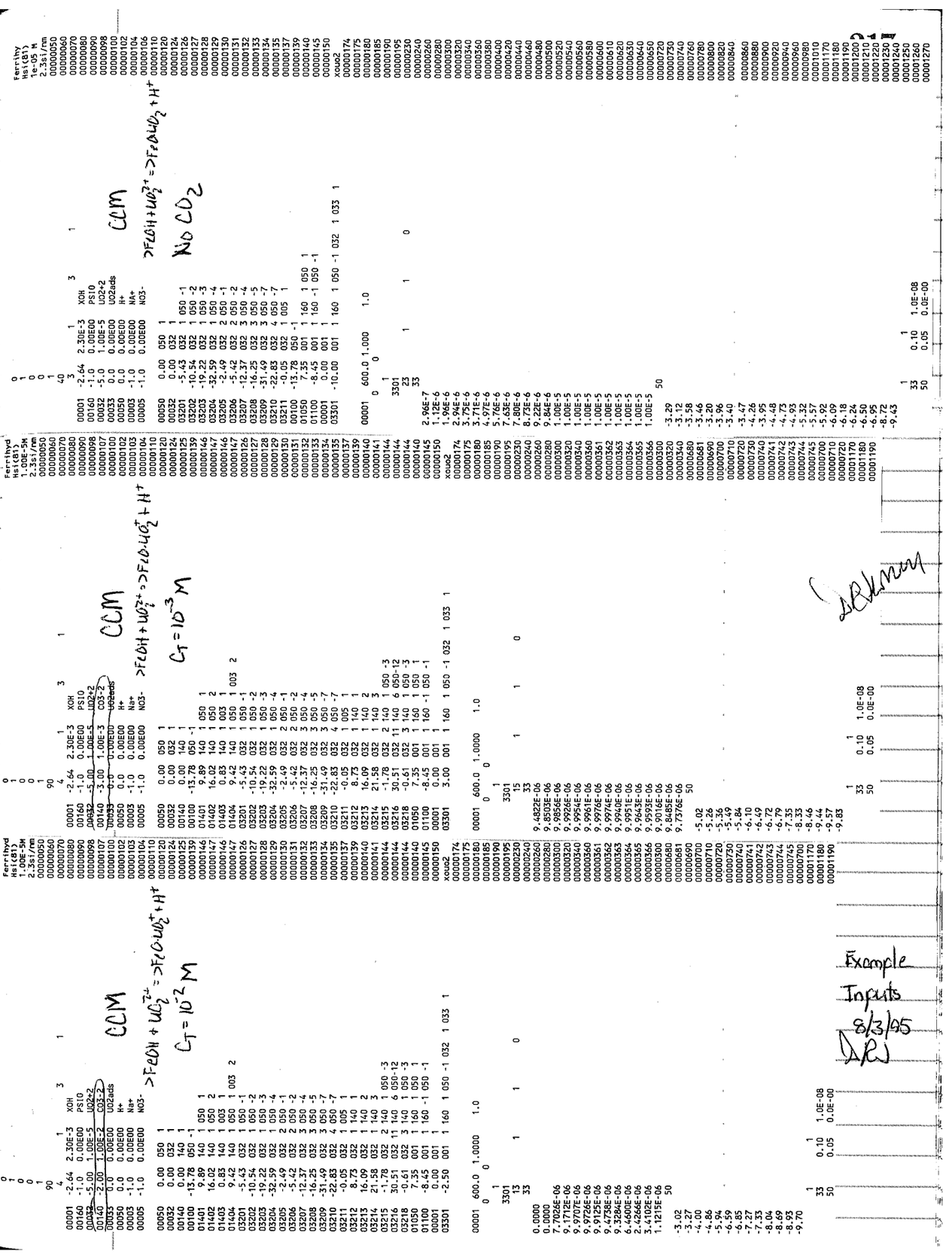
Hsi, C-K.D. 1981. *Sorption of Uranium(VI) by Iron Oxides.* Ph.D. Dissertation. Golden, CO: Colorado School of Mines.

Also:

Hsi, C-K.D, and D. Langmuir. 1985. Adsorption of uranyl onto ferric oxyhydroxides: Application of the surface complexation site-binding model. *Geochimica et Cosmochimica Acta* 49: 1931-1941.

Hsi (1981)	U(VI)-Ferrihydrite	Hsi and Langmuir (1985)
Figures 11 & 28		Figure 2(a)
Asp=600 m2/g	M/V=1 g/L	
0.1 M NaNO3	1E-5 M	
pH	%sorbed	mol sorbed
No CO2		
3.29	2.96	2.96E-7
3.12	11.20	1.12E-6
3.58	19.60	1.96E-6
3.46	29.40	2.94E-6
3.20	37.50	3.75E-6
3.96	37.10	3.71E-6
3.40	49.70	4.97E-6
3.47	57.60	5.76E-6
4.26	76.30	7.63E-6
3.95	78.00	7.80E-6
4.48	87.30	8.73E-6
4.73	92.20	9.22E-6
4.93	98.40	9.84E-6
4.32	100.00	1.00E-5
5.57	100.00	1.00E-5
5.92	100.00	1.00E-5
6.09	100.00	1.00E-5
6.18	100.00	1.00E-5
6.24	100.00	1.00E-5
6.50	100.00	1.00E-5
6.95	100.00	1.00E-5
8.72	100.00	1.00E-5
9.43	100.00	1.00E-5
pH	%sorbed	mol sorbed
C(t)=0.001 M		
5.02	94.82	9.48E-06
5.26	98.50	9.85E-06
5.36	99.86	9.99E-06
5.49	99.93	9.99E-06
5.84	99.95	1.00E-05
6.11	99.96	1.00E-05
6.49	99.98	1.00E-05
6.72	99.97	1.00E-05
6.79	99.94	1.00E-05
7.35	99.95	1.00E-05
8.33	99.64	9.96E-06
8.46	99.59	9.96E-06
9.44	99.02	9.90E-06
9.57	98.49	9.85E-06
9.83	97.38	9.74E-06



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 0
 1
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00032  -5.0   1.00E-5   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   NA+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
00100  -13.78  050 -1
01050    7.18  001  1 160  1 050  1
01100   -8.82  001  1 160 -1 050 -1
00001    0.00  001  1
03301  -10.00  001  1 160  1 050 -1 032  1 033  1


00002   600.0 1.000
0.1    1.0
         1
      3301
        23          1          1          0
        33
2.96E-7
1.12E-6
1.96E-6
2.94E-6
3.75E-6
3.71E-6
4.97E-6
5.76E-6
7.63E-6
7.80E-6
8.73E-6
9.22E-6
9.84E-6
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1.00E-5
1.00E-5
1.00E-5
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1.00E-5
1.00E-5
1.00E-5
1.00E-5
1.00E-5
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-3.29
-3.12
-3.58
-3.46
-3.20
-3.96
-3.40
-3.47
-4.26
-3.95
-4.48
-4.73
-4.93
-5.32
-5.57
-5.92
-6.09
-6.18
-6.24
-6.50
-6.95
-8.72
-9.43
         1          1
        33       0.10    1.0E-08
        50       0.05    0.0E-00
```

DLM

$>FeOH^{+} + UO_2^{2+} = >FeO\cdot UO_2^{+} + H^{+}$

No CO_2

```
Ferrihy
Hsi(81)
1e-05 M
2.3si/nm
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00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000137
00000139
00000140
00000145
00000150
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00000180
00000185
00000190
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00000240
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00000320
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00000640
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00000720
00000730
00000740
00000760
00000780
00000800
00000820
00000840
00000860
00000880
00000900
00000920
00000940
00000960
00000980
00001010
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00001240
00001250
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00032  -5.00  1.00E-5   UO2+2
00140  -3.00  1.00E-3   CO3-2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
00140    0.00  140  1
00100  -13.78  050 -1
01401    9.89  140  1 050  1
01402   16.02  140  1 050  2
01403    0.83  140  1 003  1
01404    9.42  140  1 050  1 003  2
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
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03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
03212    8.73  032  1 140  1
03213   16.09  032  1 140  2
03214   21.58  032  1 140  3
03215   -1.78  032  2 140  1 050 -3
03216   30.51  032 11 140  6 050-12
03218   -0.61  032  3 140  1 050 -3
01050    7.18  001  1 160  1 050  1
01100   -8.82  001  1 160 -1 050 -1
00001    0.00  001  1
03301    3.00  001  1 160  1 050 -1 032  1 033  1


00002   600.0  1.0000
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      3301
        15          1          1          0
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9.9940E-6
9.9951E-6
9.9643E-6
9.9593E-6
9.9016E-6
9.8485E-6
9.7376E-6
      50
-5.02
-5.26
-5.36
-5.49
-5.84
-6.10
-6.49
-6.72
-6.79
-7.35
-8.33
-8.46
-9.44
-9.57
-9.83
         1          1
        33       0.10    1.0E-08
        50       0.05    0.0E-00
```

DLM

$>FeOH + UO_2^{2+} = >FeO\cdot UO_2^{+} + H^{+}$

$C_T = 10^{-3}$ M

```
Ferrihyd
Hsi(81)
1.00E-5M
2.3si/nm
00000050
00000060
00000070
00000080
00000090
00000098
00000107
00000100
00000102
00000103
00000104
00000110
00000120
00000124
00000126
00000139
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00000137
00000139
00000140
00000141
00000144
00000144
00000144
00000140
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000361
00000362
00000363
00000364
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00000366
00000300
00000320
00000340
00000680
00000681
00000690
00000700
00000710
00000720
00000730
00000740
00000741
00000742
00000743
00000744
00000745
00000700
00001170
00001180
00001190
```

```
 0
 1
 0
 0
 1
90
 4          1          3          1
00001  -2.64  2.30E-3   XOH
00160  -1.0   0.00E00   PSIO
00032  -5.00  1.00E-5   UO2+2
00140  -2.00  1.00E-2   CO3-2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
00140    0.00  140  1
00100  -13.78  050 -1
01401    9.89  140  1 050  1
01402   16.02  140  1 050  2
01403    0.83  140  1 003  1
01404    9.42  140  1 050  1 003  2
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
03212    8.73  032  1 140  1
03213   16.09  032  1 140  2
03214   21.58  032  1 140  3
03215   -1.78  032  2 140  1 050 -3
03216   30.51  032 11 140  6 050-12
03218   -0.61  032  3 140  1 050 -3
01050    7.18  001  1 160  1 050  1
01100   -8.82  001  1 160 -1 050 -1
00001    0.00  001  1
03301   -2.50  001  1 160  1 050 -1 032  1 033  1


00002   600.0  1.0000
0.1    1.0
         1
      3301
        13          1          1          0
        33
0.0000
0.0000
7.7026E-6
9.1712E-6
9.9707E-6
9.9726E-6
9.9125E-6
9.4738E-6
9.3284E-6
6.4600E-6
2.4266E-6
3.4102E-6
1.1215E-6
      50
-3.02
-3.27
-4.00
-4.86
-5.94
-6.59
-6.85
-7.27
-7.33
-8.04
-8.69
-8.93
-9.70
         1          1
        33       0.10    1.0E-08
        50       0.05    0.0E-00
```

DLM

$>FeOH + UO_2^{2+} = >FeO\cdot UO_2^{+} + H^{+}$

$C_T = 10^{-2}$ M

```
Ferrihyd
Hsi(81)
1.00E-5M
2.3si/nm
00000050
00000060
00000070
00000080
00000090
00000098
00000107
00000100
00000102
00000103
00000104
00000110
00000120
00000124
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00000139
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00000150
xouo2
00000174
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00000680
00000681
00000690
00000700
00000710
00000720
00000730
00000740
00000741
00000742
00000743
00000744
00000745
00000700
00001170
00001180
00001190
```

Example FITEQL Input Files

8/3/95

```
Ferrihyd
Hsi(81)
1.00E-5M
2.3si/rm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098
00000107
00000100
00000102
00000103
00000104
00000110
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xouo2
00000174
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00000340
00000360
00000361
00000362
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00000700
00000710
00000720
00000730
00000740
00000741
00000742
00000743
00000744
00000745
00000700
00001170
00001180
00001190
```

```
        0
        1
        0
        0
        1
       90
        6          1          3          1
00001  -2.64   2.30E-3   XOH
00160  -1.0    0.00E00   PSIO
00161  -0.5    0.00E00   PSIB
00162  -0.1    0.00E00   PSID
00032  -5.00   1.00E-5   UO2+2
00140  -2.00   1.00E-2   CO3-2
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   Na+
00005  -1.0    0.00E00   NO3-

00050    0.00   050   1
00032    0.00   032   1
00140    0.00   140   1
00100  -13.78   050  -1
01401    9.89   140   1 050   1
01402   16.02   140   1 050   2
01403    0.83   140   1 003   1
01404    9.42   140   1 050   1 003   2
03201   -5.43   032   1 050  -1
03202  -10.54   032   1 050  -2
03203  -19.22   032   1 050  -3
03204  -32.59   032   1 050  -4
03205   -2.49   032   2 050  -1
03206   -5.42   032   2 050  -2
03207  -12.37   032   3 050  -4
03208  -16.25   032   3 050  -5
03209  -31.49   032   3 050  -7
03210  -22.83   032   4 050  -7
03211   -0.05   032   1 005   1
03212    8.73   032   1 140   1
03213   16.09   032   1 140   2
03214   21.58   032   1 140   3
03215   -1.78   032   2 140   1 050  -3
03216   30.51   032  11 140   6 050-12
03218   -0.61   032   3 140   1 050  -3
01050    5.89   001   1 160   1 050   1
01100   -9.89   001   1 160  -1 050  -1
01055    8.21   001   1 160   1 161  -1 050   1 005   1
01103   -7.66   001   1 160  -1 161   1 050  -1 003   1
00001    0.00   001   1
03301   -2.50   001   1 160  -1 161   2 050  -1 032   1 033   1

00004  600.0  1.0000  0.8   0.2
0.1    1.0
          1
       3301
         13          1          1          0
         33
0.0000
0.0000
7.7026E-06
9.1712E-06
9.9707E-06
9.9726E-06
9.9125E-06
9.4738E-06
9.3284E-06
6.4600E-06
2.4266E-06
3.4102E-06
1.1215E-06
         50
-3.02
-3.27
-4.00
-4.86
-5.94
-6.59
-6.85
-7.27
-7.33
-8.04
-8.69
-8.93
-9.70
          1          1
         33       0.10    1.0E-08
         50       0.05    0.0E-00
```

TLM

$>FeOH + UO_2^{2+} = >FeOUO_2^{+} + H^{+}$

$C_T = 10^{-2}$ M

```
        0
        1
        0
        0
        1
       90
        6          1          3          1
00001  -2.64   2.30E-3   XOH
00160  -1.0    0.00E00   PSIO
00161  -0.5    0.00E00   PSIB
00162  -0.1    0.00E00   PSID
00032  -5.00   1.00E-5   UO2+2
00140  -3.00   1.00E-3   CO3-2
00033   0.0    0.00E00   UO2ads
00050   0.0    0.00E00   H+
00003  -1.0    0.00E00   Na+
00005  -1.0    0.00E00   NO3-

00050    0.00   050   1
00032    0.00   032   1
00140    0.00   140   1
00100  -13.78   050  -1
01401    9.89   140   1 050   1
01402   16.02   140   1 050   2
01403    0.83   140   1 003   1
01404    9.42   140   1 050   1 003   2
03201   -5.43   032   1 050  -1
03202  -10.54   032   1 050  -2
03203  -19.22   032   1 050  -3
03204  -32.59   032   1 050  -4
03205   -2.49   032   2 050  -1
03206   -5.42   032   2 050  -2
03207  -12.37   032   3 050  -4
03208  -16.25   032   3 050  -5
03209  -31.49   032   3 050  -7
03210  -22.83   032   4 050  -7
03211   -0.05   032   1 005   1
03212    8.73   032   1 140   1
03213   16.09   032   1 140   2
03214   21.58   032   1 140   3
03215   -1.78   032   2 140   1 050  -3
03216   30.51   032  11 140   6 050-12
03218   -0.61   032   3 140   1 050  -3
01050    5.89   001   1 160   1 050   1
01100   -9.89   001   1 160  -1 050  -1
01055    8.21   001   1 160   1 161  -1 050   1 005   1
01103   -7.66   001   1 160  -1 161   1 050  -1 003   1
00001    0.00   001   1
03301   -2.50   001   1 160  -1 161   2 050  -1 032   1 033   1

00004  600.0  1.0000  0.8   0.2
0.1    1.0
          1
       3301
         15          1          1          0
         33
9.4822E-06
9.8503E-06
9.9856E-06
9.9926E-06
9.9954E-06
9.9961E-06
9.9976E-06
9.9974E-06
9.9940E-06
9.9951E-06
9.9643E-06
9.9593E-06
9.9016E-06
9.8485E-06
9.7376E-06
         50
-5.02
-5.26
-5.36
-5.49
-5.84
-6.10
-6.49
-6.72
-6.79
-7.35
-8.33
-8.46
-9.44
-9.57
-9.83
          1          1
         33       0.10    1.0E-08
         50       0.05    0.0E-00
```

TLM

$>FeOH + UO_2^{2+} = >FeOUO_2^{+} + H^{+}$

$C_T = 10^{-3}$ M

```
Ferrihyd
Hsi(81)
1.00E-5M
2.3si/rm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098
00000107
00000100
00000102
00000103
00000104
00000110
00000120
00000124
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00000144
00000144
00000140
00000145
00000150
xouo2
00000174
00000175
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00000230
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00000720
00000730
00000740
00000741
00000742
00000743
00000744
00000745
00000700
00000710
00000720
00001170
00001180
00001190
```

```
        0
        1
        0
        0
        1
       90
        5          1          3          1
00000070  00001  -2.64   2.30E-3   XOH
00000080  00160  -1.0    0.00E00   PSIO
00000090  00161  -0.5    0.00E00   PSIB
00000092  00162  -0.1    0.00E00   PSID
00000094  00032  -5.0    1.00E-5   UO2+2
00000098  00033   0.0    0.00E00   UO2ads
00000107  00050   0.0    0.00E00   H+
00000100  00003  -1.0    0.00E00   NA+
00000102  00005  -1.0    0.00E00   NO3-
00000103

00000104  00050    0.00   050   1
00000110  00032    0.00   032   1
00000120  03201   -5.43   032   1 050  -1
00000124  03202  -10.54   032   1 050  -2
00000125  03203  -19.22   032   1 050  -3
00000139  03204  -32.59   032   1 050  -4
00000146  03205   -2.49   032   2 050  -1
00000147  03206   -5.42   032   2 050  -2
00000146  03207  -12.37   032   3 050  -4
00000147  03208  -16.25   032   3 050  -5
00000126  03209  -31.49   032   3 050  -7
00000127  03210  -22.83   032   4 050  -7
00000128  03211   -0.05   032   1 005   1
00000129  00100  -13.78   050  -1
00000130  01050    5.89   001   1 160   1 050   1
00000131  01100   -9.89   001   1 160  -1 050  -1
00000132  01103   -7.66   001   1 160  -1 161   1 050  -1 003   1
00000133  01055    8.21   001   1 160   1 161  -1 050   1 005   1
00000134  00001    0.00   001   1
00000135  03301   -7.60   001   1 160  -1 161   2 050  -1 032   1 033   1
00000137
00000139
00000140  00004  600.0 1.000   0.8   0.2
00000141  0.1    1.0
00000144          1
00000144       3301
00000144         23          1          1          0
00000140         33
00000145  2.96E-7
00000140  1.12E-6
00000145  1.96E-6
00000150  2.94E-6
xouo2     3.75E-6
00000174  3.71E-6
00000175  4.97E-6
00000180  5.76E-6
00000185  7.63E-6
00000190  7.80E-6
00000195  8.73E-6
00000230  9.22E-6
00000240  9.84E-6
00000260  1.00E-5
00000280  1.00E-5
00000300  1.00E-5
00000320  1.00E-5
00000340  1.00E-5
00000360  1.00E-5
00000361  1.00E-5
00000362  1.00E-5
00000363  1.00E-5
00000364  1.00E-5
00000365         50
00000366  -3.29
00000300  -3.12
00000320  -3.58
00000340  -3.46
00000680  -3.20
00000681  -3.96
00000690  -3.40
00000700  -3.47
00000710  -4.26
00000720  -3.95
00000730  -4.48
00000740  -4.73
00000741  -4.93
00000742  -5.32
00000743  -5.57
00000744  -5.92
00000745  -6.09
00000700  -6.18
00000710  -6.24
00000720  -6.50
00001170  -6.95
00001180  -8.72
00001190  -9.43
          1          1
         33       0.10    1.0E-08
         50       0.05    0.0E-00
```

TLM

$>FeOH + UO_2^{2+} = >FeOUO_2^{+} + H^{+}$

NO CO_2

```
Hsi(81)
1e-05 M
2.3si/rm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000124
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00000146
00000147
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
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00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000380
00000400
00000420
00000440
00000460
00000480
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00000520
00000540
00000560
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00000610
00000680
00000690
00000700
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00000720
00000730
00000740
00000760
00000780
00000800
00000820
00000840
00000860
00000880
00000900
00000920
00000940
00000960
00000980
00001010
00001170
00001180
00001190
00001200
00001210
00001220
00001230
00001240
00001250
00001260
00001270
```

Example FITEQL Inputs 8/3/95 DKN

D. Kent Nordstrom

8/3/95 DRL

Uranium (VI)-Ferrihydrite Sorption Binding Constants. Monodentate: mononuclear compounds.

Solid: Ferrihydrite A_{SP}: 600 m^2/g Data Source: Hsi and Langmuir (1985); Hsi (1981) Concentration: [U(VI)] = 1E-5 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-8	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

No CO_2	DLM Log K_+ = 7.29 Log K_- = -8.93			CCM Log K_+ = 7.35 Log K_- = -8.45			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	2.51	13.8	.0314	2.86	13.8	.0314	-4.59	80.2	.0239
$XOH\text{-}UO_2^{2+}$	8.62	25.6	.0221	10.14	14.1	.0286	3.04	82.4	.0259
$XO\text{-}UO_2OH^o$	-3.65	17.1	.0423	-4.40	14.3	.0337	-8.21	25.4	.0234
$XOH\text{-}UO_2OH^+$	2.51	13.8	.0314	2.86	13.8	.0314	-0.53	28.9	.0222
$XO\text{-}UO_2(OH)_2^-$	-9.67	21.4	.0521	-11.65	14.9	.0360	-12.14	14.2	.0345
$XOH\text{-}UO_2(OH)_2^o$	-3.65	17.1	.0423	-4.40	14.3	.0337	-4.51	14.2	.0332
$XOH_2\text{-}UO_2(OH)_2^+$	2.51	13.8	.0314	2.86	13.8	.0314	3.17	13.7	.0322
$XOH\text{-}UO_2(OH)_3^-$	-9.67	21.4	.0521	-11.65	14.9	.0360	-8.43	17.8	.0448
$XOH_2\text{-}UO_2(OH)_3^o$	-3.65	17.1	.0423	-4.40	14.3	.0337	-0.90	17.8	.0436
$XOH\text{-}UO_2(OH)_4^{2-}$	-15.56	23.5	.0575	-18.91	15.6	.0384	-12.21	21.0	.0555
$XOH_2\text{-}UO_2(OH)_4^-$	-9.67	21.4	.0521	-11.65	14.9	.0360	-4.52	21.9	.0525

Uranium (VI)-Ferrihydrite Sorption Binding Constants. Monodentate: mononuclear compounds.

Solid: Ferrihydrite A_{SP}: 600 m^2/g Data Source: Hsi and Langmuir (1985); Hsi (1981) Concentration: [U(VI)] = 1E-5 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-8	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

C(t) = 0.001 M	DLM Log K_+ = 7.29 Log K_- = -8.93			CCM Log K_+ = 7.35 Log K_- = -8.45			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	4.95	0.02	1.449	4.85	0.02	1.476	7.60	0.02	1.394
$XOH\text{-}UO_2^{2+}$	13.43	0.02	1.413	13.14	0.02	1.456	15.96	0.02	1.412
$XO\text{-}UO_2OH^o$	-3.52	0.02	1.414	-3.43	0.02	1.449	-2.11	0.01	1.398
$XOH\text{-}UO_2OH^+$	4.95	0.02	1.449	4.85	0.02	1.476	6.10	0.02	1.397
$XO\text{-}UO_2(OH)_2^-$	-12.07	0.01	.8520	-11.75	0.02	1.231	-11.56	0.02	1.395
$XOH\text{-}UO_2(OH)_2^o$	-3.52	0.02	1.414	-3.43	0.02	1.449	-3.49	0.02	1.454
$XOH_2\text{-}UO_2(OH)_2^+$	4.95	0.02	1.449	4.85	0.02	1.476	4.73	0.02	1.481
$XOH\text{-}UO_2(OH)_3^-$	-12.07	0.01	.8520	-11.75	0.02	1.231	-10.57	0.01	.8360
$XOH_2\text{-}UO_2(OH)_3^o$	-3.52	0.02	1.414	-3.43	0.02	1.449	-2.84	0.01	.8346
$XOH\text{-}UO_2(OH)_4^{2-}$	-19.55	0.01	.7971	-20.00	0.01	.8638	-15.76	0.01	..8388
$XOH_2\text{-}UO_2(OH)_4^-$	-12.07	0.01	.8520	-11.75	0.02	1.231	-8.17	0.01	..8216
$XOH\text{-}UO_2CO_3^o$	19.96	0.02	.9753	20.04	0.02	.9745	19.98	0.02	.9745
$XOH_2\text{-}UO_2(CO_3)_2^-$	35.17	0.02	1.034	35.45	0.02	1.041	32.47	0.02	.8383
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	n.c.	n.c.	n.c.	n.c.	n.c.	n.c.	n.c.	n.c.	n.c.
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^o$	n.c.	n.c.	n.c.	n.c.	n.c.	n.c.	16.77	0.02	1.930

8/3/95 DRL

FITEQL Results

Uranium (VI)-Ferrihydrite Sorption Binding Constants. Monodentate: mononuclear compounds.

Solid: Ferrihydrite A_{SP}: 600 m^2/g Data Source: Hsi and Langmuir (1985); Hsi (1981) Concentration: [U(VI)] = 1E-5 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-8	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

C(t) = 0.01 M	DLM Log K_+ = 7.29 Log K_- = -8.93			CCM Log K_+ = 7.35 Log K_- = -8.45			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	1.49	77.9	.0648	1.87	76.1	.0609	-7.29	87.8	2.110
$XOH\text{-}UO_2^{2+}$	6.85	87.4	.0217	8.99	81.2	.0696	0.23	87.8	2.688
$XO\text{-}UO_2OH^o$	-3.53	20.5	.0366	-5.17	66.6	.0506	-9.83	87.1	.0160
$XOH\text{-}UO_2OH^+$	1.49	77.9	.0648	1.87	76.1	.0609	-2.32	87.4	.0211
$XO\text{-}UO_2(OH)_2^-$	-11.44	12.8	.0300	-11.91	36.0	.0352	-12.80	6.0	.0456
$XOH\text{-}UO_2(OH)_2^o$	-3.53	20.5	.0366	-5.17	66.6	.0506	-5.32	68.3	.0518
$XOH_2\text{-}UO_2(OH)_2^+$	1.49	77.9	.0648	1.87	76.1	.0609	2.22	73.7	.0577
$XOH\text{-}UO_2(OH)_3^-$	-11.44	12.8	.0300	-11.91	36.0	.0352	-12.40	71.1	.0397
$XOH_2\text{-}UO_2(OH)_3^o$	-3.53	20.5	.0366	-5.17	66.6	.0506	-4.15	64.1	.0341
$XOH\text{-}UO_2(OH)_4^{2-}$	-19.81	23.2	.0297	-19.60	22.7	.0282	-22.38	80.2	..0739
$XOH_2\text{-}UO_2(OH)_4^-$	-11.44	12.8	.0300	-11.91	36.0	.0352	-14.26	80.1	..0706
$XOH\text{-}UO_2CO_3^o$	14.47	56.1	.0975	13.34	70.4	.0444	13.21	71.1	.0447
$XOH_2\text{-}UO_2(CO_3)_2^-$	n.c.	n.c.	n.c.	24.79	68.1	.0465	30.52	9.7	.0290
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	n.c.	n.c.	n.c.	29.05	62.7	.0503	34.48	27.2	.0242
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^o$	13.53	42.7	.0577	11.90	56.3	.0610	n.c.	n.c.	n.c.

FITEQL Results plotted using MINTEQA2, version 3.11 and CALRA radionuclide database

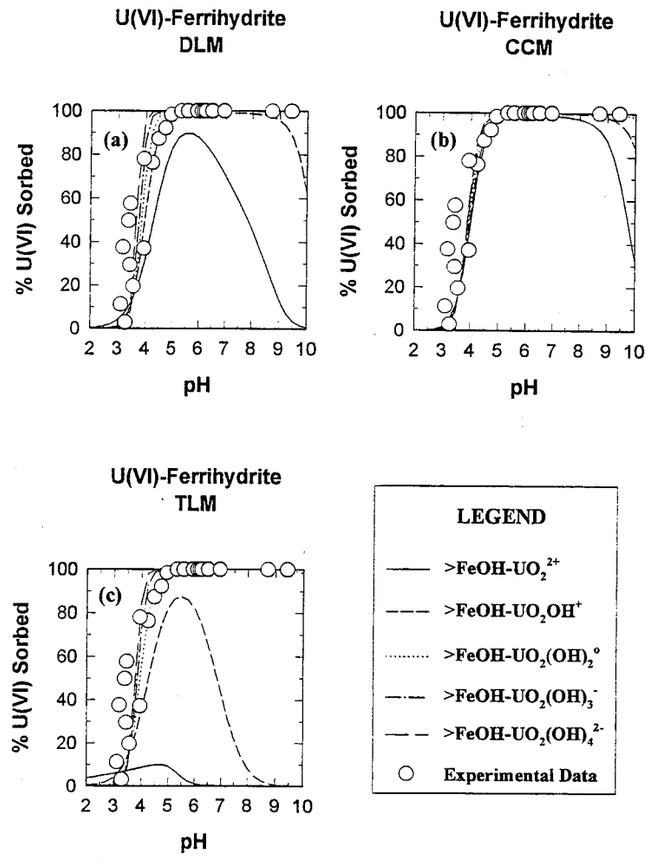

Figure 4-18. U(VI) sorption on ferrihydrite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $U(VI)_T = 1 \times 10^{-5}$ M, 0.1 M $NaNO_3$, M/V=1 g/L. Model parameters from Tables 3-1 and B-18. Data from Hsi and Langmuir (1985).

8/11/95
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Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 1: Retention of U(VI) onto silica and muscovite mica... and Figure 2: Log Kd in ml/g...) is from the following reference:

Della Mea, G. J.C. Dran, V. Moulin, J.C. Petit, J.D.F. Ramsay, and M. Theyssier. "Scavenging Properties of Inorganic Particles Toward Heavy Elements." Radiochimica Acta. Vols. 58 and 59. pp. 219-223. 1992.

8/11/95
DRJ

Della Mea, G., J.C. Dran, V. Moulin, J.C. Petit, J.D.F. Ramsay, and M. Theyssier. 1992. Scavenging properties of inorganic particles toward heavy elements. *Radiochimica Acta* 58/59:219-223.

Della Mea et al. (1992)	**U(VI)-SiO2**	
Figure 1 (page 220)		
Asp=50 m2/g	atm CO2 (?)	
U(VI)=5E-06	M/V=250 ppm=0.25 g/L	
0.1 M NaClO4		
pH	%sorbed	mol sorbed
4.70848	16.88736	8.444E-07
5.49578	43.80982	2.190E-06
6.05272	58.09594	2.905E-06
6.43351	57.25198	2.863E-06
6.90823	67.87060	3.394E-06
7.46014	77.38157	3.869E-06
7.99832	83.01599	4.151E-06
0.001 M NaClO4		
pH	%sorbed	mol sorbed
4.19846	43.69988	2.185E-06
4.45498	44.29351	2.215E-06
5.21773	55.62592	2.781E-06
5.26561	57.54081	2.877E-06
6.07645	52.01259	2.601E-06
6.25076	45.75504	2.288E-06
7.05559	29.41093	1.471E-06
7.11124	27.81505	1.391E-06
7.97127	15.05877	7.529E-07

Digitized Results

Della Mea, G., J.C. Dran, V. Moulin, J.C. Petit, J.D.F. Ramsay, and M. Theyssier. 1992. Scavenging properties of inorganic particles toward heavy elements. *Radiochimica Acta* 58/59:219-223.

Della Mea et al. (1992)	**U(VI)-Muscovite**	
Figure 1 (page 220)		
Asp=3 m2/g	atm CO2 (?)	
U(VI)=5E-06	M/V=250 ppm=0.25 g/L	
0.1 M NaClO4	Si:Al = 3:1 (tetra. site)	
pH	%sorbed	mol sorbed
4.33883	4.54684	2.273E-07
5.24792	9.99108	4.996E-07
5.95506	32.71527	1.636E-06
6.49187	37.61510	1.881E-06
6.94439	52.27614	2.614E-06
7.19866	39.97197	1.999E-06
7.80117	23.72417	1.186E-06

No FITEQL Results. Not modeled yet

8/26/95 DRJ

U(VI) - Ferrohydrite

Payne et al. (1992)

Information potentially subject to copyright protection was redacted from this location. The redacted material (4 graphs) is from the following reference:

Payne, T.E., K. Sekine, J.A. Davis, and T.D. Waite. "Modeling of Radionuclide Sorption Processes in the Weathered Zone of the Koongarra Ore Body." Alligator Rivers Analogue Project Annual Report, 1990-1991. P. Duerden, ed. Australian Nuclear Science and Technology Organization. pp. 57-85. 1992.

Payne, T.E., K. Sekine, J.A. Davis, and T.D. Waite. 1992. Modeling of radionuclide sorption processes in the weathered zone of the Koongarra ore body. P. Duerden, ed. *Alligator Rivers Analogue Project Annual Report, 1990-1991*. Australian Nuclear Science and Technology Organization (ANSTO):57-85.

Payne et al. (1992)	U(VI)-Ferrihydrite	
Figure 1 (page 72)		
Asp=600 m2/g (assumed)	No CO2	
0.1M NaNO3		
U(VI)=1E-08		
pH	%sorbed	mol sorbed
4.02	28.16	2.816e-09
4.29	43.39	4.339e-09
4.49	69.97	6.997e-09
4.77	88.13	8.813e-09
5.06	95.69	9.569e-09
U(VI)=1E-06		
pH	%sorbed	mol sorbed
3.06	1.6046	1.605e-08
3.29	5.3101	5.310e-08
3.57	2.2437	2.244e-08
3.83	15.323	1.532e-07
4.08	15.955	1.596e-07
4.25	28.482	2.848e-07
4.54	51.461	5.146e-07
4.76	74.337	7.434e-07
5.01	86.917	8.692e-07
5.24	94.297	9.430e-07
5.51	97.404	9.740e-07
5.73	99.634	9.963e-07
5.95	99.64	9.964e-07
U(VI)=1E-05		
pH	%sorbed	mol sorbed
3.99	7.177	7.177e-07
4.25	16	1.600e-06
4.49	30	3.000e-06
4.7	49	4.900e-06
4.75	53	5.300e-06
4.98	72	7.200e-06
5.61	94	9.400e-06
U(VI)=1E-04		
pH	%sorbed	mol sorbed
4.01	0.4313	4.313e-07
4.28	1.2387	1.239e-06
4.54	7.7947	7.795e-06
4.76	25.647	2.565e-05
4.89	33.824	3.482e-05
5.02	46.500	4.650e-05
5.52	78.207	7.921e-05

DRJ

Payne, T.E., K. Sekine, J.A. Davis, and T.D. Waite. 1992. Modeling of radionuclide sorption processes in the weathered zone of the Koongarra ore body. P. Duerden, ed. *Alligator Rivers Analogue Project Annual Report, 1990-1991*. Australian Nuclear Science and Technology Organization (ANSTO):57-85.

Payne et al. (1992)	U(VI)-Ferrihydrite	
Figure 3 (page 73)		
Asp=600 m2/g (assumed)	p(CO2)=1e-3.5 atm	
0.1M NaNO3		
U(VI)=1E-06		
pH	%sorbed	mol sorbed
3.06	1.6046	1.605e-08
3.29	5.3101	5.310e-08
3.57	2.2437	2.244e-08
3.83	15.323	1.532e-07
4.08	15.955	1.596e-07
4.25	28.482	2.848e-07
4.54	51.461	5.146e-07
4.76	74.337	7.434e-07
5.01	86.917	8.692e-07
5.24	94.297	9.430e-07
5.51	97.404	9.740e-07
5.73	99.634	9.963e-07
5.93	99.64	9.964e-07
6.21	99.573	9.957e-07
6.51	99.681	9.968e-07
6.89	99.117	9.912e-07
7.46	98.533	9.853e-07
7.74	98.291	9.829e-07
7.98	97.423	9.742e-07
8.29	83.535	8.354e-07
8.63	35.979	3.598e-07
8.94	1.6198	1.620e-08
9.22	2.5026	2.503e-08
9.62	1.8388	1.839e-08
U(VI)=1E-04		
pH	%sorbed	mol sorbed
4.01	0.43134	4.313e-07
4.28	1.2387	1.239e-06
4.54	7.7947	7.795e-06
4.76	25.647	2.565e-05
4.89	34.824	3.482e-05
5.02	46.5	4.650e-05
5.52	79.207	7.921e-05
6.41	96.079	9.608e-05
6.72	96.588	9.659e-05
7.17	94.251	9.425e-05
7.47	87.96	8.796e-05
8.00	31.662	3.166e-05
8.35	13.326	1.333e-05
8.51	4.4572	4.457e-06
8.64	0.086632	8.663e-08

8/26/95 DRJ

Digitized Data

DRJ/mm

Payne, T.E., K. Sekine, J.A. Davis, and T.D. Waite. 1992. Modeling of radionuclide sorption processes in the weathered zone of the Koongarra ore body. P. Duerden, ed. *Alligator Rivers Analogue Project Annual Report, 1990-1991*. Australian Nuclear Science and Technology Organization (ANSTO):57-85.

Payne et al. (1992)	U(VI)-Ferrihydrite	
Figure 4 (page 73)		
Asp=600 m2/g (assumed)	U(VI)=1E-06	
0.1M NaNO3		
pCO2=.03%=1e-3.5 atm		
pH	%sorbed	mol sorbed
3.06	1.6046	1.605e-08
3.29	5.3101	5.310e-08
3.57	2.2437	2.244e-08
3.83	15.323	1.532e-07
4.08	15.955	1.596e-07
4.25	28.482	2.848e-07
4.54	51.461	5.146e-07
4.76	74.337	7.434e-07
5.01	86.917	8.692e-07
5.24	94.297	9.430e-07
5.51	97.404	9.740e-07
5.73	99.634	9.963e-07
5.93	99.64	9.964e-07
6.21	99.573	9.957e-07
6.51	99.681	9.968e-07
6.89	99.117	9.912e-07
7.46	98.533	9.853e-07
7.74	98.291	9.829e-07
7.98	97.423	9.742e-07
8.29	83.535	8.354e-07
8.63	35.979	3.598e-07
8.94	1.6198	1.620e-08
9.22	2.5026	2.503e-08
9.62	1.8388	1.839e-08
pCO2=1%=1e-2 atm		
pH	%sorbed	mol sorbed
3.68	3.1389	3.139e-08
4.25	37.709	3.771e-07
4.86	91.732	9.173e-07
5.19	96.736	9.674e-07
5.61	95.806	9.581e-07
6	99.407	9.941e-07
6.42	99.328	9.933e-07
6.86	98.097	9.810e-07
7.33	71.579	7.158e-07
7.53	36.051	3.605e-07
7.86	0	0.000
8.22	0	0.000

DRJ/mm

Payne, T.E., K. Sekine, J.A. Davis, and T.D. Waite. 1992. Modeling of radionuclide sorption processes in the weathered zone of the Koongarra ore body. P. Duerden, ed. *Alligator Rivers Analogue Project Annual Report, 1990-1991*. Australian Nuclear Science and Technology Organization (ANSTO):57-85.

Payne et al. (1992)	U(VI)-Ferrihydrite	
Figure 5 (page 74)		
Asp=600 m2/g (assumed)	U(VI)=1E-06	
0.1M NaNO3	pCO2=.03% =1e-3.5 atm	
M/V=1E-3 M Fe		
pH	%sorbed	mol sorbed
3.06	1.6046	1.605e-08
3.29	5.3101	5.310e-08
3.57	2.2437	2.244e-08
3.83	15.323	1.532e-07
4.08	15.955	1.596e-07
4.25	28.482	2.848e-07
4.54	51.461	5.146e-07
4.76	74.337	7.434e-07
5.01	86.917	8.692e-07
5.24	94.297	9.430e-07
5.51	97.404	9.740e-07
5.73	99.634	9.963e-07
5.93	99.64	9.964e-07
6.21	99.573	9.957e-07
6.51	99.681	9.968e-07
6.89	99.117	9.912e-07
7.46	98.533	9.853e-07
7.74	98.291	9.829e-07
7.98	97.423	9.742e-07
8.29	83.535	8.354e-07
8.63	35.979	3.598e-07
8.94	1.6198	1.620e-08
9.22	2.5026	2.503e-08
9.62	1.8388	1.839e-08
M/V=2.1E-2 M Fe		
pH	%sorbed	mol sorbed
3.84	0.6459	6.459e-09
4.15	9.0459	9.046e-08
4.45	42.071	4.207e-07
4.72	70.678	7.068e-07
4.96	91.325	9.133e-07
5.29	98.29	9.829e-07
5.51	99.426	9.943e-07
5.93	99.727	9.973e-07
6.42	99.823	9.982e-07
6.92	99.672	9.967e-07
7.48	99.744	9.974e-07
7.83	99.778	9.978e-07
8.14	99.768	9.977e-07
8.36	99.671	9.967e-07
8.75	97.102	9.710e-07
9.07	77.357	7.736e-07
9.33	34.379	3.438e-07
9.7	0.077	7.700e-10

DRJ/mm

8/26/95 DRJ

```
      0
      1
      0
      0
      1
     90
      5          1          3          1
00001  -3.69  2.05E-4   XOH
00160  -1.0   0.00E00   PSI0
00161  -0.5   0.00E00   PSIB
00162  -0.1   0.00E00   PSID
00032  -8.0   1.00E-8   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00005  -1.0   0.00E00   NO3-
00003  -1.0   0.00E00   Na+

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
00100  -13.78  050 -1
01050    5.89  001  1 160  1 050  1
01100   -9.89  001  1 160 -1 050 -1
01055    8.21  001  1 160  1 161 -1 050  1 005  1
01103   -7.66  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
03301   -7.60  001  1 160 -1 161  2 050 -1 032  1 033  1

00004  600.0  0.089   0.8   0.2
0.1      1.0
         1
      3301
         5        1         1         0
        33
2.816E-9
4.339E-9
6.997E-9
8.813E-9
9.569E-9
        50
-4.02
-4.29
-4.49
-4.77
-5.06
         1        1
        33     0.10   1.0E-11
        50     0.05   0.0E-00
```

Fig. 1-1
TLM
XOH° + UO₂²⁺ = XO·UO₂⁺ − H⁺

DRJmm

```
      0
      1
      0
      0
      1
     90
      5          1          3          1
00001  -3.69  2.05E-4   XOH
00160  -1.0   0.00E00   PSI0
00161  -0.5   0.00E00   PSIB
00162  -0.1   0.00E00   PSID
00032  -6.0   1.00E-6   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
00100  -13.78  050 -1
01050    5.89  001  1 160  1 050  1
01100   -9.89  001  1 160 -1 050 -1
01055    8.21  001  1 160  1 161 -1 050  1 005  1
01103   -7.66  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
03301   -7.60  001  1 160 -1 161  2 050 -1 032  1 033  1

00004  600.0  0.089   0.8   0.2
0.1      1.0
         1
      3301
        13        1         1         0
        33
1.605E-8
5.310E-8
2.244E-8
1.532E-7
1.596E-7
2.848E-7
5.146E-7
7.434E-7
8.692E-7
8.430E-7
9.740E-6
9.963E-6
9.964E-6
        50
-3.06
-3.29
-3.57
-3.83
-4.08
-4.25
-4.54
-4.76
-5.01
-5.24
-5.51
-5.73
-5.95
         1        1
        33     0.10   1.0E-10
        50     0.05   0.0E-00
```

Fig. 1-2
TLM
XOH° + UO₂²⁺ = XO·UO₂⁺ − H⁺

DRJmm

```
      0
      1
      0
      0
      1
     90
      5          1          3          1
00001  -3.69  2.05E-4   XOH
00160  -1.0   0.00E00   PSI0
00161  -0.5   0.00E00   PSIB
00162  -0.1   0.00E00   PSID
00032  -5.0   1.00E-5   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
00100  -13.78  050 -1
01050    5.89  001  1 160  1 050  1
01100   -9.89  001  1 160 -1 050 -1
01055    8.21  001  1 160  1 161 -1 050  1 005  1
01103   -7.66  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
03301   -7.60  001  1 160 -1 161  2 050 -1 032  1 033  1

00004  600.0  0.089   0.8   0.2
0.1      1.0
         1
      3301
         7        1         1         0
        33
7.177E-7
1.600E-6
3.000E-6
4.900E-6
5.300E-6
7.200E-6
9.400E-6
        50
-3.99
-4.25
-4.49
-4.70
-4.75
-4.98
-5.61
         1        1
        33     0.10   1.0E-08
        50     0.05   0.0E-00
```

Fig. 1-3
TLM
XOH + UO₂²⁺ = XO·UO₂⁺ − H⁺

DRJmm

```
      0
      1
      0
      0
      1
     90
      5          1          3          1
00001  -3.69  2.05E-4   XOH
00160  -1.0   0.00E00   PSI0
00161  -0.5   0.00E00   PSIB
00162  -0.1   0.00E00   PSID
00032  -4.0   1.00E-4   UO2+2
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
03211   -0.05  032  1 005  1
00100  -13.78  050 -1
01050    5.89  001  1 160  1 050  1
01100   -9.89  001  1 160 -1 050 -1
01055    8.21  001  1 160  1 161 -1 050  1 005  1
01103   -7.66  001  1 160 -1 161  1 050 -1 003  1
00001    0.00  001  1
03301   -7.60  001  1 160 -1 161  2 050 -1 032  1 033  1

00004  600.0  0.089   0.8   0.2
0.1      1.0
         1
      3301
         7        1         1         0
        33
4.313E-7
1.239E-6
7.795E-6
2.565E-5
3.482E-5
4.650E-5
7.921E-5
        50
-4.01
-4.28
-4.52
-4.76
-4.89
-5.03
-5.54
         1        1
        33     0.10   1.0E-09
        50     0.05   0.0E-00
```

Fig. 1-4
TLM
XOH° + UO₂²⁺ = XO·UO₂⁺ − H⁺

DRJmm

DRJ 8/26/95

Example FITEQL Inputs (TLM)

8/26/95 DRJ

Fig. 4-2
TLM
XOH° + UO₂²⁺ = XO·UO₂⁺ + H⁺

DRJmm

Fig. 4-1
TLM
XOH° + UO₂²⁺ = XO·UO₂⁺ + H⁺

DRJmm

Fig. 3-2
TLM
XOH° + UO₂²⁺ = XO·UO₂⁺ + H⁺

DRJmm

Example FITEQL Inputs

Fig. 3-1
TLM
XOH° + UO₂²⁺ = XO·UO₂⁺ + H⁺

DRJmm

```
0
:
0
0
1
90
6 1 3 1
00001 -3.69 2.05E-4 XOH
00160 -1.0 0.00E00 PSI0
00161 -0.5 0.00E00 PSI8
00162 -0.1 0.00E00 PSI5
00032 -6.00 1.00E-6 UO2+2
00140 -3.52 3.02E-4 CO2g
00033 0.0 0.00E00 UO2ads
00050 0.0 0.00E00 H+
00003 -1.0 0.00E00 Na+
00005 -1.0 0.00E00 NO3-

00050 0.00 050 1
00032 0.00 032 1
00140 0.00 140 1
03201 -5.43 032 1 050 -1
03202 -10.54 032 1 050 -2
03203 -19.22 032 1 050 -3
03204 -32.59 032 1 050 -4
03205 -2.49 032 2 050 -1
03206 -5.42 032 2 050 -2
03207 -12.37 032 3 050 -4
03208 -16.25 032 3 050 -5
03209 -31.49 032 3 050 -7
03210 -22.83 032 4 050 -7
03211 -0.05 032 1 005 1
03212 -8.77 032 1 140 1 050 -2
03213 -19.35 032 1 140 2 050 -4
03214 -30.81 032 1 140 3 050 -6
03215 -51.09 032 3 140 6 050-12
03216 -70.09 032 11 140 6 050-24
03217 -19.28 032 2 140 1 050 -5
03218 -18.11 032 3 140 1 050 -5
01401 -17.50 140 1 050 -2
01402 -7.61 140 1 050 -1
01403 -1.48 140 1
01404 -16.67 140 1 050 -1 003 1
01405 -8.08 140 1 050 -2 003 1
00100 -13.78 050 -1
01050 5.89 001 1 160 1 050 1
01100 -9.89 001 1 160 -1 050 -1
01055 8.21 001 1 160 1 161 -1 050 1 005 1
01103 -7.66 001 1 160 -1 161 1 050 -1 003 1
00001 0.00 001 1
03301 -4.60 001 1 160 -1 161 2 050 -1 032 1 033 1

00004 600.0 0.089 0.8 0.2
0.1 1.0
1
3301
24 1 1 0
33
1.6046E-08
5.3101E-08
2.2437E-08
1.5323E-07
1.5955E-07
2.8482E-07
5.1461E-07
7.4337E-07
8.6917E-07
9.4297E-07
9.7404E-07
9.9634E-07
9.9640E-07
9.9573E-07
9.9481E-07
9.9117E-07
9.8533E-07
9.8291E-07
9.7423E-07
9.3535E-07
3.5979E-07
1.6198E-08
2.5026E-08
1.8388E-08
50
-3.06
-3.29
-3.57
-3.83
-4.08
-4.25
-4.54
-4.76
-5.01
-5.24
-5.51
-5.73
-5.93
-6.21
-6.51
-6.89
-7.46
-7.74
-7.98
-8.29
-8.63
-8.94
-9.22
-9.62
1 1
33 0.10 1.0E-10
50 0.05 0.0E-00
```

Fig 5-1
TLM
$XOH^0 + UO_2^{2+} = XO\text{-}UO_2^+ + H^+$

```
Ferryhid 0
Payne(92 1
1.00e-6M 0
2.3si/rm 0
00000050 1
00000060 90
00000070 6 1 3 1
00000080 00001 -2.39 4.10E-3 XOH
00000090 00160 -1.0 0.00E00 PSI0
00000092 00161 -0.5 0.00E00 PSI8
00000094 00162 -0.1 0.00E00 PSI5
00000098 00032 -6.0 1.00E-6 UO2+2
00000107 00140 -3.52 3.02E-4 CO2g
00000100 00033 0.0 0.00E00 UO2ads
00000102 00050 0.0 0.00E00 H+
00000103 00003 -1.0 0.00E00 Na+
00000104 00005 -1.0 0.00E00 NO3-
00000110
00000120 00050 0.00 050 1
00000124 00032 0.00 032 1
00000125 00140 0.00 140 1
00000126 03201 -5.43 032 1 050 -1
00000127 03202 -10.54 032 1 050 -2
00000128 03203 -19.22 032 1 050 -3
00000129 03204 -32.59 032 1 050 -4
00000130 03205 -2.49 032 2 050 -1
00000131 03206 -5.42 032 2 050 -2
00000132 03207 -12.37 032 3 050 -4
00000133 03208 -16.25 032 3 050 -5
00000134 03209 -31.49 032 3 050 -7
00000135 03210 -22.83 032 4 050 -7
00000137 03211 -0.05 032 1 005 1
00000139 00100 -13.78 050 -1
00000140 01050 7.35 001 1 160 1 050 1
00000145 01100 -8.45 001 1 160 -1 050 -1
00000150 00001 0.00 001 1
xouo2 03301 -7.60 001 1 160 -1 161 2 050 -1 032 1 033 1
00000174
00000175
00000180 00004 600.0 1.78 0.8 0.2
00000185 0.1 1.0
00000190 1
00000195 3301
00000230 18 1 1 0
00000240 33
00000260 6.4590E-09
00000280 9.0459E-08
00000300 4.2071E-07
00000320 7.0678E-07
00000340 9.1325E-07
00000341 9.8290E-07
00000342 9.9426E-07
00000343 9.9727E-07
00000344 9.9823E-07
00000345 9.9672E-07
00000346 9.9744E-07
00000347 9.9778E-07
00000348 9.9768E-07
00000349 9.9671E-07
00000350 9.7102E-07
00000351 7.7357E-07
00000352 3.4379E-07
00000353 7.7000E-10
00000354 50
00000355 -3.84
00000356 -4.15
00000357 -4.45
00000358 -4.72
00000359 -4.96
00000680 -5.29
00000690 -5.51
00000700 -5.93
00000710 -6.42
00000720 -6.92
00000730 -7.48
00000731 -7.83
00000732 -8.14
00000734 -8.36
00000735 -8.75
00000736 -9.07
00000737 -9.33
00000738 -9.70
00000739 1 1
00000740 33 0.10 1.0E-09
00000741 50 0.05 0.0E-00
00000742
00000743
00000744
00000745
00000746
00000747
00000748
00000749
00001170
00001180
00001190
```

Fig 5-2
-LM
$XOH^0 + UO_2^{2+} = XO\text{-}UO_2^+ + H^+$

```
Ferryhid 0
Payne(92 1
1.00e-6M 0
2.3si/rm 0
00000050 1
00000060 90
00000070 3 1 3 1
00000080 00001 -3.69 2.05E-4 XOH
00000090 00160 -1.0 0.00E00 PSI0
00000092 00032 -8.0 1.00E-8 UO2+2
00000094 00033 0.0 0.00E00 UO2ads
00000098 00050 0.0 0.00E00 H+
00000107 00003 -1.0 0.00E00 Na+
00000100 00005 -1.0 0.00E00 NO3-
00000102
00000103 00050 0.00 050 1
00000104 00032 0.00 032 1
00000110
00000120 03201 -5.43 032 1 050 -1
00000124 03202 -10.54 032 1 050 -2
00000125 03203 -19.22 032 1 050 -3
00000126 03204 -32.59 032 1 050 -4
00000127 03205 -2.49 032 2 050 -1
00000128 03206 -5.42 032 2 050 -2
00000129 03207 -12.37 032 3 050 -4
00000130 03208 -16.25 032 3 050 -5
00000131 03209 -31.49 032 3 050 -7
00000132 03210 -22.83 032 4 050 -7
00000133 03211 -0.05 032 1 005 1
00000134 00100 -13.78 050 -1
00000135 01050 7.35 001 1 160 1 050 1
00000137 01100 -8.45 001 1 160 -1 050 -1
00000139 00001 0.00 001 1
00000140 03301 1.60 001 1 160 1 050 -1 032 1 033 1
00000141
00000142 00001 600.0 0.089 1.0
00000143 0 0
00000144 1
00000145 3301
00000146 7 1 1 0
00000147 33
00000148 7.177E-7
00000146 1.600E-6
00000147 3.000E-6
00000139 4.900E-6
00000140 5.300E-6
00000145 7.200E-6
00000140 9.400E-6
00000141 50
00000150 -3.99
xouo2 -4.25
-4.49
-4.70
-4.75
-4.98
-5.61
1 1
33 0.10 1.0E-08
50 0.05 0.0E-00
```

Fig 5-3
LCM
$XOH^0 + UO_2^{2+} = XO\text{-}UO_2^+ + H^+$

```
Ferryhid 0
Payne(92 1
1.00e-6M 0
2.3si/rm 0
00000050 1
00000060 90
00000070 3 1 3 1
00000080 00001 -3.69 2.05E-4 XOH
00000090 00160 -1.0 0.00E00 PSI0
00000098 00032 -5.0 1.00E-5 UO2+2
00000100 00033 0.0 0.00E00 UO2ads
00000102 00050 0.0 0.00E00 H+
00000103 00003 -1.0 0.00E00 Na+
00000104 00005 -1.0 0.00E00 NO3-
00000110
00000120 00050 0.00 050 1
00000124 00032 0.00 032 1
00000126 03201 -5.43 032 1 050 -1
00000127 03202 -10.54 032 1 050 -2
00000128 03203 -19.22 032 1 050 -3
00000129 03204 -32.59 032 1 050 -4
00000130 03205 -2.49 032 2 050 -1
00000131 03206 -5.42 032 2 050 -2
00000132 03207 -12.37 032 3 050 -4
00000133 03208 -16.25 032 3 050 -5
00000134 03209 -31.49 032 3 050 -7
00000135 03210 -22.83 032 4 050 -7
00000137 03211 -0.05 032 1 005 1
00000139 00100 -13.78 050 -1
00000140 01050 7.35 001 1 160 1 050 1
00000145 01100 -8.45 001 1 160 -1 050 -1
00000150 00001 0.00 001 1
xouo2 03301 2.20 001 1 160 1 050 -1 032 1 033 1
00000174
00000175
00000180 00001 600.0 0.089 1.0
00000185 0 0
00000190 1
00000195 3301
00000230 13 1 1 0
00000240 33
00000260 1.605E-8
00000280 5.310E-8
00000300 2.244E-8
00000320 1.532E-7
00000340 1.596E-7
00000680 2.848E-7
00000690 5.146E-7
00000700 7.434E-7
00000710 8.692E-7
00000720 8.430E-7
00000730 9.740E-6
00001170 9.963E-6
00001180 9.964E-6
00001190 50
-3.06
-3.29
Ferryhid -3.57
Payne(91 -3.83
1.00e-6M -4.08
2.3si/rm -4.25
00000050 -4.54
00000060 -4.76
00000070 -5.01
00000080 -5.24
00000090 -5.51
00000098 -5.73
00000100 -5.95
00000102 1 1
00000103 33 0.10 1.0E-10
00000104 50 0.05 0.0E-00
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000137
00000139
00000140
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000370
00000680
00000690
00000700
00000710
00000720
00000730
00000740
00000750
00001170
00001180
00001190
```

Fig 1-1
LCM
$XOH^0 + UO_2^{2+} = XO\text{-}UO_2^+ + H^+$

```
Ferryhid 0
Payne(91 1
1.00e-6M 0
2.3si/rm 0
00000050 1
00000060 90
00000070 3 1 3 1
00000080 00001 -3.69 2.05E-4 XOH
00000090 00160 -1.0 0.00E00 PSI0
00000098 00032 -6.0 1.00E-6 UO2+2
00000100 00033 0.0 0.00E00 UO2ads
00000102 00050 0.0 0.00E00 H+
00000103 00003 -1.0 0.00E00 Na+
00000104 00005 -1.0 0.00E00 NO3-
00000110
00000120 00050 0.00 050 1
00000124 00032 0.00 032 1
00000126 03201 -5.43 032 1 050 -1
00000127 03202 -10.54 032 1 050 -2
00000128 03203 -19.22 032 1 050 -3
00000129 03204 -32.59 032 1 050 -4
00000130 03205 -2.49 032 2 050 -1
00000131 03206 -5.42 032 2 050 -2
00000132 03207 -12.37 032 3 050 -4
00000133 03208 -16.25 032 3 050 -5
00000134 03209 -31.49 032 3 050 -7
00000135 03210 -22.83 032 4 050 -7
00000137 03211 -0.05 032 1 005 1
00000139 00100 -13.78 050 -1
00000140 01050 7.35 001 1 160 1 050 1
00000145 01100 -8.45 001 1 160 -1 050 -1
00000150 00001 0.00 001 1
xouo2 03301 2.60 001 1 160 1 050 -1 032 1 033 1
00000174
00000175
00000180 00001 600.0 0.089 1.0
00000185 0 0
00000190 1
00000195 3301
00000230 5 1 1 0
00000240 33
00000260 2.816E-9
00000280 4.339E-9
00000300 6.997E-9
00000320 8.813E-9
00000340 9.569E-9
00000680 50
00000690 -4.02
00000700 -4.29
00000710 -4.49
00000720 -4.77
00000730 -5.06
00001170 1 1
00001180 33 0.10 1.0E-11
00001190 50 0.05 0.0E-00
```

Fig 1-3
LCM
$XOH^0 + UO_2^{2+} = XO\text{-}UO_2^+ + H^+$

```
Ferryhid 0
Payne(91 1
1.00e-6M 0
2.3si/rm 0
00000050 1
00000060 90
00000070 3 1 3 1
00000080 00001 -3.69 2.05E-4 XOH
00000090 00160 -1.0 0.00E00 PSI0
00000098 00032 -6.0 1.00E-6 UO2+2
00000100 00033 0.0 0.00E00 UO2ads
00000102 00050 0.0 0.00E00 H+
00000103 00003 -1.0 0.00E00 Na+
00000104 00005 -1.0 0.00E00 NO3-
00000110
00000120 00050 0.00 050 1
00000124 00032 0.00 032 1
00000126 03201 -5.43 032 1 050 -1
00000127 03202 -10.54 032 1 050 -2
00000128 03203 -19.22 032 1 050 -3
00000129 03204 -32.59 032 1 050 -4
00000130 03205 -2.49 032 2 050 -1
00000131 03206 -5.42 032 2 050 -2
00000132 03207 -12.37 032 3 050 -4
00000133 03208 -16.25 032 3 050 -5
00000134 03209 -31.49 032 3 050 -7
00000135 03210 -22.83 032 4 050 -7
00000137 03211 -0.05 032 1 005 1
00000139 00100 -13.78 050 -1
00000140 01050 7.35 001 1 160 1 050 1
00000145 01100 -8.45 001 1 160 -1 050 -1
00000150 00001 0.00 001 1
xouo2 03301 2.20 001 1 160 1 050 -1 032 1 033 1
00000174
00000175
00000180 00001 600.0 0.089 1.0
00000185 0 0
00000190 1
00000195 3301
00000230 13 1 1 0
00000240 33
00000260 1.605E-8
00000280 5.310E-8
00000300 2.244E-8
00000320 1.532E-7
00000340 1.596E-7
00000680 2.848E-7
00000690 5.146E-7
00000700 7.434E-7
00000710 8.692E-7
00000720 8.430E-7
00000730 9.740E-6
00001170 9.963E-6
00001180 9.964E-6
00001190 50
-3.06
-3.29
Ferryhid -3.57
Payne(91 -3.83
1.00e-6M -4.08
2.3si/rm -4.25
00000050 -4.54
00000060 -4.76
00000070 -5.01
00000080 -5.24
00000090 -5.51
00000098 -5.73
00000100 -5.95
00000102 1 1
00000103 33 0.10 1.0E-10
00000104 50 0.05 0.0E-00
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000137
00000139
00000140
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000370
00000680
00000690
00000700
00000710
00000720
00000730
00000740
00000750
00001170
00001180
00001190
```

Fig 1-2
LCM
$XOH + UO_2^{2+} = XO\text{-}UO_2^+ + H^+$

Example FITEQL Inputs

8228

5/4/95

LCM

```
0
1
0
0
1
90
3
301 -3.69  2.05E-4   XOH
160 -1.0   0.00E00   PS10
302 -4.0   1.00E-4   UO2+2
333  0.0   0.00E00   UO2ads
350  0.0   0.00E00   H+
303 -1.0   0.00E00   Na+
305 -1.0   0.00E00   NO3-

350    0.00   050  1
332    0.00   032  1
201   -5.43   032  1 050 -1
202  -10.54   032  1 050 -2
203  -19.22   032  1 050 -3
204  -32.59   032  1 050 -4
205   -2.49   032  2 050 -1
206   -5.42   032  2 050 -2
207  -12.37   032  3 050 -4
208  -16.25   032  3 050 -5
209  -31.49   032  3 050 -7
210  -22.83   032  4 050 -7
211   -0.05   032  1 005  1
100  -13.78   050 -1
050    7.35   001  1 160  1 050  1
100   -8.45   001  1 160 -1 050 -1
001    0.00   001  1
301    0.60   001  1 160  1 050 -1 032  1 033  1


001  600.0  0.089     1.0
   0    0
     1
  3301
     7          1          1          0
    33
313E-7
239E-6
795E-6
565E-5
482E-5
650E-5
921E-5
    50
.01
.28
.52
.76
.89
.03
.54
     1          1
    33      0.10    1.0E-09
    50      0.05    0.0E-00
```

Fig 1-4
LCM
$XOH^0 + UO_2^{2+} = XOUO_2^+ + H^+$

Example FITEQL Inputs

```
Ferryhid        0
Payne(91        1
1.00e-6M        0
2.3si/nm        0
00000050        1
00000060       90
00000070        4
00000080 00001 -3.69  2.05E-4   XOH          3          1
00000090 00160 -1.0   0.00E00   PS10
00000098 00032 -6.00  1.00E-6   UO2+2
00000100 00140 -3.52  3.02E-4   CO2g
00000102 00033  0.0   0.00E00   UO2ads
00000103 00050  0.0   0.00E00   H+
00000104 00003 -1.0   0.00E00   Na+
00000110 00005 -1.0   0.00E00   NO3-
00000120
00000124 00050    0.00   050  1
00000126 00032    0.00   032  1
00000127 00140    0.00   140  1
00000128 03201   -5.43   032  1 050 -1
00000129 03202  -10.54   032  1 050 -2
00000130 03203  -19.22   032  1 050 -3
00000131 03204  -32.59   032  1 050 -4
00000132 03205   -2.49   032  2 050 -1
00000133 03206   -5.42   032  2 050 -2
00000134 03207  -12.37   032  3 050 -4
00000135 03208  -16.25   032  3 050 -5
00000134 03209  -31.49   032  3 050 -7
00000139 03210  -22.83   032  4 050 -7
00000140 03211   -0.05   032  1 005  1
00000145 03212   -8.77   032  1 140  1 050 -2
00000150 03213  -19.35   032  1 140  2 050 -4
xouo2    03214  -30.81   032  1 140  3 050 -6
00000174 03215  -51.09   032  3 140  6 050-12
00000175 03216  -70.09   032 11 140  6 050-24
00000180 03217  -19.28   032  2 140  1 050 -5
00000185 03218  -18.11   032  3 140  1 050 -5
00000190 01401  -17.50   140  1 050 -2
00000195 01402   -7.61   140  1 050 -1
00000230 01403   -1.48   140  1
00000240 01404  -16.67   140  1 050 -1 003  1
00000260 01405   -8.08   140  1 050 -2 003  1
00000280 00100  -13.78   050 -1
00000300 01050    7.35   001  1 160  1 050  1
00000320 01100   -8.45   001  1 160 -1 050 -1
00000340 00001    0.00   001  1
00000360 03301    0.60   001  1 160  1 050 -1 032  1 033  1
00000370
00000680
00000690 00001  600.0  0.089     1.0
00000700      0    0
00000710        1
00000720     3301
00000730       24          1          1          0
00000740       33
00000750 1.6046E-08
00001170 5.3101E-08
00001180 2.2437E-08
00001190 1.5323E-07
         1.5955E-07
         2.8482E-07
         5.1461E-07
         7.4337E-07
         8.6917E-07
         9.4297E-07
         9.7404E-07
         9.9634E-07
         9.9640E-07
         9.9573E-07
         9.9681E-07
         9.9117E-07
         9.8533E-07
         9.8291E-07
         9.7423E-07
         8.3535E-07
         3.5979E-07
         1.6198E-08
         2.5026E-08
         1.8388E-08
           50
        -3.06
        -3.29
        -3.57
        -3.83
        -4.08
        -4.25
        -4.54
        -4.76
        -5.01
        -5.24
        -5.51
        -5.73
        -5.93
        -6.21
        -6.51
        -6.89
        -7.46
        -7.74
        -7.98
        -8.29
        -8.63
        -8.94
        -9.22
        -9.62
           1          1
          33      0.10    1.0E-10
          50      0.05    0.0E-00
```

Fig 3-1
LCM
$XOH^0 + UO_2^{2+} = XOUO_2^+ + H^+$

```
Ferryhid        0
Payne(92        1
1.00e-6M        0
2.3si/nm        0
00000050        1
00000060       90
00000070        4
00000080 00001 -3.69  2.05E-4   XOH          3          1
00000090 00160 -1.0   0.00E00   PS10
00000098 00032 -4.00  1.00E-4   UO2+2
00000107 00140 -3.52  3.02E-4   CO2g
00000100 00033  0.0   0.00E00   UO2ads
00000102 00050  0.0   0.00E00   H+
00000103 00003 -1.0   0.00E00   Na+
00000104 00005 -1.0   0.00E00   NO3-
00000110
00000120 00050    0.00   050  1
00000124 00032    0.00   032  1
00000125 00140    0.00   140  1
00000126 03201   -5.43   032  1 050 -1
00000127 03202  -10.54   032  1 050 -2
00000128 03203  -19.22   032  1 050 -3
00000129 03204  -32.59   032  1 050 -4
00000130 03205   -2.49   032  2 050 -1
00000131 03206   -5.42   032  2 050 -2
00000132 03207  -12.37   032  3 050 -4
00000133 03208  -16.25   032  3 050 -5
00000134 03209  -31.49   032  3 050 -7
00000135 03210  -22.83   032  4 050 -7
00000137 03211   -0.05   032  1 005  1
00000139 03212   -8.77   032  1 140  1 050 -2
00000140 03213  -19.35   032  1 140  2 050 -4
00000141 03214  -30.81   032  1 140  3 050 -6
00000142 03215  -51.09   032  3 140  6 050-12
00000143 03216  -70.09   032 11 140  6 050-24
00000144 03217  -19.28   032  2 140  1 050 -5
00000145 03218  -18.11   032  3 140  1 050 -5
00000146 01401  -17.50   140  1 050 -2
00000147 01402   -7.61   140  1 050 -1
00000148 01403   -1.48   140  1
00000146 01404  -16.67   140  1 050 -1 003  1
00000147 01405   -8.08   140  1 050 -2 003  1
00000139 00100  -13.78   050 -1
00000140 01050    7.35   001  1 160  1 050  1
00000145 01100   -8.45   001  1 160 -1 050 -1
00000150 00001    0.00   001  1
xouo2    03301    3.60   001  1 160  1 050 -1 032  1 033  1
00000174
00000175
00000180 00001  600.0  0.089     1.0
00000185      0    0
00000190        1
00000195     3301
00000230       15          1          1          0
00000240       33
00000260 4.3134E-07
00000280 1.2387E-06
00000300 7.7947E-06
00000320 2.5647E-05
00000340 3.4824E-05
00000341 4.6500E-05
00000342 7.9207E-05
00000343 9.6079E-05
00000344 9.6588E-05
00000345 9.4251E-05
00000346 8.7969E-05
00000347 3.1662E-05
00000348 1.3326E-05
00000349 4.4572E-06
00000350 8.6632E-08
00000351      50
00000352   -4.01
00000353   -4.28
00000354   -4.54
00000355   -4.76
00000356   -4.89
00000357   -5.02
00000358   -5.52
00000359   -6.41
00000680   -6.72
00000690   -7.17
00000700   -7.47
00000710   -8.00
00000720   -8.35
00000730   -8.51
00000731   -8.64
00000732
00000733        1          1
00000734       33      0.10    1.0E-09
00000735       50      0.05    0.0E-00
00000736
00000737
00000738
00000739
00000740
00000741
00000742
00000743
00000744
00000745
00000746
00000747
00000748
00000749
00001170
00001180
00001190
```

Fig. 3-2
CCM
$XOH^0 + UO_2^{2+} = XO\text{-}UO_2^+ + H^+$

```
Ferryhid        0
Payne(92        1
1.00e-6M        0
2.3si/nm        0
00000050        1
00000060       90
00000070        4
00000080 00001 -3.69  2.05E-4   XOH          3          1
00000090 00160 -1.0   0.00E00   PS10
00000098 00032 -6.00  1.00E-6   UO2+2
00000107 00140 -3.52  3.02E-4   CO2g
00000100 00033  0.0   0.00E00   UO2ads
00000102 00050  0.0   0.00E00   H+
00000103 00003 -1.0   0.00E00   Na+
00000104 00005 -1.0   0.00E00   NO3-
00000110
00000120 00050    0.00   050  1
00000124 00032    0.00   032  1
00000125 00140    0.00   140  1
00000126 03201   -5.43   032  1 050 -1
00000127 03202  -10.54   032  1 050 -2
00000128 03203  -19.22   032  1 050 -3
00000129 03204  -32.59   032  1 050 -4
00000130 03205   -2.49   032  2 050 -1
00000131 03206   -5.42   032  2 050 -2
00000132 03207  -12.37   032  3 050 -4
00000133 03208  -16.25   032  3 050 -5
00000134 03209  -31.49   032  3 050 -7
00000135 03210  -22.83   032  4 050 -7
00000137 03211   -0.05   032  1 005  1
00000139 03212   -8.77   032  1 140  1 050 -2
00000140 03213  -19.35   032  1 140  2 050 -4
00000141 03214  -30.81   032  1 140  3 050 -6
00000142 03215  -51.09   032  3 140  6 050-12
00000143 03216  -70.09   032 11 140  6 050-24
00000144 03217  -19.28   032  2 140  1 050 -5
00000145 03218  -18.11   032  3 140  1 050 -5
00000146 01401  -17.50   140  1 050 -2
00000147 01402   -7.61   140  1 050 -1
00000148 01403   -1.48   140  1
00000146 01404  -16.67   140  1 050 -1 003  1
00000147 01405   -8.08   140  1 050 -2 003  1
00000139 00100  -13.78   050 -1
00000140 01050    7.35   001  1 160  1 050  1
00000145 01100   -8.45   001  1 160 -1 050 -1
00000150 00001    0.00   001  1
xouo2    03301    0.60   001  1 160  1 050 -1 032  1 033  1
00000174
00000175
00000180 00001  600.0  0.089     1.0
00000185      0    0
00000190        1
00000195     3301
00000230       24          1          1          0
00000240       33
00000260 1.6046E-08
00000280 5.3101E-08
00000300 2.2437E-08
00000320 1.5323E-07
00000340 1.5955E-07
00000341 2.8482E-07
00000342 5.1461E-07
00000343 7.4337E-07
00000344 8.6917E-07
00000345 9.4297E-07
00000346 9.7404E-07
00000347 9.9634E-07
00000348 9.9640E-07
00000349 9.9573E-07
00000350 9.9681E-07
00000680 9.9117E-07
00000690 9.8533E-07
00000700 9.8291E-07
00000710 9.7423E-07
00000720 8.3535E-07
00000730 3.5979E-07
00000731 1.6198E-08
00000732 2.5026E-08
00000733 1.8388E-08
00000734       50
00000735    -3.06
00000736    -3.29
00000737    -3.57
00000738    -3.83
00000739    -4.08
00000740    -4.25
00001170    -4.54
00001180    -4.76
00001190    -5.01
            -5.24
            -5.51
            -5.73
            -5.93
            -6.21
            -6.51
            -6.89
            -7.46
            -7.74
            -7.98
            -8.29
            -8.63
            -8.94
            -9.22
            -9.62
               1          1
              33      0.10    1.0E-10
              50      0.05    0.0E-00
```

Fig 4-1
LCM
$XOH^0 + UO_2^{2+} = XO\text{-}UO_2^+ + H^+$

```
Ferryhid
Payne(92
1.00e-6M
2.3si/nm
00000050
00000060
00000070
00000080
00000090
00000098
00000107
00000100
00000102
00000103
00000104
00000110
00000120
00000124
00000125
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000137
00000139
00000140
00000141
00000142
00000143
00000144
00000145
00000146
00000147
00000148
00000146
00000147
00000139
00000140
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000341
00000342
00000343
00000344
00000345
00000346
00000347
00000348
00000349
00000350
00000351
00000352
00000353
00000354
00000355
00000356
00000357
00000358
00000359
00000680
00000690
00000700
00000710
00000720
00000730
00000731
00000732
00000733
00000734
00000735
00000736
00000737
00000738
00000739
00000740
00000741
00000742
00000743
00000744
00000745
00000746
00000747
00000748
00000749
00001170
00001180
00001190
```

Example FITEQL Inputs

Fig. 4-2

CCM

XOH° + UO$_2^{2+}$ = XOUO$_2^+$ + H$^+$

```
       0
       1
       0
       0
       1
      90
       4         1          3          1
)0001  -3.69  2.05E-4   XOH
)0160  -1.0   0.00E00   PSIO
)0032  -6.00  1.00E-6   UO2+2
)0140  -2.00  1.00E-2   CO2g
)0033   0.0   0.00E00   UO2ads
)0050   0.0   0.00E00   H+
)0003  -1.0   0.00E00   Na+
)0005  -1.0   0.00E00   NO3-

)0050    0.00  050  1
)0032    0.00  032  1
)0140    0.00  140  1
3201    -5.43  032  1 050 -1
3202   -10.54  032  1 050 -2
3203   -19.22  032  1 050 -3
3204   -32.59  032  1 050 -4
3205    -2.49  032  2 050 -1
3206    -5.42  032  2 050 -2
3207   -12.37  032  3 050 -4
3208   -16.25  032  3 050 -5
3209   -31.49  032  3 050 -7
3210   -22.83  032  4 050 -7
3211    -0.05  032  1 005  1
3212    -8.77  032  1 140  1 050 -2
3213   -19.35  032  1 140  2 050 -4
3214   -30.81  032  1 140  3 050 -6
3215   -51.09  032  3 140  6 050-12
3216   -70.09  032 11 140  6 050-24
3217   -19.28  032  2 140  1 050 -5
3218   -18.11  032  3 140  1 050 -5
1401   -17.50  140  1 050 -2
1402    -7.61  140  1 050 -1
1403    -1.48  140  1
1404   -16.67  140  1 050 -1 003  1
1405    -8.08  140  1 050 -2 003  1
0100   -13.78  050 -1
1050     7.35  001  1 160  1 050  1
1100    -8.45  001  1 160 -1 050 -1
0001     0.00  001  1
3301     2.60  001  1 160  1 050 -1 032  1 033  1

)001  600.0  0.089      1.0
    0      0
      1
   3301
     10        1         1         0
     33
.1389E-08
.7709E-07
.1732E-07
.6736E-07
.5806E-07
.9407E-07
.9328E-07
.8097E-07
.1579E-07
.6051E-07
     50
.68
.25
.86
.19
.61
.00
.42
.86
.33
.53
      1         1
     33      0.10   1.0E-09
     50      0.05   0.0E-00
```

Fig. 5-1

CCM

XOH° + UO$_2^{2+}$ = XO-UO$_2^+$ + H$^+$

```
Ferryhid       0
Payne(92       1
1.00e-6M       0
2.3si/nm       0
00000050       1
00000060      90
00000070       4         1          3          1
00000080 00001  -3.69  2.05E-4   XOH
00000090 00160  -1.0   0.00E00   PSIO
00000098 00032  -6.00  1.00E-6   UO2+2
00000107 00140  -3.52  3.02E-4   CO2g
00000100 00033   0.0   0.00E00   UO2ads
00000102 00050   0.0   0.00E00   H+
00000102 00003  -1.0   0.00E00   Na+
00000102 00005  -1.0   0.00E00   NO3-
00000110
00000120 00050    0.00  050  1
00000124 00032    0.00  032  1
00000125 00140    0.00  140  1
00000126 03201   -5.43  032  1 050 -1
00000127 03202  -10.54  032  1 050 -2
00000128 03203  -19.22  032  1 050 -3
00000129 03204  -32.59  032  1 050 -4
00000130 03205   -2.49  032  2 050 -1
00000131 03206   -5.42  032  2 050 -2
00000132 03207  -12.37  032  3 050 -4
00000133 03208  -16.25  032  3 050 -5
00000134 03209  -31.49  032  3 050 -7
00000135 03210  -22.83  032  4 050 -7
00000137 03211   -0.05  032  1 005  1
00000139 03212   -8.77  032  1 140  1 050 -2
00000140 03213  -19.35  032  1 140  2 050 -4
00000141 03214  -30.81  032  1 140  3 050 -6
00000142 03215  -51.09  032  3 140  6 050-12
00000143 03216  -70.09  032 11 140  6 050-24
00000144 03217  -19.28  032  2 140  1 050 -5
00000145 03218  -18.11  032  3 140  1 050 -5
00000146 01401  -17.50  140  1 050 -2
00000147 01402   -7.61  140  1 050 -1
00000148 01403   -1.48  140  1
00000146 01404  -16.67  140  1 050 -1 003  1
00000147 01405   -8.08  140  1 050 -2 003  1
00000139 00100  -13.78  050 -1
00000140 01050    7.35  001  1 160  1 050  1
00000145 01100   -8.45  001  1 160 -1 050 -1
00000150 00001    0.00  001  1
xouo2    03301    0.60  001  1 160  1 050 -1 032  1 033  1
00000174
00000175
00000180 00001  600.0  0.089      1.0
00000185          0      0
00000190            1
00000195         3301
00000230           24        1         1         0
00000240           33
00000260 1.6046E-08
00000280 5.3101E-08
00000300 2.2437E-08
00000320 1.5323E-07
00000340 1.5955E-07
00000360 2.8482E-07
00000361 5.1461E-07
00000362 7.4337E-07
00000363 8.6917E-07
00000364 9.4297E-07
00000680 9.7404E-07
00000681 9.9634E-07
00000690 9.9640E-07
00000700 9.9573E-07
00000710 9.9681E-07
00000720 9.9117E-07
00000730 9.8533E-07
00000740 9.8291E-07
00000741 9.7423E-07
00000742 8.3535E-07
00000743 3.5979E-07
00001170 1.6198E-08
00001180 2.5026E-08
00001190 1.8388E-08
                   50
          -3.06
          -3.29
          -3.57
          -3.83
          -4.08
          -4.25
          -4.54
          -4.76
          -5.01
          -5.24
          -5.51
          -5.73
          -5.93
          -6.21
          -6.51
          -6.89
          -7.46
          -7.74
          -7.98
          -8.29
          -8.63
          -8.94
          -9.22
          -9.62
                    1         1
                   33      0.10   1.0E-10
                   50      0.05   0.0E-00
```

Fig. 5-2

CCM

XOH° + UO$_2^{2+}$ = XOUO$_2^+$ + H$^+$

```
Ferryhid       0
Payne(92       1
1.00e-6M       0
2.3si/nm       0
00000050       1
00000060      90
00000070       4         1          3          1
00000080 00001  -2.39  4.10E-3   XOH
00000090 00160  -1.0   0.00E00   PSIO
00000098 00032  -6.0   1.00E-6   UO2+2
00000107 00140  -3.52  3.02E-4   CO2g
00000100 00033   0.0   0.00E00   UO2ads
00000102 00050   0.0   0.00E00   H+
00000103 00003  -1.0   0.00E00   Na+
00000104 00005  -1.0   0.00E00   NO3-
00000110
00000120 00050    0.00  050  1
00000124 00032    0.00  032  1
00000125 00140    0.00  140  1
00000126 03201   -5.43  032  1 050 -1
00000127 03202  -10.54  032  1 050 -2
00000128 03203  -19.22  032  1 050 -3
00000129 03204  -32.59  032  1 050 -4
00000130 03205   -2.49  032  2 050 -1
00000131 03206   -5.42  032  2 050 -2
00000132 03207  -12.37  032  3 050 -4
00000133 03208  -16.25  032  3 050 -5
00000134 03209  -31.49  032  3 050 -7
00000135 03210  -22.83  032  4 050 -7
00000137 03211   -0.05  032  1 005  1
00000139 03212   -8.77  032  1 140  1 050 -2
00000140 03213  -19.35  032  1 140  2 050 -4
00000141 03214  -30.81  032  1 140  3 050 -6
00000142 03215  -51.09  032  3 140  6 050-12
00000143 03216  -70.09  032 11 140  6 050-24
00000144 03217  -19.28  032  2 140  1 050 -5
00000145 03218  -18.11  032  3 140  1 050 -5
00000146 01401  -17.50  140  1 050 -2
00000147 01402   -7.61  140  1 050 -1
00000148 01403   -1.48  140  1
00000146 01404  -16.67  140  1 050 -1 003  1
00000147 01405   -8.08  140  1 050 -2 003  1
00000139 00100  -13.78  050 -1
00000140 01050    7.35  001  1 160  1 050  1
00000145 01100   -8.45  001  1 160 -1 050 -1
00000150 00001    0.00  001  1
xouo2    03301   -1.60  001  1 160  1 050 -1 032  1 033  1
00000174
00000175
00000180 00001  600.0  1.78       1.0
00000185          0      0
00000190            1
00000195         3301
00000230           18        1         1         0
00000240           33
00000260 6.4590E-09
00000280 9.0459E-08
00000300 4.2071E-07
00000320 7.0678E-07
00000340 9.1325E-07
00000341 9.8290E-07
00000342 9.9426E-07
00000343 9.9727E-07
00000344 9.9823E-07
00000345 9.9672E-07
00000346 9.9744E-07
00000347 9.9778E-07
00000348 9.9768E-07
00000349 9.9671E-07
00000350 9.7102E-07
00000351 7.7357E-07
00000352 3.4379E-07
00000353 7.7000E-10
00000354           50
00000355 -3.84
00000356 -4.15
00000357 -4.45
00000358 -4.72
00000359 -4.96
00000680 -5.29
00000690 -5.51
00000700 -5.93
00000710 -6.42
00000720 -6.92
00000730 -7.48
00000731 -7.83
00000732 -8.14
00000733 -8.36
00000734 -8.75
00000735 -9.07
00000736 -9.33
00000737 -9.70
00000738            1         1
00000739           33      0.10   1.0E-09
00000740           50      0.05   0.0E-00
00000741
00000742
00000743
00000744
00000745
00000746
00000747
00000748
00000749
00001170
00001180
00001190
```

Fig. 1-1

DLM

XOH° + UO$_2^{2+}$ = XO-UO$_2^+$ + H$^+$

```
                   0
                   1
                   0
                   0
                   1
                  90
                   3         1          3          1
Ferryhid 00001  -3.69  2.05E-4   XOH
Payne(91 00160  -1.0   0.00E00   PSIO
1.00e-6M 00032  -8.0   1.00E-8   UO2+2
2.3si/nm 00033   0.0   0.00E00   UO2ads
00000050 00050   0.0   0.00E00   H+
00000060 00003  -1.0   0.00E00   Na+
00000070 00005  -1.0   0.00E00   NO3-
00000080
00000090 00050    0.00  050  1
00000098 00032    0.00  032  1
00000107 03201   -5.43  032  1 050 -1
00000100 03202  -10.54  032  1 050 -2
00000102 03203  -19.22  032  1 050 -3
00000103 03204  -32.59  032  1 050 -4
00000104 03205   -2.49  032  2 050 -1
00000110 03206   -5.42  032  2 050 -2
00000120 03207  -12.37  032  3 050 -4
00000124 03208  -16.25  032  3 050 -5
00000125 03209  -31.49  032  3 050 -7
00000126 03210  -22.83  032  4 050 -7
00000127 03211   -0.05  032  1 005  1
00000128 00100  -13.78  050 -1
00000129 01050    7.18  001  1 160  1 050  1
00000130 01100   -8.82  001  1 160 -1 050 -1
00000131 00001    0.00  001  1
00000132 03301    2.60  001  1 160  1 050 -1 032  1 033  1
00000133
00000134
00000135 00002  600.0  0.089
00000137 0.1    1.0
00000139          1
00000140       3301
00000141          5        1         1         0
00000142         33
00000143 2.816E-9
00000144 4.339E-9
00000145 6.997E-9
00000146 8.813E-9
00000147 9.569E-9
00000148         50
00000146 -4.02
00000147 -4.29
00000139 -4.49
00000140 -4.77
00000145 -5.06
00000150          1         1
xouo2            33      0.10   1.0E-11
00000174         50      0.05   0.0E-00
00000175
00000180          0
00000185          1
00000190          0
00000195          0
00000230          1
00000240         90
00000260          3         1          3          1
00000280 00001  -3.69  2.05E-4   XOH
00000300 00160  -1.0   0.00E00   PSIO
00000320 00032  -6.0   1.00E-6   UO2+2
00000340 00033   0.0   0.00E00   UO2ads
00000341 00050   0.0   0.00E00   H+
00000342 00003  -1.0   0.00E00   Na+
00000343 00005  -1.0   0.00E00   NO3-
00000344
00000345 00050    0.00  050  1
00000346 00032    0.00  032  1
00000347 03201   -5.43  032  1 050 -1
00000348 03202  -10.54  032  1 050 -2
00000349 03203  -19.22  032  1 050 -3
00000350 03204  -32.59  032  1 050 -4
00000351 03205   -2.49  032  2 050 -1
00000352 03206   -5.42  032  2 050 -2
00000353 03207  -12.37  032  3 050 -4
00000680 03208  -16.25  032  3 050 -5
00000690 03209  -31.49  032  3 050 -7
00000700 03210  -22.83  032  4 050 -7
00000710 03211   -0.05  032  1 005  1
00000720 00100  -13.78  050 -1
00000730 01050    7.18  001  1 160  1 050  1
00000731 01100   -8.82  001  1 160 -1 050 -1
00000732 00001    0.00  001  1
00000733 03301    2.60  001  1 160  1 050 -1 032  1 033  1
00000734
00000735
00000736 00002  600.0  0.089
00000737 0.1    1.0
00000738          1
00000739       3301
00000740         13        1         1         0
00000741         33
00000742 1.605E-8
00000743 5.310E-8
00001170 2.244E-8
00001180 1.532E-7
00001190 1.596E-7
         2.848E-7
         5.146E-7
         7.434E-7
         8.692E-7
         8.430E-7
         9.740E-6
         9.963E-6
         9.964E-6
                 50
         -3.06
         -3.29
         -3.57
         -3.83
         -4.08
         -4.25
         -4.54
         -4.76
         -5.01
         -5.24
         -5.51
         -5.73
         -5.95
                  1         1
                 33      0.10   1.0E-10
                 50      0.05   0.0E-00
```

Fig. 1-2

DLM

XOH° + UO$_2^{2+}$ = XO UO$_2^-$ + H$^+$

```
Ferryhid
Payne(91
1.00e-6M
2.3si/nm
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000103
00000104
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000137
00000139
00000140
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000680
00000690
00000700
00000710
00000720
00000730
00001170
00001180
00001190

Ferryhid
Payne(91
1.00e-6M
2.3si/nm
00000050
00000060
00000070
00000080
00000090
00000098
00000100
00000102
00000103
00000104
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000137
00000139
00000140
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
00000260
00000280
00000300
00000320
00000340
00000360
00000370
00000371
00000372
00000373
00000374
00000375
00000376
00000680
00000690
00000700
00000710
00000720
00000730
00000740
00000750
00000751
00000752
00000753
00000754
00000755
00000756
00001170
00001180
00001190
```

230

8/24/95 JRJ

```
0
1
0
0
1
90
3 1 3 1
00001 -3.69 2.05E-4 XOH
00160 -1.0 0.00E00 PSI0
00032 -6.0 1.00E-6 UO2+2
00033 0.0 0.00E00 UO2ads
00050 0.0 0.00E00 H+
00003 -1.0 0.00E00 NO3-
00005 -1.0 0.00E00 Na+

00050 0.00 050 1
00032 0.00 032 1
03201 -5.43 032 1 050 -1
03202 -10.54 032 1 050 -2
03203 -19.22 032 1 050 -3
03204 -32.59 032 1 050 -4
03205 -2.49 032 2 050 -1
03206 -5.42 032 2 050 -2
03207 -12.37 032 3 050 -4
03208 -16.25 032 3 050 -5
03209 -31.49 032 3 050 -7
03210 -22.83 032 4 050 -7
03211 -0.05 032 1 005 1
00100 -13.78 050 -1
01050 7.18 001 1 160 1 050 1
01100 -8.82 001 1 160 -1 050 -1
00001 0.00 001 1
03301 1.60 001 1 160 1 050 -1 032 1 033 1

00002 600.0 0.089
0.1 1.0
1
3301
7 1 1 0
33
7.177E-7
1.600E-6
3.000E-6
4.900E-6
5.300E-6
7.200E-6
9.400E-6
50
-3.99
-4.25
-4.49
-4.70
-4.75
-4.98
-5.61
1 1
33 0.10 1.0E-08
50 0.05 0.0E-00
```

Fig. 1-3
DLM
$XOH^0 + UO_2^{2+} = XO \cdot UO_2^+ + H^+$

```
0
1
0
0
1
90
3 1 3 1
10001 -3.69 2.05E-4 XOH
10160 -1.0 0.00E00 PSI0
10032 -4.0 1.00E-6 UO2+2
10033 0.0 0.00E00 UO2ads
10050 0.0 0.00E00 H+
10003 -1.0 0.00E00 NO3-
10005 -1.0 0.00E00 Na+

10050 0.00 050 1
10032 0.00 032 1
13201 -5.43 032 1 050 -1
13202 -10.54 032 1 050 -2
13203 -19.22 032 1 050 -3
13204 -32.59 032 1 050 -4
13205 -2.49 032 2 050 -1
13206 -5.42 032 2 050 -2
13207 -12.37 032 3 050 -4
13208 -16.25 032 3 050 -5
13209 -31.49 032 3 050 -7
13210 -22.83 032 4 050 -7
13211 -0.05 032 1 005 1
10100 -13.78 050 -1
11050 7.18 001 1 160 1 050 1
11100 -8.82 001 1 160 -1 050 -1
10001 0.00 001 1
13301 0.60 001 1 160 1 050 -1 032 1 033 1

10002 600.0 0.089
0.1 1.0
1
3301
7 1 1 0
33
4.313E-7
1.239E-6
7.795E-6
2.565E-5
3.482E-5
4.650E-5
7.921E-5
50
-4.01
-4.28
-4.52
-4.76
-4.89
-5.03
-5.54
1 1
33 0.10 1.0E-09
50 0.05 0.0E-00
```

Fig. 1-4
DLM
$XOH^0 + UO_2^{2+} = XO \cdot UO_2^+ + H^+$

```
Ferryhid
Paynet(91
1.00e-6M
2.3si/nm
00000050
00000060
00000070
00000080 00001 -3.69 2.05E-4 XOH
00000090 00160 -1.0 0.00E00 PSI0
00000098 00032 -6.00 1.00E-6 UO2+2
00000100 00140 -3.52 3.02E-4 CO2g
00000102 00033 0.0 0.00E00 UO2ads
00000103 00050 0.0 0.00E00 H+
00000104 00003 -1.0 0.00E00 Na+
00000110 00005 -1.0 0.00E00 NO3-
00000120
00000124 00050 0.00 050 1
00000126 00032 0.00 032 1
00000127 00140 0.00 140 1
00000128 03201 -5.43 032 1 050 -1
00000129 03202 -10.54 032 1 050 -2
00000130 03203 -19.22 032 1 050 -3
00000131 03204 -32.59 032 1 050 -4
00000132 03205 -2.49 032 2 050 -1
00000133 03206 -5.42 032 2 050 -2
00000134 03207 -12.37 032 3 050 -4
00000135 03208 -16.25 032 3 050 -5
00000137 03209 -31.49 032 3 050 -7
00000139 03210 -22.83 032 4 050 -7
00000140 03211 -0.05 032 1 005 1
00000145 03212 -8.77 032 1 140 1 050 -2
00000150 03213 -19.35 032 1 140 2 050 -4
xouo2 03214 -30.81 032 1 140 3 050 -6
00000174 03215 -51.09 032 3 140 6 050-12
00000175 03216 -70.09 032 11 140 6 050-24
00000180 03217 -19.28 032 2 140 1 050 -5
00000185 03218 -18.11 032 3 140 1 050 -5
00000190 01401 -17.50 140 1 050 -2
00000195 01402 -7.61 140 1 050 -1
00000230 01403 -1.48 140 1
00000240 01404 -16.67 140 1 050 -1 003 1
00000260 01405 -8.08 140 1 050 -2 003 1
00000280 00100 -13.78 050 -1
00000300 01050 7.18 001 1 160 1 050 1
00000320 01100 -8.82 001 1 160 -1 050 -1
00000340 00001 0.00 001 1
00000360 03301 0.60 001 1 160 1 050 -1 032 1 033 1
00000370
00000680
00000690 00002 600.0 0.089
00000700 0.1 1.0
00000710 1
00000720 3301
00000730 24 1 1 0
00000740 33
00000750 1.6046E-08
00001170 5.3101E-08
00001180 2.2437E-08
00001190 1.5323E-07
1.5955E-07
2.8482E-07
5.1461E-07
7.4337E-07
8.6917E-07
9.4297E-07
9.7404E-07
9.9634E-07
9.9640E-07
9.9573E-07
9.9681E-07
9.9117E-07
9.8533E-07
9.8291E-07
9.7423E-07
8.3535E-07
3.5979E-07
1.6198E-08
2.5026E-08
1.8388E-08
50
-3.06
-3.29
-3.57
-3.83
-4.08
-4.25
-4.54
-4.76
-5.01
-5.24
-5.51
-5.73
-5.93
-6.21
-6.51
-6.89
-7.46
-7.74
-7.98
-8.29
-8.63
-8.94
-9.22
-9.62
1 1
33 0.10 1.0E-10
50 0.05 0.0E-00
```

Fig. 3-1
DLM
$XOH^0 + UO_2^{2+} = XO \cdot UO_2^+ + H^+$

```
Ferryhid
Paynet(92
1.00e-6M
2.3si/nm
00000050
00000060
00000070
00000080 00001 -3.69 2.05E-4 XOH
00000090 00160 -1.0 0.00E00 PSI0
00000098 00032 -4.0 1.00E-4 UO2+2
00000107 00140 -3.52 3.02E-4 CO2g
00000100 00033 0.0 0.00E00 UO2ads
00000102 00050 0.0 0.00E00 H+
00000103 00003 -1.0 0.00E00 Na+
00000104 00005 -1.0 0.00E00 NO3-
00000110
00000120 00050 0.00 050 1
00000124 00032 0.00 032 1
00000125 00140 0.00 140 1
00000126 03201 -5.43 032 1 050 -1
00000127 03202 -10.54 032 1 050 -2
00000128 03203 -19.22 032 1 050 -3
00000129 03204 -32.59 032 1 050 -4
00000130 03205 -2.49 032 2 050 -1
00000131 03206 -5.42 032 2 050 -2
00000132 03207 -12.37 032 3 050 -4
00000133 03208 -16.25 032 3 050 -5
00000134 03209 -31.49 032 3 050 -7
00000135 03210 -22.83 032 4 050 -7
00000137 03211 -0.05 032 1 005 1
00000139 03212 -8.77 032 1 140 1 050 -2
00000140 03213 -19.35 032 1 140 2 050 -4
00000141 03214 -30.81 032 1 140 3 050 -6
00000142 03215 -51.09 032 3 140 6 050-12
00000143 03216 -70.09 032 11 140 6 050-24
00000144 03217 -19.28 032 2 140 1 050 -5
00000145 03218 -18.11 032 3 140 1 050 -5
00000146 01401 -17.50 140 1 050 -2
00000147 01402 -7.61 140 1 050 -1
00000148 01403 -1.48 140 1
00000146 01404 -16.67 140 1 050 -1 003 1
00000147 01405 -8.08 140 1 050 -2 003 1
00000139 00100 -13.78 050 -1
00000140 01050 7.18 001 1 160 1 050 1
00000145 01100 -8.82 001 1 160 -1 050 -1
00000150 00001 0.00 001 1
xouo2 03301 -7.60 001 1 160 1 050 -1 032 1 033 1
00000174
00000175
00000180 00002 600.0 0.089
00000185 0.1 1.0
00000190 1
00000195 3301
00000230 15 1 1 0
00000240 33
00000260 4.3134E-07
00000280 1.2387E-06
00000300 7.7947E-06
00000320 2.5647E-05
00000340 3.4824E-05
00000341 4.6508E-05
00000342 7.9207E-05
00000343 9.6079E-05
00000344 9.6588E-05
00000345 9.4251E-05
00000346 8.7968E-05
00000347 3.1662E-05
00000348 1.3326E-05
00000349 4.4572E-06
00000350 8.6632E-08
00000351 50
00000352 -4.01
00000353 -4.28
00000354 -4.54
00000355 -4.76
00000356 -4.89
00000357 -5.02
00000358 -5.52
00000359 -6.41
00000680 -6.72
00000690 -7.17
00000700 -7.47
00000710 -8.00
00000720 -8.35
00000730 -8.51
00000731 -8.64
00000732
00000733 1 1
00000734 33 0.10 1.0E-09
00000735 50 0.05 0.0E-00
00000736
00000737
00000738
00000739
00000740
00000741
00000742
00000743
00000744
00000745
00000746
00000747
00000748
00000749
00001170
00001180
00001190
```

Fig. 3-2
DLM
$XOH^0 + UO_2^{2+} = XO \cdot UO_2^+ + H^+$

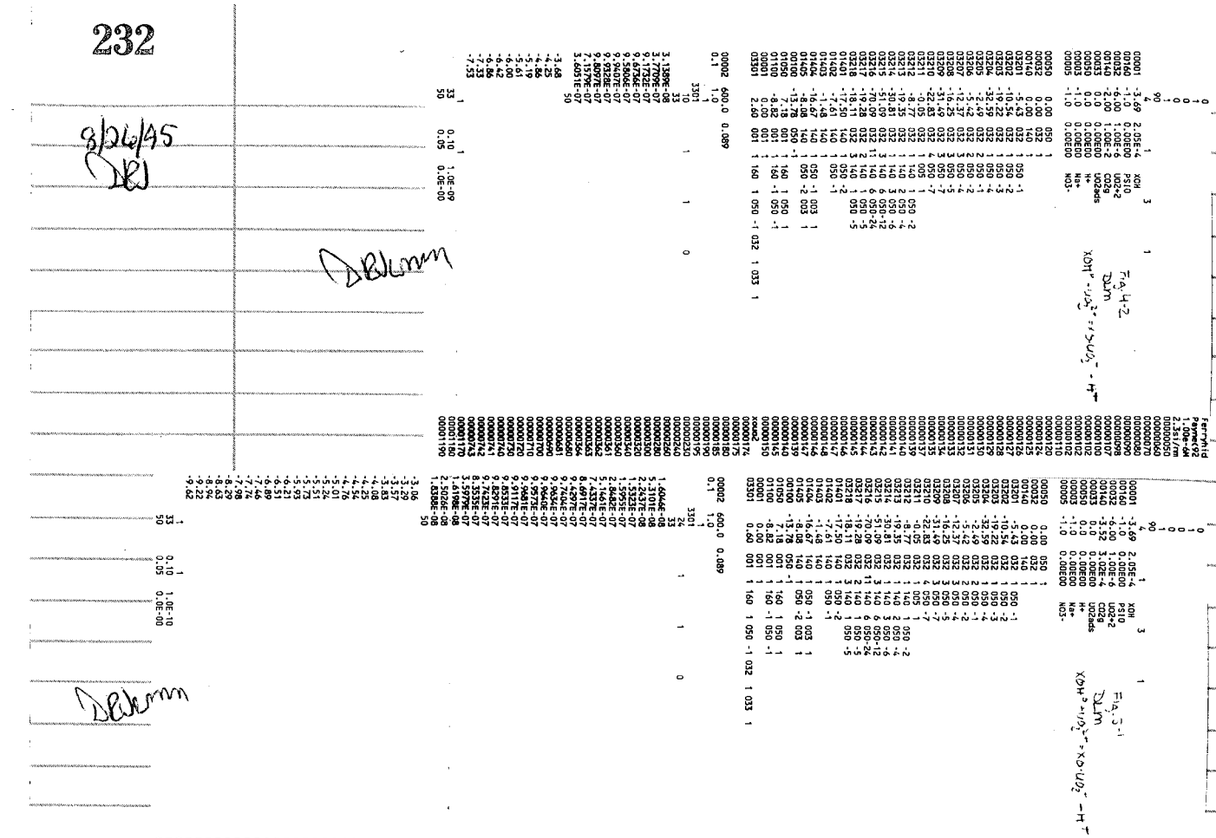
```
Ferryhid
Paynet(92
1.00e-6M
2.3si/nm
00000050
00000060
00000070
00000080 00001 -3.69 2.05E-4 XOH
00000090 00160 -1.0 0.00E00 PSI0
00000098 00032 -6.00 1.00E-6 UO2+2
00000107 00140 -3.52 3.02E-4 CO2g
00000100 00033 0.0 0.00E00 UO2ads
00000102 00050 0.0 0.00E00 H+
00000103 00003 -1.0 0.00E00 Na+
00000104 00005 -1.0 0.00E00 NO3-
00000110
00000120 00050 0.00 050 1
00000124 00032 0.00 032 1
00000125 00140 0.00 140 1
00000126 03201 -5.43 032 1 050 -1
00000127 03202 -10.54 032 1 050 -2
00000128 03203 -19.22 032 1 050 -3
00000129 03204 -32.59 032 1 050 -4
00000130 03205 -2.49 032 2 050 -1
00000131 03206 -5.42 032 2 050 -2
00000132 03207 -12.37 032 3 050 -4
00000133 03208 -16.25 032 3 050 -5
00000134 03209 -31.49 032 3 050 -7
00000135 03210 -22.83 032 4 050 -7
00000159 03211 -0.05 032 1 005 1
00000139 03212 -8.77 032 1 140 1 050 -2
00000140 03213 -19.35 032 1 140 2 050 -4
00000141 03214 -30.81 032 1 140 3 050 -6
00000142 03215 -51.09 032 3 140 6 050-12
00000143 03216 -70.09 032 11 140 6 050-24
00000144 03217 -19.28 032 2 140 1 050 -5
00000145 03218 -18.11 032 3 140 1 050 -5
00000146 01401 -17.50 140 1 050 -2
00000147 01402 -7.61 140 1 050 -1
00000148 01403 -1.48 140 1
00000146 01404 -16.67 140 1 050 -1 003 1
00000147 01405 -8.08 140 1 050 -2 003 1
00000139 00100 -13.78 050 -1
00000140 01050 7.18 001 1 160 1 050 1
00000145 01100 -8.82 001 1 160 -1 050 -1
00000150 00001 0.00 001 1
xouo2 03301 0.60 001 1 160 1 050 -1 032 1 033 1
00000174
00000175
00000180 00002 600.0 0.089
00000185 0.1 1.0
00000190 1
00000195 3301
00000230 24 1 1 0
00000240 33
00000260 1.6046E-08
00000280 5.3101E-08
00000300 2.2437E-08
00000320 1.5323E-07
00000340 1.5955E-07
00000341 2.8482E-07
00000342 5.1461E-07
00000343 7.4337E-07
00000344 8.6917E-07
00000345 9.4297E-07
00000346 9.7404E-07
00000347 9.9634E-07
00000348 9.9640E-07
00000349 9.9573E-07
00000350 9.9681E-07
00000680 9.9117E-07
00000690 9.8533E-07
00000700 9.8291E-07
00000710 9.7423E-07
00000720 8.3535E-07
00000730 3.5979E-07
00000731 1.6198E-08
00000732 2.5026E-08
00000733 1.8388E-08
00000734 50
00000735
00000736 -3.06
00000737 -3.29
00000738 -3.57
00000739 -3.83
00000740 -4.08
00001170 -4.25
00001180 -4.54
00001190 -4.76
-5.01
-5.24
-5.51
-5.73
-5.93
-6.21
-6.51
-6.89
-7.46
-7.74
-7.98
-8.29
-8.63
-8.94
-9.22
-9.62
1 1
33 0.10 1.0E-10
50 0.05 0.0E-00
```

Example FIREAL Inputs

5/26/95 DLM

3/26/95 DBL

DBLumm



DBLumm

DBLumm

3/26/95 DBL

DBLumm

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-8 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-11	Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 10^{-3} M Fe = 0.089 g/L HFO

Fig 1.1 Binduf.8	DLM			CCM			TLM		
	Log K_+ = 7.29 Log K_- = -8.93			Log K_+ = 7.35 Log K_- = -8.45			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-UO_2^+	2.80	0.75	.0533	3.15	0.81	.0541	-2.80	19.4	.0388
XOH-UO_2^{2+}	9.52	2.1	.0449	10.54	0.61	.0517	4.92	22.4	.0387
XO-UO_2OH^o	-3.91	2.8	.0635	-4.25	1.2	.0566	-7.15	1.4	.0464
XOH-UO_2OH^+	2.80	0.75	.0533	3.15	0.81	.0541	-0.58	2.0	.0454
XO-$UO_2(OH)_2^-$	-10.63	5.9	.0752	-11.64	1.8	.0592	-11.37	1.8	.0595
XOH-$UO_2(OH)_2^o$	-3.91	2.8	.0635	-4.25	1.2	.0566	-3.75	1.5	.0582
XOH_2-$UO_2(OH)_2^+$	2.80	0.75	.0533	3.15	0.81	.0541	3.98	1.2	.0570
XOH-$UO_2(OH)_3^-$	-10.63	5.9	.0752	-11.64	1.8	.0592	-8.06	5.6	.0742
XOH_2-$UO_2(OH)_3^o$	-3.91	2.8	.0635	-4.25	1.2	.0566	-0.33	5.1	.0726
XOH-$UO_2(OH)_4^{2-}$	-17.34	9.3	.0887	-19.03	2.4	.0620	-12.81	10.9	.0956
XOH_2-$UO_2(OH)_4^-$	-10.63	5.9	.0752	-11.64	1.8	.0592	-4.64	9.9	.0916

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-10	Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 10^{-3} M Fe = 0.089 g/L HFO

fig 1.2 Binduf.4	DLM			CCM			TLM		
	Log K_+ = 7.29 Log K_- = -8.93			Log K_+ = 7.35 Log K_- = -8.45			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-UO_2^+	2.58	33.6	.0304	2.94	33.7	.0308	-4.01	73.1	.0229
XOH-UO_2^{2+}	9.06	33.7	.0210	10.30	31.5	.0281	3.62	75.7	.0240
XO-UO_2OH^o	-4.07	42.6	.0425	-4.44	36.0	.0336	-7.49	31.4	.0230
XOH-UO_2OH^+	2.58	33.6	.0304	2.94	33.7	.0308	0.21	35.2	.0228
XO-$UO_2(OH)_2^-$	-10.85	50.4	.0569	-11.81	38.2	.0366	-11.61	37.6	.0367
XOH-$UO_2(OH)_2^o$	-4.07	42.6	.0425	-4.44	36.0	.0336	-3.82	35.1	.0355
XOH_2-$UO_2(OH)_2^+$	2.58	33.6	.0304	2.94	33.7	.0308	4.00	32.9	.0346
XOH-$UO_2(OH)_3^-$	-10.85	50.4	.0569	-11.81	38.2	.0366	-8.59	48.3	.0556
XOH_2-$UO_2(OH)_3^o$	-4.07	42.6	.0425	-4.44	36.0	.0336	-0.18	41.6	.0505
XOH-$UO_2(OH)_4^{2-}$	-17.66	54.6	.0709	-19.18	40.4	.0397	-13.06	55.0	.0764
XOH_2-$UO_2(OH)_4^-$	-10.85	50.4	.0569	-11.81	38.2	.0366	-4.62	50.7	.0719

DBLumm

Example FITEQL Inputs

8/26/95 DRL

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-5 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-08	Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 10^{-3} M Fe = 0.089 g/L HFO

fig 1.3 Binduf.14

	DLM: Log K_+ = 7.29, Log K_- = -8.93			CCM: Log K_+ = 7.35, Log K_- = -8.45			TLM: Log K_+ = 6.00, Log K_- = -10.00, Log K_{Cat} = -7.66, Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	2.17	0.38	.0337	2.50	0.54	.0347	-3.35	53.2	.0359
$XOH\text{-}UO_2^{2+}$	8.99	8.5	.0275	9.96	0.40	.0327	4.70	55.8	.0562
$XO\text{-}UO_2OH^\circ$	-4.71	5.7	.0424	-4.94	1.7	.0370	-7.50	15.3	.0369
$XOH\text{-}UO_2OH^+$	2.17	0.38	.0337	2.50	0.54	.0347	-0.58	30.9	.0568
$XO\text{-}UO_2(OH)_2^-$	-11.61	12.9	.0529	12.34	2.6	.0400	-11.88	0.49	.0455
$XOH\text{-}UO_2(OH)_2^\circ$	-4.71	5.7	.0425	-4.94	1.7	.0370	-3.64	10.5	.0611
$XOH_2\text{-}UO_2(OH)_2^+$	2.17	0.38	.0337	2.50	0.54	.0347	4.76	24.3	.0905
$XOH\text{-}UO_2(OH)_3^-$	-11.61	12.9	.0529	-12.34	2.6	.0400	-8.82	1.1	.0616
$XOH_2\text{-}UO_2(OH)_3^\circ$	-4.71	5.7	.0425	-4.94	1.7	.0370	-0.53	10.9	.0932
$XOH\text{-}UO_2(OH)_4^{2[18]}$	-18.51	18.1	.0637	-19.70	2.7	.0435	-13.35	7.4	.0758
$XOH_2\text{-}UO_2(OH)_{11}^{-4[1]}$	-11.61	12.9	.0529	-12.34	2.6	.0400	-3.80	3.3	.0988

FITEQL Results

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-4 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-09	Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 10^{-3} M Fe = 0.089 g/L HFO

fig 1.4 Binduf.1

	DLM: Log K_+ = 7.29, Log K_- = -8.93			CCM: Log K_+ = 7.35, Log K_- = -8.45			TLM: Log K_+ = 6.00, Log K_- = -10.00, Log K_{Cat} = -7.66, Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	1.23	45.0	.0277	1.59	40.5	.0277	-4.81	85.9	.0375
$XOH\text{-}UO_2^{2+}$	7.71	72.0	.0302	8.90	55.3	.0305	3.05	86.4	.0490
$XO\text{-}UO_2OH^\circ$	-5.43	10.9	.0285	-5.75	27.2	.0270	-8.88	73.1	.0372
$XOH\text{-}UO_2OH^+$	1.23	45.0	.0277	1.59	40.5	.0277	-1.05	78.1	.0499
$XO\text{-}UO_2(OH)_2^-$	-12.20	6.1	.0376	-13.16	29.1	.0314	-13.02	55.8	.0429
$XOH\text{-}UO_2(OH)_2^\circ$	-5.43	10.9	.0285	-5.75	27.2	.0270	-5.16	68.4	.0562
$XOH_2\text{-}UO_2(OH)_2^+$	1.23	45.0	.0277	1.59	40.5	.0277	2.80	74.8	.0754
$XOH\text{-}UO_2(OH)_3^-$	-12.20	6.1	.0376	-13.16	29.1	.0314	-9.84	48.5	.0578
$XOH_2\text{-}UO_2(OH)_3^\circ$	-5.43	10.9	.0285	-5.75	27.2	.0270	-1.31	68.6	.0834
$XOH\text{-}UO_2(OH)_4^{2-}$	-18.88	10.4	.0496	-20.55	35.8	.0370	-13.44	48.7	.0747
$XOH_2\text{-}UO_2(OH)_4^-$	-12.20	6.1	.0376	-13.16	29.1	.0314	-5.42	62.0	.0927

Uranium (VI) Sorption Binding Constants; Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-10	Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 10^{-3} M Fe = 0.089 g/L HFO

fig. 3.1 $P(CO_2)$ = 0.03% Binduf.5

	DLM: Log K_+ = 7.29, Log K_- = -8.93			CCM: Log K_+ = 7.35, Log K_- = -8.45			TLM: Log K_+ = 6.00, Log K_- = -10.00, Log K_{Cat} = -7.66, Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	0.97	70.0	.0202	0.86	77.0	.0215	-4.00	84.3	.0227
$XOH\text{-}UO_2^{2+}$	9.11	29.8	.0159	9.20	54.7	.0193	3.63	85.8	.0239
$XO\text{-}UO_2OH^\circ$	-7.56	86.6	.0253	-7.47	86.2	.0250	-7.35	33.1	.0192
$XOH\text{-}UO_2OH^+$	0.97	70.0	.0202	0.86	77.0	.0215	0.33	42.9	.0198
$XO\text{-}UO_2(OH)_2^-$	-15.94	89.2	.0268	-15.72	88.9	.0267	-15.95	89.5	.0271
$XOH\text{-}UO_2(OH)_2^\circ$	-7.56	86.6	.0253	-7.47	86.2	.0250	-7.84	89.1	.0272
$XOH_2\text{-}UO_2(OH)_2^+$	0.97	70.0	.0202	0.86	77.0	.0215	0.29	88.4	.0274
$XOH\text{-}UO_2(OH)_3^-$	-15.94	89.2	.0268	-15.72	88.9	.0267	-17.17	90.4	.0282
$XOH_2\text{-}UO_2(OH)_3^\circ$	-7.56	86.6	.0253	-7.47	86.2	.0250	-9.03	90.1	.0282
$XOH\text{-}UO_2(OH)_4^{2-}$	-24.28	89.4	.0265	-23.94	89.6	.0270	-26.85	94.6	.0404
$XOH_2\text{-}UO_2(OH)_4^-$	-15.94	89.2	.0268	-15.72	88.9	.0267	-18.69	94.3	.0395
$XOH\text{-}UO_2CO_3^\circ$	17.89	56.8	.0231	17.48	58.7	.0188	17.39	58.9	.0186
$XOH_2\text{-}UO_2(CO_3)_2^-$	32.97	70.5	.0278	31.83	71.3	.0200	37.95	60.8	.0322
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	41.23	76.0	.0374	38.85	75.5	.0222	50.85	60.2	.0480
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^\circ$	15.88	47.9	.0458	15.50	48.2	.0398	17.29	62.4	.0169

Uranium (VI) Sorption Binding Constants; Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-4 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-09	Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 10^{-3} M Fe = 0.089 g/L HFO

fig. 3.2 $P(CO_2)$ = 0.03% Binduf.13

	DLM: Log K_+ = 7.29, Log K_- = -8.93			CCM: Log K_+ = 7.35, Log K_- = -8.45			TLM: Log K_+ = 6.00, Log K_- = -10.00, Log K_{Cat} = -7.66, Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	-0.76	98.0	.0449	-0.88	98.5	.0461	-4.81	92.5	.0375
$XOH\text{-}UO_2^{2+}$	7.60	81.4	.0261	7.39	96.8	.0423	3.05	92.7	.0490
$XO\text{-}UO_2OH^\circ$	-9.02	98.9	.0468	-8.94	98.9	.0467	-8.81	81.9	.0325
$XOH\text{-}UO_2OH^+$	-0.76	98.0	.0449	-0.88	98.5	.0461	-0.94	85.8	.0446
$XO\text{-}UO_2(OH)_2^-$	-17.25	99.0	.0468	-16.91	99.0	.0468	-17.24	99.0	.0477
$XOH\text{-}UO_2(OH)_2^\circ$	-9.02	98.9	.0468	-8.94	98.9	.0467	-9.14	99.0	.0500
$XOH_2\text{-}UO_2(OH)_2^+$	-0.76	98.0	.0449	-0.88	98.5	.0461	-1.03	99.0	.0540
$XOH\text{-}UO_2(OH)_3^-$	-17.25	99.0	.0468	-16.91	99.0	.0468	-17.90	99.2	.0534
$XOH_2\text{-}UO_2(OH)_3^\circ$	-9.02	98.9	.0468	-8.94	98.9	.0467	-9.79	99.2	.0567
$XOH\text{-}UO_2(OH)_4^{2-}$	-25.48	99.1	.0471	-25.20	99.0	.0469	-26.65	99.3	.0639
$XOH_2\text{-}UO_2(OH)_4^-$	-17.25	99.0	.0468	-16.91	99.0	.0468	-18.54	99.3	.0662
$XOH\text{-}UO_2CO_3^\circ$	16.30	77.6	.0229	15.85	81.8	.0230	15.76	82.0	.0229
$XOH_2\text{-}UO_2(CO_3)_2^-$	31.37	80.3	.0271	30.20	84.9	.0252	36.33	77.7	.0345
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	39.88	79.1	.0370	37.24	85.8	.0290	49.60	80.7	.0657
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^\circ$	12.00	62.4	.0245	11.75	63.5	.0235	15.76	85.1	.0249

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Uranium (VI) Sorption Binding Constants; Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-10			Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 10^{-3} M Fe = 0.089 g/L HFO		
fig 4.1 $P(CO_2)$ = 0.03% Binduf.9	DLM Log K_+ = 7.29 Log K_- = -8.93			CCM Log K_+ = 7.35 Log K_- = -8.45			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	0.97	70.0	.0202	0.86	77.0	.0215	-4.00	84.3	.0227
$XOH\text{-}UO_2^{2+}$	9.11	29.8	.0159	9.20	54.7	.0193	3.63	85.8	.0239
$XO\text{-}UO_2OH^\circ$	-7.56	86.6	.0253	-7.47	86.2	.0250	-7.35	33.1	.0192
$XOH\text{-}UO_2OH^+$	0.97	70.0	.0202	0.86	77.0	.0215	0.33	42.9	.0198
$XO\text{-}UO_2(OH)_2^-$	-15.94	89.2	.0268	-15.72	88.9	.0267	-15.95	89.5	.0271
$XOH\text{-}UO_2(OH)_2^\circ$	-7.56	86.6	.0253	-7.47	86.2	.0250	-7.84	89.1	.0272
$XOH_2\text{-}UO_2(OH)_2^+$	0.97	70.0	.0202	0.86	77.0	.0215	0.29	88.4	.0274
$XOH\text{-}UO_2(OH)_3^-$	-15.94	89.2	.0268	-15.72	88.9	.0267	-17.17	90.4	.0282
$XOH_2\text{-}UO_2(OH)_3^\circ$	-7.56	86.6	.0253	-7.47	86.2	.0250	-9.03	90.1	.0282
$XOH\text{-}UO_2(OH)_4^{2-}$	-24.28	89.4	.0265	-23.94	89.6	.0270	-26.85	94.6	.0404
$XOH_2\text{-}UO_2(OH)_4^-$	-15.94	89.2	.0268	-15.72	88.9	.0267	-18.69	94.3	.0395
$XOH\text{-}UO_2CO_3^\circ$	17.89	56.8	.0231	17.48	58.7	.0188	17.39	58.9	.0186
$XOH_2\text{-}UO_2(CO_3)_2^-$	32.97	70.5	.0278	31.83	71.3	.0200	37.95	60.8	.0322
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	41.23	76.0	.0374	38.85	75.5	.0222	50.85	60.2	.0480
$XOH_3\text{-}(UO_2)_2CO_3(OH)_3^\circ$	15.88	47.9	.0458	15.50	48.2	.0398	17.29	62.4	.0169

FITEQL Results

8/26/95 DRJ

Uranium (VI) Sorption Binding Constants; Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-10			Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 10^{-3} M Fe = 0.089 g/L HFO		
fig. 5.1 $P(CO_2)$ = 0.03% Binduf.10	DLM Log K_+ = 7.29 Log K_- = -8.93			CCM Log K_+ = 7.35 Log K_- = -8.45			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	0.97	70.0	.0202	0.86	77.0	.0215	-4.00	84.3	.0227
$XOH\text{-}UO_2^{2+}$	9.11	29.8	.0159	9.20	54.7	.0193	3.63	85.8	.0239
$XO\text{-}UO_2OH^\circ$	-7.56	86.6	.0253	-7.47	86.2	.0250	-7.35	33.1	.0192
$XOH\text{-}UO_2OH^+$	0.97	70.0	.0202	0.86	77.0	.0215	0.33	42.9	.0198
$XO\text{-}UO_2(OH)_2^-$	-15.94	89.2	.0268	-15.72	88.9	.0267	-15.95	89.5	.0271
$XOH\text{-}UO_2(OH)_2^\circ$	-7.56	86.6	.0253	-7.47	86.2	.0250	-7.84	89.1	.0272
$XOH_2\text{-}UO_2(OH)_2^+$	0.97	70.0	.0202	0.86	77.0	.0215	0.29	88.4	.0274
$XOH\text{-}UO_2(OH)_3^-$	-15.94	89.2	.0268	-15.72	88.9	.0267	-17.17	90.4	.0282
$XOH_2\text{-}UO_2(OH)_3^\circ$	-7.56	86.6	.0253	-7.47	86.2	.0250	-9.03	90.1	.0282
$XOH\text{-}UO_2(OH)_4^{2-}$	-24.28	89.4	.0265	-23.94	89.6	.0270	-26.85	94.6	.0404
$XOH_2\text{-}UO_2(OH)_4^-$	-15.94	89.2	.0268	-15.72	88.9	.0267	-18.69	94.3	.0395
$XOH\text{-}UO_2CO_3^\circ$	17.89	56.8	.0231	17.48	58.7	.0188	17.39	58.9	.0186
$XOH_2\text{-}UO_2(CO_3)_2^-$	32.97	70.5	.0278	31.83	71.3	.0200	37.95	60.8	.0322
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	41.23	76.0	.0374	38.85	75.5	.0222	50.85	60.2	.0480
$XOH_3\text{-}(UO_2)_2CO_3(OH)_3^\circ$	15.88	47.9	.0458	15.50	48.2	.0398	17.29	62.4	.0169

FITEQL Results

Uranium (VI) Sorption Binding Constants; Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-09			Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 10^{-3} M Fe = 0.089 g/L HFO		
fig. 4.2 $P(CO_2)$ = 1% Binduf.11	DLM Log K_+ = 7.29 Log K_- = -8.93			CCM Log K_+ = 7.35 Log K_- = -8.45			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	1.96	21.8	.0528	2.64	29.6	.0627	-3.90	91.6	.0446
$XOH\text{-}UO_2^{2+}$	9.14	22.3	.0277	9.86	16.2	.0475	3.76	92.8	.0475
$XO\text{-}UO_2OH^\circ$	-4.00	34.8	.0650	-4.49	33.6	.0560	-7.41	22.8	.0304
$XOH\text{-}UO_2OH^+$	1.96	21.8	.0528	2.64	29.6	.0627	0.30	37.7	.0317
$XO\text{-}UO_2(OH)_2^-$	-10.60	37.4	.0836	-11.80	34.5	.0578	-11.62	34.6	.0583
$XOH\text{-}UO_2(OH)_2^\circ$	-4.00	34.8	.0650	-4.49	33.6	.0560	-3.89	34.4	.0583
$XOH_2\text{-}UO_2(OH)_2^+$	1.96	21.8	.0528	2.64	29.6	.0627	3.78	33.2	.0610
$XOH\text{-}UO_2(OH)_3^-$	-10.60	37.4	.0836	-11.80	34.5	.0578	-13.70	79.8	.0701
$XOH_2\text{-}UO_2(OH)_3^\circ$	-4.00	34.8	.0650	-4.49	33.6	.0560	-5.33	83.1	.0794
$XOH\text{-}UO_2(OH)_4^{2-}$	-22.17	68.9	.0576	-19.14	34.8	.0610	-21.49	85.5	.0800
$XOH_2\text{-}UO_2(OH)_4^-$	-10.60	37.4	.0836	-11.80	34.5	.0578	-13.25	84.4	.0900
$XOH\text{-}UO_2CO_3^\circ$	16.48	45.0	.0346	15.98	54.1	.0290	15.88	76.5	.0407
$XOH_2\text{-}UO_2(CO_3)_2^-$	30.12	62.1	.0425	28.80	72.6	.0320	35.14	71.8	.0666
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	37.01	67.9	.0605	34.31	77.1	.0362	47.06	69.3	.0973
$XOH_3\text{-}(UO_2)_2CO_3(OH)_3^\circ$	14.84	8.1	.0480	14.57	13.7	.0456	15.85	55.2	.0803

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: Ferrihydrite A_{sp}: 600 m²/g Data Source: Payne et al. (1992) Concentration: [U(VI)] = 1E-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0E00 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-09			Ionic Strength (electrolyte): 0.1 $NaNO_3$ N_s = 2.31 sites/nm² 2 x 10^{-2} M Fe = 1.78 g/L HFO		
fig. 5.2 $P(CO_2)$ = 0.03% Binduf.6	DLM Log K_+ = 7.29 Log K_- = -8.93			CCM Log K_+ = 7.35 Log K_- = -8.45			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Cat} = -7.66 Log K_{An} = 8.43		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	n.c.	n.c.	n.c.	0.07	59.6	.0270	-5.85	88.9	.0636
$XOH\text{-}UO_2^{2+}$	7.04	75.9	.0265	8.26	36.7	.0252	1.83	89.2	.0667
$XO\text{-}UO_2OH^\circ$	-9.68	97.1	.0725	-7.43	29.9	.0319	-9.30	62.7	.0276
$XOH\text{-}UO_2OH^+$	n.c.	n.c.	n.c.	0.07	59.6	.0270	-1.65	69.0	.0288
$XO\text{-}UO_2(OH)_2^-$	-18.27	97.8	.0886	-15.73	45.9	.0323	-17.59	90.8	.1106
$XOH\text{-}UO_2(OH)_2^\circ$	-9.68	97.1	.0725	-7.43	29.9	.0319	-7.86	48.1	.0329
$XOH_2\text{-}UO_2(OH)_2^+$	n.c.	n.c.	n.c.	0.07	59.6	.0270	-1.07	89.1	.0669
$XOH\text{-}UO_2(OH)_3^-$	-18.27	97.8	.0886	-15.73	45.9	.0323	-19.80	91.7	.3863
$XOH_2\text{-}UO_2(OH)_3^\circ$	-9.68	97.1	.0725	-7.43	29.9	.0319	-11.64	91.7	.3707
$XOH\text{-}UO_2(OH)_4^{2-}$	-26.80	98.0	.0942	-25.70	91.1	.1323	-29.74	91.7	.5170
$XOH_2\text{-}UO_2(OH)_4^-$	-18.27	97.8	.0886	-15.73	45.9	.0323	-21.59	91.7	.5112
$XOH\text{-}UO_2CO_3^\circ$	16.02	62.9	.0237	15.53	72.3	.0223	15.43	73.1	.0224
$XOH_2\text{-}UO_2(CO_3)_2^-$	31.14	70.3	.0273	29.74	82.3	.0271	35.97	59.4	.0295
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	39.55	69.4	.0340	36.78	83.1	.0290	48.59	56.6	.0437
$XOH_3\text{-}(UO_2)_2CO_3(OH)_3^\circ$	13.80	44.9	.0419	13.41	47.5	.0375	15.48	72.4	.0210

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Corrections to CNWRA Radionuclide Database (12/4/95)

Several entry errors were identified with the Database:

1. ID number 3086400 was used for both $NaTcO_4$(s) and $KTcO_4$(s). The new ID number 3086401 was assigned to NaTcO4(s) in both THERMO.DBS and TYPE6.DBS

2. The sign was wrong for the equilibrium constant (log K) for the formation of Th2Se3(s). The value was changed from -73.6817 to + 73.6817 in both THERMO.DBS and TYPE6.DBS

3. The stoichiometric factor and the component ID number for H_2O are entered one space too far to the right for $Th_6(OH)_{15}^{9+}$. These were corrected in THERMO.DBS.

All other radionuclide data remain as before. With the exception of the species mentioned here, these corrections should have no affect on earlier runs using MINTEQA2. After correcting these mistakes, the UNFRMT.EXE program was run to create the binary files THERMO.UNF and TYPE6.UNF. The corrected files and the new binary files were copied onto the disk enclosed in the envelope at the back of this scientific notebook.

12/18/95 DRWinn

U(VI)-Montmorillonite Sorption

U(VI)-Montmorillonite sorption was revisited to use the DLM to investigate the effect of using the Al:Si ratio of 0.83 proposed for edge sites by White and Zelazny (1988) as used by Zachara and McKinley (1993) and Zachara and Smith (1994) in their U(VI)- and Cd-montmorillonite sorption modeling. In this study, an approach has been adopted such that the simplest model that can describe the observed sorption behavior is used.

The U(VI)-montmorillonite sorption data for the conditions:

U_{total}=504.24 ppb=2.164e-6 M
M/V=0.28 g/L
$P(CO_2)=10^{-3.5}$ atm

were modeled for the DLM using FITEQL, version 2.0. Only the data from pH ~3.5 to 7.5 was modeled because this is where most of the sorption occurred. Including the data at higher and lower pH values where sorption is essentially zero tends to bias the data, resulting in an underprediction of the sorption maximum.

Experiments conducted in this study were at relatively high ionic strength (0.1 M $NaNO_3$), which suppressed ion-exchange of UO_2^{2+} with interlayer cations. Therefore, in modeling U(6+) sorption on montmorillonite, it was assumed in this study that the edge sites dominate the sorption behavior, and ion-exchange was not explicitly incorporated in the model construction.

In order to develop a DLM for the U(6+)-montmorillonite system, it is necessary to calculate the total number of sorption sites ($T_{>XOH}$). In this study, the decrease in K_d observed for M/V=0.28 g/L with an order of magnitude increase in ΣU suggested approaching saturation of available sorption sites (Dzombak and Morel, 1990). It unlikely that such behavior would be observed if the measured (N_2/BET) external surface area of 97 m^2/g were entirely attributed to pH-dependent edge sites, given the potentially large number of sites (~10^{-4} moles sites/L) relative to the uranium concentration (ΣU = 2.16×10^{-7} M to 2.16×10^{-6} M). The crystallite edges were therefore assumed to comprise 10 percent of the N_2-BET specific surface area, consistent with observations of Wanner et al. (1994). This effective surface area of 9.7 m^2/g, together with a "standard" site density of 2.3 sites/nm^2 recommended for all minerals by Davis and Kent (1990) based on the ferrihydrite work of Dzombak and Morel (1990), was used to calculate the total number of available edge sites. In the absence of more quantitative information, it was also assumed that the ratio of >AlOH° to >SiOH° sites is 0.83 as proposed for montmorillonite by White and Zelazny (1988). The acidity constants used for the protonation and deprotonation of the >SiOH° and >AlOH° edge sites were derived based on potentiometric titration data for SiO_2 and α-Al_2O_3, as described in Turner and Sassman (1994).

FITEQL requires the input of an equilibrium aqueous speciation model. For this reason, the resultant binding constants are dependent on the quality and extent of the thermodynamic data available for the system of interest. For U(6+), the equilibrium constants used in the chemical equilibrium models submitted to FITEQL are listed below. These values were taken from the NEA thermodynamic database (Wanner and Forrest, 1992) with the exception of the value for the neutral hydroxy complex, $UO_2(OH)_2°$(aq). Due to experimental uncertainties, Wanner and Forrest (1992) could only recommend an upper limit to the stability constant of $UO_2(OH)_2°$(aq). The equilibrium constant for $UO_2(OH)_2°$(aq) used with FITEQL and listed in the table below was taken from Fuger (1992). This value is 2.7 log units lower than the upper limit recommended by Wanner and Forrest (1992), but as pointed out by Fuger (1992), a lower value is consistent with the work of Choppin and Mathur (1991). Assuming a lower

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equilibrium constant for $UO_2(OH)_2°$(aq) also provides for a much better fit to the available sorption data.

There is typically a lack of independent analytical data supporting the formation of a particular surface complex. In the absence of these data, the exact form of the surface reaction is selected by the modeler based on analogous speciation reactions in the aqueous phase. If the postulated reaction does not contribute significantly to the sorption behavior, FITEQL will iterate towards a large negative binding constant and fail to converge. In this way, the modeler can identify those reactions that dominate sorption in the conceptual model.

Based on FITEQL optimization runs, the following four inner-sphere complex reactions proved to be most capable of reproducing the M4 experiment data:

$$>SiOH° + UO_2^{2+} = >SiO\text{-}UO_2^{+} + H^+$$

$$>SiOH° + 3UO_2^{2+} + 5H_2O = >SiO\text{-}(UO_2)_3(OH)_5^{\circ} + 6H^+$$

$$>AlOH° + UO_2^{2+} = >AlO\text{-}UO_2^{+} + H^+$$

$$>AlOH° + 3UO_2^{2+} + 5H_2O = >AlO\text{-}(UO_2)_3(OH)_5^{\circ} + 6H^+$$

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Initial values for the binding constants were adjusted in MINTEQA2 runs to give the best visual fit to the U(VI) sorption data presented here, and the U(VI)-montmorillonite sorption data of McKinley et al. (in submission). The binding constants determined for these reactions using FITEQL are given below. Only data in the pH range of U(6+) sorption were used in the optimization. These surface species are the same as those used by McKinley et al (in submission) in applying the Triple-Layer SCM to U(6+)-montmorillonite sorption.

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Choppin G.R and Mathur J.N. (1991) Hydrolysis of actinyl(VI) cations. *Radiochimica Acta*. **52/53**, 25-28.

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Turner, D.R. and S.A. Sassman. 1994. Approaches to sorption modeling for high-level waste performance assessment. *Radiochimica Acta* 66/67:745-756.

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Wanner H., Albinsson Y., Karnl O., Wieland E., Wersin P. and Charlet L. (1994) The acid/base chemistry of montmorillonite. *Radiochimica Acta* **66/67**, 733-738.

White G.N. and Zelazny L.W. (1988) Analysis and implications of the edge structure of dioctahedral phyllosilicates. *Clays and Clay Minerals* **36**, 141-146.

Zachara J.M., and McKinley J.P. (1993) Influence of hydrolysis on the sorption of metal cations by smectites: Importance of edge coordination reactions. *Aquatic Sciences* **55**, 250-261.

Zachara J.M. and Smith S.C. (1994) Edge complexation reactions of cadmium on specimen and soil-derived smectite. *Soil Science Society of America Journal* **58**, 762-769.

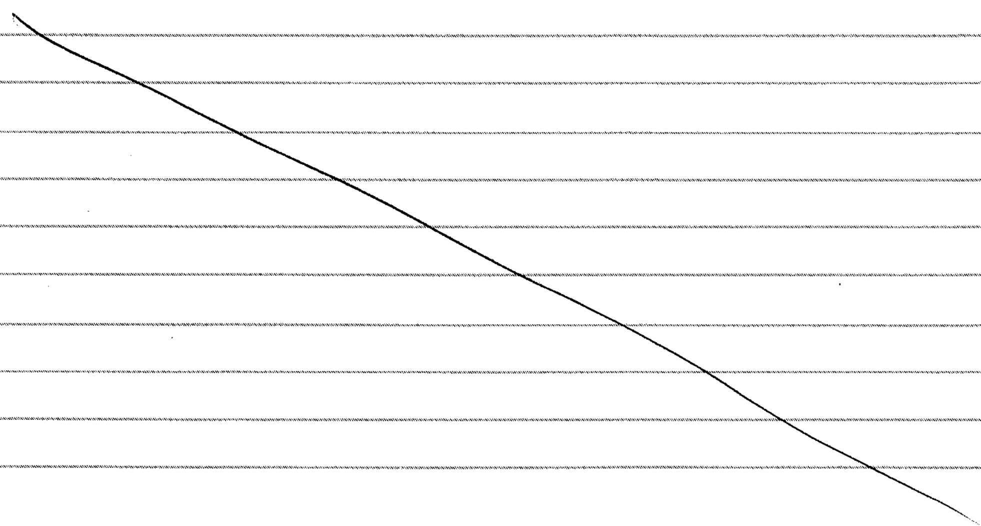
Chemical equilibrium model used in FITEQL optimization.

Reaction	Log K	Ref.
Aqueous Speciation:		
$UO_2^{2+} + H_2O \Leftrightarrow UO_2OH^+ + H^+$	-5.20	1
$UO_2^{2+} + 2H_2O \Leftrightarrow UO_2(OH)_2^{\circ} + 2H^+$	-13.0	2
$UO_2^{2+} + 3H_2O \Leftrightarrow UO_2(OH)_3^- + 3H^+$	-19.20	1
$2UO_2^{2+} + 2H_2O \Leftrightarrow (UO_2)_2(OH)_2^{2+} + 2H^+$	-5.62	1
$3UO_2^{2+} + 5H_2O \Leftrightarrow (UO_2)_3(OH)_5^+ + 5H^+$	-15.55	1
$UO_2^{2+} + CO_3^{2-} \Leftrightarrow UO_2CO_3^{\circ}$	9.68	1
$UO_2^{2+} + 2CO_3^{2-} \Leftrightarrow UO_2(CO_3)_2^{2-}$	16.94	1
$UO_2^{2+} + 3CO_3^{2-} \Leftrightarrow UO_2(CO_3)_3^{4-}$	21.60	1
$2UO_2^{2+} + CO_3^{2-} + 3H_2O \Leftrightarrow (UO_2)_2CO_3(OH)_3^- + 3H^+$	-0.86	1
$UO_2^{2+} + NO_3^- \Leftrightarrow UO_2NO_3^+$	0.30	1
Surface Reactions (DLM):		
$>SiOH^{\circ} \Leftrightarrow >SiO^- + H^+$	7.20	3
$>SiOH^{\circ} + UO_2^{2+} \Leftrightarrow >SiO\text{-}UO_2^+ + H^+$	2.60	this study
$>SiOH^{\circ} + 3UO_2^{2+} \Leftrightarrow >SiO\text{-}(UO_2)_3(OH)_5^{\circ} + 6H^+$	-15.29	this study
$>AlOH^{\circ} + H+ \Leftrightarrow >AlOH_2^+$	8.33	3
$>AlOH^{\circ} \Leftrightarrow >AlO^- + H^+$	-9.73	3
$>AlOH^{\circ} + UO_2^{2+} \Leftrightarrow >AlO\text{-}UO_2^+ + H^+$	2.70	this study
$>AlOH^{\circ} + 3UO_2^{2+} \Leftrightarrow >AlO\text{-}(UO_2)_3(OH)_5^{\circ} + 6H^+$	-14.95	this study

1. Wanner and Forest (1992).
2. Fuger (1992)
3. Turner and Sassman (1994)

After determining the binding constants for the U(VI) sorption reactions, MINTEQA2, Version 3.11/3.12 was used to predict sorption behavior over a wide range in pH, M/V, and P(CO2) conditions. The CNWRA database was used, with the exception of the log K value for UO2(OH)2o(aq) which was assigned a value of -13.00 as given in the table.

Results presented here were plotted using Sigma Plot for Windows, version 2.0



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                1
                1
                1
               30
                5        1         3         1
00001  -5.33  4.73E-6   AlOH
00002  -5.24  5.69E-6   SiOH
00160  -1.0   0.00E00   PSIO
00032  -5.67  2.16E-6   UO2+2
00140  -3.5   3.16E-4   CO2g
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
00140    0.00  140  1
00001    0.00  001  1
00002    0.00  002  1
03201   -5.43  032  1 050 -1
03202  -13.22  032  1 050 -2
03203  -19.22  032  1 050 -3
03206   -5.42  032  2 050 -2
03208  -16.25  032  3 050 -5
03211   -8.77  032  1 140  1 050 -2
03212  -18.91  032  1 140  2 050 -4
03213  -30.92  032  1 140  3 050 -6
03216  -19.28  032  2 140  1 050 -5
03218   -0.05  032  1 005  1
01401  -17.50  140  1 050 -2
01402   -7.61  140  1 050 -1
01403   -1.48  140  1
01404  -16.67  140  1 003  1 050 -2
01405   -8.08  140  1 003  1 050 -1
00100  -13.78  050 -1
01050    8.22  001  1 160  1 050  1
01100   -9.62  001  1 160 -1 050 -1
02100   -7.09  002  1 160 -1 050 -1
03306    2.27  002  1 160  1 050 -1 032  1 033  1
03307    2.37  001  1 160  1 050 -1 032  1 033  1
03308  -15.69  002  1 160  0 050 -6 032  3 033  3
03309  -15.37  001  1 160  0 050 -6 032  3 033  3


00002   9.70  0.28
0.1    1.0
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      3308
        18          1          1          0
        33
1.568E-07
2.738E-07
3.336E-07
7.297E-07
1.452E-06
1.563E-06
1.611E-06
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1.563E-06
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1.493E-06
1.493E-06
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1.470E-06
1.396E-06
1.236E-06
1.100E-06
7.100E-07
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-3.96
-4.20
-4.84
-5.56
-5.93
-5.85
-6.31
-6.40
-6.24
-6.39
-6.45
-6.31
-6.47
-6.47
-6.82
-7.17
-7.30
         1          1
        33       0.04   2.1E-09
        50       0.05   0.0E-00
```

Al:Si = 0.83

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montmori
CNWRA
2.16e-6M
dlm
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alouo2
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alou3oh5
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00000230
00000240

00000760
00000770
00000790
```

FITEQL Input File:

FITEQL input strategy: solve for $>SiO\text{-}UO_2$ + $>AlOUO_2^+$ then add $(UO_2)_3(OH)_5$ surface complexes.

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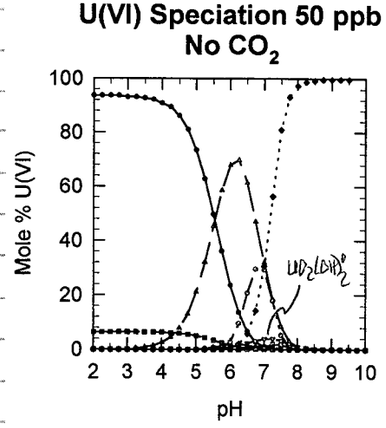
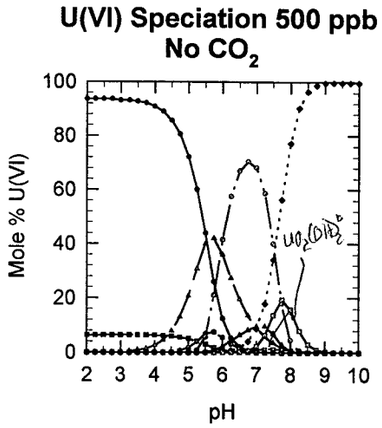
U(VI) speciation with $UO_2(OH)_2^0$ log K reduced to -13.00

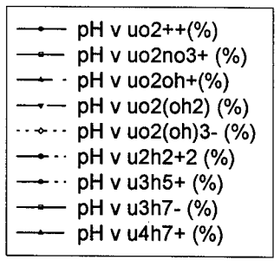
(see text on page 238

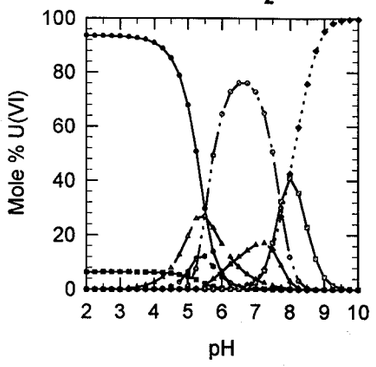




DBL mm

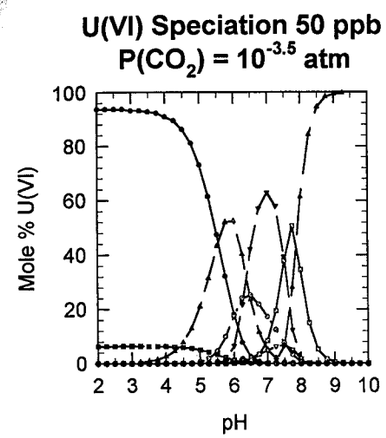
MINTEQA2

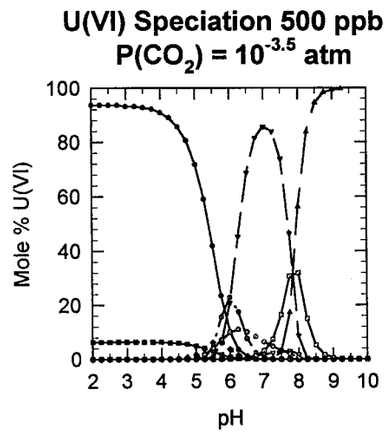




U(VI) speciation: $\log K_{UO_2(OH)_2^0} = -13.0$

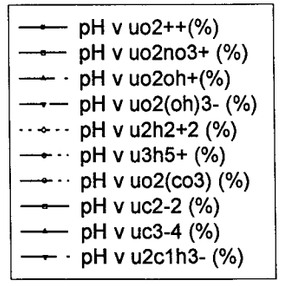
12/18/95 DBL

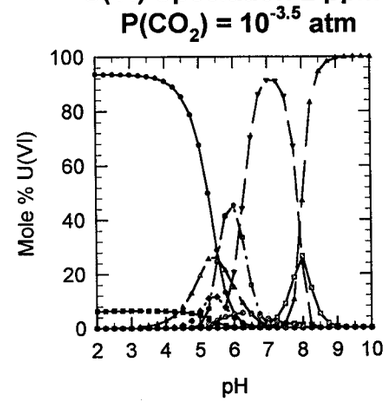




DBL mm

MINTEQA2

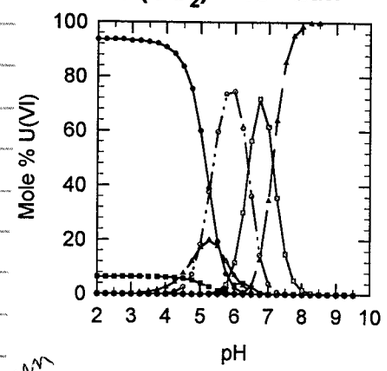




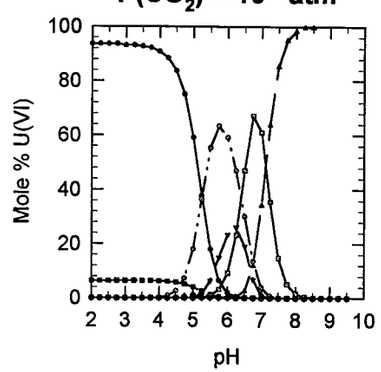
12/18/95
DRL

U(VI) speciation: $\log K_{UO_2(OH)_2^0} = -13.0$

U(VI) Speciation 50 ppb
$P(CO_2) = 10^{-2}$ atm

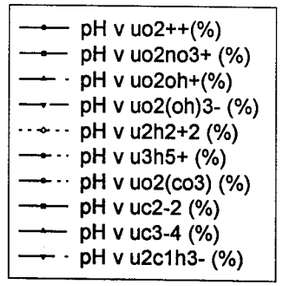


U(VI) Speciation 500 ppb
$P(CO_2) = 10^{-2}$ atm

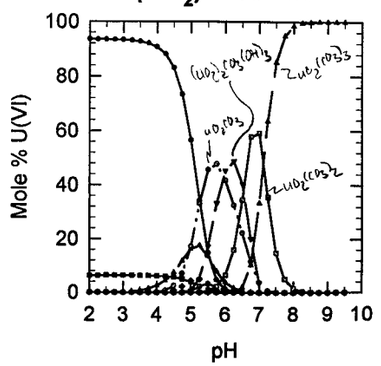


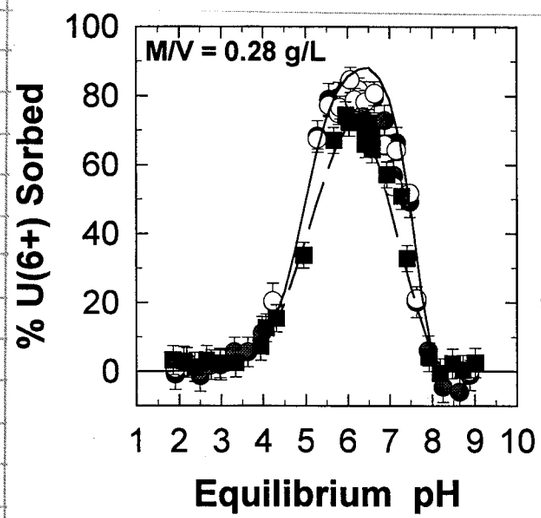
DRLmann

MINTEQA2



U(VI) Speciation 2 ppm
$P(CO_2) = 10^{-2}$ atm





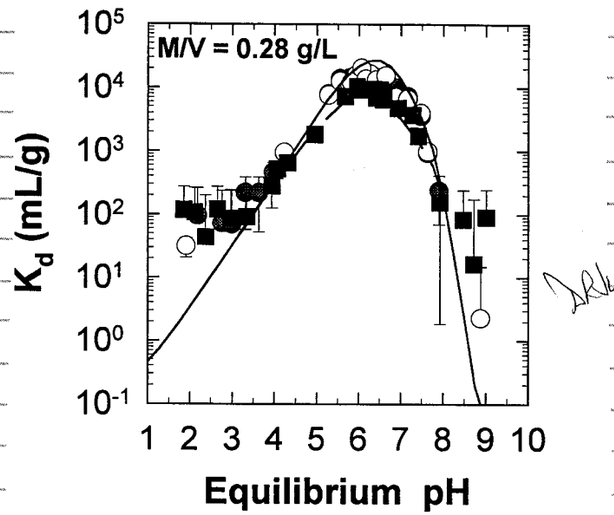
ED:

12/18/95
DRLmann

DLM Results
Effects of $U(VI)_{tot}$
U(VI) - montmorillonite
CNLBRA data

DRLmann

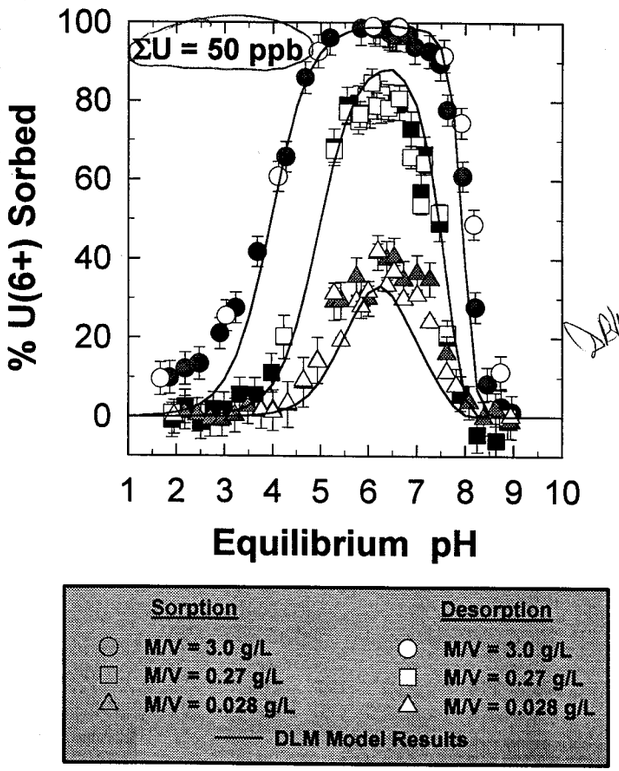
ln % $U(VI)_{total}$



DRLmann

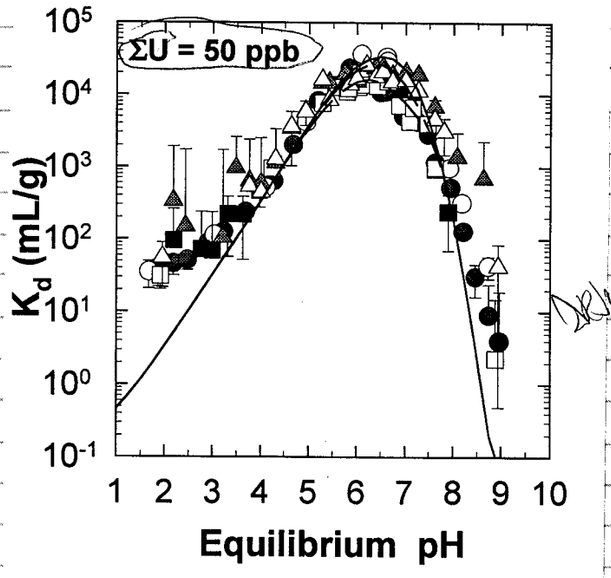
ln K_d

12/18/95
DRLumm



DLM Results
Effects of m/v
U(VI)-montmorillonite
CNWRA data
In % U(VI)$_{total}$

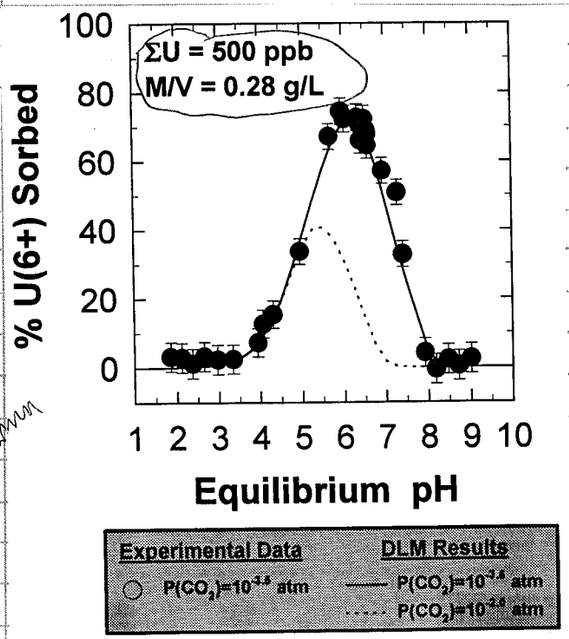
DRLumm



In K_d

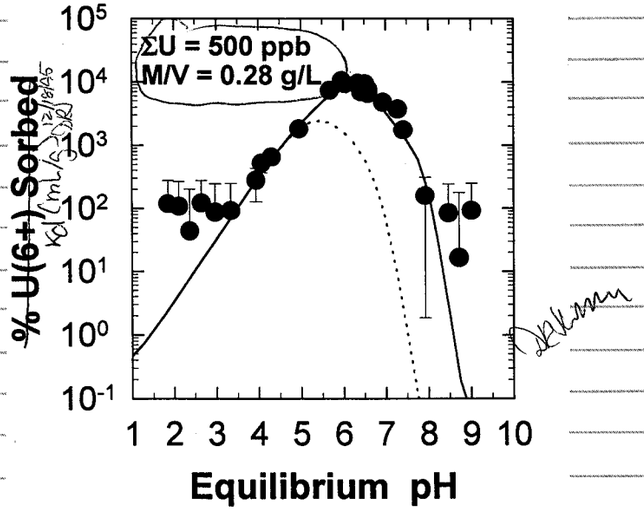
DRLumm

12/18/95
DRL



DLM results
Effects of $P(CO_2)$
U(VI)-montmorillonite
CNWRA data
In % U(VI)$_{tot}$

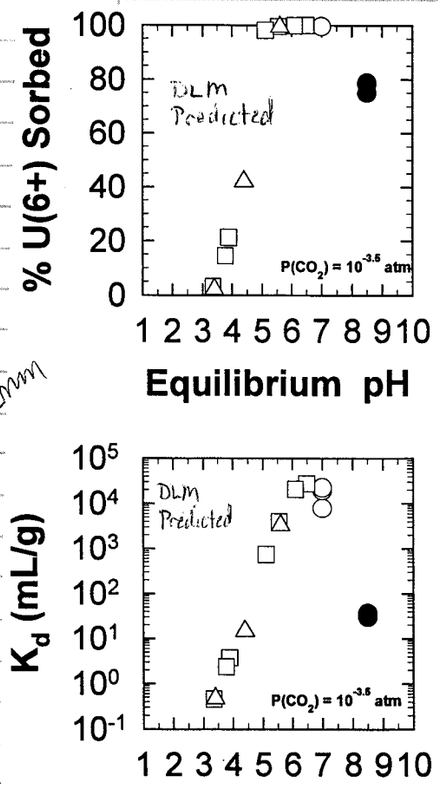
DRLumm

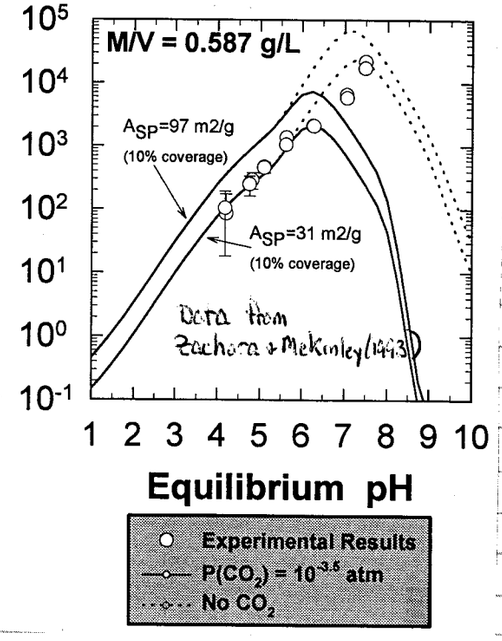


In K_d

DRLumm

12/18/95
DRJ





DLM results compared to other U(VI)-montmorillonite sorption studies

Project 5704-472 closed due to CNWRA reorganization. Research assigned to 5708-871 KTI Radionuclide Transport effective 1/30/96 DRJ
Update CNWRA/MINTEQA2 radionuclide database

2/2/96
DRJ

Updating the CNWRA MINTEQA2 Radionuclide Database (2/2/96)

The Americium data was updated to use the new NEA Americium thermodynamic database. The reference for the data is:

Silva, R.J., G. Bidoglio, M.H. Rand, P.B. Robouch, H. Wanner, and I. Puigdomenich. 1995. *Chemical Thermodynamics Series, Volume 2: Chemical Thermodynamics of Americium*. Nuclear Energy Agency (NEA), Organization for Economic Cooperation and Development (OECD). New York: Elsevier. 95NEA/1

The database was also modified to correct equilibrium constants for the uranium species UO_2CO_3(aq), UO_2CO_3 (s-rutherfordine), and $U(CO_3)_5^{-6}$. The corrections were reported in:

Grenthe, I., I Puigdomenech, M.C.A. Sandino, and M.H. Rand. 1995. *Appendix D, Corrections to the NEA-TDB Review. Chemical Thermodynamics Series, Volume 2: Chemical Thermodynamics of Americium*. Nuclear Energy Agency (NEA), Organization for Economic Cooperation and Development (OECD). New York: Elsevier. 95NEA/2

2/2/96 DRS

Calculating Log K Values from Free Energies

Log K	Del G(r) (kJ/mol)	Del H(r) (kJ/mol)	M.W. (g/mol)	Del G(f) (kJ/mol)	Del H(f) (kJ/mol)	Mineral/Species
AM(III) AQUEOUS:						
-6.4003	36.5310	57.7300	260.0697	-799.3070	-844.8000	AmOH++
-14.1008	80.4830	76.3600	277.0781	-992.4950	-1110.0000	Am(OH)2+
-25.7015	146.6960	84.1900	294.0834	-1163.4220	-1380.0000	Am(OH)3 (aq)
3.4001	-19.4070	19.0100	262.0598	-898.6280	-933.0400	AmF++
5.8004	-33.1070	18.4000	281.0582	-1194.8510	-1269.0000	AmF2+
1.0502	-5.9940	-15.6200	278.5144	-735.9090	-789.4000	AmCl++
3.9502	-21.9760	21.0400	339.1230	-1364.9780	-1505.0000	AmSO4+
5.4004	-30.8240	44.3800	435.1846	-2117.5300	-2391.0000	Am(SO4)2-
1.3300	-7.5910	##########	305.0683	-717.0930	##########	AmNO3++
22.5634	-128.7950	##########	340.0487	-1752.9740	##########	AmH2PO4++
7.8005	-44.5230	14.8300	303.0708	-1171.1200	-1277.0000	AmCO3+
12.3009	-70.2100	10.1800	363.0802	-1724.7080	-1957.0000	Am(CO3)2-
15.2012	-86.7640	##########	423.0896	-2269.1580	##########	Am(CO3)3-3
AM(IV) AQUEOUS:						
38.3108	-224.3740	##########	543.1084	-3210.2270	##########	Am(CO3)5-6
AM(III) SOLIDS:						
-51.7715	295.4860	400.4900	534.1210	-1613.3200	-1890.4000	Am2O3(c)
-17.0009	97.0360	202.1900	294.0834	-1213.0820	-1272.0000	Am(OH)3 (am)
-15.2009	86.7620	202.1800	294.0834	-1223.3560	-1272.0000	Am(OH)3 (c)
13.2393	-75.5660	34.7500	300.0586	-1518.8330	-1588.0000	AmF3 (c)
-14.3138	81.6990	140.1400	349.4204	-910.6500	-977.8000	AmCl3 (c)
-11.3035	64.5170	119.8100	294.5138	-902.5380	-949.8000	AmOCl (c)
-21.6755	123.7170	170.9300	482.7734	-786.5310	-810.0000	AmBr3 (c)
-13.7211	78.3180	130.9400	338.9848	-861.3720	-893.0000	AmOBr (c)
-24.6266	140.5610	175.0400	623.7746	-813.3090	-812.0000	AmI3 (c)
33.4023	-190.6500	38.0900	666.1510	-2971.7430	-3221.0000	Am2(CO3)3 (c)
7.1992	-41.0910	42.7600	320.0781	-1404.8280	-1535.0000	AmCO3(OH) (c)
-104.8832	598.6980	616.7000	243.0614	0.0000	0.0000	Am-metal
AM(IV) SOLIDS:						
9.4353	-53.8540	45.4600	275.0802	-874.4920	-932.2000	AmO2(c)
25.2962	-144.3830	37.4000	319.0550	-1616.8330	-1710.0000	AmF4 (c)
REDOX REACTIONS:						
-44.2105	252.3400	210.7000	0.0000			Am+++/Am++
-58.3742	333.1820	384.1000	0.0000			AmO2+/Am+++
-85.3545	487.1770	537.6000	0.0000			AmO2++/Am+++

Reaction Stoichiometries

	e-	H+	Cl-	F-	CO3--	SO4--	PO4-3	NO3-	Br-	I-	H2O(l)	Am+++	Am++++	AmO2+	AmO2++	COMMENTS		
M.W.	0	1.0079	35.4530	18.9984	60.0094	96.0616	94.9714	62.0049	79.9040	126.9044	18.0153	243.0614	243.0614	275.0802	275.0802	All Auxilliary Data from NEA95 (Silva et al., 1995)		
Del G(f)(kJ/mol)	0	0.0000	-131.2170	-281.5230	-527.8990	-744.0040	-1025.4910	-110.7940	-103.9500	-51.7240	-237.1400	-598.6980	-348.3560	-739.7960	-585.9010			
Del H(f)(kJ/mol)	0	0.0000	-167.0800	-335.3500	-675.2300	-909.3400	-1284.4000	-206.8500	-121.4100	-58.7800	-285.8300	-616.7000	-406.0000	-804.2600	-650.7600			
	-1	-1									1	1						
	-2	-2									2	1				del Gf: NEA95'	del Hf: PHI88'	
	-3	-3									3	1				del Gf: NEA95'	del Hf: PHI88'	
				1								1				del Gf: NEA95'	del Hf: PHI88'	
				2								1				del Gf: NEA95'	del Hf: PHI88'	
			1									1				del Gf: NEA95'	del Hf: PHI88'	
			2									1				del Gf: NEA95'	del Hf: PHI88'	
					1							1				del Gf: NEA95'	del Hf: PHI88'	
					2							1				del Gf: NEA95'	del Hf: PHI88'	
					3							1				del Gf: NEA95'	del Hf: PHI88'	
					5							1				del Gf: NEA95'	del Hf: PHI88'	
													1			del Gf: NEA95'	del Hf: PHI88'	
	-6										3	2						
	-3										3	1				del Gf: NEA95'	del Hf: NEA95'	
	-3										3	1				del Gf: NEA95'	del Hf: PHI88'-(Only identified as Am(OH)3 (s)	
				3							3	1				del Gf: NEA95'	del Hf: PHI88'-(Only identified as Am(OH)3 (s)	
		3										1				del Gf: NEA95'	del Hf: NEA95'	
	-2	1										1				del Gf: NEA95'	del Hf: NEA95'	
											1	1				del Gf: NEA95'	del Hf: NEA95'	
	-2							3				1				del Gf: NEA95'	del Hf: NEA95'	
									1		1	1				del Gf: NEA95'	del Hf: NEA95'	
					3					3		1				del Gf: NEA95'	del Hf: NEA95'	
	-1				1							2				del Gf: NEA95'	del Hf: PHI88'	
3											1	1				del Gf: NEA95'	del Hf: PHI88'	
												1				del Gf: NEA95'	del Hf: NEA95'	
	-4																	
				4							2		1			del Gf: NEA95'	del Hf: NEA95'	
													1			del Gf: NEA95'	del Hf: NEA95'	
-1																		
-2	-4										2	1	-1			del Gf: NEA95'	del Hf: NEA95'	
-3	-4										2	1		-1		del Gf: NEA95'	del Hf: NEA95'	
														-1		del Gf: NEA95'	del Hf: NEA95'	

Comparison: for spreadsheet Log $K_{AmF_2^+}$ = 5.8004 vs. 5.800

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Table III.2 (continued)

Selected americium data

Species	Reaction	$\log_{10} K^\circ$	$\Delta_r G_m^\circ$ (kJ · mol^{-1})	$\Delta_r H_m^\circ$ (kJ · mol^{-1})	$\Delta_r S_m^\circ$ (J · K^{-1} · mol^{-1})
✓ $Am(OH)_3(aq)$	$Am^{3+} + 3\ H_2O(l) \rightleftharpoons Am(OH)_3(aq) + 3\ H^+$	−25.700 ±0.500	146.697 ±2.854		
✓ $Am(OH)_3(cr)$	$Am^{3+} + 3\ H_2O(l) \rightleftharpoons Am(OH)_3(cr) + 3\ H^+$	−15.200 ±0.600	86.762 ±3.425		
✓ AmF^{2+}	$Am^{3+} + F^- \rightleftharpoons AmF^{2+}$	3.400 ±0.400	−19.407 ±2.283		
✓ AmF_2^+	$Am^{3+} + 2\ F^- \rightleftharpoons AmF_2^+$	5.800 ±0.200	−33.107 ±1.142		
$AmF_3(g)$	$AmF_3(cr) \rightleftharpoons AmF_3(g)$	−62.982[c] ±1.333	359.502[a] ±7.609	421.100 ±7.000	206.600 ±10.000
✓ $AmCl^{2+}$	$Am^{3+} + Cl^- \rightleftharpoons AmCl^{2+}$	1.050 ±0.060	−5.993 ±0.342		
✓ $AmSO_4^+$	$Am^{3+} + SO_4^{2-} \rightleftharpoons AmSO_4^+$	3.850 ±0.030	−21.976 ±0.171		
✓ $Am(SO_4)_2^-$	$Am^{3+} + 2\ SO_4^{2-} \rightleftharpoons Am(SO_4)_2^-$	5.400 ±0.800	−30.823 ±3.996		
AmN_3^{2+}	$Am^{3+} + N_3^- \rightleftharpoons AmN_3^{2+}$	1.670 ±0.100	−9.532 ±0.571		
✓ $AmNO_2^{2+}$	$Am^{3+} + NO_2^- \rightleftharpoons AmNO_2^{2+}$	2.100 ±0.200	−11.987 ±1.142		
✓ $AmNO_3^{2+}$	$Am^{3+} + NO_3^- \rightleftharpoons AmNO_3^{2+}$	1.330 ±0.200	−7.592 ±1.142		

2/13/96
DPJ

Correct error in THERMO.DBS and TYPE6.DBS

Species ID # 3089300 - Uraninite
components should be '2' not '3'

$$UO_2^{++} + 2e^- = UO_2(c)$$

Change made in both THERMO.UNF and TYPE6.DBS. Recompiled using UNFRMT.EXE. Copies of the 4 affected files in envelope at the back of this notebook - THERMO.DBS
THERMO.UNF
TYPE6.DBS
TYPE6.UNF

4/16/96
DBJ

U(VI)-Quartz Sorption

U(VI)-Quartz sorption was revisited using the DLM and a simplified container sorption model to evaluate the effect of mineral-container competition in U(VI) sorption experiments for minerals with low surface areas (fewer sorption sites). In this study, an approach has been adopted such that the simplest model that can describe the observed sorption behavior is used.

U(VI)-Container Sorption

To develop the necessary pH dependence for U(VI)-container sorption, two reactions were postulated that bind the positively charge species UO_2OH^+ and $(UO_2)_3(OH)_5^+$ to a hypothetical, negatively charged site represented as X$^-$:

$$X^- + UO_2^{2+} + H_2O \Leftrightarrow XUO_2OH^o + H^+ \qquad (K_{XUO_2OH}) \qquad (5)$$

$$X^- + 3UO_2^{2+} + 5H_2O \Leftrightarrow X(UO_2)_3OH_5^o + 5H^+ \qquad (K_{X(UO_2)_3OH_5}) \qquad (6)$$

Using FITEQL to interpret the U(6+) loss to the container from an average of three control experiments for U_{total} = 50 ppb, and simultaneously determining site density and binding constants for the sorption reactions resulted in binding constants (log K) of 2.73 and -5.62 for Equations (5) and (6), respectively and a total site concentration (T_x) of about 2.3 x 10^{-8} M (based on a rough estimate of wetted container surface area of ~60 cm^2, an assumed site density of 0.1 sites/nm^2, with subsequent optimization of T_x using FITEQL). No electrostatic terms were included in the mass action. These binding constants were adjusted slightly by trial-and-error [log K = 2.85 and -5.25 for (5) and (6), respectively] to produce the best fit to the observed container sorption at U_{total} = 5, 50, and 500 ppb. Despite the large number of assumptions made, the model was successful in reproducing observed container sorption.

U(VI)-Quartz Sorption

The U(VI)-quartz sorption data for the conditions (Experiment Q2):

U_{total}=49.24 ppb=2.11e-7 M
M/V=20 g/L
PCO_2=$10^{-3.5}$ atm

were modeled for the DLM using FITEQL, version 2.0. Only the data from pH ~4 to 8 was modeled because this is where most sorption occurred. Including data at higher and lower pH where sorption is essentially zero tends to bias the data, resulting in an underprediction of the sorption maximum.

In order to develop a DLM for the U(6+)-quartz system, it is necessary to calculate the total number of sorption sites ($T_{>XOH}$). The N_2/BET surface area of 0.03 m^2/g, together with a "standard" site density of 2.3 sites/nm^2 recommended for all minerals by Davis and Kent (1990) based on the ferrihydrite work of Dzombak and Morel (1990), was used to calculate the total number of available sites. The acidity constant used to describe the deprotonation of the >SiOH^o sites was derived based on potentiometric titration data for amorphous SiO_2, as described in Turner and Sassman (1994).

FITEQL requires the input of an equilibrium aqueous speciation model. For this reason, the resultant binding constants are dependent on the quality and extent of the thermodynamic data available for the system of interest. For U(6+), the equilibrium constants used in the chemical equilibrium models submitted to FITEQL are listed below. These values were taken from the NEA thermodynamic database (Wanner and Forrest, 1992) with the exception of the value for the neural hydroxy complex, $UO_2(OH)_2$°(aq). Due to experimental uncertainties, Wanner and Forrest (1992) could only recommend an upper limit to the stability constant of $UO_2(OH)_2$°(aq). The equilibrium constant for $UO_2(OH)_2$°(aq) used with FITEQL and listed in the table below was taken from Fuger (1992). This value is 2.7 log units lower than the upper limit recommended by Wanner and Forrest (1992), but as pointed out by Fuger (1992), a lower value is consistent with the work of Choppin and Mathur (1991). Assuming a lower equilibrium constant for $UO_2(OH)_2$°(aq) also provides for a much better fit to the available sorption data.

There is typically a lack of independent analytical data supporting the formation of a particular surface complex. In the absence of these data, the exact form of the surface reaction is selected by the modeler based on analogous speciation reactions in the aqueous phase. If the postulated reaction does not contribute significantly to the sorption behavior, FITEQL will iterate towards a large negative binding constant and fail to converge. In this way, the modeler can identify those reactions that dominate sorption in the conceptual model.

Based on FITEQL optimization runs, the following three inner-sphere complex reactions proved to be most capable of reproducing the Q2 experiment data:

$$>SiOH^o + UO_2^{2+} = >SiO\text{-}UO_2^+ + H^+$$

$$>SiOH^o + UO_2^{2+} + H_2O = >SiO\text{-}UO_2OH^o + 2H^+$$

$$>SiOH^o + 3UO_2^{2+} + 5H_2O = >SiO\text{-}(UO_2)_3(OH)_5^o + 6H^+$$

Typically, FITEQL would not converge if the three binding constants were simultaneously optimized. The approach taken was to fit a binding constant to one reaction first, fix this binding constant in the geochemical equilibrium model and optimize the remaining reaction(s). In most cases, the first two reactions dominated the sorption behavior. The FITEQL results (binding constants) for each of the five experimental runs differed only slightly. Initial values for the binding constants were adjusted in MINTEQA2 runs to the values in Table 1 to provide the best visual fit to the U(VI) sorption data presented here for a variety of pH, M/V, and U_{total} conditions. The final binding constants determined for these reactions are given below.

4/16/96
DBJ

Table 1. FITEQL model conditions used to determine DLM binding constants for U(6+) sorption on quartz.

DLM Parameters and Chemical Model Reactions:	Quartz
Site density[a]	2.3 sites/nm^2
Surface area	0.03 m^2/g
Ionic strength	0.1 M $NaNO_3$
PCO_2	$10^{-3.5}$ atm
Sorption Reactions:	**Log K**
>SiOH° ⇔ >SiO$^-$ + H$^+$	-7.20[b]
>SiOH° + UO_2^{2+} ⇔ >SiO-UO_2^+ + H$^+$	0.30[c]
>SiOH° + UO_2^{2+} + H_2O ⇔ >SiO-UO_2OH° + 2H$^+$	-5.65[c]
>SiOH° + 3UO_2^{2+} + 5H_2O ⇔ >SiO-$(UO_2)_3(OH)_5$° + 6H$^+$	-16.75[c]
Aqueous Speciation Reactions:	**Log K**
UO_2^{2+} + H_2O ⇔ UO_2OH^+ + H$^+$	-5.20
UO_2^{2+} + 2H_2O ⇔ $UO_2(OH)_2$° (aq)+ 2H$^+$	-13.0[d]
UO_2^{2+} + 3H_2O ⇔ $UO_2(OH)_3^-$ + 3H$^+$	-19.20
2UO_2^{2+} + 2H_2O ⇔ $(UO_2)_2(OH)_2^{2+}$ +2H$^+$	-5.62
3UO_2^{2+} + 5H_2O ⇔ $(UO_2)_3(OH)_5^+$ + 5H$^+$	-15.55
UO_2^{2+} + CO_3^{2-} ⇔ UO_2CO_3°	9.68
UO_2^{2+} + 2CO_3^{2-} ⇔ $UO_2(CO_3)_2^{2-}$	16.94
UO_2^{2+} + 3CO_3^{2-} ⇔ $UO_2(CO_3)_3^{4-}$	21.60
2UO_2^{2+} + CO_3^{2-} + 3H_2O ⇔ $(UO_2)_2CO_3(OH)_3^-$ + 3H$^+$	-0.86
UO_2^{2+} + NO_3^- ⇔$UO_2NO_3^+$	0.30

a. Site density recommended for all minerals by Davis and Kent (1990), based on ferrihydrite work of Dzombak and Morel (1990).
b. Acidity constants for am-SiO_2 from Turner and Sassman (1996).
c. This study. Binding constants determined using FITEQL, Version 2.0 (Westall, 1982a,b).
d. All aqueous speciation Log K values from NEA Uranium Thermodynamic Database (Wanner and Forrest, 1992), except for $UO_2(OH)_2$° (aq) which is taken from Fuger (1992).

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DBJ

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
1	Quartz sand sorption data compilation																				
2		equil cont pH	= pH for container sorption																		
3		initial cont sorp	= percent U sorbed onto container (no substrate)																		
4		equil fin pH	= pH at end of sorption phase																		
5		final cont sorp	= percent sorbed on container after addition of quartz (total sorp - qtz sorp)																		
6		cont desorp	= percent sorbed on container after addition of quartz (desorption of container)																		
7		tot sorp	= percent total sorption																		
8		qtz desorp	= percent sorbed on quartz (from quartz desorption)																		
9		equiv sol conc	= final conc U in solution based on qtz desorp data ((1-%sorbed/100)*initial concentration)																		
10																					
11	Q1 conditions:	48.88 ppb		solution=	4.99E-08	g/mL			Q2 conditions:	49.24 ppb		solution=	4.92E-08	g/mL			Q3 conditions:	501.54 ppb		solution=	
12		0.1 g qtz								1.0 g qtz									2.5 g qtz		
13		50 mL solution								50 mL solution									50 mL solution		
14								equivalent								equivalent					
15		equil	initial	equil	final			solution		equil	initial	equil	final			solution		equil	initial	equil	final
16	exp samp	cont pH	cont sorp	fin pH	cont sorp	tot sorp	qtz desor	conc (g/mL)		cont pH	cont sorp	fin pH	cont sorp	tot sorp	qtz desor	conc (g/mL)		cont pH	cont sorp	fin pH	cont sorp
17	Q-pH2	2.02	-0.93	1.95		-1.31				1.95	-0.29	1.96		-0.98				1.96	1.94	1.97	
18	Q-pH 2.25	2.24	3.37	2.19		2.23				2.20	1.44	2.21		-0.71				2.18	-0.18	2.21	
19	Q-pH 2.5	2.49	0.98	2.44		-1.01	0.00	4.99E-08		2.46	1.95	2.46		-0.52	0.11	4.92E-08		2.45	0.00	2.49	
20	Q-pH 2.75	2.74	1.13	2.70		1.05				2.73	1.32	2.74		0.64				2.46	-0.30	2.49	
21	Q-pH3	2.97	1.07	2.93		-0.11				2.95	3.40	2.97		1.31				2.96	-0.30	3.01	
22	Q-pH 3.25	3.20	3.91	3.17		1.32	0.00	4.99E-08		3.20	0.56	3.23		-2.58	0.00	4.92E-08		3.21	0.31	3.23	
23	Q-pH 3.5	3.45	0.93	3.41		-0.32				3.45	2.91	3.45		0.52				3.48	0.49	3.53	
24	Q-pH 3.75	3.63	0.41	3.60		1.00				3.71	1.75	3.74		1.69				3.73	-0.54	3.78	
25	Q-pH 4	3.84	-1.45	3.80	0.98	1.15	0.17	4.98E-08		3.95	2.27	3.99	1.53	3.72	2.19	4.82E-08		4.01	1.68	4.09	-0.14
26	Q-pH 4.25	4.32	-0.28	4.24	2.83	2.94	0.31	4.97E-08		4.16	2.16	4.14	1.13	3.41	2.28	4.81E-08		4.37	3.78	4.50	3.04
27	Q-pH 4.5	4.48	2.25	4.38	2.82	3.29	0.47	4.96E-08		4.48	4.59	4.41	0.91	4.67	3.76	4.74E-08		4.76	1.58	4.86	3.91
28	Q-pH 4.75	4.62	5.52	4.50	1.41	1.86	0.45	4.97E-08		4.83	8.84	4.71	4.20	11.17	8.97	4.58E-08		4.93	4.89	5.05	4.98
29	Q-pH 5	4.78	6.24	4.60	4.48	5.43	0.95	4.94E-08		5.03	7.27	4.86	3.37	11.63	8.26	4.52E-08		5.61	6.58	5.84	6.38
30	Q-pH 5.25	5.04	6.61	4.80	5.91	7.11	1.20	4.93E-08		5.00	11.13	4.70	5.54	12.42	8.58	4.60E-08		6.05	8.97	6.11	6.01
31	Q-pH 5.5	5.15	7.40	4.81	3.02	3.99	0.97	4.94E-08		5.55	13.60	5.07	6.98	17.64	10.66	4.40E-08		6.19	6.05	6.30	1.60
32	Q-pH 5.75	5.35	9.14	4.98	5.63	7.27	1.64	4.91E-08		5.84	13.04	5.19	6.79	18.73	11.94	4.34E-08		6.36	6.62	6.47	
33	Q-pH 6	5.51	10.66	5.01	7.07	8.39	1.32	4.92E-08		6.09	16.58	5.38	9.75	24.51	14.76	4.20E-08		6.41	4.42	6.63	1.98
34	Q-pH 6.25	5.90	14.22	5.26	11.76	13.75	1.99	4.89E-08		6.29	23.82	5.39	17.76	30.72	12.96	4.29E-08		6.68	7.60	6.79	1.98
35	Q-pH 6.5	6.24	14.32	5.68	10.99	13.43	2.44	4.87E-08		6.58	23.25	6.12	19.07	46.91	27.84	3.55E-08		6.75	7.11	6.87	4.08
36	Q-pH 6.75	6.66	13.73	6.40	16.40	21.18	4.78	4.75E-08		6.82	12.62	6.43	-2.01	43.46	45.47	2.69E-08		6.80	7.79	6.95	2.48
37	Q-pH 7	6.89	10.98	6.71	10.08	14.53	4.45	4.77E-08		7.10	15.12	6.81	1.29	43.62	42.33	2.84E-08		7.00	7.18	7.04	2.95
38	Q-pH 7.25	7.09	7.52	6.96	5.76	10.63	4.87	4.75E-08		7.35	6.51	7.12	-3.89	34.54	38.43	3.03E-08		7.15	6.28	7.17	-0.32
39	Q-pH 7.5	7.40	4.14	7.31	1.90	5.64	3.74	4.80E-08		7.56	4.79	7.38	-1.81	29.62	31.23	3.39E-08		7.38	2.93	7.40	0.01
40	Q-pH 7.75	7.70	1.92	7.62	0.83	3.35	2.52	4.86E-08		7.83	4.53	7.64	-2.01	16.54	18.55	4.01E-08		7.74	-0.46	7.78	-2.61
41	Q-pH 8	7.98	-0.97	7.91	-1.72	-0.57	1.15	4.93E-08		8.09	0.57	7.91	-1.84	6.55	8.39	4.51E-08		7.97	0.52	7.98	5.56
42	Q-pH 8.25	8.25	0.81	8.21		-0.30				8.31	-0.37	8.16		-1.58				8.17	0.29	8.20	
43	Q-pH 8.5	8.52	-1.97	8.53		-2.27				8.56	0.83	8.45		0.68				8.42	1.88	8.43	
44	Q-pH 8.75	8.75	0.88	8.73		-0.87				8.77	-0.52	8.68		-1.34				8.68	0.00	8.70	
45	Q-pH 9	8.98	-1.18	8.96		-2.00				8.99	0.60	8.95		-0.68				8.94	1.07	8.95	

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	AQ	AR	AS	AT	AU	AV	AW	AX	AY	AZ	BA	BB	BC	BD	BE	BF	BG	BH	BI	BJ	BK
1																					
2																					
3																					
4																					
5																					
6																					
7																					
8																					
9																					
10																					
11																					
12																					
13	Container loss					Container+Quartz					Container Only (no substrate)						Quartz Only (from Qz desorption)				
14	Avg. of 50ppb data		2.11E-07		5ppb	50ppb(a)	50ppb(b)	50ppb(c)	500ppb		5ppb	50ppb(a)	50ppb(b)	50ppb(c)	500ppb		5ppb	50ppb(a)	50ppb(b)	50ppb(c)	500ppb
15					2E-08	2.14E-07	2.11E-07	2.06E-07	2.15E-06		2E-08	2.14E-07	2.11E-07	2.06E-07	2.15E-06		2E-08	2.14E-07	2.11E-07	2.06E-07	2.15E-06
16	pH	% sorbed	mol sorbed		mol sorb	mol sorb	mol sorb	molsorb	mol sorb		mol sorb	mol sorb	mol sorb	molsorb	mol sorb		mol sorb	mol sorb	mol sorb	molsorb	mol sorb
17	1.99	-0.69	-1.4E-09		-2.6E-10	-2.8E-09	-2.1E-09	-8.3E-09	4.24E-08		-5.7E-10	-2E-09	-6.1E-10	-1.7E-09	4.18E-08		0	0	0	0	0
18	2.23	1.65	3.47E-09		8.4E-10	4.77E-09	-1.5E-09	-4E-09	4.76E-08		3.13E-10	7.21E-09	3.04E-09	2.89E-10	-3.9E-09		0	0	0	0	0
19	2.48	1.48	3.07E-09		-1.9E-10	-2.2E-09	-1.1E-09	-1.8E-09	5.36E-08		5.85E-10	2.1E-09	4.12E-09	2.99E-09	0		-1E-11	0	2.32E-10	3.51E-10	-1.7E-09
20	2.74	0.95	2E-09		1.12E-09	2.25E-09	1.35E-09	-5.6E-09	5.96E-08		2E-11	2.42E-09	2.79E-09	8.25E-10	-1.5E-09		0	0	0	0	0
21	2.97	3.73	7.86E-09		3.17E-10	-2.4E-10	2.77E-09	7.3E-09	6.48E-08		4.35E-10	2.29E-09	7.19E-09	1.39E-08	-6.5E-09		0	0	0	0	0
22	3.22	1.66	3.49E-09		7.06E-10	2.83E-09	-5.5E-09	-1.4E-10	6.95E-08		4.87E-10	8.37E-09	1.18E-09	1.05E-09	6.67E-09		0	0	0	2.19E-09	0
23	3.49	2.03	4.27E-09		7.24E-10	-6.9E-10	1.1E-09	1.86E-10	7.5E-08		9.2E-10	1.99E-09	6.15E-09	4.62E-09	1.05E-08		0	0	0	0	0
24	3.71	1.69	3.56E-09		3.23E-10	2.14E-09	3.57E-09	1E-08	8.14E-08		-4.1E-10	8.78E-10	3.7E-09	6E-09	-1.2E-08		0	0	0	0	0
25	3.94	1.36	2.86E-09		1.61E-09	2.46E-09	7.86E-09	9.4E-09	8.8E-08		2.67E-10	-3.1E-09	4.8E-09	5.72E-09	3.62E-08		6.89E-10	3.64E-10	4.63E-09	9.07E-09	3.55E-08
26	4.26	3.02	6.37E-09		2.52E-09	6.29E-09	7.21E-09	2.58E-08	9.69E-08		1.2E-09	-8E-10	4.56E-09	1.48E-08	8.09E-08		1.37E-09	6.64E-10	4.82E-09	1.64E-08	9.23E-08
27	4.51	4.84	1.02E-08		3.76E-09	7.04E-09	9.87E-09	3.97E-08	1.05E-07		1.79E-09	4.82E-09	9.7E-09	1.58E-08	3.4E-08		2.51E-09	1.01E-09	7.95E-09	2.88E-08	1.63E-07
28	4.76	8.77	1.85E-08		6.09E-09	3.98E-09	2.36E-08	5.28E-08	1.09E-07		2.74E-09	1.18E-08	1.87E-08	2.46E-08	1.05E-07		4.08E-09	9.63E-10	1.47E-08	4.17E-08	2.16E-07
29	4.96	10.10	2.13E-08		9.4E-09	1.16E-08	2.46E-08	7.1E-08	1.26E-07		4.9E-09	1.34E-08	1.54E-08	3.46E-08	1.42E-07		6E-09	2.03E-09	1.75E-08	5.44E-08	5.87E-07
30	5.13	12.15	2.56E-08		1.17E-08	1.52E-08	2.62E-08	8.52E-08	1.32E-07		6.33E-09	1.42E-08	2.35E-08	3.86E-08	1.93E-07		7.53E-09	2.57E-09	1.39E-08	6.8E-08	5.85E-07
31	5.44	15.18	3.2E-08		1.18E-08	8.54E-09	3.73E-08	1.13E-07	1.36E-07		4.77E-09	1.58E-08	2.87E-08	5.06E-08	1.3E-07		8.73E-09	2.08E-09	2.25E-08	7.92E-08	7.52E-07
32	5.67	16.28	3.42E-08		1.34E-08	1.56E-08	3.96E-08	1.27E-07	1.39E-07		6.11E-09	1.96E-08	2.76E-08	5.48E-08	1.42E-07		9.59E-09	3.51E-09	2.52E-08	1.04E-07	0
33	5.86	20.02	4.21E-08		1.42E-08	1.8E-08	5.18E-08	1.54E-07	1.43E-07		7.92E-09	2.28E-08	3.5E-08	6.76E-08	9.51E-08		9.83E-09	2.83E-09	3.12E-08	1.02E-07	7.79E-07
34	6.13	21.57	4.54E-08		1.47E-08	2.94E-08	6.49E-08	1.56E-07	1.46E-07		7.96E-09	3.04E-08	5.03E-08	5.5E-08	1.64E-07		1.09E-08	4.26E-09	2.74E-08	1.08E-07	7.59E-07
35	6.42	22.38	4.71E-08		1.48E-08	2.88E-08	9.91E-08	1.6E-07	1.48E-07		6.76E-09	3.07E-08	4.91E-08	6.1E-08	1.53E-07		1.15E-08	5.22E-09	5.88E-08	1.18E-07	7.2E-07
36	6.73	14.22	2.99E-08		1.44E-08	4.53E-08	9.18E-08	1.56E-07	1.5E-07		4.46E-09	2.94E-08	2.67E-08	3.36E-08	1.68E-07		1.19E-08	1.02E-08	9.61E-08	1.4E-07	7.36E-07
37	7.01	12.72	2.68E-08		1.37E-08	3.11E-08	9.22E-08	1.45E-07	1.52E-07		3.04E-09	2.35E-08	3.2E-08	2.48E-08	1.55E-07		1.16E-08	9.53E-09	8.95E-08	1.34E-07	7.51E-07
38	7.24	7.71	1.62E-08		1.28E-08	2.28E-08	7.3E-08	1.29E-07	1.54E-07		2.24E-09	1.61E-08	1.38E-08	1.58E-08	1.35E-07		1.05E-08	1.04E-08	8.12E-08	1.19E-07	7.32E-07
39	7.51	4.28	9E-09		9.97E-09	1.21E-08	6.26E-08	8.18E-08	1.59E-07		2.57E-10	8.66E-09	1.01E-08	8.04E-09	6.31E-08		9.71E-09	8.01E-09	6.8E-08	8.22E-08	6.07E-07
40	7.78	2.42	5.09E-09		7.57E-09	7.17E-09	3.5E-08	7.32E-08	1.67E-07		-6E-11	3.9E-09	9.57E-09	1.88E-08	-9.9E-09		7.4E-09	5.39E-09	3.92E-08	7.04E-08	3.55E-07
41	8.05	-0.15	-3.2E-10		3.13E-09	-1.2E-09	1.38E-08	3.41E-08	1.72E-07		-1.2E-10	-2.1E-09	1.2E-09	-1E-10	1.12E-08		3.52E-09	2.46E-09	1.77E-08	3.6E-08	2.48E-08
42	8.28	0.02	4.91E-11		6.57E-10	-6.4E-10	-3.3E-09	8.16E-09	1.77E-07		7.22E-11	1.73E-09	-7.8E-10	-7.6E-10	6.24E-09		0	0	0	0	0
43	8.52	-0.32	-6.8E-10		-1.4E-10	-4.9E-09	1.44E-09	-5E-09	1.81E-07		-5.6E-10	-4.2E-09	1.75E-09	3.51E-10	4.05E-08		0	0	0	0	0
44	8.75	-0.08	-1.6E-10		4.47E-10	-1.9E-09	-2.8E-09	-1.8E-09	1.87E-07		-2.5E-10	1.88E-09	-1.1E-09	-1.2E-09	0		0	0	0	0	0
45	8.99	0.70	1.47E-09		-3.8E-10	-4.3E-09	-1.4E-09	-4.1E-10	1.93E-07		-1.3E-10	-2.5E-09	1.27E-09	5.51E-09	2.3E-08		0	0	0	0	0

	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP
1																					
2																					
3																					
4																					
5																					
6																					
7																					
8																					
9																					
10																					
11	5.02E-07	g/mL			Q4 conditions:	4.67 ppb		solution=	4.67E-09	g/mL				Q5 conditions:	48.04 ppb		solution=	4.8E-08	g/mL		
12						1.0 g qtz									2.5 g qtz						
13						50 mL solution									50 mL solution						
14			equivalent									equivalent									equivalent
15	tot sorp	qtz desor	solution		equil	initial	equil	final				solution		equil	initial	equil	final				solution
16			conc (g/mL)		cont pH	cont sorp	fin pH	cont sorp	cont deso	tot sorp	qtz desorp	conc (g/mL)		cont pH	cont sorp	fin pH	cont sorp	cont deso	tot sorp	qtz desor	conc (g/mL)
17	0.53				1.97	-2.86	1.97			-1.32				2.01	-0.84	1.93			-4.01		
18	3.03				2.21	1.56	2.21			4.19				2.25	0.14	2.26			-1.95		
19	0.26	-0.06	5.02E-07		2.43	2.92	2.47		0.54	-0.94	-0.05	4.67E-09		2.50	1.45	2.51		0.00	-0.85	0.17	4.80E-08
20	1.79				2.89	0.10	2.72			5.60				2.76	0.40	2.78			-2.71		
21	1.08				2.96	2.17	2.97			1.58				3.00	6.73	3.01			3.54		
22	1.63	0.00	5.02E-07		3.22	2.43	3.26			3.52	0.00	4.67E-09		3.26	0.51	3.24		0.00	-0.07	1.06	4.75E-08
23	2.01				3.47	4.59	3.49			3.61				3.56	2.24	3.56			0.09		
24	0.42				3.74	-2.05	3.79			1.61				3.80	2.91	3.84			4.87		
25	1.51	1.65	4.93E-07		3.94	1.33	4.01	4.61	0.49	8.05	3.44	4.51E-09		4.03	3.26	4.05	0.16	0.20	4.56	4.40	4.59E-08
26	7.33	4.29	4.80E-07		4.23	6.01	4.30	5.77	0.99	12.59	6.82	4.35E-09		4.29	7.19	4.34	4.50	0.50	12.44	7.94	4.42E-08
27	11.49	7.58	4.64E-07		4.51	8.93	4.60	6.21	3.83	18.75	12.54	4.08E-09		4.58	7.67	4.66	5.31	0.20	19.26	13.95	4.13E-08
28	15.01	10.03	4.51E-07		4.82	13.69	4.91	10.03	6.49	30.38	20.35	3.72E-09		4.84	11.95	4.89	5.39	3.36	25.62	20.23	3.83E-08
29	33.64	27.26	3.65E-07		5.17	24.47	5.25	16.99	9.68	46.91	29.92	3.27E-09		5.08	16.80	5.02	8.05	5.70	34.45	26.40	3.54E-08
30	33.31	27.20	3.65E-07		5.51	31.56	5.55	20.80	17.57	58.37	37.57	2.92E-09		5.36	18.70	5.26	8.34	5.63	41.30	32.96	3.22E-08
31	36.54	34.94	3.28E-07		5.77	23.80	5.86	15.32	11.81	58.88	43.56	2.64E-09		5.62	24.54	5.62	16.21	12.94	54.64	38.43	2.96E-08
32	41.07		5.02E-07		5.97	30.46	6.04	19.05	14.56	66.88	47.83	2.44E-09		5.83	26.60	5.86	11.38	9.88	61.58	50.20	2.39E-08
33	38.15	36.17	3.20E-07		6.11	39.53	6.19	21.55	19.09	70.60	49.05	2.38E-09		5.98	32.81	6.03	25.29	22.65	74.76	49.47	2.43E-08
34	37.26	35.28	3.25E-07		6.30	39.83	6.40	19.17	16.92	73.31	54.14	2.14E-09		6.21	26.68	6.24	23.30	20.26	75.63	52.33	2.29E-08
35	37.55	33.47	3.34E-07		6.51	33.74	6.60	16.28	14.63	73.88	57.59	1.98E-09		6.44	29.58	6.49	20.18	18.04	77.40	57.22	2.06E-08
36	38.67	34.19	3.30E-07		6.73	22.23	6.78	12.50	10.77	71.96	59.46	1.89E-09		6.71	16.32	6.64	7.95	7.20	75.72	67.77	1.55E-08
37	37.86	34.91	3.26E-07		6.92	15.15	6.98	10.59	6.55	68.57	57.98	1.96E-09		7.03	12.05	6.86	5.23	4.25	70.18	64.95	1.68E-08
38	33.67	33.99	3.31E-07		7.19	11.20	7.20	11.77	10.46	63.98	52.21	2.23E-09		7.27	9.11	7.13	5.05	3.40	62.71	57.66	2.03E-08
39	28.19	28.18	3.60E-07		7.44	1.28	7.48	1.30	0.20	49.74	48.44	2.41E-09		7.56	3.90	7.57	-0.20	0.35	39.68	39.88	2.89E-08
40	13.86	16.47	4.19E-07		7.69	-0.30	7.72	0.86	0.90	37.77	36.91	2.95E-09		7.81	0.91	7.68	1.37	0.00	35.51	34.14	3.16E-08
41	6.71	1.15	4.96E-07		7.99	-0.60	7.99	-1.94	0.35	15.61	17.55	3.85E-09		8.08	-0.05	8.03	-0.92	0.00	16.56	17.48	3.96E-08
42	2.00				8.24	0.36	8.24			3.28				8.27	-0.37	8.27			3.96		
43	1.64				8.46	-2.77	8.51			-0.70				8.49	0.17	8.48			-2.41		
44	0.53				8.71	-1.23	8.77			2.23				8.73	-0.59	8.73			-0.88		
45	1.00				8.95	-0.63	9.02			-1.91				9.01	2.67	9.02			-0.20		

CNWRA-generated U(VI)-Qz-Container sorption Data.

4/16/96
DRJ

Example FITEQL Input files:

Container

```
         1
         1
         1
         1
         1
        30
         3          1          3
00001  -6.30  2.30E-8   X-
00032  -6.68  2.11E-7   UO2+2
00140  -3.48  3.31E-4   CO2g
00033   0.0   0.00E00   UO2ads
00050   0.0   0.00E00   H+
00003  -1.0   0.00E00   Na+
00005  -1.0   0.00E00   NO3-

00050    0.00  050  1
00032    0.00  032  1
00140    0.00  140  1
00001    0.00  001  1
03201   -5.43  032  1 050 -1
03202  -13.22  032  1 050 -2
03203  -19.22  032  1 050 -3
03206   -5.42  032  2 050 -2
03208  -16.25  032  3 050 -5
03211   -8.77  032  1 140  1 050 -2
03212  -18.91  032  1 140  2 050 -4
03213  -30.92  032  1 140  3 050 -6
03216  -19.28  032  2 140  1 050 -5
03218   -0.05  032  1 005  1
01401  -17.50  140  1 050 -2
01402   -7.61  140  1 050 -1
01403   -1.48  140  1
01404  -16.67  140  1 003  1 050 -2
01405   -8.08  140  1 003  1 050 -1
00100  -13.78  050 -1
03301    2.40  001  1 032  1 033  1 050 -1
03302   -6.39  001  1 032  3 033  3 050 -5


         2          1
      3301
      3302
       001
        13          1          1          0
        33
4.56E-09
9.70E-09
1.87E-08
1.54E-08
2.35E-08
2.87E-08
2.76E-08
3.50E-08
5.03E-08
4.91E-08
2.67E-08
3.20E-08
1.38E-08
        50
-4.05
-4.37
-4.72
-4.92
-4.89
-5.44
-5.73
-5.98
-6.18
-6.47
-6.71
-6.99
-7.24
         1          1
        33       0.05   2.1E-10
        50       0.05   0.0E-00
```

Quartz Only

```
containr           1
CNWRA/Q2           1
2.11e-7M           1
                   1
                   1
00000060          30
00000070           4          1          3          1
00000085  00002   -5.64  2.30E-6   SiOH
00000097  00160   -1.0   0.00E00   PSIO
00000098  00032   -6.68  2.11E-7   UO2+2
00000100  00140   -3.5   3.16E-4   CO2g
00000102  00033    0.0   0.00E00   UO2ads
00000104  00050    0.0   0.00E00   H+
00000106  00003   -1.0   0.00E00   Na+
00000110  00005   -1.0   0.00E00   NO3-
00000120
00000122  00050    0.00  050  1
00000124  00032    0.00  032  1
00000168  00140    0.00  140  1
00000126  00002    0.00  002  1
00000128  03201   -5.43  032  1 050 -1
00000130  03202  -13.22  032  1 050 -2
00000136  03203  -19.22  032  1 050 -3
00000140  03206   -5.42  032  2 050 -2
00000146  03208  -16.25  032  3 050 -5
00000148  03211   -8.77  032  1 140  1 050 -2
00000150  03212  -18.91  032  1 140  2 050 -4
00000156  03213  -30.92  032  1 140  3 050 -6
00000159  03216  -19.28  032  2 140  1 050 -5
00000161  03218   -0.05  032  1 005  1
00000162  01401  -17.50  140  1 050 -2
00000163  01402   -7.61  140  1 050 -1
00000164  01403   -1.48  140  1
00000165  01404  -16.67  140  1 003  1 050 -2
00000160  01405   -8.08  140  1 003  1 050 -1
xuo2oh    00100  -13.78  050 -1
xuo23oh5  01100   -7.09  002  1 160 -1 050 -1
00000180  03301   -0.08  002  1 160  1 050 -1 032  1 033  1
00000182  03302   -6.03  002  1 160  0 050 -2 032  1 033  1
00000190  03303  -13.00  002  1 160  0 050 -6 032  3 033  3
00000192
00000192
00000192  00002   0.03  20.0
00000230  0.1     1.0
00000240             3
                  3301
                  3302
                  3303
                    17          1          1          0
                    33
          4.63E-09
          4.82E-09
          7.95E-09
          1.47E-08
          1.75E-08
          1.39E-08
          2.25E-08
          2.52E-08
          3.12E-08
          2.74E-08
          5.88E-08
          9.61E-08
          8.95E-08
          8.12E-08
          6.60E-08
          3.92E-08
          1.77E-08
                    50
          -3.88
          -4.03
          -4.30
          -4.60
00000760  -4.75
00000770  -4.59
00000780  -4.96
          -5.08
          -5.27
          -5.28
          -6.01
          -6.32
          -6.70
          -7.01
          -7.27
          -7.53
          -7.80
                     1          1
                    33       0.10   1.9E-11
                    50       0.05   0.0E-00
```


```
CNWRA/Q2
2.11e-7M
dlm
20 g/L
00000060
00000070
00000085
00000090
00000097
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000124
00000168
00000126
00000128
00000130
00000136
00000140
00000146
00000148
00000150
00000156
00000159
00000161
00000162
00000163
00000164
00000165
00000160
00000170
siouo2+
siouo2oh
siou3oh5
00000180
00000182
00000184
00000185
00000190
00000192
00000192
00000192
00000230
00000240

00000760
00000770
00000780
```


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DRJ

Example MINTEQA2, v 3.11/3.11 Input files

Container Only

```
Container sorption. U(t)=49.24 ppb; pCO2=1E-3.5; X- exchange; fitted sites
X2UO2 & X(UO2)3(OH)5; 2/13/96 CNWRA Radionuclide Database; wgted logK
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 2 3
ACTIVITY   330 33
  0.25
contain7.123   38930   38931
0   0   0
    330  0.000E-01   -2.00 y                          /H+1
    893  2.113E-07   -6.67 y                          /UO2+2
    492  1.000E-01   -1.00 y                          /NO3-1
    500  1.000E-01   -1.00 y                          /Na+1
    140  0.000E-01  -16.00 y                          /CO3-2
      3  2.300E-08   -7.56 y                          /X-

  2   1
8933301   -13.0000   18.0940                          /UO2(OH)2
  3   2
3301403    21.6600   -0.5300                          /CO2 (g)
    330     2.0000    0.0000                          /H+1

  2   2
  38930 XUO2OH           0.0000    2.8500   0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000    3   1.000 893   1.000    2  -1.000 330   0.000   0   0.000   0
  0.000    0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
  38931 X(UO2)3(OH)5     0.0000   -5.2500   0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000    3   3.000 893   5.000    2  -5.000 330   0.000   0   0.000   0
  0.000    0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

Qz-Only

```
U(VI)-Quartz sorption. U(t)=49.24 ppb; pCO2=1E-3.5; 20 g/L; 2.31 sites/nm2
XOUO2+, XOUO2OH & XO(UO2)3(OH)5; 2/13/96 CNWRA Radionuclide Database; wgted logK
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 3 3
ACTIVITY   330 33
  0.25
quartz9.123  8118930 8118931 8118932
4   1   7
2.000E+01     0.03 0.000 0.000 81
    330  0.000E-01   -2.00 y                          /H+1
    893  2.113E-07   -6.68 y                          /UO2+2
    492  1.000E-01   -1.00 y                          /NO3-1
    500  1.000E-01   -1.00 y                          /Na+1
    140  0.000E-01  -16.00 y                          /CO3-2
    813  0.000E-01    0.00 y                          /ADS1PSIo
    811  2.301E-06   -5.64 y                          /ADS1TYP1

  2   1
8933301   -13.0000   18.0940                          /uo2(oh)2
  3   2
3301403    21.6600   -0.5300                          /co2 (g)
    330     2.0000    0.0000                          /H+1
  6   1
    813     0.0000    0.0000                          /ADS1PSIo

  2   4
8113300 >sio-            0.0000   -7.2000   0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 3    1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000    0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118930 >siouo2+         0.0000    0.3000   0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000 811   1.000 893  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000    0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118931 >siouo2oh        0.0000   -5.6500   0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000 811   1.000 893   1.000    2  -2.000 330   0.000   0   0.000   0
  0.000    0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118932 >siou3(oh)5      0.0000  -16.7500   0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000 811   3.000 893   5.000    2  -6.000 330   0.000   0   0.000   0
  0.000    0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

7/16/96 DR

Example MINTEQA2 (v. 3.10/3.11) input files

```
U(VI)-Qz-Cont sorption. U(t)=49.24 ppb; pCO2=1E-3.5; 20 g/L; 2.31 sites/nm2
XOUO2+, XOUO2OH & XO(UO2)3(OH)5; 2/13/96 CNWRA Radionuclide Database; wgted logK
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 5 3
ACTIVITY   330 33
  0.25
qzcont8.123  8118930 8118931 8118932   38930   38931
4   1   7
2.000E+01     0.03 0.000 0.000 81
     330  0.000E-01   -2.00 y                    /H+1
     893  2.113E-07   -6.68 y                    /UO2+2
     492  1.000E-01   -1.00 y                    /NO3-1
     500  1.000E-01   -1.00 y                    /Na+1
     140  0.000E-01  -16.00 y                    /CO3-2
       3  2.300E-08   -7.64 y                    /X-
     813  0.000E-01    0.00 y                    /ADS1PSIo
     811  2.301E-06   -5.64 y                    /ADS1TYP1

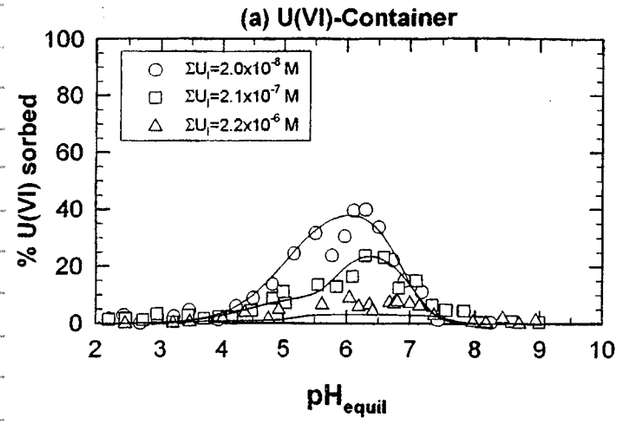
   2   1
8933301    -13.0000     18.0940                  /uo2(oh)2
   3   2
3301403     21.6600     -0.5300                  /co2 (g)
     330     2.0000      0.0000                  /H+1
   6   1
     813     0.0000      0.0000                  /ADS1PSIo

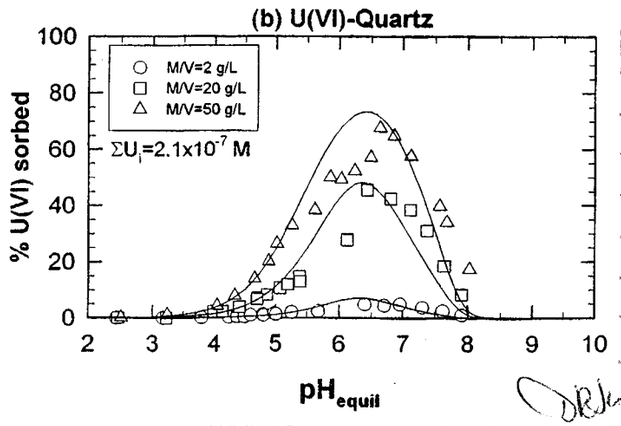
   2   6
8113300 >sio-              0.0000    -7.2000    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 3    1.000 811   -1.000 330   -1.000 813    0.000    0    0.000    0    0.000    0
   0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118930 >siouo2+           0.0000     0.3000    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000 811    1.000 893   -1.000 330    1.000 813    0.000    0    0.000    0
   0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118931 >siouo2oh          0.0000    -5.6500    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000 811    1.000 893    1.000    2   -2.000 330    0.000    0    0.000    0
   0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118932 >siou3(oh)5        0.0000   -16.7500    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000 811    3.000 893    5.000    2   -6.000 330    0.000    0    0.000    0
   0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38930 xuo2oh            0.0000     2.8500    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000    3    1.000 893    1.000    2   -1.000 330    0.000    0    0.000    0
   0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38931 x(uo2)3(oh)5      0.0000    -5.2500    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000    3    3.000 893    5.000    2   -5.000 330    0.000    0    0.000    0
   0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
```

Qz + Container

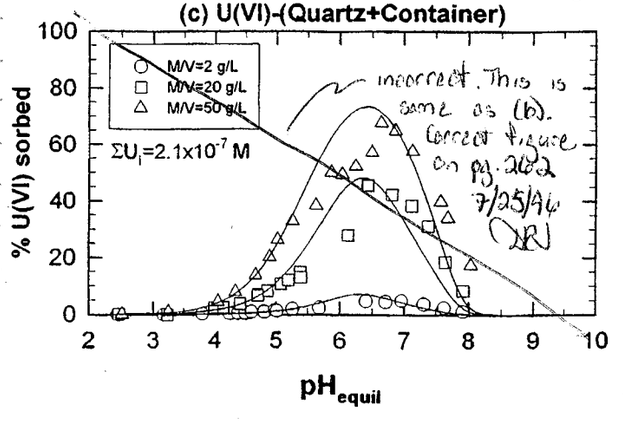
DRLamm

7/16/96 DR





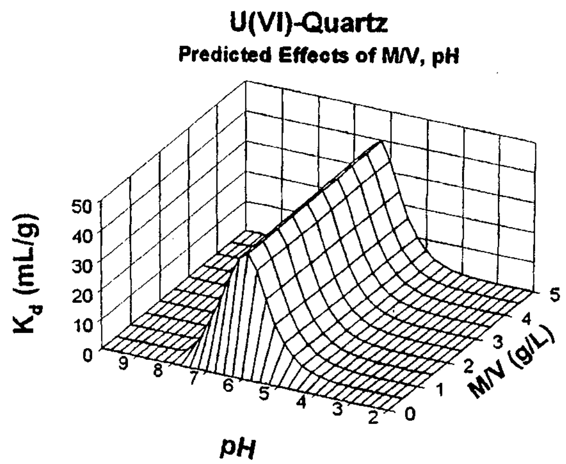
DRLamm



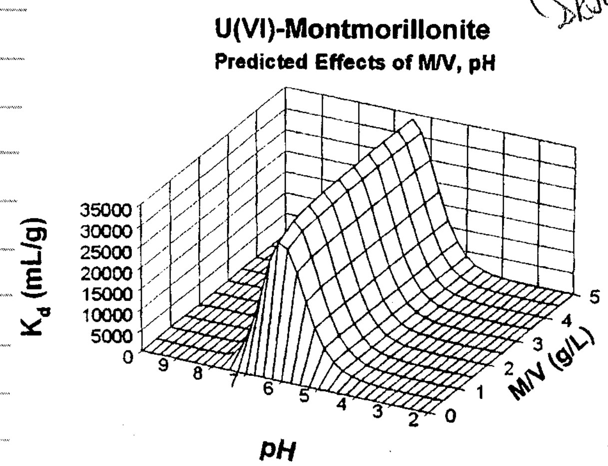
incorrect. This is same as (b). Correct figure on pg. 262 7/25/96 DR

DLM Model Results

DRJ 7/16/96 DRJ



– U(VI) = 50 ppb = 2.15e-7
– $p(CO_2) = 10^{-3.5}$ atm
– Qz + Container, Model parameters given above



U(VI) = 50 ppb = 2.15×10^{-7} M
$p(CO_2) = 10^{-3.5}$
No Container Sorption

DLM Model Predictions on U(VI)-Quartz
U(VI)-Montmorillonite

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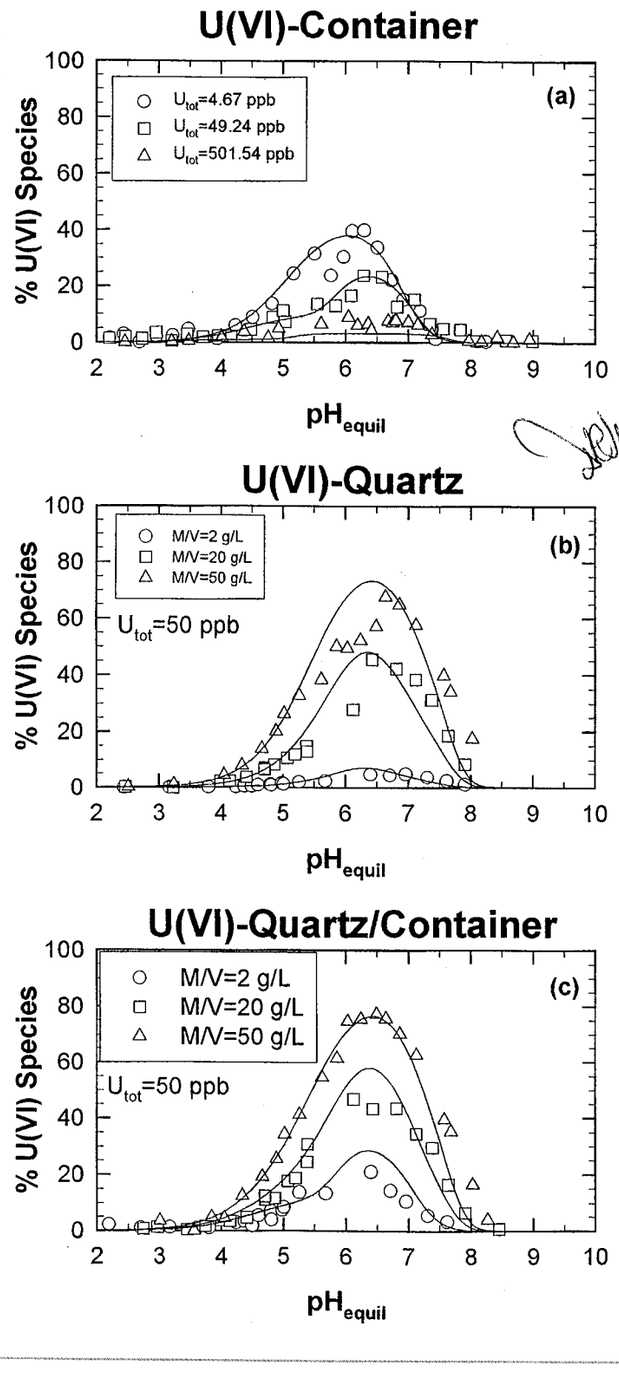
Wanner, H., and Forest, I., eds. 1992. "Chemical Thermodynamics of Uranium." Elsevier, New York, New York.

Westall, J. C. 1982. FITEQL: A Computer Program for Determination of Chemical Equilibrium Constants From Experimental Data, Version 2.0. Rpt. 82-02. Department of Chemistry, Oregon State University, Corvallis, Oregon.

Wolery, T. J. 1992. EQ3NR, A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: Theoretical Manual, User's Guide, and Related Documentation (Version 7.0). UCRL-MA-110662- Pt.3. Lawrence Livermore National Laboratory, Livermore, California.

7/25/96 DR

Corrected figure for Quartz-U(VI) sorption. Using data plotted in (c) on pg. 254



9/5/96 DRJ

Updating the CNWRA MINTEQA2 Radionuclide Database (9/5/96)

The Neptunium and Plutonium data has been updated to include new data from the EQ3/6 database (Data0.alt.r2, release 02aug95). Although the data have all been taken from EQ3/6, the original source of the data as documented in the EQ3/6 database is:

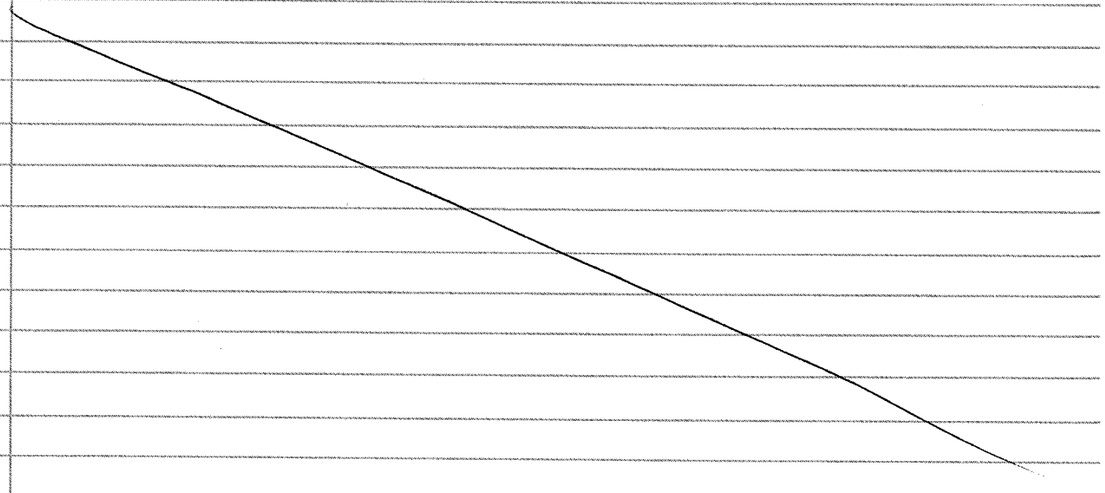
Palmer, C.E.A., R.J. Silva, and C.W. Miller. 1992. Speciation Calculations of Pu, Np, Am, and U in J-13 Water. Effects of Anion Concentration and pH (LLNL Unpub. ms.). 92PAL/SIL

Spreadsheets in Excel for Windows, Version 4.0 were prepared to take free energies of formation for both Np-, Pu and auxiliary species from Palmer et al. (1992) and calculate equilibrium constants (Log K) for Np- and Pu-aqueous specis and solids. As expected, agreement between the calculated equilibrium constants and those reported in the EQ3/6 database (Data0.alt.r2) was typically accurate to the third decimal place. In entering the data into the MINTEQA2 database, accuracy in Log K was carried to the second decimal place. The spreadsheet was also used to calculate enthalpies of reaction and molecular weights (see attachment below). The source for the enthalpies of formation is taken from: DRJ

Phillips, S. L., F. V. Hale, L. F. Silvester, and M. D. Siegel. 1988. Thermodynamic Tables for Nuclear Waste Isolation. NUREG/CR-4864. Washington, D. C.: NRC. 88PHI

The databases updated include THERMO.DBS, TYPE6.DBS, and REDOX.DBS. With the exception of the neptunium and plutonium data, all other radionuclide data remain as before (2/10/96 version). ~~In addition, all species, and solids titles were converted to lower case to make the databases easier to read.~~ With the exception of the species mentioned here, these modifications should have no affect on earlier runs using MINTEQA2, version 3.11. After updating the database, the UNFRMT.EXE program was run to create the binary files THERMO.UNF and TYPE6.UNF. The corrected files and the new binary files were copied onto the disk enclosed in the envelope at the back of this scientific notebook.

9/5/96 DRJ Done earlier



(1)

```
+--------------------------------------------------------
NpHPO4++
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  23-nov-1988
*    mol.wt. = 333.027 g/mol
*    DHazero =   4.5
     charge  =   2.0
****
     4 element(s):
      1.0000 H              1.0000 Np            4.0000 O
      1.0000 P
****
     3 species in aqueous dissociation reaction:
    -1.0000  NpHPO4++                     1.0000  HPO4--
     1.0000  Np++++
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000  -16.0000  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpHPO4++                    -1.0000  HPO4--
*   -1.0000  Np++++
*    ref-state data:
*         logK   =      16.000          [source: 92pal/sil ]
*         delG0f =    -402.334 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      1.094 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpNO3++
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  06-dec-1993
*    mol.wt. = 299.053 g/mol
*    DHazero =   4.5
     charge  =   2.0
****
     3 element(s):
      1.0000 N              1.0000 Np            3.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  NpNO3++                      1.0000  NO3-
     1.0000  Np+++
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000  -1.4100  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpNO3++                     -1.0000  NO3-
*   -1.0000  Np+++
*    ref-state data:
*         logK   =      1.410           [source: 92pal/sil ]
*         delG0f =    -152.020 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      1.094 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpNO3+++
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  06-dec-1993
*    mol.wt. = 299.053 g/mol
*    DHazero =   5.0
     charge  =   3.0
****
     3 element(s):
      1.0000 N              1.0000 Np            3.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  NpNO3+++                     1.0000  NO3-
     1.0000  Np++++
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000  -1.5000  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpNO3+++                    -1.0000  NO3-
*   -1.0000  Np++++
*    ref-state data:
*         logK   =      1.500           [source: 92pal/sil ]
*         delG0f =    -148.749 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      1.094 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpO2(CO3)2--
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  14-dec-1993
*    mol.wt. = 389.065 g/mol
*    DHazero =   4.0
     charge  =  -2.0
****
     3 element(s):
      2.0000 C              1.0000 Np            8.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  NpO2(CO3)2--                -2.0000  H+
     1.0000  NpO2++                       2.0000  HCO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000   3.6976  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(CO3)2--                -2.0000  CO3--
*   -1.0000  NpO2++
*    ref-state data:
*         logK   =      16.960          [source: 92pal/sil ]
*         delG0f =    -465.720 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.851 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpO2(CO3)2---
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  13-dec-1993
*    mol.wt. = 389.065 g/mol
*    DHazero =   4.0
     charge  =  -3.0
****
     3 element(s):
      2.0000 C              1.0000 Np            8.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  NpO2(CO3)2---               -2.0000  H+
     1.0000  NpO2+                        2.0000  HCO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000  14.0376  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(CO3)2---               -2.0000  CO3--
*   -1.0000  NpO2+
*    ref-state data:
*         logK   =      6.620           [source: 92pal/sil ]
*         delG0f =    -480.104 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      1.043 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpO2(CO3)3(5-)
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  13-dec-1993
*    mol.wt. = 449.074 g/mol
*    DHazero =   4.0
     charge  =  -5.0
****
     3 element(s):
      3.0000 C              1.0000 Np           11.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  NpO2(CO3)3(5-)              -3.0000  H+
     1.0000  NpO2+                        3.0000  HCO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000  22.4364  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(CO3)3(5-)              -3.0000  CO3--
```

EQ3/6 data · original data · different components · DLWmm

```
*   -1.0000  NpO2+
*    ref-state data:
*         logK   =      8.550           [source: 92pal/sil ]
*         delG0f =    -608.928 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      1.043 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpO2(CO3)3----
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  13-dec-1993
*    mol.wt. = 449.074 g/mol
*    DHazero =   4.0
     charge  =  -4.0
****
     3 element(s):
      3.0000 C              1.0000 Np           11.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  NpO2(CO3)3----              -3.0000  H+
     1.0000  NpO2++                       3.0000  HCO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000   9.4064  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(CO3)3----              -3.0000  CO3--
*   -1.0000  NpO2++
*    ref-state data:
*         logK   =      21.580          [source: 92pal/sil ]
*         delG0f =    -598.214 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.851 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpO2(H2PO4)2(aq)
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  07-dec-1993
*    mol.wt. = 463.021 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     4 element(s):
      4.0000 H              1.0000 Np           10.0000 O
      2.0000 P
****
     4 species in aqueous dissociation reaction:
    -1.0000  NpO2(H2PO4)2(aq)             1.0000  NpO2++
     2.0000  H+                           2.0000  HPO4--
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000  -21.9609  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(H2PO4)2(aq)            -2.0000  H2PO4-
*   -1.0000  NpO2++
*    ref-state data:
*         logK   =      7.550           [source: 92pal/sil ]
*         delG0f =    -740.781 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.851 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpO2(NO3)2(aq)
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  06-dec-1993
*    mol.wt. = 393.057 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     3 element(s):
      2.0000 N              1.0000 Np            8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  NpO2(NO3)2(aq)               1.0000  NpO2++
     2.0000  NO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000  -0.0100  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(NO3)2(aq)              -2.0000  NO3-
*   -1.0000  NpO2++
*    ref-state data:
*         logK   =      0.010           [source: 92pal/sil ]
*         delG0f =    -243.228 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.851 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpO2(NO3)2-
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  06-dec-1993
*    mol.wt. = 393.057 g/mol
*    DHazero =   4.0
     charge  =  -1.0
****
     3 element(s):
      2.0000 N              1.0000 Np            8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  NpO2(NO3)2-                  1.0000  NpO2+
     2.0000  NO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000   2.1200  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(NO3)2-                 -2.0000  NO3-
*   -1.0000  NpO2+
*    ref-state data:
*         logK   =     -2.120           [source: 92pal/sil ]
*         delG0f =    -268.812 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.851 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpO2(OH)2(aq)
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  08-dec-1993
*    mol.wt. = 303.061 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     3 element(s):
      2.0000 H              1.0000 Np            4.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  NpO2(OH)2(aq)               -2.0000  H+
     1.0000  NpO2++                       2.0000  H2O
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
      500.0000  12.0202  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(OH)2(aq)               -2.0000  OH-
*   -1.0000  NpO2++
*    ref-state data:
*         logK   =      15.970          [source: 92pal/sil ]
*         delG0f =    -287.178 kcal/mol  [calculated]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.851 cal/(mol*K) [source: 72kes    ]
+--------------------------------------------------------
NpO2(OH)3-
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  08-dec-1993
*    mol.wt. = 320.069 g/mol
*    DHazero =   4.0
     charge  =  -1.0
****
     3 element(s):
      3.0000 H              1.0000 Np            5.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  NpO2(OH)3-                  -3.0000  H+
     1.0000  NpO2++                       3.0000  H2O
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
```

(2) · DLWmm

EQ3/6 (Data0.alt.r2) Highlighted numbers are LogK values

Note: EQ3/6 writes reactions as dissassociation as opposed to formation reactions in MINTEQA so LogK signs will be opposite. Also, EQ3/6 uses different components in some cases (e.g. HCO_3^- instead of CO_3^{2-}, HPO_4^{2-} instead of PO_4^{3-}) and Log Ks are different.

9/5/96 DLW

```
@Psat-H2O]:
       500.0000   20.2652  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(OH)3-                    -3.0000  OH-
*   -1.0000  NpO2++
*    ref-state data:
*         logK   =      21.720              [source: 92pal/sil ]
*         delG0f =   -332.617 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     0.851 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
NpO2(OH)4--
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  08-dec-1993
*    mol.wt. = 337.076 g/mol
*    DHazero =   4.0
     charge  =  -2.0
****
     3 element(s):
      4.0000 H                1.0000 Np               6.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  NpO2(OH)4--                    -4.0000  H+
     1.0000  NpO2++                          4.0000  H2O
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000   33.0503  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  NpO2(OH)4--                   -4.0000  OH-
*   -1.0000  NpO2++
*    ref-state data:
*         logK   =      22.930              [source: 92pal/sil ]
*         delG0f =   -371.863 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     0.851 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuNO3+++
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  09-dec-1993
*    mol.wt. = 306.005 g/mol
*    DHazero =   5.0
     charge  =   3.0
****
     3 element(s):
      1.0000 N                3.0000 O                1.0000 Pu
****
     3 species in aqueous dissociation reaction:
    -1.0000  PuNO3+++                       1.0000  NO3-
     1.0000  Pu++++
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000   -1.8700  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuNO3+++                      -1.0000  NO3-
*   -1.0000  Pu++++
*    ref-state data:
*         logK   =       1.870              [source: 92pal/sil ]
*         delG0f =   -144.163 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(CO3)2--
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  15-dec-1993
*    mol.wt. = 396.017 g/mol
*    DHazero =   4.0
     charge  =  -2.0
****
     3 element(s):
      2.0000 C                8.0000 O                1.0000 Pu
****
     4 species in aqueous dissociation reaction:
    -1.0000  PuO2(CO3)2--                   -2.0000  H+
      1.0000  PuO2++                         2.0000  HCO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000    6.5576  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuO2(CO3)2--                  -2.0000  CO3--
*   -1.0000  PuO2++
*    ref-state data:
*         logK   =      14.100              [source: 92pal/sil ]
*         delG0f =   -452.521 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(CO3)2---
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  09-dec-1993
*    mol.wt. = 396.017 g/mol
*    DHazero =   4.0
     charge  =  -3.0
****
     3 element(s):
      2.0000 C                8.0000 O                1.0000 Pu
****
     4 species in aqueous dissociation reaction:
    -1.0000  PuO2(CO3)2---                  -2.0000  H+
      1.0000  PuO2+                          2.0000  HCO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000   14.0376  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuO2(CO3)2---                 -2.0000  CO3--
*   -1.0000  PuO2+
*    ref-state data:
*         logK   =       6.620              [source: 92pal/sil ]
*         delG0f =   -464.368 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(CO3)3(5-)
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  09-dec-1993
*    mol.wt. = 456.026 g/mol
*    DHazero =   4.0
     charge  =  -5.0
****
     3 element(s):
      3.0000 C                11.0000 O               1.0000 Pu
****
     4 species in aqueous dissociation reaction:
    -1.0000  PuO2(CO3)3(5-)                 -3.0000  H+
      1.0000  PuO2+                          3.0000  HCO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000   23.6264  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuO2(CO3)3(5-)                -3.0000  CO3--
*   -1.0000  PuO2+
*    ref-state data:
*         logK   =       7.360              [source: 92pal/sil ]
*         delG0f =   -591.769 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(CO3)3----
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  09-dec-1993
*    mol.wt. = 456.026 g/mol
*    DHazero =  -4.0
     charge  =  -4.0
****
     3 element(s):
      3.0000 C                11.0000 O               1.0000 Pu
```



```
****
     4 species in aqueous dissociation reaction:
    -1.0000  PuO2(CO3)3----                 -3.0000  H+
      1.0000  PuO2++                         3.0000  HCO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000   12.6364  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuO2(CO3)3----                -3.0000  CO3--
*   -1.0000  PuO2++
*    ref-state data:
*         logK   =      18.350              [source: 92pal/sil ]
*         delG0f =   -584.510 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(H2PO4)2(aq)
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  09-dec-1993
*    mol.wt. = 469.973 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     4 element(s):
      4.0000 H               10.0000 O                2.0000 P
      1.0000 Pu
****
     4 species in aqueous dissociation reaction:
    -1.0000  PuO2(H2PO4)2(aq)               1.0000  PuO2++
     2.0000  H+                             2.0000  HPO4--
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000  -21.9609  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuO2(H2PO4)2(aq)              -2.0000  H2PO4-
*   -1.0000  PuO2++
*    ref-state data:
*         logK   =       7.550              [source: 92pal/sil ]
*         delG0f =   -731.483 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(NO3)2(aq)
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  09-dec-1993
*    mol.wt. = 400.009 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     3 element(s):
      2.0000 N                8.0000 O                1.0000 Pu
****
     3 species in aqueous dissociation reaction:
    -1.0000  PuO2(NO3)2(aq)                 1.0000  PuO2++
     2.0000  NO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000   -0.0100  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuO2(NO3)2(aq)                -2.0000  NO3-
*   -1.0000  PuO2++
*    ref-state data:
*         logK   =       0.010              [source: 92pal/sil ]
*         delG0f =   -233.931 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(NO3)2-
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  09-dec-1993
*    mol.wt. = 400.009 g/mol
*    DHazero =   4.0
     charge  =  -1.0
****
     3 element(s):
      2.0000 N                8.0000 O                1.0000 Pu
****
     3 species in aqueous dissociation reaction:
    -1.0000  PuO2(NO3)2-                    1.0000  PuO2+
     2.0000  NO3-
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000    2.1200  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuO2(NO3)2-                   -2.0000  NO3-
*   -1.0000  PuO2+
*    ref-state data:
*         logK   =      -2.120              [source: 92pal/sil ]
*         delG0f =   -253.277 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(OH)2(aq)
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  09-dec-1993
*    mol.wt. = 310.013 g/mol
*    DHazero =   3.0
     charge  =   0.0
****
     3 element(s):
      2.0000 H                4.0000 O                1.0000 Pu
****
     4 species in aqueous dissociation reaction:
    -1.0000  PuO2(OH)2(aq)                  -2.0000  H+
     1.0000  PuO2++                         2.0000  H2O
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000   12.4502  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuO2(OH)2(aq)                 -2.0000  OH-
*   -1.0000  PuO2++
*    ref-state data:
*         logK   =      15.540              [source: 92pal/sil ]
*         delG0f =   -277.294 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(OH)3-
     sp.type =  aqueous
*    EQ3/6   =  alt
     revised =  09-dec-1993
*    mol.wt. = 327.021 g/mol
*    DHazero =   4.0
     charge  =  -1.0
****
     3 element(s):
      3.0000 H                5.0000 O                1.0000 Pu
****
     4 species in aqueous dissociation reaction:
    -1.0000  PuO2(OH)3-                     -3.0000  H+
     1.0000  PuO2++                         3.0000  H2O
*
****  logK  grid  [0-25-60-100C  @1.0132bar;  150-200-250-300C
@Psat-H2O]:
       500.0000   20.2652  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 3 [reported logK data used]
*    reference reaction:
*    1.0000  PuO2(OH)3-                    -3.0000  OH-
*   -1.0000  PuO2++
*    ref-state data:
*         logK   =      21.720              [source: 92pal/sil ]
*         delG0f =   -323.320 kcal/mol      [calculated]
*         delH0f =       N/A
*         S0PrTr =       N/A
*         Selec  =     1.043 cal/(mol*K) [source: 72kes    ]
+-------------------------------------------------------------------------------
PuO2(OH)4--
     sp.type =  aqueous
*    EQ3/6   =  alt
```

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DRJ

Excel Spreadsheet (Windows v4.0)

Compare to Np, Pu highlighted Data in EQ3/6 (pg. 264-265)

[signature]

Np Data

Calculating Log K Values from Free Energies

Log K	Del G(r) (kJ/mol)	Del G(r) (kcal/mol)	Del H(r) (kJ/mol)	Del H(r) (kcal/mol)	M.W. (g/mol)	Del G(f) (kJ/mol)	Del H(f) (kJ/mol)	Mineral/Species
Np(III) AQUEOUS:								
7.90	-46.0916	-10.7771	############	############	297.0576	-1090.1747	############	NpCO3+
12.20	-69.6391	-16.6441	############	############	357.0670	-1642.7053	############	Np(CO3)2-1
12.70	-72.4925	-17.3261	############	############	417.0764	-2173.5420	############	Np(CO3)3-3
21.92	-125.1022	-29.9001	-49.6248	-11.8606	334.0355	-1661.0062	-1854.2000	NpH2PO4++
42.78	-244.2123	-58.3681	-113.3496	-27.0912	431.0228	-2798.9203	-3196.3000	Np(H2PO4)2+
64.22	-366.5775	-87.6141	-190.2744	-45.4767	528.0100	-3940.0895	-4549.6000	Np(H2PO4)3(aq)
83.66	-477.5247	-114.1311	############	############	624.9973	-5069.8407	############	Np(H2PO4)4-1
1.41	-8.0455	-1.9232	############	############	299.0531	-636.0517	############	NpNO3++
1.92	-10.9586	-2.6192	############	############	361.0580	-749.8690	############	Np(NO3)2+
2.52	-14.3854	-3.4382	############	############	423.0629	-864.2010	############	Np(NO3)3(aq)
-6.80	38.8437	9.2839	60.1383	11.9833	254.0555	-716.4389	-762.9000	NpOH++
-16.01	91.3864	21.8419	############	############	271.0629	-900.0788	############	Np(OH)2+
-23.91	136.4554	32.6139	############	############	288.0702	-1092.1914	############	Np(OH)3(aq)
3.93	-22.4310	-5.3611	############	############	333.1098	-1283.9901	############	NpSO4+
5.45	-31.1086	-7.4351	############	############	429.1714	-2037.1268	############	Np(SO4)2-
1.07	-6.0940	-1.4565	############	############	272.5012	-654.4838	############	NpCl++
0.82	-4.6825	-1.1191	############	############	307.9542	-784.3619	############	NpCl2+
3.73	-21.2888	-5.0881	############	############	256.0462	-820.1393	############	NpF++
7.83	-44.6940	-10.6821	############	############	275.0442	-1125.2952	############	NpF2+
11.08	-63.2459	-15.1161	############	############	294.0422	-1425.5976	############	NpF3(aq)
Np(IV) AQUEOUS:								
12.30	-70.2076	-16.7800	############	############	297.0576	-1101.0907	############	NpCO3++
23.36	-133.2814	-31.8550	############	############	357.0670	-1692.1477	############	Np(CO3)2(aq)
30.00	-171.2386	-40.9270	############	############	417.0764	-2258.0881	############	Np(CO3)3-2
33.00	-188.3637	-45.0200	############	############	477.0858	-2803.1963	############	Np(CO3)4-4
34.00	-194.0707	-46.3840	19.9642	4.7716	537.0952	-3335.8854	-3912.3100	Np(CO3)5-6
24.45	-139.5448	-33.3520	############	############	334.0355	-1661.2488	############	NpH2PO4+++
47.35	-270.2990	-64.6030	############	############	431.0228	-2810.8070	############	Np(H2PO4)2++
91.96	-524.9038	-125.4550	############	############	624.9973	-5103.0198	############	Np(H2PO4)4(aq)
28.32	-161.6615	-38.6380	-7.4248	-1.7746	333.0275	-1583.3666	-1840.9000	NpHPO4++
52.77	-301.2313	-71.9960	-65.0496	-15.5472	429.0069	-2841.7393	-3176.9000	Np(HPO4)2(aq)
74.86	-427.3329	-102.1360	-89.9744	-21.5044	524.9862	-3966.6449	-4478.2000	Np(HPO4)3(-2)
94.93	-541.9034	-129.5180	-126.7992	-30.3057	620.9656	-5120.0194	-5792.4000	Np(HPO4)4(-4)
110.21	-629.0728	-150.3520	-157.5240	-37.6491	716.9449	-6225.9928	-7100.6000	Np(HPO4)5(-6)
1.50	-8.5606	-2.0460	############	############	299.0531	-622.3658	############	NpNO3+++
2.31	-13.1840	-3.1511	############	############	361.0580	-737.8944	############	Np(NO3)2++
3.51	-20.0333	-4.7881	############	############	423.0629	-855.6489	############	Np(NO3)3+
2.75	-15.6968	-3.7521	############	############	485.0678	-962.2198	############	Np(NO3)4(aq)
-1.05	5.9663	1.4260	51.3963	12.2845	254.0555	-734.1163	-790.6400	NpOH+++
0.21	-1.1967	-0.2860	77.3767	18.4936	271.0629	-978.4619	-1060.4000	Np(OH)2++
-3.14	17.8991	4.2780	99.9100	23.8791	288.0702	-1198.6487	-1313.7050	Np(OH)3+
-4.53	25.8554	6.1620	-0.4467	-0.1068	305.0776	-1425.7649	-1699.9000	Np(OH)4(aq)
-16.18	92.3368	22.0690	121.9416	29.1446	322.0849	-1596.4763	-1863.3500	Np(OH)5-1
6.58	-37.5598	-8.9770	20.9116	4.9980	333.1098	-1284.9190	-1444.7900	NpSO4++
9.79	-55.8816	-13.3560	40.7032	9.7283	429.1714	-2047.6998	-2334.6000	Np(SO4)2(aq)
8.30	-47.3755	-11.3230	############	############	525.2330	-2783.6529	############	Np(SO4)3-2
1.15	-6.5648	-1.5690	19.7047	4.7095	272.5012	-640.7545	-703.4750	NpCl+++
1.68	-9.5898	-2.2920	94.4643	22.5775	307.9542	-776.0693	-795.7950	NpCl2++
2.41	-13.7571	-3.2880	############	############	343.4072	-910.5263	############	NpCl3+
8.68	-49.5470	-11.8420	-3.3524	-0.8012	256.0462	-834.1976	-894.6000	NpF+++
15.70	-89.6172	-21.4190	############	############	275.0442	-1156.0183	############	NpF2++
21.35	-121.9218	-29.1400	############	############	294.0422	-1470.0735	############	NpF3+
25.25	-144.1263	-34.4470	############	############	313.0402	-1774.0286	############	NpF4(aq)
26.83	-153.1470	-36.6030	############	############	332.0382	-2064.7998	############	NpF5-1
28.86	-164.7325	-39.3720	############	############	351.0362	-2358.1359	############	NpF6-2
Np(V) AQUEOUS:								
-9.11	52.0291	12.4352	43.9383	10.5015	286.0543	-1100.1535	-1220.1000	NpO2OH(aq)
5.07	-28.9397	-6.9168	53.5348	12.7951	329.0564	-1471.9228	-1699.9000	NpO2CO3-1
6.62	-37.7888	-9.0318	29.8597	7.1390	389.0658	-2008.7551	-2298.8000	NpO2(CO3)2-3
8.55	-48.8063	-11.6648	26.2045	6.2630	449.0752	-2547.7546	-2977.7000	NpO2(CO3)3-5
-1.42	8.1054	1.9372	############	############	331.0519	-1017.7998	############	NpO2NO3(aq)
-2.12	12.1010	2.8922	############	############	393.0568	-1124.7094	############	NpO2(NO3)2-1
-1.51	8.6201	2.0602	15.3877	3.6777	304.5000	-1037.5697	-1129.8920	NpO2Cl(aq)
-3.00	17.1220	4.0922	############	############	339.9530	-1160.4575	############	NpO2Cl2-1
0.82	-4.6809	-1.1188	28.8476	6.8947	288.0450	-1201.4314	-1284.7000	NpO2F(aq)
6.76	-38.7010	-9.2498	############	############	364.0184	-1972.6050	############	NpO2PO4-2
15.66	-89.3985	-21.3668	34.3752	8.2159	365.0263	-2023.2026	-2221.2000	NpO2HPO4-1
20.57	-117.3978	-28.0588	-37.1248	-8.8730	366.0343	-2051.2018	-2292.7000	NpO2H2PO4(aq)
1.53	-8.7352	-2.0878	31.4016	7.5052	365.1086	-1568.1943	-1856.4000	NpO2SO4-1
Np(VI) AQUEOUS:								
-5.09	29.0820	6.9508	43.4483	10.3844	286.0543	-1003.9006	-1102.9900	NpO2OH+
-12.02	68.6124	16.3988	############	############	303.0617	-1201.5528	############	NpO2(OH)2(aq)
-20.27	115.6762	27.6478	############	############	320.0690	-1391.6695	############	NpO2(OH)3-1
-33.06	188.6556	45.0898	############	############	337.0764	-1555.8748	############	NpO2(OH)4-2
-2.82	16.0588	3.8405	############	############	556.1013	-1812.7138	############	(NpO2)2OH+++
-5.67	32.3596	7.7365	46.5567	11.1536	572.1087	-2033.5955	-2248.2100	(NpO2)2(OH)2++
-11.96	68.2172	16.3043	############	############	876.1704	-3267.9132	############	(NpO2)3(OH)4++
-15.63	89.1957	21.3183	113.4416	27.1132	892.1777	-3484.1172	-3897.5600	(NpO2)3(OH)5+
-31.09	177.4447	42.4103	############	############	926.1924	-3870.2336	############	(NpO2)3(OH)7-
-21.99	125.5035	29.9961	############	############	1195.2394	-4717.9746	############	(NpO2)4(OH)7+
9.68	-55.2549	-13.2062	-4.1662	-0.9956	329.0564	-1379.0380	-1640.0000	NpO2CO3(aq)
16.96	-96.8062	-23.1372	-10.6303	-2.5407	389.0658	-1946.5726	-2221.7000	NpO2(CO3)2-2
21.58	-123.1779	-29.4402	-41.5955	-9.9416	449.0752	-2502.9274	-2927.9000	NpO2(CO3)3-4
53.76	-306.8031	-73.3277	############	############	1167.1974	-5862.1020	############	(NpO2)3(CO3)6(6-)
20.86	-119.0776	-28.4602	-21.0248	-5.0250	365.0263	-1933.6816	-2169.0000	NpO2HPO4(aq)
21.96	-125.3327	-29.9552	-46.9248	-11.2153	366.0343	-1939.9357	-2184.9000	NpO2H2PO4+1
46.60	-266.0197	-63.5802	############	############	463.0216	-3099.4277	############	NpO2(H2PO4)2(aq)
-0.30	1.7144	0.4097	############	############	331.0519	-904.9906	############	NpO2NO3+
0.01	-0.0556	-0.0133	############	############	393.0568	-1017.6660	############	NpO2(NO3)2(aq)
2.00	-11.4149	-2.7282	16.7016	3.9918	365.1086	-1561.6741	-1753.6000	NpO2SO4(aq)
4.64	-26.4867	-6.3302	26.0032	6.2149	461.1702	-2311.2039	-2653.6000	NpO2(SO4)2-2
0.20	-1.1432	-0.2732	12.1397	2.9015	304.5000	-928.2330	-1015.5400	NpO2Cl+
0.10	-0.5700	-0.1362	19.4593	4.6509	339.9530	-1058.9495	-1175.3000	NpO2Cl2(aq)
5.10	-29.1091	-6.9572	1.5476	0.3699	288.0450	-1106.6596	-1194.4000	NpO2F+
7.56	-43.1506	-10.3132	3.5602	0.8509	307.0430	-1402.4517	-1527.7350	NpO2F2(aq)
9.67	-55.1963	-13.1922	############	############	326.0410	-1696.2480	############	NpO2F3-1
11.54	-65.8697	-15.7432	############	############	345.0390	-1988.6719	############	NpO2F4-2
Np(IV) SOLIDS:								
-88.10	502.9000	120.1960	556.1000	132.9111	237.0482	0.0000	0.0000	Np(metal)
55.62	-317.4920	-75.8824	############	############	429.0069	-2858.0000	############	Np(HPO4)2
-0.81	4.6304	1.1067	78.0683	18.6536	305.0776	-1447.0000	-1621.3650	Np(OH)4
7.80	-44.5346	-10.6441	53.7767	12.8529	269.0470	-1021.8000	-1074.0000	NpO2
Np(V) SOLIDS:								
-9.60	54.2278	12.9607	94.8773	22.6762	554.0934	-2012.9550	-2147.3610	Np2O5
-4.24	24.1826	5.7796	39.9383	9.5455	286.0543	-1128.0000	-1224.1000	NpO2OH(am)
11.56	-65.9970	-15.7737	############	############	415.0997	-2601.0000	############	NaNpCO3:3.5H2O
Np(VI) SOLIDS:								
-5.99	34.1652	8.1657	############	############	303.0617	-1236.0000	############	NpO2(OH)2
REDOX REACTIONS:								
2.49	-14.2000	-3.3939	28.9000	6.9073	0.0000			Np+++/Np++++
-10.91	62.2662	14.8817	149.5767	35.7497	0.0000			NpO2+/Np++++
-31.79	181.4662	43.3712	267.1767	63.8558	0.0000			NpO2++/Np++++

Reaction Stoichiometries

Mineral/Species	e-	H+	Cl-	F-	CO3--	SO4--	PO4-3	NO3-	Br-	I-	H2O(l)	Np+++	Np++++	NpO2+	NpO2++	Na+	Charge	dbha(zero)	dbhb	COMMENTS	
Del G(f)(kJ/mol)	0	0.0000	-131.2170	-281.5230	-527.9831	-744.0040	-1025.4910	-110.7940	-103.8500	-51.7240	-237.1400	-517.1000	-502.9000	-915.0000	-795.8000	-261.9530				NEA Basis/Auxiliary species data	
Del H(f)(kJ/mol)	0	0.0000	-167.0800	-335.3500	-675.2300	-909.3400	-1284.4000	-206.8500	-121.4100	-56.7800	-285.8300	-527.2000	-556.1000	-978.2000	-860.6000	-240.3400				NEA Basis/Auxiliary species data	
M.W.	0	1.0079	35.4530	18.9980	60.0094	96.0616	94.9714	62.0049	79.9040	126.9044	18.0153	237.0482	237.0482	269.0470	269.0470	22.9898				Data from EQ3/6 database (Dat0.alt.r2 release, 02aug95)	
Del G(f)(kJ/mol)	0	0.0000	-131.2897	-281.7606	-527.9831	-744.4691	-1018.8040	-110.9052	-104.0561	-51.9234	-237.1826	-517.1000	-502.9000	-915.0000	-795.8000	-261.8807				Original data source is from draft NEA data Palmer et al. (1992)	
Del H(f)(kJ/mol)	0	0.0000	-167.0797	-335.3476	-675.2348	-909.6016	-1277.3752	-206.8109	-121.5034	-56.9024	-285.8363	-527.2000	-556.1000	-978.2000	-860.6000	-240.2997				del Hf for Np+++,Np++++,NpO2+,NpO2++ from PHI88	
NpCO3+					1							1					1.0000	4.0	0.0	del Gf: Pal92'	
Np(CO3)2-1					2							1					-1.0000	4.0	0.0	del Gf: Pal92'	
Np(CO3)3-3					3							1					-3.0000	4.0	0.0	del Gf: Pal92'	
NpH2PO4++		2					1					1					2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(H2PO4)2+		4					2					1					1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(H2PO4)3(aq)		6					3					1					0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(H2PO4)4-1		8					4					1					-1.0000	4.0	0.0	del Gf: Pal92'	
NpNO3++								1				1					2.0000	4.5	0.0	del Gf: Pal92'	
Np(NO3)2+								2				1					1.0000	4.0	0.0	del Gf: Pal92'	
Np(NO3)3(aq)								3				1					0.0000	3.0	0.0	del Gf: Pal92'	
NpOH++		-1									1	1					2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(OH)2+		-2									2	1					1.0000	4.0	0.0	del Gf: Pal92'	
Np(OH)3(aq)		-3									3	1					0.0000	3.0	0.0	del Gf: Pal92'	
NpSO4+						1						1					1.0000	4.0	0.0	del Gf: Pal92'	
Np(SO4)2-						2						1					-1.0000	4.0	0.0	del Gf: Pal92'	
NpCl++			1									1					2.0000	4.5	0.0	del Gf: Pal92'	
NpCl2+			2									1					1.0000	4.0	0.0	del Gf: Pal92'	
NpF++				1								1					2.0000	4.5	0.0	del Gf: Pal92'	
NpF2+				2								1					1.0000	4.0	0.0	del Gf: Pal92'	
NpF3(aq)				3								1					0.0000	3.0	0.0	del Gf: Pal92'	
NpCO3++					1								1				2.0000	4.5	0.0	del Gf: Pal92'	
Np(CO3)2(aq)					2								1				0.0000	3.0	0.0	del Gf: Pal92'	
Np(CO3)3-2					3								1				-2.0000	4.0	0.0	del Gf: Pal92'	
Np(CO3)4-4					4								1				-4.0000	4.0	0.0	del Gf: Pal92'	
Np(CO3)5-6					5								1				-6.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpH2PO4+++		2					1						1				3.0000	6.0	0.0	del Gf: Pal92'	
Np(H2PO4)2++		4					2						1				2.0000	4.5	0.0	del Gf: Pal92'	
Np(H2PO4)4(aq)		8					4						1				0.0000	3.0	0.0	del Gf: Pal92'	
NpHPO4++		1					1						1				2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(HPO4)2(aq)		2					2						1				0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(HPO4)3(-2)		3					3						1				-2.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(HPO4)4(-4)		4					4						1				-4.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(HPO4)5(-6)		5					5						1				-6.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpNO3+++								1					1				3.0000	6.0	0.0	del Gf: Pal92'	
Np(NO3)2++								2					1				2.0000	4.5	0.0	del Gf: Pal92'	
Np(NO3)3+								3					1				1.0000	4.0	0.0	del Gf: Pal92'	
Np(NO3)4(aq)								4					1				0.0000	3.0	0.0	del Gf: Pal92'	
NpOH+++		-1									1		1				3.0000	6.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(OH)2++		-2									2		1				2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(OH)3+		-3									3		1				1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(OH)4(aq)		-4									4		1				0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(OH)5-1		-5									5		1				-1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpSO4++						1							1				2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(SO4)2(aq)						2							1				0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Np(SO4)3-2						3							1				-2.0000	4.0	0.0	del Gf: Pal92'	
NpCl+++			1										1				3.0000	6.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpCl2++			2										1				2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
NpCl3+			3										1				1.0000	4.0	0.0	del Gf: Pal92'	
NpF+++				1									1				3.0000	6.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpF2++				2									1				2.0000	4.5	0.0	del Gf: Pal92'	
NpF3+				3									1				1.0000	4.0	0.0	del Gf: Pal92'	
NpF4(aq)				4									1				0.0000	3.0	0.0	del Gf: Pal92'	
NpF5-1				5									1				-1.0000	4.0	0.0	del Gf: Pal92'	
NpF6-2				6									1				-2.0000	4.0	0.0	del Gf: Pal92'	
NpO2OH(aq)		-1									1			1			0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2CO3-1					1									1			-1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2(CO3)2-3					2									1			-3.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2(CO3)3-5					3									1			-5.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2NO3(aq)								1						1			0.0000	3.0	0.0	del Gf: Pal92'	
NpO2(NO3)2-1								2						1			-1.0000	4.0	0.0	del Gf: Pal92'	
NpO2Cl(aq)			1											1			0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2Cl2-1			2											1			-1.0000	4.0	0.0	del Gf: Pal92'	
NpO2F(aq)				1										1			0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2PO4-2							1							1			-2.0000	4.0	0.0	del Gf: Pal92'	
NpO2HPO4-1		1					1							1			-1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2H2PO4(aq)		2					1							1			0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2SO4-1						1								1			-1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2OH+		-1									1				1		1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2(OH)2(aq)		-2									2				1		0.0000	3.0	0.0	del Gf: Pal92'	
NpO2(OH)3-1		-3									3				1		-1.0000	4.0	0.0	del Gf: Pal92'	
NpO2(OH)4-2		-4									4				1		-2.0000	4.0	0.0	del Gf: Pal92'	
(NpO2)2OH+++		-1									1				2		3.0000	6.0	0.0	del Gf: Pal92'	
(NpO2)2(OH)2++		-2									2				2		2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
(NpO2)3(OH)4++		-4									4				3		2.0000	4.5	0.0	del Gf: Pal92'	
(NpO2)3(OH)5+		-5									5				3		1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
(NpO2)3(OH)7-		-7									7				3		-1.0000	4.0	0.0	del Gf: Pal92'	
(NpO2)4(OH)7+		-7									7				4		1.0000	4.0	0.0	del Gf: Pal92'	
NpO2CO3(aq)					1										1		0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2(CO3)2-2					2										1		-2.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2(CO3)3-4					3										1		-4.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
(NpO2)3(CO3)6(6-)					6										3		-6.0000	4.0	0.0	del Gf: Pal92'	
NpO2HPO4(aq)		1					1								1		0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2H2PO4+1		2					1								1		1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2(H2PO4)2(aq)		4					2								1		0.0000	3.0	0.0	del Gf: Pal92'	
NpO2NO3+								1							1		1.0000	4.0	0.0	del Gf: Pal92'	
NpO2(NO3)2(aq)								2							1		0.0000	3.0	0.0	del Gf: Pal92'	
NpO2SO4(aq)						1									1		0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2(SO4)2-2						2									1		-2.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2Cl+			1												1		1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2Cl2(aq)			2												1		0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2F+				1											1		1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2F2(aq)				2											1		0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
NpO2F3-1				3											1		-1.0000	4.0	0.0	del Gf: Pal92'	
NpO2F4-2				4											1		-2.0000	4.0	0.0	del Gf: Pal92'	
Np(metal)	4												1							del Gf: Lem84'	del Hf: PHI88'
Np(HPO4)2		2					2						1							del Gf: Lem84'	
Np(OH)4		-4									4		1							del Gf: Lem84'	del Hf: PHI88'
NpO2		-4									2		1							del Gf: Lem84'	del Hf: PHI88'
Np2O5		-2									1			2						del Gf: Lem84'	del Hf: PHI88'
NpO2OH(am)		-1									1			1						del Gf: Lem84'	del Hf: PHI88'
NaNpCO3:3.5H2O					1						3.5			1		1				del Gf: Lem84'	
NpO2(OH)2		-2									2				1					del Gf: Lem84'	
Np+++/Np++++	1											-1	1							del Gf: Lem84'	del Hf: PHI88'
NpO2+/Np++++	-1	-4									2		1	-1						del Gf: Lem84'	del Hf: PHI88'
NpO2++/Np++++	-2	-4									2		1		-1					del Gf: Lem84'	del Hf: PHI88'

Note: Np + Pu Log K values as given in the EQ3/6 database (Data0.alt.R2) are identical — 9/5/94 (DR)

DRJ 9/5/94 ~~Np~~ Pu · Data

DRJ 10/30/94

Log K	Del G(r) (kJ/mol)	Del G(r) (kcal/mol)	Del H(r) (kJ/mol)	Del H(r) (kcal/mol)	M.W. (g/mol)	Del G(f) (kJ/mol)	Del H(f) (kJ/mol)	Mineral/Species
Calculating Log K Values from Free Energies								
Pu(III) AQUEOUS:								
7.90	-45.0921	-10.7773	############	############	304.0094	-1151.6763	############	PuCO3+
12.20	-69.6355	-16.6433	############	############	364.0188	-1704.2018	############	Pu(CO3)2-1
12.70	-72.4932	-17.3263	############	############	424.0282	-2235.0426	############	Pu(CO3)3-3
22.21	-126.7696	-30.2963	############	############	340.9873	-1724.1636	############	PuH2PO4++
43.13	-246.2128	-58.8463	############	############	437.9746	-2862.4208	############	Pu(H2PO4)2+
63.62	-363.1615	-86.7953	############	############	534.9618	-3998.1635	############	Pu(H2PO4)3(aq)
83.76	-478.0985	-114.2683	############	############	631.9491	-5131.9145	############	Pu(H2PO4)4-1
1.09	-6.2229	-1.4873	############	############	306.0049	-595.7281	############	PuNO3++
2.22	-12.6705	-3.0283	############	############	368.0098	-813.0809	############	Pu(NO3)2+
2.52	-14.3860	-3.4383	############	############	430.0147	-925.7016	############	Pu(NO3)3(aq)
-5.49	31.3119	7.4837	53.2383	12.7243	261.0073	-764.4707	-824.6000	PuOH++
-16.01	91.3899	21.8427	############	############	278.0147	-961.5752	############	Pu(OH)2+
-23.91	136.4558	32.6137	############	############	295.0220	-1153.6920	############	Pu(OH)3(aq)
3.78	-21.5761	-5.1573	14.4016	3.4421	340.0616	-1344.6372	-1487.2000	PuSO4+
6.32	-36.0756	-8.6223	############	############	436.1232	-2103.5939	############	Pu(SO4)2-
0.98	-5.5962	-1.3373	############	############	279.4530	-715.4849	############	PuCl++
0.82	-4.6789	-1.1183	############	############	314.9060	-845.8564	############	PuCl2+
3.73	-21.2894	-5.0883	############	############	262.9980	-881.6399	############	PuF++
7.83	-44.6947	-10.6823	############	############	281.9960	-1186.7958	############	PuF2+
11.08	-63.2465	-15.1163	############	############	300.9940	-1487.0982	############	PuF3(aq)
Pu(IV) AQUEOUS:								
12.30	-70.2068	-16.7798	-16.1662	-3.8636	304.0094	-1079.7900	-1227.8000	PuCO3++
23.35	-133.2806	-31.8548	############	############	364.0188	-1670.8469	############	Pu(CO3)2(aq)
30.00	-171.2379	-40.9258	############	############	424.0282	-2236.7873	############	Pu(CO3)3-2
33.00	-188.3630	-45.0198	############	############	484.0376	-2781.8956	############	Pu(CO3)4-4
34.00	-194.0700	-46.3838	############	############	644.0470	-3316.5857	############	Pu(CO3)5-6
24.46	-139.6441	-33.3518	############	############	340.9873	-1639.9481	############	PuH2PO4+++
47.36	-270.2963	-64.6028	############	############	437.9746	-2769.5063	############	Pu(H2PO4)2++
91.96	-524.9030	-125.4548	############	############	631.9491	-5081.7190	############	Pu(H2PO4)4(aq)
28.32	-161.6607	-38.6378	############	############	339.9793	-1662.0647	############	PuHPO4++
52.77	-301.2306	-71.9958	############	############	435.9587	-2620.4385	############	Pu(HPO4)2(aq)
74.86	-427.3322	-102.1346	############	############	531.9380	-3965.3442	############	Pu(HPO4)3(-2)
94.93	-541.9026	-129.5176	############	############	627.9174	-5096.7186	############	Pu(HPO4)4(-4)
110.21	-629.0721	-150.3516	############	############	723.8967	-6204.6921	############	Pu(HPO4)5(-6)
1.87	-10.6728	-2.5509	############	############	306.0049	-603.1780	############	PuNO3+++
3.36	-19.1790	-4.5839	############	############	368.0098	-722.5894	############	Pu(NO3)2++
3.15	-17.9824	-4.2979	############	############	430.0147	-832.2980	############	Pu(NO3)3+
-0.33	1.8584	0.4442	48.2383	11.5292	261.0073	-716.9242	-774.0000	PuOH+++
0.21	-1.1959	-0.2858	74.3767	17.7764	278.0147	-957.1611	-1033.7000	Pu(OH)2++
-3.14	17.8998	4.2782	96.6160	23.0915	295.0220	-1175.2479	-1297.3000	Pu(OH)3+
-6.78	38.7069	9.2512	109.1633	26.0893	312.0294	-1391.6235	-1670.5000	Pu(OH)4(aq)
-16.18	92.3332	22.0682	125.6916	30.0410	329.0367	-1575.1798	-1839.9000	Pu(OH)5-1
6.76	-38.5842	-9.2218	12.5016	2.9880	340.0616	-1264.6433	-1433.6000	PuSO4++
10.36	-59.1360	-14.1338	############	############	436.1232	-2029.6542	############	Pu(SO4)2(aq)
8.30	-47.3748	-11.3228	############	############	532.1848	-2762.3521	############	Pu(SO4)3-2
1.16	-6.6226	-1.5828	17.1797	4.1060	279.4530	-619.5123	-686.3000	PuCl+++
2.16	-12.3298	-2.9468	############	############	314.9060	-756.5090	############	PuCl2++
0.09	-0.5140	-0.1228	############	############	350.3590	-875.9632	############	PuCl3+
8.45	-48.2325	-11.5278	21.8276	5.2169	262.9980	-811.5830	-849.9200	PuF+++
16.82	-90.3026	-21.5828	############	############	281.9960	-1135.4037	############	PuF2++
20.70	-118.1665	-28.2398	############	############	300.9940	-1445.0072	############	PuF3+
25.00	-142.6988	-34.1058	############	############	319.9920	-1751.3011	############	PuF4(aq)
26.83	-153.1463	-36.6028	############	############	338.9900	-2043.4991	############	PuF5-1
28.86	-164.7318	-39.3718	############	############	357.9880	-2336.8351	############	PuF6-2
Pu(V) AQUEOUS:								
-9.54	54.4291	13.0089	68.9343	16.4757	293.0061	-1032.7535	-1131.5040	PuO2OH(aq)
5.07	-28.9412	-6.9171	############	############	338.0082	-1408.9244	############	PuO2CO3-1
6.62	-37.7737	-9.0281	############	############	398.0176	-1943.7400	############	PuO2(CO3)2-3
7.36	-42.0121	-10.0411	############	############	458.0270	-2475.9615	############	PuO2(CO3)3-5
-1.42	8.1038	1.9369	############	############	338.0037	-952.6014	############	PuO2NO3(aq)
-2.12	12.0994	2.8918	############	############	400.0086	-1059.7110	############	PuO2(NO3)2-1
-1.51	8.6185	2.0599	############	############	311.4518	-972.6712	############	PuO2Cl(aq)
-3.00	17.1246	4.0929	############	############	346.9048	-1096.4549	############	PuO2Cl2-1
0.89	-5.0799	-1.2141	############	############	294.9958	-1136.8305	############	PuO2F(aq)
6.78	-38.6963	-9.2491	############	############	370.9702	-1907.5023	############	PuO2PO4-2
15.13	-86.3708	-20.6431	############	############	371.9781	-1955.1748	############	PuO2HPO4-1
20.57	-117.3994	-28.0591	############	############	372.9861	-1986.2034	############	PuO2H2PO4(aq)
1.53	-8.7325	-2.0871	############	############	372.0604	-1603.1916	############	PuO2SO4-1
Pu(VI) AQUEOUS:								
-5.38	30.6831	7.3334	45.4383	10.6600	293.0061	-963.3995	-1062.6000	PuO2OH+
-12.45	71.0671	16.9854	############	############	310.0135	-1160.1981	############	PuO2(OH)2(aq)
-20.27	115.6777	27.6476	############	############	327.0208	-1352.7701	############	PuO2(OH)3-1
-33.05	188.6542	45.0894	############	############	344.0282	-1516.9761	############	PuO2(OH)4-2
-2.82	16.0703	3.8409	############	############	569.0049	-1734.9123	############	(PuO2)2OH+++
-7.81	44.5842	10.6559	58.1767	13.9046	586.0123	-1943.5810	-2167.9000	(PuO2)2(OH)2++
-11.95	68.2173	16.3043	############	############	896.0258	-3161.2131	############	(PuO2)3(OH)4++
-20.23	115.4547	27.5943	139.4916	33.3393	913.0331	-3341.1583	-3766.3000	(PuO2)3(OH)5+
-31.09	177.4446	42.4103	############	############	947.0478	-3763.5333	############	(PuO2)3(OH)7-
-21.99	125.5023	29.9958	############	############	1223.0466	-4562.3759	############	(PuO2)4(OH)7+
9.31	-53.1433	-12.7016	############	############	336.0082	-1338.0266	############	PuO2CO3(aq)
14.10	-80.4816	-19.2356	23.1597	5.5377	396.0176	-1893.3479	-2149.5000	PuO2(CO3)2-2
18.36	-104.7404	-25.0336	-38.2955	-9.1528	456.0270	-2445.5898	-2886.2000	PuO2(CO3)3-4
53.75	-306.8030	-73.3277	############	############	1188.0528	-5745.4019	############	(PuO2)3(CO3)6(6-)
20.86	-119.0790	-28.4606	############	############	371.9781	-1894.7830	############	PuO2HPO4(aq)
24.02	-137.0911	-32.7656	############	############	372.9861	-1912.7951	############	PuO2H2PO4+1
46.60	-266.0169	-63.5796	############	############	469.9734	-3060.6249	############	PuO2(H2PO4)2(aq)
0.24	-1.3706	-0.3276	############	############	338.0037	-869.1768	############	PuO2NO3+
0.01	-0.0569	-0.0136	############	############	400.0086	-976.7673	############	PuO2(NO3)2(aq)
3.38	-19.2948	-4.6116	16.1016	3.8484	372.0604	-1520.6539	-1716.7000	PuO2SO4(aq)
3.99	-22.7768	-5.4436	43.0032	10.2780	468.1220	-2268.5941	-2598.4000	PuO2(SO4)2-2
0.60	-2.8558	-0.6826	11.1797	2.6720	311.4518	-891.0458	-976.1000	PuO2Cl+
-0.18	1.0269	0.2454	############	############	346.9048	-1018.4525	############	PuO2Cl2(aq)
4.68	-26.7130	-6.3846	-5.2524	-1.2554	294.9958	-1065.3636	-1162.6000	PuO2F+
8.37	-47.7752	-11.4186	-41.7048	-9.9677	313.9948	-1368.1764	-1534.5000	PuO2F2(aq)
10.78	-61.5322	-14.7066	-29.4572	-7.0404	332.9928	-1663.6839	-1857.7000	PuO2F3-1
11.54	-65.8710	-15.7436	-40.0096	-9.5625	351.9908	-1949.7733	-2203.6000	PuO2F4-2
Pu(III) SOLIDS:								
-22.45	128.1478	30.6281	152.9160	36.5476	295.0220	-1162.0000	-1296.6000	Pu(OH)3
-48.13	274.7478	65.6663	385.5160	92.1400	535.9982	-1594.0000	-1656.0000	Pu2O3
10.19	-58.1483	-13.8978	12.3428	2.9500	300.9940	-1462.0000	-1585.7000	PuF3
Pu(IV) SOLIDS:								
-84.37	481.6000	115.1052	536.4000	128.2027	244.0000	0.0000	0.0000	Pu(metal)
52.34	-298.7920	-71.4130	5.9604	1.4246	435.9587	-2818.0000	-3085.1900	Pu(HPO4)2
-0.76	4.3304	1.0350	64.6333	15.4477	312.0294	-1426.0000	-1615.1200	Pu(OH)4
7.36	-42.0348	-10.0466	51.8847	12.4007	275.9988	-998.0000	-1056.1920	PuO2
13.21	-75.3978	-18.0205	31.7904	7.5981	319.9920	-1684.0000	-1646.0000	PuF4
Pu(V) SOLIDS:								
-5.46	31.1826	7.4528	42.2783	10.1048	293.0061	-1056.0000	-1158.1600	PuO2OH(am)
Pu(VI) SOLIDS:								
-3.55	20.2552	4.8435	36.9767	8.8376	310.0135	-1211.0000	-1358.9000	PuO2(OH)2
24.93	-142.2950	-34.0096	-3.6348	-0.8687	371.9781	-1918.0000	-2103.2100	PuO2HPO4
REDOX REACTIONS:								
16.99	-97.0000	-23.1836	-55.6000	-13.2887	0.0000			Pu+++/Pu++++
-18.56	105.9652	25.3263	193.4767	46.2420	0.0000			PuO2+/Pu++++
-34.87	199.0652	47.5777	285.8767	68.3262	0.0000			PuO2++/Pu++++

Mineral/Species	e-	H+	Cl-	F-	CO3--	SO4--	PO4-3	NO3-	Br-	I-	H2O(l)	Pu+++	Pu++++	PuO2+	PuO2++	Charge	dbha(zero)	dbhb	COMMENTS	
		Reaction Stoichiometries																		
Del G(f)(kJ/mol)	0	0.0000	-131.2170	-281.5230	-527.9831	-744.0040	-1025.4910	-110.7940	-103.8500	-51.7240	-237.1400	~~-517.1000~~	~~-502.9000~~	~~-915.6000~~	~~-795.8000~~				NEA Basis/Auxiliary species data	
Del H(f)(kJ/mol)	0	0.0000	-167.0800	-335.3500	-675.2300	-909.3400	-1284.4000	-206.8500	-121.4100	-56.7600	-285.8300	~~-527.2000~~	~~-556.1000~~	~~-978.2000~~	~~-860.6000~~				NEA Basis/Auxiliary species data	
M.W.	0	1.0079	35.4530	18.9980	60.0094	96.0616	94.9714	62.0049	79.9040	126.9044	18.0153	244.0000	244.0000	275.9988	275.9988				Data from EQ3/6 database (Dat0.alt.r2 release, 02aug95)	
Del G(f)(kJ/mol)	0	0.0000	-131.2897	-281.7506	-527.9831	-744.4591	-1018.8040	-110.9052	-104.0561	-51.9234	-237.1826	-578.6000	-481.6000	-850.0000	-756.9000				Original data source is from draft NEA data Palmer et al. (1992)	
Del H(f)(kJ/mol)	0	0.0000	-167.0797	-335.3476	-675.2348	-909.6016	-1277.3752	-206.8109	-121.6034	-56.9024	-285.8383	-592.0000	-536.4000	-914.6000	-822.2000				del Hf for Pu+++,Pu++++,PuO2+,PuO2++ from PHI88	
PuCO3+					1							1				1.0000	4.0	0.0	del Gf: Pal92'	
Pu(CO3)2-1					2							1				-1.0000	4.0	0.0	del Gf: Pal92'	
Pu(CO3)3-3					3							1				-3.0000	4.0	0.0	del Gf: Pal92'	
PuH2PO4++		2					1					1				2.0000	4.5	0.0	del Gf: Pal92'	
Pu(H2PO4)2+		4					2					1				1.0000	4.0	0.0	del Gf: Pal92'	
Pu(H2PO4)3(aq)		6					3					1				0.0000	3.0	0.0	del Gf: Pal92'	
Pu(H2PO4)4-1		8					4					1				-1.0000	4.0	0.0	del Gf: Pal92'	
PuNO3++								1				1				2.0000	4.5	0.0	del Gf: Pal92'	
Pu(NO3)2+								2				1				1.0000	4.0	0.0	del Gf: Pal92'	
Pu(NO3)3(aq)								3				1				0.0000	3.0	0.0	del Gf: Pal92'	
PuOH++		-1									1	1				2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
Pu(OH)2+		-2									2	1				1.0000	4.0	0.0	del Gf: Pal92'	
Pu(OH)3(aq)		-3									3	1				0.0000	3.0	0.0	del Gf: Pal92'	
PuSO4+						1						1				1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Pu(SO4)2-						2						1				-1.0000	4.0	0.0	del Gf: Pal92'	
PuCl++			1									1				2.0000	4.5	0.0	del Gf: Pal92'	
PuCl2+			2									1				1.0000	4.0	0.0	del Gf: Pal92'	
PuF++				1								1				2.0000	4.5	0.0	del Gf: Pal92'	
PuF2+				2								1				1.0000	4.0	0.0	del Gf: Pal92'	
PuF3(aq)				3								1				0.0000	3.0	0.0	del Gf: Pal92'	
PuCO3++					1								1			2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
Pu(CO3)2(aq)					2								1			0.0000	3.0	0.0	del Gf: Pal92'	
Pu(CO3)3-2					3								1			-2.0000	4.0	0.0	del Gf: Pal92'	
Pu(CO3)4-4					4								1			-4.0000	4.0	0.0	del Gf: Pal92'	
Pu(CO3)5-6					5								1			-6.0000	4.0	0.0	del Gf: Pal92'	
PuH2PO4+++		2					1						1			3.0000	5.0	0.0	del Gf: Pal92'	
Pu(H2PO4)2++		4					2						1			2.0000	4.5	0.0	del Gf: Pal92'	
Pu(H2PO4)4(aq)		8					4						1			0.0000	3.0	0.0	del Gf: Pal92'	
PuHPO4++		1					1						1			2.0000	4.5	0.0	del Gf: Pal92'	
Pu(HPO4)2(aq)		2					2						1			0.0000	3.0	0.0	del Gf: Pal92'	
Pu(HPO4)3(-2)		3					3						1			-2.0000	4.0	0.0	del Gf: Pal92'	
Pu(HPO4)4(-4)		4					4						1			-4.0000	4.0	0.0	del Gf: Pal92'	
Pu(HPO4)5(-6)		5					5						1			-6.0000	4.0	0.0	del Gf: Pal92'	
PuNO3+++								1					1			3.0000	5.0	0.0	del Gf: Pal92'	
Pu(NO3)2++								2					1			2.0000	4.5	0.0	del Gf: Pal92'	
Pu(NO3)3+								3					1			1.0000	4.0	0.0	del Gf: Pal92'	
PuOH+++		-1									1		1			3.0000	5.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Pu(OH)2++		-2									2		1			2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
Pu(OH)3+		-3									3		1			1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Pu(OH)4(aq)		-4									4		1			0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Pu(OH)5-1		-5									5		1			-1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuSO4++						1							1			2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
Pu(SO4)2(aq)						2							1			0.0000	3.0	0.0	del Gf: Pal92'	
Pu(SO4)3-2						3							1			-2.0000	4.0	0.0	del Gf: Pal92'	
PuCl+++			1										1			3.0000	5.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuCl2++			2										1			2.0000	4.5	0.0	del Gf: Pal92'	
PuCl3+			3										1			1.0000	4.0	0.0	del Gf: Pal92'	
PuF+++				1									1			3.0000	5.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuF2++				2									1			2.0000	4.5	0.0	del Gf: Pal92'	
PuF3+				3									1			1.0000	4.0	0.0	del Gf: Pal92'	
PuF4(aq)				4									1			0.0000	3.0	0.0	del Gf: Pal92'	
PuF5-1				5									1			-1.0000	4.0	0.0	del Gf: Pal92'	
PuF6-2				6									1			-2.0000	4.0	0.0	del Gf: Pal92'	
PuO2OH(aq)		-1									1			1		0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuO2CO3-1					1									1		-1.0000	4.0	0.0	del Gf: Pal92'	
PuO2(CO3)2-3					2									1		-3.0000	4.0	0.0	del Gf: Pal92'	
PuO2(CO3)3-5					3									1		-6.0000	4.0	0.0	del Gf: Pal92'	
PuO2NO3(aq)								1						1		0.0000	3.0	0.0	del Gf: Pal92'	
PuO2(NO3)2-1								2						1		-1.0000	4.0	0.0	del Gf: Pal92'	
PuO2Cl(aq)			1											1		0.0000	3.0	0.0	del Gf: Pal92'	
PuO2Cl2-1			2											1		-1.0000	4.0	0.0	del Gf: Pal92'	
PuO2F(aq)				1										1		0.0000	3.0	0.0	del Gf: Pal92'	
PuO2PO4-2							1							1		-2.0000	4.0	0.0	del Gf: Pal92'	
PuO2HPO4-1		1					1							1		-1.0000	4.0	0.0	del Gf: Pal92'	
PuO2H2PO4(aq)		2					1							1		0.0000	3.0	0.0	del Gf: Pal92'	
PuO2SO4-1						1								1		-1.0000	4.0	0.0	del Gf: Pal92'	
PuO2OH+		-1									1				1	1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuO2(OH)2(aq)		-2									2				1	0.0000	3.0	0.0	del Gf: Pal92'	
PuO2(OH)3-1		-3									3				1	-1.0000	4.0	0.0	del Gf: Pal92'	
PuO2(OH)4-2		-4									4				1	-2.0000	4.0	0.0	del Gf: Pal92'	
(PuO2)2OH+++		-1									1				2	3.0000	5.0	0.0	del Gf: Pal92'	
(PuO2)2(OH)2++		-2									2				2	2.0000	4.5	0.0	del Gf: Pal92'	del Hf: PHI88'
(PuO2)3(OH)4++		-4									4				3	2.0000	4.5	0.0	del Gf: Pal92'	
(PuO2)3(OH)5+		-5									5				3	1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
(PuO2)3(OH)7-		-7									7				3	-1.0000	4.0	0.0	del Gf: Pal92'	
(PuO2)4(OH)7+		-7									7				4	1.0000	4.0	0.0	del Gf: Pal92'	
PuO2CO3(aq)					1										1	0.0000	3.0	0.0	del Gf: Pal92'	
PuO2(CO3)2-2					2										1	-2.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuO2(CO3)3-4					3										1	-4.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
(PuO2)3(CO3)6(6-)					6										3	-6.0000	4.0	0.0	del Gf: Pal92'	
PuO2HPO4(aq)		1					1								1	0.0000	3.0	0.0	del Gf: Pal92'	
PuO2H2PO4+1		2					1								1	1.0000	4.0	0.0	del Gf: Pal92'	
PuO2(H2PO4)2(aq)		4					2								1	0.0000	3.0	0.0	del Gf: Pal92'	
PuO2NO3+								1							1	1.0000	4.0	0.0	del Gf: Pal92'	
PuO2(NO3)2(aq)								2							1	0.0000	3.0	0.0	del Gf: Pal92'	
PuO2SO4(aq)						1									1	0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuO2(SO4)2-2						2									1	-2.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuO2Cl+			1												1	1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuO2Cl2(aq)			2												1	0.0000	3.0	0.0	del Gf: Pal92'	
PuO2F+				1											1	1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuO2F2(aq)				2											1	0.0000	3.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuO2F3-1				3											1	-1.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
PuO2F4-2				4											1	-2.0000	4.0	0.0	del Gf: Pal92'	del Hf: PHI88'
Pu(OH)3		-3									3	1							del Gf: Pal92'	del Hf: PHI88'
Pu2O3		-6									3	2							del Gf: Pal92'	del Hf: PHI88'
PuF3				3								1							del Gf: Pal92'	del Hf: PHI88'
Pu(metal)	4												1						del Gf: Pal92'	del Hf: PHI88'
Pu(HPO4)2		2					2						1						del Gf: Pal92'	del Hf: PHI88'
Pu(OH)4		-4									4		1						del Gf: Pal92'	del Hf: PHI88'
PuO2		-4									2		1						del Gf: Pal92'	del Hf: PHI88'
PuF4				4									1						del Gf: Pal92'	del Hf: PHI88'
PuO2OH(am)		-1									1			1					del Gf: Pal92'	del Hf: PHI88'
PuO2(OH)2		-2									2				1				del Gf: Pal92'	del Hf: PHI88'
PuO2HPO4		1					1								1				del Gf: Pal92'	del Hf: PHI88'
Pu+++/Pu++++	1											-1	1						del Gf: Pal92'	del Hf: PHI88'
PuO2+/Pu++++	-1	-4									2		1	-1					del Gf: Pal92'	del Hf: PHI88'
PuO2++/Pu++++	-2	-4									2		1		-1				del Gf: Pal92'	del Hf: PHI88'

Np(V)-Montmorillonite Sorption

Np(V)-Montmorillonite sorption was revisited to use the DLM to investigate the effect of using the Al:Si ratio of 0.83 proposed for edge sites by White and Zelazny (1988) as used by Zachara and McKinley (1993) and Zachara and Smith (1994) in their Np(V)- and Cd-montmorillonite sorption modeling. In this study, an approach has been adopted such that the simplest model that can describe the observed sorption behavior is used.

The Np(V)-montmorillonite sorption data for experiment NpM1, the conditions were:

Np_{total}=8.785e-7 M
M/V=3.97 g/L
I=0.1 m $NaNO_3$
Capped vials (25 mL headspace, $C_T = 3.3x10^{-7}$ M based on ideal gas law PV=nRT)

were modeled for the DLM using FITEQL, version 2.0. All data were used in the FITEQL regression, and because carbon was so low, Np(V)-carbonate species were neglected in the thermodynamic model. Experiments conducted in this study were at relatively high ionic strength (0.1 M $NaNO_3$), which suppressed ion-exchange of NpO_2^+ with interlayer cations. Therefore, in modeling Np(V) sorption on montmorillonite, it was assumed that the edge sites dominate the sorption behavior, and ion-exchange was not explicitly incorporated in the model construction.

In order to develop a DLM for the Np(V)-montmorillonite system, it is necessary to calculate the total number of sorption sites (T>XOH). The crystallite edges were assumed to comprise 10 percent of the N_2-BET specific surface area, consistent with observations of Wanner et al. (1994). This effective surface area of 9.7 m^2/g, together with a "standard" site density of 2.3 sites/nm^2 recommended for all minerals by Davis and Kent (1990) based on the ferrihydrite work of Dzombak and Morel (1990), was used to calculate the total number of available edge sites. In the absence of more quantitative information, it was also assumed that the ratio of >AlOH° to >SiOH° sites is 0.83 as proposed for montmorillonite by White and Zelazny (1988). The acidity constants used for the protonation and deprotonation of the >SiOH° and >AlOH° edge sites were derived based on potentiometric titration data for SiO_2 and α-Al_2O_3, as described in Turner and Sassman (1996).

FITEQL requires the input of an equilibrium aqueous speciation model. For this reason, the resultant binding constants are dependent on the quality and extent of the thermodynamic data available for the system of interest. For Np(V), the equilibrium constants used in the chemical equilibrium models submitted to FITEQL are listed below in Table 1. These constants are different from the thermodynamic data in the 9/5/96 modification of the MINTEQA2 database, but are consistent with earlier versions of the EQ3/6 database. There is typically a lack of independent analytical data supporting the formation of a particular surface complex.

In the absence of these data, the exact form of the surface reaction is selected by the modeler based on analogous speciation reactions in the aqueous phase. Based on the goodness-of-fit results from the FITEQL regression to the NpM1 experimental dataset, two surface complexation reactions in the DLM conceptual model best describe observed Np(V)-montmorillonite sorption behavior:

$$>SiOH^\circ + NpO_2^+ = >SiOH\text{-}NpO_2^+$$

$$>AlOH^\circ + NpO_2^+ + H_2O = >AlO\text{-}NpO_2(OH)^- + 2H^+$$

The binding constants for these reactions are given below in Table 1. These binding constants were then used to predict sorption under the experimental conditions of Experiments NpM2(forward), NpM2(reverse), and NpM3 (See Table 2).

Table 1. FITEQL model conditions used to determine DLM binding constants for Np(V) sorption on montmorillonite.

Solid concentration (M/V)	3.97 g/L
Site density	2.3 sites/nm^2
Surface area[a]	9.7 m^2/g
Ionic strength	0.1 M $NaNO_3$
$\Sigma^{237}Np(V)$	8.79×10^{-7} M
Edge-Site Reactions:	**Log K**
$>AlOH^\circ + H^+ \rightleftharpoons >AlOH_2^+$	8.33[b]
$>AlOH^\circ \rightleftharpoons >AlO^- + H^+$	-9.73[b]
$>AlOH^\circ + NpO_2^+ + H_2O \Leftrightarrow >AlO\text{-}NpO_2(OH)^- + 2H^+$	-13.79[c]
$>SiOH^\circ \rightleftharpoons >SiO^- + H^+$	-7.20[b]
$>SiOH^\circ + NpO_2^+ \Leftrightarrow >SiOH\text{-}NpO_2^+ +$	4.05[c]
Aqueous Speciation Reactions:	**Log K**
$NpO_2^+ + H_2O \Leftrightarrow NpO_2OH^\circ + H^+$	-10.0[d]
$NpO_2^+ + 2H_2O \Leftrightarrow NpO_2(OH)_2^- + 2H^+$	-22.4[d,e]
$NpO_2^+ + CO_3^{2-} \Leftrightarrow NpO_2CO_3^-$	4.6[e,f,g]
$NpO_2^+ + 2CO_3^{2-} \Leftrightarrow NpO_2(CO_3)_2^{3-}$	7.0[e,f,g]
$NpO_2^+ + 3CO_3^{2-} \Leftrightarrow NpO_2(CO_3)_3^{5-}$	8.5[f,g]
$NpO_2^+ + NO_3^- \Leftrightarrow NpO_2NO_3^\circ$ (aq)	-0.5[h]

a. Effective edge site surface area assumed to be 10 percent of total N_2-BET surface area (97 m^2/g). See text for detailed discussion.
b. Acidity constants for am-SiO_2 and α-Al_2O_3 from Turner and Sassman (1996).
c. This study. Binding constants determined using FITEQL, Version 2.0 (Westall, 1982a,b).
d. Lemire and Garisto (1989)
e. Fuger (1992)
f. Lemire (1984)
g. Lemire et al. (1993)
h. Danesi et al. (1971)

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Table 2. CNWRA Np(V)-montmorillonite experimental conditions.

Experiment	Atmosphere	Initial Np(V) conc. (M)	Mass of solid (g, ± 1σ)	Volume of solution (mL, ± 1σ)	Approx. M/V (g/L, ± 1σ)
NpM1	capped vial (Trace CO_2)	8.79×10^{-7}	0.0999±0.0005	25.2±0.1	3.97±0.02
NpM2 (forward)	open vial ($P_{CO_2}=10^{-3.5}$atm)	9.25×10^{-7}	0.0996±0.0004	24.9±0.1	4.01±0.02
NpM2 (reverse)	open vial ($P_{CO_2}=10^{-3.5}$atm)	9.25×10^{-7}	0.0996±0.0004	23.5±0.3	4.24±0.07
NpM3	glove box (No CO_2)	9.46×10^{-7}	0.1001±0.0006	23.8±0.2	4.20±0.05

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CNWRA Experimental Data

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M1 Kd calculations		capped vials									
Np(t)=	8.785E-07										
M/V=	3.971			Al:Si=0.83	Al:Si=1.68						
S(a)=	97.000		T(sioh)=	8.073E-05	5.513E-05						
T(xoh)	1.477E-04		T(aloh)=	6.701E-05	9.261E-05						
I = 0.1 M NaNO3											
exp soln	fwd equil solution pH	fwd equil volume of solution	mass of solid (g)	M/V (g/L)	fwd equil mass of Np in soln.	fwd equil Np soln (M)	desorp fwd equil mass Np on solid	desorp fwd equil Np on solid (M)	Np(total) (M)	calculated Kd ml/g	Ukd uncert in kd
pH-5	7.08	25.0865	0.1007	4.0141	4.623E-06	7.776E-07	0.000E+00	0.000E+00	7.776E-07		
pH-5.25	7.20	25.0328	0.0990	3.9548	4.601E-06	7.755E-07	5.892E-07	9.932E-08	8.748E-07	32.38	1.86
pH-5.5	7.27	25.3607	0.0999	3.9392	4.707E-06	7.831E-07	5.991E-07	9.968E-08	8.828E-07	32.31	1.92
pH-5.75	7.30	25.2722	0.1004	3.9727	4.656E-06	7.774E-07	6.469E-07	1.080E-07	8.854E-07	34.97	2.03
pH-6	7.37	25.1381	0.0994	3.9542	4.448E-06	7.466E-07	7.669E-07	1.287E-07	8.753E-07	43.61	2.52
pH-6.25	7.42	25.2522	0.0998	3.9521	4.447E-06	7.431E-07	6.952E-07	1.162E-07	8.593E-07	39.55	2.35
pH-6.5	7.62	25.1173	0.0998	3.9734	4.226E-06	7.098E-07	9.702E-07	1.630E-07	8.728E-07	57.79	3.29
pH-6.75	7.52	24.9552	0.0995	3.9871	4.429E-06	7.489E-07	7.970E-07	1.348E-07	8.836E-07	45.13	2.69
pH-7	7.70	25.2167	0.0996	3.9498	4.267E-06	7.140E-07	9.237E-07	1.546E-07	8.686E-07	54.80	3.10
pH-7.25	7.61	24.9669	0.0997	3.9933	4.266E-06	7.210E-07	8.710E-07	1.472E-07	8.682E-07	51.13	2.92
pH-7.5	7.73	25.1191	0.1008	4.0129	4.307E-06	7.234E-07	8.997E-07	1.511E-07	8.745E-07	52.06	2.96
pH-7.75	7.56	25.2395	0.1000	3.9620	4.415E-06	7.380E-07	9.652E-07	1.614E-07	8.994E-07	55.18	3.11
pH-8	7.62	25.0854	0.0998	3.9784	4.282E-06	7.202E-07	9.470E-07	1.593E-07	8.795E-07	55.60	3.27
pH-8.25	7.60	25.3733	0.1006	3.9648	4.430E-06	7.367E-07	8.950E-07	1.488E-07	8.855E-07	50.96	3.05
pH-8.5	7.62	25.0081	0.1007	4.0267	4.264E-06	7.194E-07	9.576E-07	1.616E-07	8.810E-07	55.77	3.33
pH-8.75	7.64	25.0562	0.0998	3.9830	4.196E-06	7.066E-07	9.859E-07	1.660E-07	8.726E-07	58.99	3.54
pH-9	7.68	25.1260	0.1006	4.0038	4.184E-06	7.026E-07	1.028E-06	1.726E-07	8.751E-07	61.35	3.49
pH-9.25	7.76	25.2581	0.1004	3.9750	4.135E-06	6.908E-07	1.130E-06	1.888E-07	8.796E-07	68.77	3.96
pH-9.5	7.93	25.3040	0.0999	3.9480	3.869E-06	6.452E-07	1.359E-06	2.266E-07	8.718E-07	88.97	4.97
pH-9.75	7.80	25.2360	0.0997	3.9507	4.089E-06	6.836E-07	1.203E-06	2.011E-07	8.847E-07	74.45	4.14
pH-10	8.75	25.1031	0.0996	3.9676	3.089E-06	5.192E-07	2.202E-06	3.702E-07	8.894E-07	179.70	9.72
pH-10.25	9.13	25.0457	0.1000	3.9927	2.820E-06	4.750E-07	2.427E-06	4.089E-07	8.839E-07	215.60	11.68
pH-10.5	9.56	25.2823	0.0994	3.9316	2.620E-06	4.373E-07	2.602E-06	4.342E-07	8.715E-07	252.58	13.66
pH-10.75	9.98	25.1857	0.1003	3.9824	2.052E-06	3.437E-07	3.279E-06	5.494E-07	8.931E-07	401.35	21.57
pH-11	10.54	25.3360	0.1001	3.9509	1.203E-06	2.003E-07	4.029E-06	6.710E-07	8.713E-07	847.82	45.65
Average Values		25.1696	0.0999	3.9711					8.785E-07		
S.D.		0.1239	4.5968E-04	2.3691E-02					8.9015E-09		

M2 Kd calculations		open to atmosphere									
Np(t)=	9.257E-07	(excluding 3 highest pH due to ppt)									
M/V=	4.007			Al:Si=0.83	Al:Si=1.68						
S(a)=	97.00		T(sioh)=	8.145E-05	5.562E-05						
T(xoh)	1.491E-04		T(aloh)=	6.760E-05	9.344E-05						
I = 0.1 M NaNO3											
exp soln	fwd equil solution pH	fwd equil solution volume(g)	equil mass solid (g)	M/V (g/L)	fwd equil mass of Np in soln.	fwd equil solution volume(M)	fwd equil mass Np on solid(g)	fwd equil mass Np on solid(M)	fwd equil Total Np (M)	calculated Kd ml/g	fwd Kd uncert
pH-5	7.31	24.8152	0.0985	3.9693	4.691E-06	7.977E-07	7.218E-07	1.227E-07	9.204E-07	38.75	2.23
pH-5.25	7.34	24.9625	0.0995	3.9860	4.626E-06	7.820E-07	8.548E-07	1.445E-07	9.265E-07	46.36	2.76
pH-5.5	7.38	24.8393	0.0999	4.0219	4.624E-06	7.855E-07	8.138E-07	1.382E-07	9.237E-07	43.78	2.54
pH-5.75	7.41	25.0221	0.0995	3.9765	4.533E-06	7.645E-07	9.383E-07	1.582E-07	9.227E-07	52.05	3.01
pH-6	7.48	24.8762	0.0996	4.0038	4.534E-06	7.690E-07	9.310E-07	1.579E-07	9.269E-07	51.29	3.04
pH-6.25	7.51	25.0600	0.0993	3.9625	4.539E-06	7.643E-07	9.298E-07	1.566E-07	9.209E-07	51.69	2.94
pH-6.5	7.46	24.9652	0.0995	3.9855	4.612E-06	7.794E-07	8.502E-07	1.437E-07	9.231E-07	46.26	2.78
pH-6.75	7.54	24.9268	0.0993	3.9837	4.597E-06	7.781E-07	8.795E-07	1.489E-07	9.270E-07	48.03	2.72
pH-7	7.56	24.9754	0.1002	4.0119	4.556E-06	7.697E-07	9.065E-07	1.531E-07	9.229E-07	49.59	2.83
pH-7.25	7.67	24.7750	0.0994	4.0121	4.418E-06	7.525E-07	1.037E-06	1.766E-07	9.291E-07	58.50	3.33
pH-7.5	7.72	24.6874	0.0994	4.0296	4.313E-06	7.378E-07	1.119E-06	1.914E-07	9.292E-07	64.37	3.63
pH-7.75	7.87	24.6710	0.0993	4.0250	4.113E-06	7.035E-07	1.319E-06	2.256E-07	9.291E-07	79.69	4.69
pH-8	8.05	24.6474	0.0994	4.0329	4.076E-06	6.976E-07	1.369E-06	2.344E-07	9.321E-07	83.29	4.99
pH-8.25	8.22	24.8476	0.1001	4.0286	4.001E-06	6.793E-07	1.432E-06	2.432E-07	9.225E-07	88.85	5.30
pH-8.5	8.46	24.6699	0.0999	4.0495	4.021E-06	6.878E-07	1.409E-06	2.410E-07	9.288E-07	86.54	5.19
pH-8.75	8.69	24.7487	0.1001	4.0447	4.133E-06	7.047E-07	1.312E-06	2.236E-07	9.283E-07	78.47	4.46
pH-9	9.01	25.1362	0.0995	3.9584	4.179E-06	7.015E-07	1.294E-06	2.171E-07	9.187E-07	78.19	4.50
pH-9.25	9.40	24.8316	0.1002	4.0352	4.517E-06	7.675E-07	9.568E-07	1.626E-07	9.301E-07	52.50	2.93
pH-9.5	10.44	25.0423	0.1014	4.0491	2.718E-06	4.580E-07	2.718E-06	4.577E-07	9.157E-07	246.80	13.71
pH-9.75	12.60	26.1210	0.0993	3.8015	8.992E-07	1.453E-07	4.565E-06	7.375E-07	8.827E-07	1335.49	72.24
pH-10	13.08	29.3677	0.0993	3.3813	1.667E-06	2.682E-07	3.580E-06	5.144E-07	7.826E-07	567.24	30.73
Mean Values		24.8576	0.0996	4.0065					9.257E-07		
S.D.		0.1454	4.2272E-04	2.9101E-02					3.8773E-09		

M2 Kd calculations		open to atmosphere							
Np(t)=	9.251E-07								
M/V=	4.243				Al:Si=0.83	Al:Si=1.68			
S(a)=	97.00			T(sioh)=	8.626E-05	5.890E-05			
T(xoh)	1.579E-04			T(aloh)=	7.160E-05	9.896E-05			
I = 0.1 M NaNO3									
desorb equil pH	des equil solution volume	M/V (g/L)	des equil mass of Np in soln.(g)	des equil mass of Np in soln (M)	des equil mass on solid	des equil mass of Np on solid(M)	des equil Total Np (M)	calculated Kd ml/g	desorp Kd uncert
2.76	24.0609	4.0938	5.089E-06	8.924E-07	1.281E-07	2.247E-08	9.148E-07	6.15	0.35
3.00	24.0778	4.1324	5.165E-06	9.052E-07	1.251E-07	2.192E-08	9.271E-07	5.66	0.35
3.31	23.6360	4.2266	5.155E-06	9.202E-07	9.072E-08	1.619E-08	9.364E-07	4.16	0.24
4.02	23.3990	4.2523	5.224E-06	9.419E-07	6.079E-08	1.096E-08	9.529E-07	2.74	0.16
5.34	23.2726	4.2797	5.093E-06	9.233E-07	1.863E-07	3.377E-08	9.571E-07	8.55	0.51
5.47	23.5328	4.2196	5.113E-06	9.167E-07	1.699E-07	3.046E-08	9.472E-07	7.87	0.45
3.41	23.9800	4.1493	5.145E-06	9.054E-07	1.274E-07	2.242E-08	9.278E-07	5.97	0.36
5.63	23.5516	4.2163	5.067E-06	9.078E-07	2.198E-07	3.938E-08	9.472E-07	10.29	0.58
3.40	23.8155	4.2073	5.186E-06	9.188E-07	8.968E-08	1.589E-08	9.347E-07	4.11	0.23
4.18	23.4670	4.2357	5.039E-06	9.059E-07	4.081E-07	7.338E-08	9.793E-07	19.12	1.09
6.94	23.2480	4.2756	4.574E-06	8.302E-07	6.788E-07	1.232E-07	9.534E-07	34.71	1.96
7.35	23.2057	4.2791	4.313E-06	7.842E-07	9.503E-07	1.728E-07	9.570E-07	51.49	3.03
7.73	23.0770	4.3073	3.925E-06	7.177E-07	1.351E-06	2.470E-07	9.647E-07	79.89	4.78
8.14	23.4134	4.2753	3.694E-06	6.657E-07	1.574E-06	2.836E-07	9.492E-07	99.65	5.85
8.45	23.2019	4.3057	3.786E-06	6.885E-07	1.478E-06	2.687E-07	9.572E-07	90.65	5.44
8.67	23.1298	4.3276	3.990E-06	7.279E-07	1.282E-06	2.338E-07	9.618E-07	74.22	4.22
8.96	23.7060	4.1969	4.299E-06	7.651E-07	1.003E-06	1.785E-07	9.436E-07	55.57	3.20
9.21	23.2438	4.3108	4.522E-06	8.208E-07	7.847E-07	1.386E-07	9.597E-07	39.23	2.19
9.55	23.4078	4.3319	4.558E-06	8.216E-07	7.652E-07	1.379E-07	9.595E-07	38.76	2.15
11.10	24.4713	4.0578	2.880E-06	4.967E-07	2.549E-06	4.394E-07	9.361E-07	218.05	11.79
12.84	20.9009	4.7510	1.020E-06	2.060E-07	4.360E-06	8.801E-07	1.088E-06	899.37	48.73
	23.4962	4.2433					9.251E-07		
	0.3112	0.0670					1.5423E-08		

M3 Kd calculations		No CO2									
Np(t)=	9.456E-07										
M/V=	4.200			Al:Si=0.83	Al:Si=1.68						
S(a)=	97.00		T(sioh)=	8.537E-05	5.830E-05						
T(xoh)	1.562E-04		T(aloh)=	7.086E-05	9.794E-05						
I = 0.1 M NaNO3											
exp soln	fwd equil solution pH	fwd equil solution volume	mass of solid (g)	M/v (g/L)	fwd equil mass of Np in soln.(g)	fwd equil mass of Np in soln.(M)	desorp fwd equil mass Np on solid(g)	desorp fwd equil mass Np on solid(M)	fwd equil Total Np (M)	calculated Kd ml/g	Ukd uncert in kd
pH-5	5.46	24.1692	0.0992	4.1044	5.159E-06	9.007E-07	2.099E-07	3.664E-08	9.373E-07	9.91	0.92
pH-5.25	5.52	23.9434	0.0995	4.1556	5.031E-06	8.866E-07	2.247E-07	3.960E-08	9.262E-07	10.75	1.30
pH-5.5	5.84	23.9445	0.1010	4.2181	4.978E-06	8.772E-07	2.537E-07	4.471E-08	9.219E-07	12.08	1.64
pH-5.75	5.96	24.1386	0.0999	4.1386	4.966E-06	8.680E-07	2.892E-07	5.056E-08	9.186E-07	14.07	1.41
pH-6	6.26	23.9666	0.0999	4.1683	4.993E-06	8.790E-07	3.312E-07	5.831E-08	9.373E-07	15.91	1.45
pH-6.25	6.64	24.1502	0.0995	4.1200	4.861E-06	8.493E-07	4.424E-07	7.730E-08	9.266E-07	22.09	1.92
pH-6.5	7.14	24.0871	0.1001	4.1558	4.703E-06	8.239E-07	6.205E-07	1.087E-07	9.326E-07	31.75	2.37
pH-6.75	7.56	23.6214	0.0999	4.2292	4.458E-06	7.964E-07	8.202E-07	1.465E-07	9.429E-07	43.50	2.95
pH-7	7.90	24.0749	0.0992	4.1205	4.083E-06	7.156E-07	1.222E-06	2.142E-07	9.299E-07	72.65	4.46
pH-7.25	8.27	23.7020	0.0990	4.1769	3.536E-06	6.295E-07	1.746E-06	3.108E-07	9.403E-07	118.19	6.86
pH-7.5	8.50	23.3603	0.1005	4.3022	3.307E-06	5.972E-07	1.959E-06	3.539E-07	9.512E-07	137.74	7.80
pH-7.75	8.48	23.6690	0.1002	4.2334	3.350E-06	5.972E-07	1.929E-06	3.439E-07	9.411E-07	136.03	7.57
pH-8	8.48	23.9409	0.1009	4.2145	3.340E-06	5.886E-07	1.889E-06	3.329E-07	9.215E-07	134.18	7.83
pH-8.25	8.52	23.9581	0.0999	4.1698	3.334E-06	5.871E-07	1.931E-06	3.401E-07	9.273E-07	138.94	7.83
pH-8.5	8.47	23.5126	0.1001	4.2573	3.293E-06	5.910E-07	1.896E-06	3.402E-07	9.311E-07	135.21	7.62
pH-8.75	8.53	23.6325	0.1009	4.2695	3.288E-06	5.871E-07	1.956E-06	3.492E-07	9.362E-07	139.31	7.70
pH-9	8.63	23.8268	0.1006	4.2221	3.289E-06	5.825E-07	2.078E-06	3.680E-07	9.505E-07	149.65	8.31
pH-9.25	8.61	23.7739	0.1009	4.2442	3.306E-06	5.867E-07	2.102E-06	3.730E-07	9.597E-07	149.81	8.49
pH-9.5	8.52	23.6872	0.1011	4.2681	3.290E-06	5.861E-07	2.112E-06	3.763E-07	9.624E-07	150.40	8.51
pH-9.75	8.74	23.9161	0.1011	4.2273	3.090E-06	5.452E-07	2.353E-06	4.151E-07	9.603E-07	180.14	10.12
pH-10	8.98	23.6136	0.0999	4.2306	2.907E-06	5.195E-07	2.509E-06	4.484E-07	9.679E-07	204.02	11.32
pH-10.25	9.08	23.7056	0.0996	4.2015	2.862E-06	5.094E-07	2.624E-06	4.670E-07	9.764E-07	218.21	12.24
pH-10.5	9.21	23.8186	0.0996	4.1816	2.898E-06	5.135E-07	2.496E-06	4.421E-07	9.555E-07	205.91	11.40
pH-10.75	9.50	23.7629	0.0996	4.1914	2.994E-06	5.317E-07	2.647E-06	4.700E-07	1.002E-06	210.91	11.59
pH-11	9.93	23.8917	0.1001	4.1897	2.608E-06	4.606E-07	2.962E-06	5.232E-07	9.838E-07	271.10	14.83
Mean Values		23.8347	0.1001	4.1996					9.456E-07		
S.D.		0.2101	6.3398E-04	5.0969E-02					2.1167E-08		

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FITEQL
Input Files
Np(V)-Montmorillonite
sorption

Np-Mont
Used for subsequent
modeling

MINTEQA2 Input files:

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Np-Montmorillonite Sorption; Exp. NpM1: Np(t)=8.785E-07(M)
DLM; Np as listed: I=0.1 m NaNO3; M/V=3.97 g/L; Capped vials
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 6 3
ACTIVITY   330 37
  0.25
npmont6.123        552 5523300 5523301 5524920 8115520 8125520
 4   1   7
3.971E+00     9.70 0.000 0.000 81
   330  0.000E-01   -2.00 y              /H+1
   552  8.785E-07   -6.06 y              /Np02+1
   500  1.000E-01   -1.00 y              /Na+1
   492  1.000E-01   -1.00 y              /NO3-1
   140  3.286E-07   -6.48 y              /CO3-2
   813  0.000E-01    0.00 y              /ADS1PSIo
   811  6.700E-05   -4.17 y              /ADS1TYP1
   812  8.073E-05   -4.09 y              /ADS1TYP2
 2   5
5523300   -10.0000    10.5015            /npo2(oh)
5521400     4.6000    12.7951            /npo2(co3)-1
5521401     7.0000     7.1390            /npo2(co3)2-3
5521402     8.5000     6.2630            /npo2(co3)3-5
5524920    -0.5000     0.0000            /npo2no3(aq)
 3   1
   330     2.0000     0.0000            /H+1
 6   2
   813     0.0000     0.0000            /ADS1PSIo
5524921    -2.1200     0.0000            /npo2(no3)2-

 2   6
5523301 npo2(oh)2-        0.0000   -22.4000    0.000   0.000-1.00 4.00 0.00   0.0000
  0.00 3   -2.000 330   1.000 552    2.000   2   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113300 >AlO-             0.0000    -9.7300    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 811   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113301 >AlOH2+           0.0000     8.3300    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 811    1.000 330    1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8115520 >AlONpO2OH-       0.0000   -13.7900    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 5   1.000 811    1.000 552    1.000   2  -2.000 330   -1.000 813   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8123300 >SiO-             0.0000    -7.2000    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 812   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8125520 >SiONpO2+         0.0000     4.0500    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 812    1.000 552    1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
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Np-Montmorillonite Sorption; Exp. NpM2(forward): Np(t)=9.257e-07(M)
DLM; 9/5/96 CNWRA database: I=0.1 m NaNO3; M/V=3.96g/L; Atmospheri
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 6 3
ACTIVITY   330 37
  0.25
npmont6.123        552 5523300 5523301 5524920 8115520 8125520
 4   1   7
4.007E+00     9.70 0.000 0.000 81
   330  0.000E-01   -2.00 y              /H+1
   552  9.257E-07   -6.03 y              /Np02+1
   500  1.000E-01   -1.00 y              /Na+1
   492  1.000E-01   -1.00 y              /NO3-1
   140  0.000E-01   -16.00               /CO3-2
   813  0.000E-01    0.00 y              /ADS1PSIo
   811  6.760E-05   -4.17 y              /ADS1TYP1
   812  8.145E-05   -4.09 y              /ADS1TYP2
 2   5
5523300   -10.0000    10.5015            /npo2(oh)
5521400     4.6000    12.7951            /npo2(co3)-1
5521401     7.0000     7.1390            /npo2(co3)2-3
5521402     8.5000     6.2630            /npo2(co3)3-5
5524920    -0.5000     0.0000            /npo2no3(aq)
 3   1
3301403    21.6600    -0.5300            /co2 (g)
   330     2.0000     0.0000            /H+1
 6   2
   813     0.0000     0.0000            /ADS1PSIo
5524921    -2.1200     0.0000            /npo2(no3)2-

 2   6
5523301 npo2(oh)2-        0.0000   -22.4000    0.000   0.000-1.00 4.00 0.00   0.0000
  0.00 3   -2.000 330   1.000 552    2.000   2   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113300 >AlO-             0.0000    -9.7300    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 811   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113301 >AlOH2+           0.0000     8.3300    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 811    1.000 330    1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8115520 >AlONpO2OH-       0.0000   -13.7900    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 5   1.000 811    1.000 552    1.000   2  -2.000 330   -1.000 813   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8123300 >SiO-             0.0000    -7.2000    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 812   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8125520 >SiONpO2+         0.0000     4.0500    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 812    1.000 552    1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
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Np-Montmorillonite Sorption; Exp. NpM2(reverse): Np(t)=9.251e-07(M)
DLM; 9/5/96 CNWRA database: I=0.1 m NaNO3; M/V=3.96g/L; Atmospheri
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 6 3
ACTIVITY   330 37
  0.25
npmont6.123        552 5523300 5523301 5524920 8115520 8125520
 4   1   7
4.243E+00     9.70 0.000 0.000 81
   330  0.000E-01   -2.00 y              /H+1
   552  9.251E-07   -6.04 y              /Np02+1
   500  1.000E-01   -1.00 y              /Na+1
   492  1.000E-01   -1.00 y              /NO3-1
   140  0.000E-01   -16.00               /CO3-2
   813  0.000E-01    0.00 y              /ADS1PSIo
   811  7.160E-05   -4.15 y              /ADS1TYP1
   812  8.626E-05   -4.06 y              /ADS1TYP2
 2   5
5523300   -10.0000    10.5015            /npo2(oh)
5521400     4.6000    12.7951            /npo2(co3)-1
5521401     7.0000     7.1390            /npo2(co3)2-3
5521402     8.5000     6.2630            /npo2(co3)3-5
5524920    -0.5000     0.0000            /npo2no3(aq)
 3   1
3301403    21.6600    -0.5300            /co2 (g)
   330     2.0000     0.0000            /H+1
 6   2
   813     0.0000     0.0000            /ADS1PSIo
5524921    -2.1200     0.0000            /npo2(no3)2-

 2   6
5523301 npo2(oh)2-        0.0000   -22.4000    0.000   0.000-1.00 4.00 0.00   0.0000
  0.00 3   -2.000 330   1.000 552    2.000   2   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113300 >AlO-             0.0000    -9.7300    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 811   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113301 >AlOH2+           0.0000     8.3300    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 811    1.000 330    1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8115520 >AlONpO2OH-       0.0000   -13.7900    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 5   1.000 811    1.000 552    1.000   2  -2.000 330   -1.000 813   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8123300 >SiO-             0.0000    -7.2000    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 812   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8125520 >SiOHNpO2+        0.0000     4.0500    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 812    1.000 552    1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
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Np-Montmorillonite Sorption; Exp. NpM3: Np(t)=9.456e-07(M)
DLM; 9/5/96 CNWRA database: I=0.1 m NaNO3; M/V=4.2 g/L; No CO2
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 6 3
ACTIVITY   330 37
  0.25
npmont6.123        552 5523300 5523301 5524920 8115520 8125520
 4   1   7
4.199E+00     9.70 0.000 0.000 81
   330  0.000E-01   -2.00 y              /H+1
   552  9.454E-07   -6.02 y              /Np02+1
   500  1.000E-01   -1.00 y              /Na+1
   492  1.000E-01   -1.00 y              /NO3-1
   813  0.000E-01    0.00 y              /ADS1PSIo
   811  7.089E-05   -4.15 y              /ADS1TYP1
   812  8.537E-05   -4.07 y              /ADS1TYP2

 2   2
5523300   -10.0000    10.5015            /npo2(oh)
5524920    -0.5000     0.0000            /npo2no3(aq)
 3   1
   330     2.0000     0.0000            /H+1
 6   2
   813     0.0000     0.0000            /ADS1PSIo
5524921    -2.1200     0.0000            /npo2(no3)2-

 2   6
5523301 npo2(oh)2-        0.0000   -22.4000    0.000   0.000-1.00 4.00 0.00   0.0000
  0.00 3   -2.000 330   1.000 552    2.000   2   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113300 >AlO-             0.0000    -9.7300    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 811   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113301 >AlOH2+           0.0000     8.3300    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 811    1.000 330    1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8115520 >AlONpO2OH-       0.0000   -13.7900    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 5   1.000 811    1.000 552    1.000   2  -2.000 330   -1.000 813   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8123300 >SiO-             0.0000    -7.2000    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 812   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8125520 >SiOHNpO2+        0.0000     4.0500    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 812    1.000 552    1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
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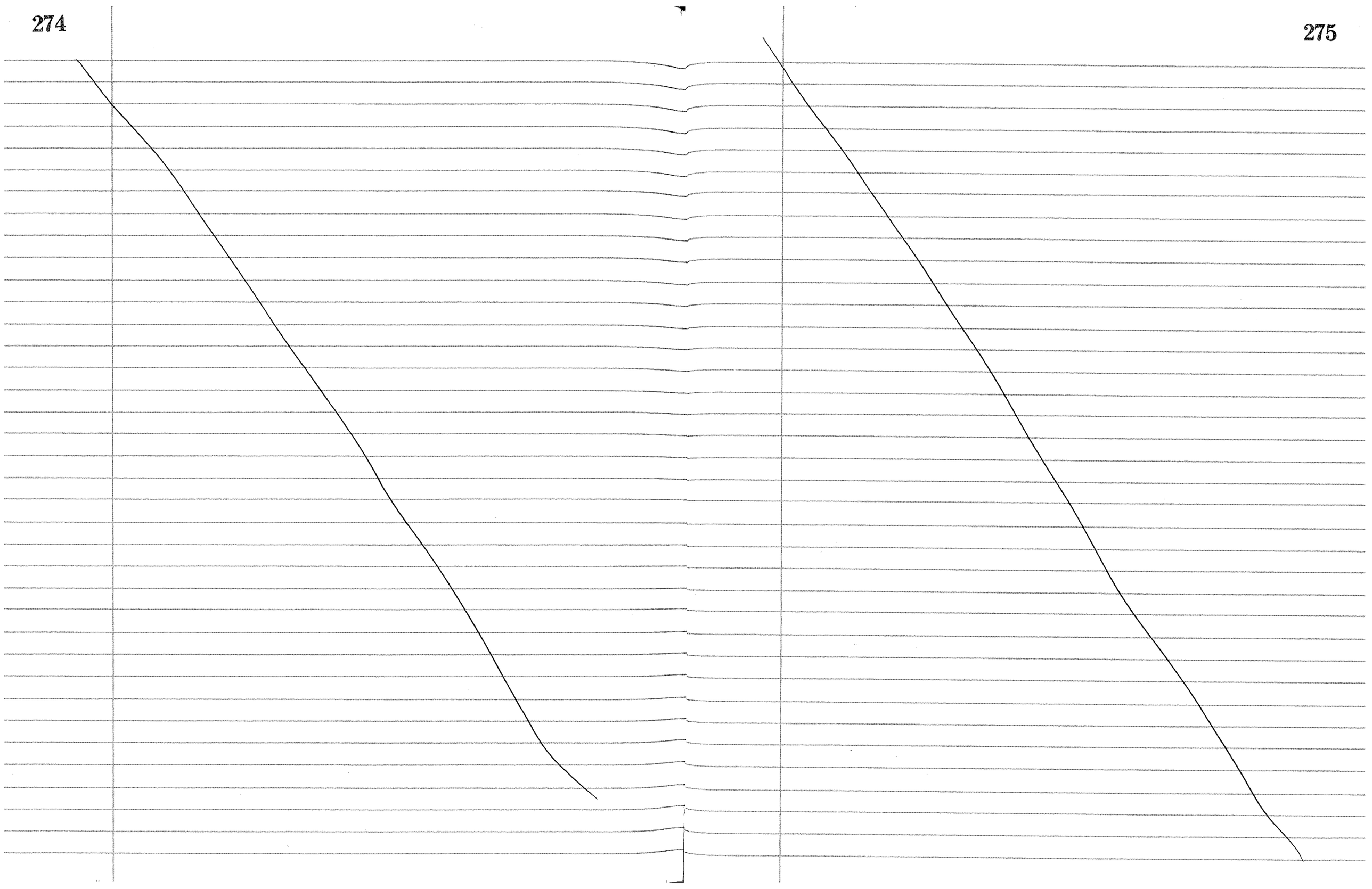

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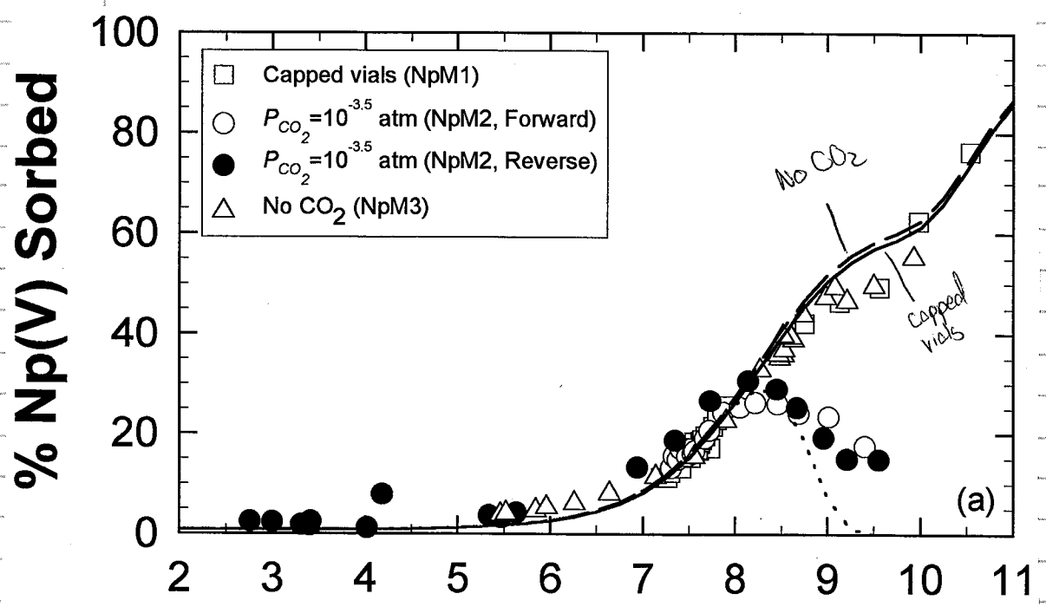
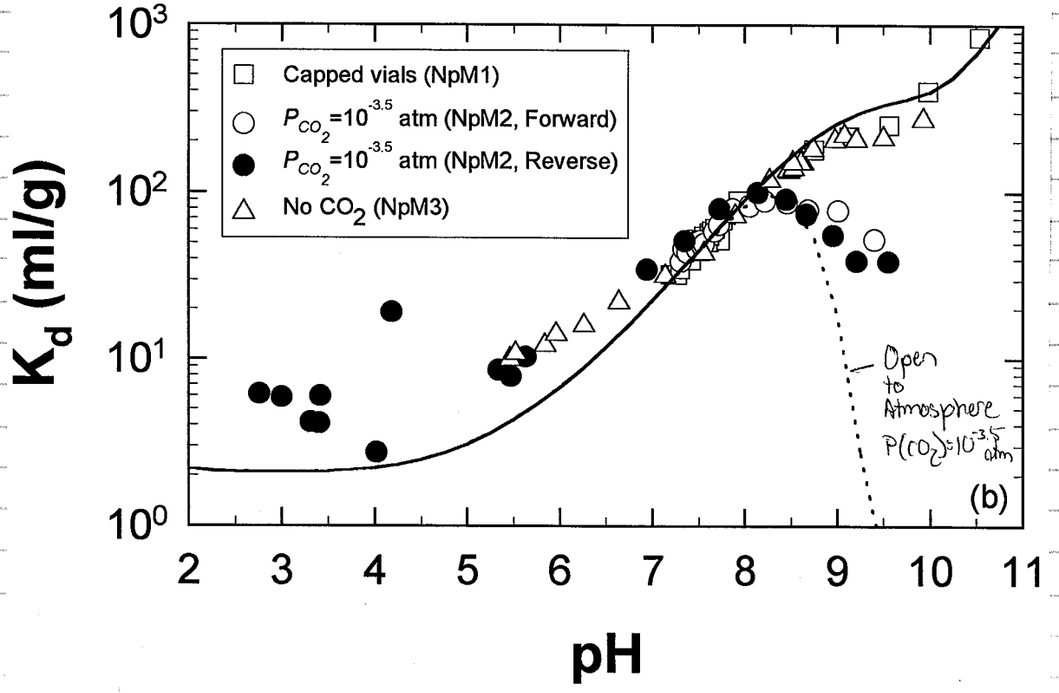


DRLemmon



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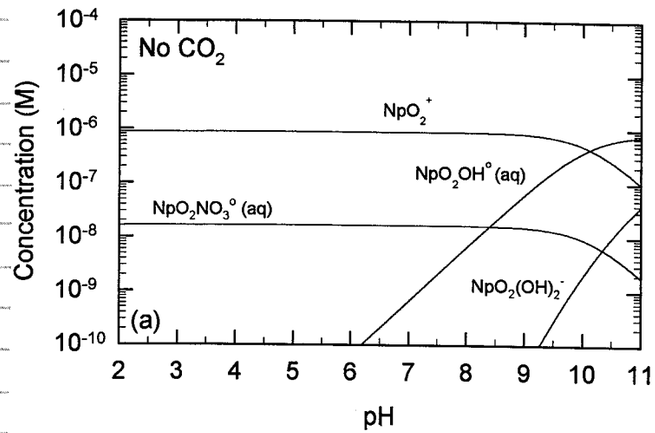
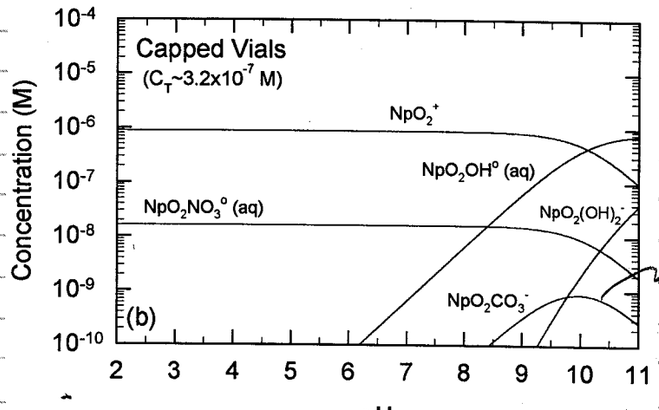
DRLemmon

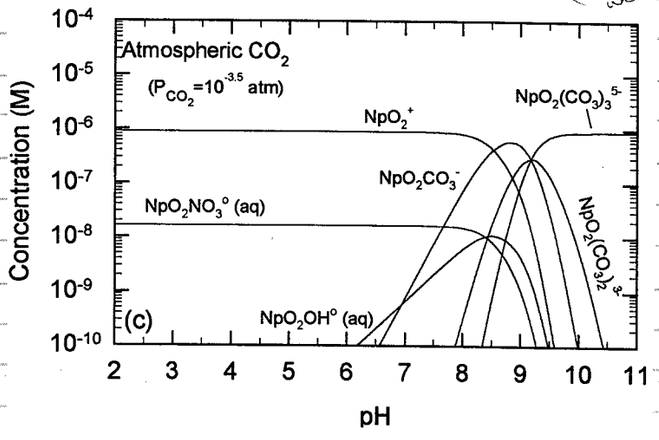


MINTEQA2 calculated speciation using Thermodynamic Log K values given in Table 1, Pg. 269 this book



Minor Np(V)-carbonate. Little to No effect on hydrolysis

DRLemmon



Strong Np(V)-carbonate greatly reduces Np(V)-hydrolysis field for pH > 8.5

U(VI)-Quartz Sorption

U(VI)-Quartz sorption was revisited yet again using the DLM, a simplified container sorption model, and the DLM acidity coefficients of Sverjensky and Sahai (1996). With these exceptions, the approach is similar to that outlined on pages 252 to 262 of this notebook.

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Acidity constants from Sverjensky and Sahai (1996)

Sverjensky and Sahai (1996) developed a method to determine DLM acidity constants using Born solvation theory. The details are provided in Sverjensky (1993, 1994) and Sverjensky and Sahai (1996). For quartz, assuming a site density of 2.3 sites/nm^2, equations (146), Figure 7b, and data from Table 1 were used to determine Log K_+ and Log K_-.

From equation (146):

$$pH_{ZPC} = (\log K_+ - \log K_-)/2$$
$$pH_{ZPC} = 21.1158(1/\epsilon_k) - 42.9148(s/r_{M\text{-}OH}) + 14.6866$$

From Table 1, for quartz:

$\epsilon_k = 4.578$
Pauling Bond Strength $s/r_{M\text{-}OH} = 0.3818$

From Figure 7b (DLM with site density = 2.3 sites/nm^2):

$$K_n = \log K_+ + \log K_-$$
$$K_n = 30.143\ (s/r_{M\text{-}OH}) - 3.214$$

Therefore, for quartz:

$pH_{ZPC} = 2.91$
$K_n = 8.29$
$K_+ = -1.24$
$K_- = -7.06$

These acidity constants were used in the FITEQL runs in the same manner described in pages 252-262 of this notebook. Three surface complexes $>SiO\text{-}UO_2^+$, $>SiO\text{-}UO_2OH^\circ$, and $>SiO\text{-}UO_2(OH)_2^-$ provided the best fit the observed data. The resulting binding constants are given below.

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Information potentially subject to copyright protection was redacted from this location. The redacted material (Figure 7: Values ... for the diffuse double layer model... and Table 1: Dielectric constants...) is from the following reference:

Sverjensky, D.A. and N. Sahai. "Theoretical Prediction of Single-Site Surface-Protonation Equilibrium Constants for Oxides and Silicates in Water." Geochimica et Cosmochimica Acta. Vol. 60. pp. 3,773-3,797. 1996.

from Sverjensky + Sahai (1996)

Table 1. FITEQL model conditions used to determine DLM binding constants for U(6+) sorption on quartz.

DLM Parameters and Chemical Model Reactions:	Quartz
Site density[a]	2.3 sites/nm^2
Surface area	0.03 m^2/g
Ionic strength	0.1 M $NaNO_3$
PCO_2	$10^{-3.5}$ atm
Sorption Reactions:	**Log K**
$>SiOH^o + H^+ \Leftrightarrow >SiOH_2^+$	-1.24[b]
$>SiOH^o \Leftrightarrow >SiO^- + H^+$	-7.06[b]
$>SiOH^o + UO_2^{2+} \Leftrightarrow >SiO\text{-}UO_2^+ + H^+$	0.31c
$>SiOH^o + UO_2^{2+} + H_2O \Leftrightarrow >SiO\text{-}UO_2OH^o + 2H^+$	-6.0[c]
$>SiOH^o + UO_2^{2+} + 2H_2O \Leftrightarrow >SiO\text{-}UO_2(OH)_2^- + 3H^+$	-12.18[c]
Aqueous Speciation Reactions:	**Log K**
$UO_2^{2+} + H_2O \Leftrightarrow UO_2OH^+ + H^+$	-5.20
$UO_2^{2+} + 2H_2O \Leftrightarrow UO_2(OH)_2^o$ (aq)$+ 2H^+$	-13.0[d]
$UO_2^{2+} + 3H_2O \Leftrightarrow UO_2(OH)_3^- + 3H^+$	-19.20
$2UO_2^{2+} + 2H_2O \Leftrightarrow (UO_2)_2(OH)_2^{2+} + 2H^+$	-5.62
$3UO_2^{2+} + 5H_2O \Leftrightarrow (UO_2)_3(OH)_5^+ + 5H^+$	-15.55
$UO_2^{2+} + CO_3^{2-} \Leftrightarrow UO_2CO_3^o$	9.68
$UO_2^{2+} + 2CO_3^{2-} \Leftrightarrow UO_2(CO_3)_2^{2-}$	16.94
$UO_2^{2+} + 3CO_3^{2-} \Leftrightarrow UO_2(CO_3)_3^{4-}$	21.60
$2UO_2^{2+} + CO_3^{2-} + 3H_2O \Leftrightarrow (UO_2)_2CO_3(OH)_3^- + 3H^+$	-0.86
$UO_2^{2+} + NO_3^- \Leftrightarrow UO_2NO_3^+$	0.30

a. Site density recommended for all minerals by Davis and Kent (1990), based on ferrihydrite work of Dzombak and Morel (1990).

b. Acidity constants for am-SiO_2 from Sverjensky and Sahai (1996).

c. This study. Binding constants determined using FITEQL, Version 2.0 (Westall, 1982a,b).

d. All aqueous speciation Log K values from NEA Uranium Thermodynamic Database (Wanner and Forrest, 1992), except for $UO_2(OH)_2^o$ (aq) which is taken from Fuger (1992).

Additional References (see page 261 for other references)

Sverjensky, D.A. 1993. Physical surface-complexation models for sorption at the mineral-water interface. *Nature* 364: 776-780.

Sverjensky, D.A. 1994. Zero-point-of-charge prediction from crystal chemistry and solvation theory. *Geochimica et Cosmochimica Acta* 58: 3123-3129.

Sverjensky, D.A., and N. Sahai. 1996. Theoretical prediction of single-site surface-protonation equilibrium constants for oxides and silicates in water. *Geochimica et Cosmochimica Acta* 60: 3773-3797.

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MINTEQA2 Input files:

```
U(VI)-Quartz sorption. U(t)=4.67 ppb; pCO2=1E-3.5; 20 g/L; 2.31 sites/nm2
XOUO2+, XOUO2OH, XOUO2(OH)2-;9/5/96 CNWRA Radionuclide Database;S&S(96)acid
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 3 3
ACTIVITY   330 33
  0.25
quartz12.123 8118930 8118931 8118932
 4   1   7
2.000E+01    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                /H+1
   893  2.004E-08   -7.70 y                /UO2+2
   492  1.000E-01   -1.00 y                /NO3-1
   500  1.000E-01   -1.00 y                /Na+1
   140  0.000E-01  -16.00 y                /CO3-2
   813  0.000E-01    0.00 y                /ADS1PSIo
   811  2.301E-06   -5.64 y                /ADS1TYP1

 2   1
8933301   -13.0000    18.0940             /uo2(oh)2
 3   2
3301403    21.6600    -0.5300             /co2 (g)
   330     2.0000     0.0000             /H+1
 6   1
   813     0.0000     0.0000             /ADS1PSIo

 2   5
8113300 >sio-              0.0000   -7.0600    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 811   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113301 >sioh2+            0.0000   -1.2400    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 811    1.000 330    1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118930 >siouo2+           0.0000    0.3100    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893   -1.000 330    1.000 813   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118931 >siouo2oh          0.0000   -6.0000    0.000    0.000 0.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893    1.000   2   -2.000 330   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 5   1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
```

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```
U(VI)-Quartz sorption. U(t)=49.88 ppb; pCO2=1E-3.5; 2 g/L; 2.31 sites/nm2
XOUO2+, XOUO2OH, XOUO2(OH)2-;9/5/96 CNWRA Radionuclide Database;S&S(96)acid
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 3 3
ACTIVITY   330 33
  0.25
quartz12.123 8118930 8118931 8118932
 4   1   7
2.000E+00    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                /H+1
   893  2.141E-07   -6.67 y                /UO2+2
   492  1.000E-01   -1.00 y                /NO3-1
   500  1.000E-01   -1.00 y                /Na+1
   140  0.000E-01  -16.00 y                /CO3-2
   813  0.000E-01    0.00 y                /ADS1PSIo
   811  2.301E-07   -6.64 y                /ADS1TYP1

 2   1
8933301   -13.0000    18.0940             /uo2(oh)2
 3   2
3301403    21.6600    -0.5300             /co2 (g)
   330     2.0000     0.0000             /H+1
 6   1
   813     0.0000     0.0000             /ADS1PSIo

 2   5
8113300 >sio-              0.0000   -7.0600    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 811   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113301 >sioh2+            0.0000   -1.2400    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 811    1.000 330    1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118930 >siouo2+           0.0000    0.3100    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893   -1.000 330    1.000 813   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118931 >siouo2oh          0.0000   -6.0000    0.000    0.000 0.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893    1.000   2   -2.000 330   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 5   1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
```

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```
U(VI)-Quartz sorption. U(t)=49.24 ppb; pCO2=1E-3.5; 20 g/L; 2.31 sites/nm2
XOUO2+, XOUO2OH, XOUO2(OH)2-;9/5/96 CNWRA Radionuclide Database;S&S(96)acid
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 3 3
ACTIVITY   330 33
  0.25
quartz12.123 8118930 8118931 8118932
 4   1   7
2.000E+01    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                /H+1
   893  2.113E-07   -6.68 y                /UO2+2
   492  1.000E-01   -1.00 y                /NO3-1
   500  1.000E-01   -1.00 y                /Na+1
   140  0.000E-01  -16.00 y                /CO3-2
   813  0.000E-01    0.00 y                /ADS1PSIo
   811  2.301E-06   -5.64 y                /ADS1TYP1

 2   1
8933301   -13.0000    18.0940             /uo2(oh)2
 3   2
3301403    21.6600    -0.5300             /co2 (g)
   330     2.0000     0.0000             /H+1
 6   1
   813     0.0000     0.0000             /ADS1PSIo

 2   5
8113300 >sio-              0.0000   -7.0600    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 811   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113301 >sioh2+            0.0000   -1.2400    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 811    1.000 330    1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118930 >siouo2+           0.0000    0.3100    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893   -1.000 330    1.000 813   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118931 >siouo2oh          0.0000   -6.0000    0.000    0.000 0.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893    1.000   2   -2.000 330   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 5   1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
```

```
U(VI)-Quartz sorption. U(t)=48.04 ppb; pCO2=1E-3.5; 50 g/L; 2.31 sites/nm2
XOUO2+, XOUO2OH, XOUO2(OH)2-;9/5/96 CNWRA Radionuclide Database;S&S(96)acid
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 3 3
ACTIVITY   330 33
  0.25
quartz12.123 8118930 8118931 8118932
 4   1   7
5.000E+01    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                /H+1
   893  2.062E-07   -6.69 y                /UO2+2
   492  1.000E-01   -1.00 y                /NO3-1
   500  1.000E-01   -1.00 y                /Na+1
   140  0.000E-01  -16.00 y                /CO3-2
   813  0.000E-01    0.00 y                /ADS1PSIo
   811  5.753E-06   -5.24 y                /ADS1TYP1

 2   1
8933301   -13.0000    18.0940             /uo2(oh)2
 3   2
3301403    21.6600    -0.5300             /co2 (g)
   330     2.0000     0.0000             /H+1
 6   1
   813     0.0000     0.0000             /ADS1PSIo

 2   5
8113300 >sio-              0.0000   -7.0600    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 811   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113301 >sioh2+            0.0000   -1.2400    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 811    1.000 330    1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118930 >siouo2+           0.0000    0.3100    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893   -1.000 330    1.000 813   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118931 >siouo2oh          0.0000   -6.0000    0.000    0.000 0.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893    1.000   2   -2.000 330   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 5   1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
```

```
U(VI)-Quartz sorption. U(t)=501.54 ppb; pCO2=1E-3.5; 50 g/L;2.31 sites/nm2
XOUO2+, XOUO2OH, XOUO2(OH)2-;9/5/96 CNWRA Radionuclide Database;S&S(96)acid
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 3 3
ACTIVITY   330 33
  0.25
quartz12.123 8118930 8118931 8118932
 4   1   7
5.000E+01    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                /H+1
   893  2.153E-06   -5.67 y                /UO2+2
   492  1.000E-01   -1.00 y                /NO3-1
   500  1.000E-01   -1.00 y                /Na+1
   140  0.000E-01  -16.00 y                /CO3-2
   813  0.000E-01    0.00 y                /ADS1PSIo
   811  5.753E-06   -5.24 y                /ADS1TYP1

 2   1
8933301   -13.0000    18.0940             /uo2(oh)2
 3   2
3301403    21.6600    -0.5300             /co2 (g)
   330     2.0000     0.0000             /H+1
 6   1
   813     0.0000     0.0000             /ADS1PSIo

 2   5
8113300 >sio-              0.0000   -7.0600    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 3   1.000 811   -1.000 330   -1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8113301 >sioh2+            0.0000   -1.2400    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 3   1.000 811    1.000 330    1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118930 >siouo2+           0.0000    0.3100    0.000    0.000 1.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893   -1.000 330    1.000 813   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118931 >siouo2oh          0.0000   -6.0000    0.000    0.000 0.00 0.00 0.00   0.0000
  0.00 4   1.000 811    1.000 893    1.000   2   -2.000 330   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000    0.000-1.00 0.00 0.00   0.0000
  0.00 5   1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
 0  0.000   0   0.000   0   0.000   0
```

MINTEQA2 Input files.

Quartz only

1/8/97 DRL

```
U(VI)-Qz-Cont sorption. U(t)=4.67 ppb; pCO2=1E-3.5; 20 g/L; 2.31 sites/nm2
XUO2+, XUO2OH, XUO2(CO3)2-; 9/5/96 CNWRA Radionuclide Database; 50b LogK
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 5 3
ACTIVITY   330 33
  0.25
qzcont12,123 8118930 8118931 8118932   38930   38931
4   1   7
2.000E+01    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                    /H+1
   893  2.004E-08   -7.70 y                    /UO2+2
   492  1.000E-01   -1.00 y                    /NO3-1
   500  1.000E-01   -1.00 y                    /Na+1
   140  0.000E-01  -16.00 y                    /CO3-2
     3  3.650E-08   -7.30 y                    /X-
   813  0.000E-01    0.00 y                    /ADS1PSIo
   811  2.301E-06   -5.64 y                    /ADS1TYP1

  2   1
8933301   -13.0000   18.0940                   /uo2(oh)2
  3   2
3301403   21.6600   -0.5300                    /co2 (g)
      3    2.0000    0.0000                    /H+1
  6   1
    813    0.0000    0.0000                    /ADS1PSIo

  2   7
8113300 >sio-              0.0000   -7.0600    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3    1.000 811   -1.000 330   -1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8113301 >siooh2+           0.0000   -1.2400    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3    1.000 811    1.000 330    1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118930 >siouo2+           0.0000    0.3100    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893   -1.000 330    1.000 813    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118931 >siouo2oh          0.0000   -6.0000    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893    1.000   2   -2.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 5    1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38930 xuo2oh            0.0000    2.6500    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    1.000 893    1.000   2   -1.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38931 x(uo2)3(oh)5      0.0000   -5.7200    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    3.000 893    5.000   2   -5.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
```

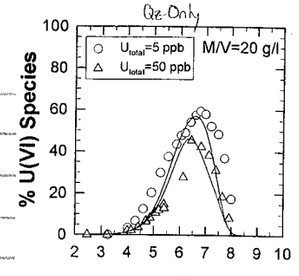
D.R.Lmm

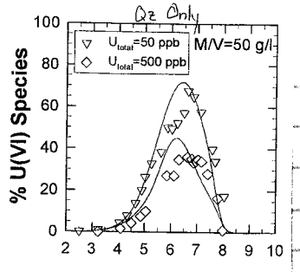
```
U(VI)-Qz-Cont sorption. U(t)=49.88 ppb; pCO2=1E-3.5; 2 g/L; 2.31 sites/nm2
XUO2+, XUO2OH, XUO2(CO3)2-; 9/5/96 CNWRA Radionuclide Database; 50b LogK
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 5 3
ACTIVITY   330 33
  0.25
qzcont12,123 8118930 8118931 8118932   38930   38931
4   1   7
2.000E+00    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                    /H+1
   893  2.141E-07   -6.67 y                    /UO2+2
   492  1.000E-01   -1.00 y                    /NO3-1
   500  1.000E-01   -1.00 y                    /Na+1
   140  0.000E-01  -16.00 y                    /CO3-2
     3  1.800E-08   -7.74 y                    /X-
   813  0.000E-01    0.00 y                    /ADS1PSIo
   811  2.301E-07   -6.64 y                    /ADS1TYP1

  2   1
8933301   -13.0000   18.0940                   /uo2(oh)2
  3   2
3301403   21.6600   -0.5300                    /co2 (g)
    330    2.0000    0.0000                    /H+1
  6   1
    813    0.0000    0.0000                    /ADS1PSIo

  2   7
8113300 >sio-              0.0000   -7.0600    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3    1.000 811   -1.000 330   -1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8113301 >siooh2+           0.0000   -1.2400    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3    1.000 811    1.000 330    1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118930 >siouo2+           0.0000    0.3100    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893   -1.000 330    1.000 813    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118931 >siouo2oh          0.0000   -6.0000    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893    1.000   2   -2.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 5    1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38930 xuo2oh            0.0000    2.6500    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    1.000 893    1.000   2   -1.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38931 x(uo2)3(oh)5      0.0000   -5.7200    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    3.000 893    5.000   2   -5.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
```

D.R.Lmm



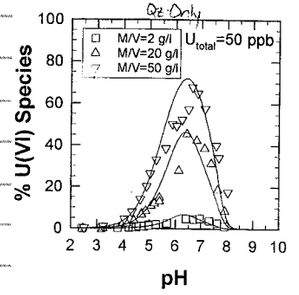


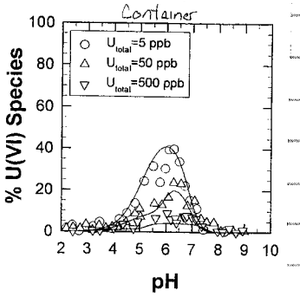
1/8/97 DRL

Qz-sorption is 0%

D.R.Lmm

MINTEQA2 U(VI)-Quartz DLM results.





Example MINTEQA2 Input files, Qz+Container

```
U(VI)-Qz-Cont sorption. U(t)=49.24 ppb; pCO2=1E-3.5; 20 g/L; 2.31 sites/nm2
XUO2+, XUO2OH, XUO2(CO3)2-; 9/5/96 CNWRA Radionuclide Database; 50b LogK
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 5 3
ACTIVITY   330 33
  0.25
qzcont12,123 8118930 8118931 8118932   38930   38931
4   1   7
2.000E+01    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                    /H+1
   893  2.113E-07   -6.68 y                    /UO2+2
   492  1.000E-01   -1.00 y                    /NO3-1
   500  1.000E-01   -1.00 y                    /Na+1
   140  0.000E-01  -16.00 y                    /CO3-2
     3  2.350E-08   -7.62 y                    /X-
   813  0.000E-01    0.00 y                    /ADS1PSIo
   811  2.301E-06   -5.64 y                    /ADS1TYP1

  2   1
8933301   -13.0000   18.0940                   /uo2(oh)2
  3   2
3301403   21.6600   -0.5300                    /co2 (g)
    330    2.0000    0.0000                    /H+1
  6   1
    813    0.0000    0.0000                    /ADS1PSIo

  2   7
8113300 >sio-              0.0000   -7.0600    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3    1.000 811   -1.000 330   -1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8113301 >siooh2+           0.0000   -1.2400    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3    1.000 811    1.000 330    1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118930 >siouo2+           0.0000    0.3100    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893   -1.000 330    1.000 813    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118931 >siouo2oh          0.0000   -6.0000    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893    1.000   2   -2.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 5    1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38930 xuo2oh            0.0000    2.6500    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    1.000 893    1.000   2   -1.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38931 x(uo2)3(oh)5      0.0000   -5.7200    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    3.000 893    5.000   2   -5.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
```

D.R.Lmm

```
U(VI)-Qz-Cont sorption. U(t)=48.04 ppb; pCO2=1E-3.5; 50 g/L; 2.31 sites/nm2
XUO2+, XUO2OH, XUO2(CO3)2-; 9/5/96 CNWRA Radionuclide Database; 50b LogK
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 5 3
ACTIVITY   330 33
  0.25
qzcont12,123 8118930 8118931 8118932   38930   38931
4   1   7
5.000E+01    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                    /H+1
   893  2.062E-07   -6.69 y                    /UO2+2
   492  1.000E-01   -1.00 y                    /NO3-1
   500  1.000E-01   -1.00 y                    /Na+1
   140  0.000E-01  -16.00 y                    /CO3-2
     3  3.500E-08   -7.46 y                    /X-
   813  0.000E-01    0.00 y                    /ADS1PSIo
   811  5.753E-06   -5.24 y                    /ADS1TYP1

  2   1
8933301   -13.0000   18.0940                   /uo2(oh)2
  3   2
3301403   21.6600   -0.5300                    /co2 (g)
    330    2.0000    0.0000                    /H+1
  6   1
    813    0.0000    0.0000                    /ADS1PSIo

  2   7
8113300 >sio-              0.0000   -7.0600    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3    1.000 811   -1.000 330   -1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8113301 >siooh2+           0.0000   -1.2400    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3    1.000 811    1.000 330    1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118930 >siouo2+           0.0000    0.3100    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893   -1.000 330    1.000 813    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118931 >siouo2oh          0.0000   -6.0000    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893    1.000   2   -2.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 5    1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38930 xuo2oh            0.0000    2.6500    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    1.000 893    1.000   2   -1.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38931 x(uo2)3(oh)5      0.0000   -5.7200    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    3.000 893    5.000   2   -5.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
```

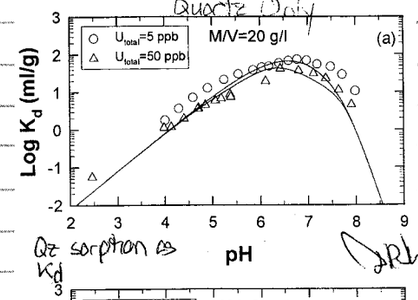
D.R.Lmm

```
U(VI)-Qz-Cont sorption. U(t)=501.54 ppb; pCO2=1E-3.5; 50 g/L;2.31 sites/nm2
XUO2+, XUO2OH, XUO2(CO3)2-; 9/5/96 CNWRA Radionuclide Database; 50b LogK
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 5 3
ACTIVITY   330 33
  0.25
qzcont12,123 8118930 8118931 8118932   38930   38931
4   1   7
5.000E+01    0.03 0.000 0.000 81
   330  0.000E-01   -2.00 y                    /H+1
   893  2.153E-06   -5.67 y                    /UO2+2
   492  1.000E-01   -1.00 y                    /NO3-1
   500  1.000E-01   -1.00 y                    /Na+1
   140  0.000E-01  -16.00 y                    /CO3-2
     3  3.000E-08   -7.52 y                    /X-
   813  0.000E-01    0.00 y                    /ADS1PSIo
   811  5.753E-06   -5.24 y                    /ADS1TYP1

  2   1
8933301   -13.0000   18.0940                   /uo2(oh)2
  3   2
3301403   21.6600   -0.5300                    /co2 (g)
    330    2.0000    0.0000                    /H+1
  6   1
    813    0.0000    0.0000                    /ADS1PSIo

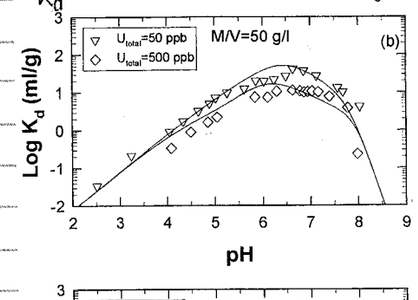
  2   7
8113300 >sio-              0.0000   -7.0600    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 3    1.000 811   -1.000 330   -1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8113301 >siooh2+           0.0000   -1.2400    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 3    1.000 811    1.000 330    1.000 813    0.000    0    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118930 >siouo2+           0.0000    0.3100    0.000   0.000 1.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893   -1.000 330    1.000 813    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118931 >siouo2oh          0.0000   -6.0000    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000 811    1.000 893    1.000   2   -2.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8118932 >siouo2(oh)2       0.0000  -12.1800    0.000   0.000-1.00 0.00 0.00   0.0000
  0.00 5    1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38930 xuo2oh            0.0000    2.6500    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    1.000 893    1.000   2   -1.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
   38931 x(uo2)3(oh)5      0.0000   -5.7200    0.000   0.000 0.00 0.00 0.00   0.0000
  0.00 4    1.000   3    3.000 893    5.000   2   -5.000 330    0.000    0    0.000    0
    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
```

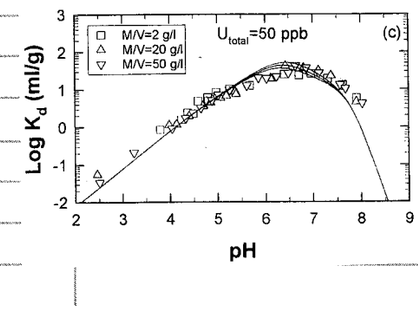
D.R.Lmm



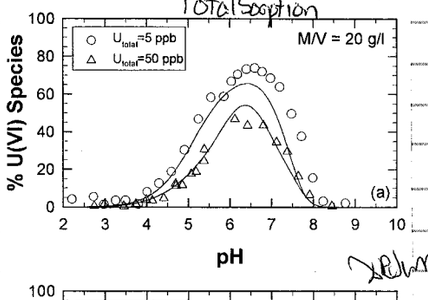
Qz sorption as Kd

D.R.Lmm





Total Sorption



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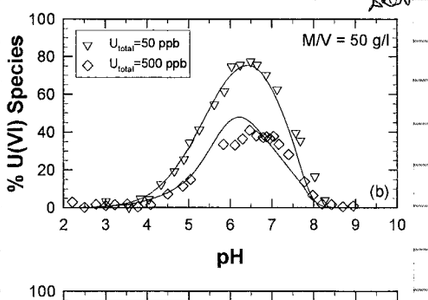

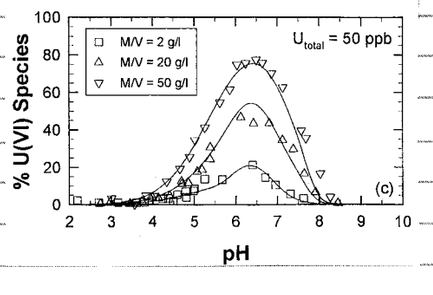

U(VI)-α-Al_2O_3 Sorption

U(VI)-α-Al_2O_3 sorption was revisited yet again using the DLM, a simplified container sorption model, and the DLM acidity coefficients of Sverjensky and Sahai (1996).

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Acidity constants from Sverjensky and Sahai (1996)

Sverjensky and Sahai (1996) developed a method to determine DLM acidity constants using Born solvation theory. The details are provided in Sverjensky (1993, 1994) and Sverjensky and Sahai (1996). For quartz, assuming a site density of 2.3 sites/nm^2, equations (146), Figure 7b, and data from Table 1 were used to determine Log K_+ and Log K_-.

From equation (146):

$$pH_{ZPC} = (\log K_+ - \log K_-)/2$$
$$pH_{ZPC} = 21.1158(1/\epsilon_k) - 42.9148(s/r_{M\text{-}OH}) + 14.6866$$

From Table 1, for α-Al_2O_3(corundum):

$$\epsilon_k = 10.43$$
Pauling Bond Strength $s/r_{M\text{-}OH} = 0.1711$

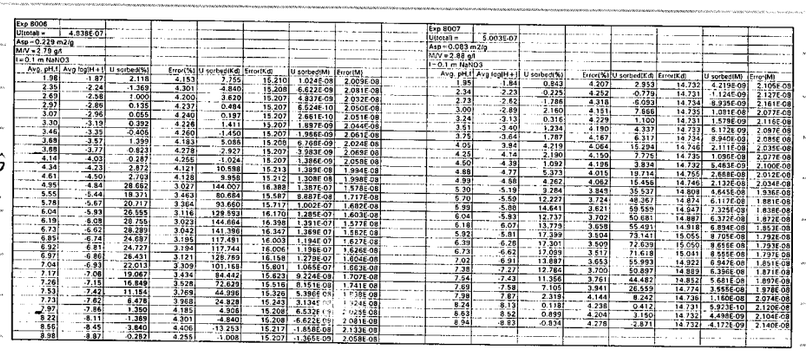
From Figure 7b (DLM with site density = 2.3 sites/nm^2):

$$K_n = \log K_+ + \log K_-$$
$$K_n = 30.143\ (s/r_{M\text{-}OH}) - 3.214$$

Therefore, for α-Al_2O_3:

$pH_{ZPC} = 9.37$
$K_n = 1.94$
$K_+ = 10.34$
$K_- = -8.40$

Like U(VI)-Quartz, three surface complexes >AlO-UO_2^+, >AlO-UO_2OH°, and >AlO-$UO_2(OH)_2^-$ provided the best fit the observed data. The resulting binding constants are given below.



CNLRA data for experiments RM 8006 & RM 8007

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Table 1. FITEQL model conditions used to determine DLM binding constants for U(6+) sorption on α-Al_2O_3:

DLM Parameters and Chemical Model Reactions:	α-Al_2O_3
Site density[a]	2.3 sites/nm^2
Surface area	0.229 and 0.083 m^2/g
Ionic strength	0.1 M $NaNO_3$
PCO_2	$10^{-3.5}$ atm
Sorption Reactions:	**Log K**
>AlOH° + H^+ ⇔ >$AlOH_2^+$	10.34[b]
>AlOH° ⇔ >AlO^- + H^+	-8.40[b]
>AlOH° + UO_2^{2+} ⇔ >AlO-UO_2^+ + H^+	4.60[c]
>AlOH° + UO_2^{2+} + H_2O ⇔ >AlO-UO_2OH° + $2H^+$	-4.39[c]
>AlOH° + UO_2^{2+} + $2H_2O$ ⇔ >AlO-$UO_2(OH)_2^-$ + $3H^+$	-13.60[c]
Aqueous Speciation Reactions:	**Log K**
UO_2^{2+} + H_2O ⇔ UO_2OH^+ + H^+	-5.20
UO_2^{2+} + $2H_2O$ ⇔ $UO_2(OH)_2^\circ$ (aq)+ $2H^+$	-13.0[d]
UO_2^{2+} + $3H_2O$ ⇔ $UO_2(OH)_3^-$ + $3H^+$	-19.20
$2UO_2^{2+}$ + $2H_2O$ ⇔ $(UO_2)_2(OH)_2^{2+}$ +$2H^+$	-5.62
$3UO_2^{2+}$ + $5H_2O$ ⇔ $(UO_2)_3(OH)_5^+$ + $5H^+$	-15.55
UO_2^{2+} + CO_3^{2-} ⇔ $UO_2CO_3^\circ$	9.68
UO_2^{2+} + $2CO_3^{2-}$ ⇔ $UO_2(CO_3)_2^{2-}$	16.94
UO_2^{2+} + $3CO_3^{2-}$ ⇔ $UO_2(CO_3)_3^{4-}$	21.60
$2UO_2^{2+}$ + CO_3^{2-} + $3H_2O$ ⇔ $(UO_2)_2CO_3(OH)_3^-$ + $3H^+$	-0.86
UO_2^{2+} + NO_3^- ⇔$UO_2NO_3^+$	0.30

a. Site density recommended for all minerals by Davis and Kent (1990), based on ferrihydrite work of Dzombak and Morel (1990).
b. Acidity constants for am-SiO_2 from Sverjensky and Sahai (1996).
c. This study. Binding constants determined using FITEQL, Version 2.0 (Westall, 1982a,b).
d. All aqueous speciation Log K values from NEA Uranium Thermodynamic Database (Wanner and Forrest, 1992), except for $UO_2(OH)_2^\circ$ (aq) which is taken from Fuger (1992).

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```
U(VI)-Al2O3 (alpha); Atmospheric CO2; 116.57 ppb; RM 8007 (0.083 m2/g)
DLM; XOUO2+; XOUO2OH & XOUO2(OH)2-; 9/5/96 CNWRA Database
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 3 3
ACTIVITY   330 33
   0.25
al2o3c.123    8118930 8118931 8118932
4   1   7
2.880E-00   0.0830 0.000 0.000 81
    330   0.000E-01   -2.00 y                 /H+1
    893   5.003E-07   -6.30 y                 /UO2+2
    500   1.000E-01   -1.00 y                 /Na+1
    492   1.000E-01   -1.00 y                 /NO3-1
    140   0.000E-01   -16.00 y                /CO3-2
    813   0.000E-01    0.00 y                 /ADS1PSIo
    811   9.168E-07   -6.04 y                 /ADS1TYP1

  2   1
8933301   -13.0000    18.0940                 /UO2(OH)2
  3   2
3301403    21.6600    -0.5300                 /CO2 (g)
    330     2.0000     0.0000                 /H+1
  6   1
    813     0.0000     0.0000                 /ADS1PSIo

  2   5
8113300 >alOH2+          0.0000   10.3400   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3    1.000 811    1.000 330    1.000 813   0.000    0   0.000    0   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
8113301 >alO-            0.0000   -8.4000   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3    1.000 811   -1.000 330   -1.000 813   0.000    0   0.000    0   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
8118930 >alouo2+         0.0000    4.6000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 4    1.000 811    1.000 893   -1.000 330    1.000 813   0.000    0   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
8118931 >alouo2oh        0.0000   -4.3900   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 4    1.000 811    1.000 893    1.000   2   -2.000 330   0.000    0   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
8118932 >alouo2(oh)2     0.0000  -13.6000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5    1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
```

```
U(VI)-Al2O3 (alpha); Atmospheric CO2; 112.72 ppb; RM 8006 (0.229 m2/g)
DLM; XOUO2+; XOUO2OH & XOUO2(OH)2-; 9/5/96 CNWRA Database
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 1 3 3
ACTIVITY   330 33
   0.25
al2o3c.123    8118930 8118931 8118932
4   1   7
2.790E-00   0.209 0.000 0.000 81
    330   0.000E-01   -2.00 y                 /H+1
    893   4.838E-07   -6.32 y                 /UO2+2
    500   1.000E-01   -1.00 y                 /Na+1
    492   1.000E-01   -1.00 y                 /NO3-1
    140   0.000E-01   -16.00 y                /CO3-2
    813   0.000E-01    0.00 y                 /ADS1PSIo
    811   2.450E-06   -5.61 y                 /ADS1TYP1

  2   1
8933301   -13.0000    18.0940                 /UO2(OH)2
  3   2
3301403    21.6600    -0.5300                 /CO2 (g)
    330     2.0000     0.0000                 /H+1
  6   1
    813     0.0000     0.0000                 /ADS1PSIo

  2   5
8113300 >alOH2+          0.0000   10.3400   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3    1.000 811    1.000 330    1.000 813   0.000    0   0.000    0   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
8113301 >alO-            0.0000   -8.4000   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3    1.000 811   -1.000 330   -1.000 813   0.000    0   0.000    0   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
8118930 >alouo2+         0.0000    4.6000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 4    1.000 811    1.000 893   -1.000 330    1.000 813   0.000    0   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
8118931 >alouo2oh        0.0000   -4.3900   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 4    1.000 811    1.000 893    1.000   2   -2.000 330   0.000    0   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
8118932 >alouo2(oh)2     0.0000  -13.6000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5    1.000 811    1.000 893    2.000   2   -3.000 330   -1.000 813   0.000   0
   0.000    0   0.000    0   0.000    0   0.000    0   0.000    0   0.000   0
 0  0.000    0   0.000    0   0.000    0
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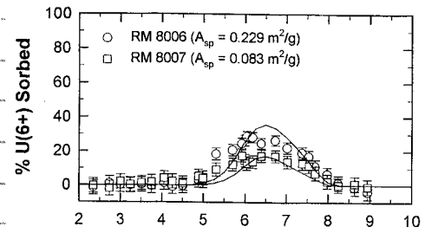
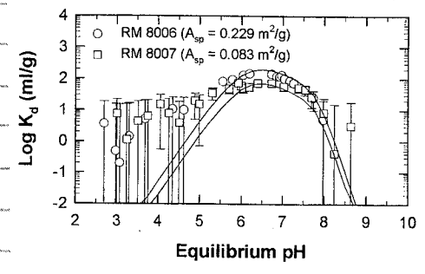


MINTEQA2
DLM Results
U(VI)-αAl_2O_3



Notebook closed due to closing of Radionuclide Transport KTI (20-5708-871). Final deliverables transmitted to NRC.

I have reviewed this notebook and find it in general compliance with QAP-001. There is sufficient information for another qualified person to conduct the activities.

E. C. [illegible]

1/13/87

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK #: 046

Document Date:	06/02/1992
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	■"Non-Sensitive" □ Sensitive □"Non-Sensitive - Copyright" □ Sensitive - Copyright
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Operating System: (including version number)	NA
Application Used: (including version number)	MINTEQA2, Version 3.11; FITEQL, Version 2.0
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	4 - 3 ½ disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Media contains: MINTEQA2 database dated 1991; analog master lists files; sorption modeling for high-level waste performance assessment.

Original MINTEQA2 Data:

GASES.DBS

1/67

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3301404 CH4 (g)      -61.0      40.1                                          16.0432
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3301403 CO2 (g)      -0.53      18.16                                         41.0100
      3      1.000 140      2.000 330     -1.000   2
3300021 O2 (g)       133.83     -83.12                                        31.9988
      3      2.000   2     -4.000 330     -4.000   1
3600001 Hg (g)       -5.265     7.8708                                        200.5900
 0.00 2      0.500 360      1.000   1
3600002 Hg2 (g)      -13.87     14.963                                        401.1800
 0.00 2      1.000 360      2.000   1
3611400 Hg(CH3)2(g) -115.4      73.724                                        230.6594
 0.00 5      1.000 361      2.000 140    16.000   1     20.000 330    -8.000   2
3601300 HgBr (g)     34.004     -16.79                                        280.4940
 0.00 2      0.500 360      1.000 130
3601800 HgCl (g)     40.098     -20.50                                        236.0430
 0.00 2      0.500 360      1.000 180
3602700 HgF (g)      60.916     -32.72                                        219.5884
 0.00 2      0.500 360      1.000 270
3603800 HgI (g)      25.264     -11.15                                        327.4945
 0.00 2      0.500 360      1.000 380
3611300 HgBr2 (g)    -14.35     18.47                                         360.3980
 0.00 4      1.000 361      2.000 130     2.000 330     -2.000   2
3612700 HgF2 (g)     0.0000     -0.38                                         238.5868
 0.00 4      1.000 361      2.000 270     2.000 330     -2.000   2
3613800 HgI2 (g)     -28.63     27.28                                         454.3990
 0.00 4      1.000 361      2.000 380     2.000 330     -2.000   2

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Original MINTEQA2 Data:

THERMO.DBS


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3300020 OH-          13.345    -13.998                    -1. 3.5  0.0  17.0074
      2     1.000    2    -1.000 330
3307700 H3SiO4 -     8.9350    -9.9300                    -1. 4.0  0.0  95.1070
      2     1.000 770    -1.000 330
3307701 H2SiO4 -2   29.7140   -21.6190                    -2. 5.4  0.0  94.0990
      2     1.000 770    -2.000 330
7702700 SiF6 -2     -16.2600  30.1800                    -2. 5.0  0.0  142.0760
      4     1.000 770     6.000 270     4.000 330    -4.000   2
3300900 H2BO3 -1     3.2240    -9.2400                    -1. 2.5  0.0  60.8250
      2     1.000  90    -1.000 330
0902700 BF(OH)3 -    1.8500    -0.3990                    -1. 2.5  0.0  80.8310
      2     1.000  90     1.000 270
0902701 BF2(OH)2 -  1.63500    7.63000                    -1. 2.5  0.0  82.8220
      4     1.000  90     2.000 270    -1.000   2     1.000 330
0902702 BF3OH -     -1.5800   13.66700                    -1. 2.5  0.0  84.8130
      4     1.000  90     3.000 270    -2.000   2     2.000 330
0902703 BF4 -       -1.7950   20.27400                    -1. 2.5  0.0  86.8040
      4     1.000  90     4.000 270    -3.000   2     3.000 330
3304900 NH3 AQ       12.4800   -9.2520                     0. 0.0  0.0  17.0300
      2     1.000 490    -1.000 330
4907320 NH4SO4 -     0.0000    1.1100                     -1. 5.0  0.0  114.1000
      2     1.000 490     1.000 732
1603300 MgOH +       15.935    -11.79                      1. 6.5  0.0  41.3190
      3     1.000 460     1.000   2    -1.000 330
4602700 MgF +        4.6740    1.8200                      1. 4.5  0.0  43.3100
      2     1.000 460     1.000 270
4601400 MgCO3 AQ     2.0220    2.9800                      0. 0.0  0.0  84.3210
 2.00 2     1.000 460     1.000 140
4601401 MgHCO3 +     -2.430    11.400                      1. 4.0  0.0  85.3290
 1.00 3     1.000 460     1.000 140     1.000 330
4607320 MgSO4 AQ     1.3990    2.2500                      0. 0.0  0.0  120.3730
      2     1.000 460     1.000 732
4605800 MgPO4 -      3.1000    6.5890                     -1. 5.4  0.0  119.2830
      2     1.000 460     1.000 580
4605801 MgH2PO4 +    -1.120    21.066                      1. 5.4  0.0  121.2990
      3     1.000 460     1.000 580     2.000 330
4605802 MgHPO4 AQ    -0.230    15.220                      0. 0.0  0.0  120.2910
      3     1.000 460     1.000 580     1.000 330
1503300 CaOH +       14.535    -12.598                     1. 6.0  0.0  57.0870
      3     1.000 150     1.000   2    -1.000 330
1501400 CaHCO3 +     1.7900    11.330                      1. 6.0  0.0  101.0970
 1.00 3     1.000 150     1.000 140     1.000 330
1501401 CaCO3 AQ     4.0300    3.1500                      0. 0.0  0.0  100.0890
 2.00 2     1.000 150     1.000 140
1507320 CaSO4 AQ     1.4700    2.3090                      0. 0.0  0.0  136.1410
      2     1.000 150     1.000 732
1505800 CaHPO4 AQ    -0.230    15.085                      0. 0.0  0.0  136.0590
      3     1.000 150     1.000 580     1.000 330
1505801 CaPO4 -      3.1000    6.4590                     -1. 5.4  0.0  135.0510
      2     1.000 150     1.000 580
1505802 CaH2PO4 +    -1.120    20.960                      1. 5.4  0.0  137.0670
      3     1.000 150     1.000 580     2.000 330
1502700 CaF +        3.7980    0.9400                      1. 5.0  0    59.0780
      2     1.000 150     1.000 270
5001400 NaCO3 -      8.9110    1.2680                     -1. 5.4  0.0  82.9990
 2.00 2     1.000 500     1.000 140
5001401 NaHCO3 AQ    0.0000    10.0800                     0. 0.0  0.0  84.0070
 1.00 3     1.000 500     1.000 140     1.000 330
5007320 NaSO4 -      1.1200    0.7000                     -1. 5.4  0.0  119.0510
      2     1.000 500     1.000 732
5005800 NaHPO4 -     0.0000    12.636                     -1. 5.4  0.0  118.9690
      3     1.000 500     1.000 580     1.000 330
5002700 NaF AQ       0.0000    -0.7900                     0. 0.0  0.0  41.9880
      2     1.000 500     1.000 270
4107320 KSO4 -       2.2500    0.8500                     -1. 5.4  0.0  135.1630
```

```
      2     1.000 410     1.000 732
4105800 KHPO4 -     0.0000    12.640                          -1. 5.4  0.0  135.0810
      3     1.000 410     1.000 580     1.000 330
0303300 AlOH +2     11.8990   -4.9900                          2. 5.4  0.0  43.9880
      3     1.000  30     1.000   2    -1.000 330
0303301 Al(OH)2 +   0.0000    -10.1000                        1. 5.4  0.0  60.9960
      3     1.000  30     2.000   2    -2.000 330
0303302 Al(OH)4 -   44.0600   -23.0000                        -1. 4.5  0.0  95.0110
      3     1.000  30     4.000   2    -4.000 330
0302700 AlF +2      0.0000    7.0100                          2. 5.4  0.0  45.9790
      2     1.000  30     1.000 270
0302701 AlF2 +      20.0000   12.7500                         1. 5.4  0.0  64.9780
      2     1.000  30     2.000 270
0302702 AlF3 AQ     2.5000    17.0200                         0. 0.0  0.0  83.9760
      2     1.000  30     3.000 270
0302703 AlF4 -      0.0000    19.7200                         -1. 4.5  0.0  102.9750
      2     1.000  30     4.000 270
0307320 AlSO4 +     2.1500    3.0200                          1. 4.5  0.0  123.0430
      2     1.000  30     1.000 732
0307321 Al(SO4)2 -  2.8400    4.9200                          -1. 4.5  0.0  219.1040
      2     1.000  30     2.000 732
0303303 Al(OH)3 AQ  0.0000    -16.0000                        0. 0.0  0.0  78.0030
      3     1.000  30     3.000   2    -3.000 330
2803300 FeOH +      13.1990   -9.5000                         1. 5.0  0.0  72.8540
      3     1.000 280     1.000   2    -1.000 330
2803301 FeOH3 -1    30.3000   -31.0000                        -1. 5.0  0.0  106.8690
      3     1.000 280     3.000   2    -3.000 330
2807320 FeSO4 AQ    3.2300    2.2500                          0. 0.0  0.0  151.9080
      2     1.000 280     1.000 732
2805800 FeH2PO4 +   0.0000    22.253                          1. 5.4  0.0  152.8340
      3     1.000 280     1.000 580     2.000 330
2803302 FeOH2 AQ    28.5650   -20.5700                        0. 0.0  0.0  89.8610
      3     1.000 280     2.000   2    -2.000 330
2805801 FeHPO4 AQ   0.0000    15.950                          0. 0.0  0.0  151.8260
      3     1.000 280     1.000 580     1.000 330
2807300 Fe(HS)2 AQ  0.0000    8.9500                          0. 0.0  0.0  121.9900
      2     1.000 280     2.000 730
2807301 Fe(HS)3 -   0.0000    10.9870                         -1. 0.0  0.0  155.0620
      2     1.000 280     3.000 730
2813300 FeOH +2     10.3990   -2.1900                         2. 5.0  0.0  72.8540
      3     1.000 281     1.000   2    -1.000 330
2815800 FeHPO4 +    -7.300    17.780                          1. 5.4  0.0  151.8260
      3     1.000 281     1.000 580     1.000 330
2817320 FeSO4 +     3.9100    3.9200                          1. 5.0  0.0  151.9080
      2     1.000 281     1.000 732
2811800 FeCl +2     5.6000    1.4800                          2. 5.0  0.0  91.3000
      2     1.000 281     1.000 180
2811801 FeCl2 +     0.0000    2.1300                          1. 5.0  0.0  126.7530
      2     1.000 281     2.000 180
2811802 FeCl3 AQ    0.0000    1.1300                          0. 0.0  0.0  162.2060
      2     1.000 281     3.000 180
2813301 FeOH2 +     0.0000    -5.6700                         1. 5.4  0.0  89.8610
      3     1.000 281     2.000   2    -2.000 330
2813302 FeOH3 AQ    0.0000    -13.6000                        0. 0.0  0.0  106.8690
      3     1.000 281     3.000   2    -3.000 330
2813303 FeOH4 -     0.0000    -21.6000                        -1. 5.4  0.0  123.8760
      3     1.000 281     4.000   2    -4.000 330
2815801 FeH2PO4 +2  0.0000    24.980                          2. 5.4  0.0  152.8340
      3     1.000 281     1.000 580     2.000 330
2812700 FeF +2      2.6990    6.1990                          2. 5.0  0.0  74.8450
      2     1.000 281     1.000 270
2812701 FeF2 +      4.8000    10.8000                         1. 5.0  0.0  93.8430
      2     1.000 281     2.000 270
2812702 FeF3 AQ     5.3990    14.000                          0. 0.0  0.0  112.8420
      2     1.000 281     3.000 270
2817321 Fe(SO4)2 -  4.6000    5.4200                          -1. 0.0  0.0  247.9700
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      2     1.000 281     2.000 732
2819900 Fe FULVATE  0.0000    9.3990                          1. 0.0  0.0  705.8470
      2     1.000 281     1.000 990
2819910 Fe HUMATE   0.0000    9.3990                          1. 0.0  0.0  2055.8460
      2     1.000 281     1.000 991
2813304 Fe2(OH)2+4  13.5000   -2.9500                          4. 0.0  0.0  145.7080
      3     2.000 281     2.000   2    -2.000 330
2813305 Fe3(OH)4+5  14.3000   -6.3000                          5. 0.0  0.0  235.5700
      3     3.000 281     4.000   2    -4.000 330
4407320 LiSO4 -     0.0000    0.6400                         -1. 5.0  0.0  103.0000
      2     1.000 440     1.000 732
8003300 SrOH +      14.495    -13.178                          1. 5.0  0.0  104.6270
      3     1.000 800     1.000   2    -1.000 330
1003300 BaOH +      15.095    -13.358                          1. 5.0  0.0  154.3470
      3     1.000 100     1.000   2    -1.000 330
4701800 MnCl +      0.0000    0.6070                           1. 5.0  0.0  90.3910
      2     1.000 470     1.000 180
4701801 MnCl2 AQ    0.0000    0.0410                           0. 0.0  0.0  125.8440
      2     1.000 470     2.000 180
4701802 MnCl3 -     0.0000    -.30500                         -1. 5.0  0.0  161.2970
      2     1.000 470     3.000 180
4703300 MnOH +      14.3990   -10.5900                         1. 5.0  0.0  161.2970
      3     1.000 470     1.000   2    -1.000 330
4703301 Mn(OH)3 -1  0.0000    -34.8000                        -1. 5.0  0.0  105.9600
      3     1.000 470     3.000   2    -3.000 330
4700020 MnO4 -      176.6200  -127.8240                       -1. 3.0  0.0  118.9350
      4     1.000 470     4.000   2    -8.000 330   -5.000   1
4700021 MnO4 -2     150.0200  -118.4400                       -2. 5.0  0.0  118.9350
      4     1.000 470     4.000   2    -8.000 330   -4.000   1
4702700 MnF +       0.0000    0.8500                           1. 5.0  0.0  73.9360
      2     1.000 470     1.000 270
4707320 MnSO4 AQ    2.1700    2.2600                           0. 0.0  0.0  150.9990
      2     1.000 470     1.000 732
4704920 Mn(NO3)2AQ  -0.3960   0.6000                           0. 0.0  0.0  178.9470
      2     1.000 470     2.000 492
4701400 MnHCO3 +    0.0000    11.600                           1. 5.0  0.0  115.9550
 1.00 3     1.000 470     1.000 140     1.000 330
2301800 CuCl2 -     -0.42     5.5                             -1. 4.0  0.0  134.452
      2     1.000 230     2.000 180
2301801 CuCl3 -2    0.26      5.70                            -2. 5.0  0.0  169.905
      2     1.000 230     3.000 180
2307300 Cu(S4)2 -3  0.0       3.39                            -3. 23.0 0.0  320.058
      4     1.000 230     2.000 730     6.000 731    -2.000 330
2307301 CuS4S5 -3   0.0       2.66                            -3. 25.0 0.0  352.122
      4     1.000 230     2.000 730     7.000 731    -2.000 330
2319921 Cu ACETATE  0.0       2.22                             1. 0.0  0.0  122.5900
      2     1.000 231     1.000 992
2319941 Cu GLYCINE  0.0       8.62                             1. 0.0  0.0  137.6100
      2     1.000 231     1.000 994
2319942 Cu2GLYCINE  0.0       15.64                            3. 0.0  0.0  201.1500
      2     2.000 231     1.000 994
2319951 Cu SALICYL  0.0       10.640                           0. 0.0  0.0  199.6600
      2     1.000 231     1.000 995
2319952 Cu2SALICYL  0.0       16.940                           2. 0.0  0.0  263.20
      2     2.000 231     1.000 995
2319961 Cu GLUTAMA  0.0       8.33                             0. 0.0  0.0  208.6700
      2     1.000 231     1.000 996
2319962 Cu2GLUTAMA  0.0       14.84                            2. 0.0  0.0  272.2100
      2     2.000 231     1.000 996
2319972 Cu2PHTHALA  0.0       5.3                              2. 0.0  0.0  291.2100
      2     2.000 231     1.000 997
2311400 CuCO3 AQ    0.0000    6.7300                           0. 0.0  0.0  123.5550
 2.00 2     1.000 231     1.000 140
2311401 Cu(CO3)2-2  0.0000    9.8300                          -2. 0.0  0.0  183.5640
 4.00 2     1.000 231     2.000 140
2311800 CuCl +      8.6500    0.4300                           1. 4.0  0.0  98.9990
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      2     1.000 231     1.000 180
2311801 CuCl2 AQ    10.5600   0.1600                          0. 0.0  0.0  134.4520
      2     1.000 231     2.000 180
2311802 CuCl3 -     13.6900   -2.2900                        -1. 4.0  0.0  169.9050
      2     1.000 231     3.000 180
2311803 CuCl4 -2   17.7800    -4.5900                        -2. 5.0  0.0  205.3580
      2     1.000 231     4.000 180
2312700 CuF +       1.6200    1.2600                          1. 0.0  0.0  82.5440
      2     1.000 231     1.000 270
2313300 CuOH +      0.0000    -8.0000                         1. 4.0  0.0  80.5530
      3     1.000 231     1.000   2    -1.000 330
2313301 Cu(OH)2 AQ  0.0000    -13.6800                        0. 0.0  0.0  97.5600
      3     1.000 231     2.000   2    -2.000 330
2313302 Cu(OH)3 -   0.0000    -26.8990                       -1. 0.0  0.0  114.5680
      3     1.000 231     3.000   2    -3.000 330
2313303 Cu(OH)4 -2  0.0000    -39.6000                       -2. 0.0  0.0  131.5750
      3     1.000 231     4.000   2    -4.000 330
2313304 Cu2(OH)2+2  17.5390   -10.3590                        2. 0.0  0.0  161.1060
      3     2.000 231     2.000   2    -2.000 330
2317320 CuSO4 AQ    1.2200    2.3100                          0. 0.0  0.0  159.6070
      2     1.000 231     1.000 732
2317300 Cu(HS)3 -   0.0000    25.8990                        -1. 0.0  0.0  162.7610
      2     1.000 231     3.000 730
2311402 CuHCO3 +    0.0000    13.000                          1. 0.0  0.0  124.5630
 1.00 3     1.000 231     1.000 140     1.000 330
2319900 Cu FULVATE  0.0000    0.0000                          0. 0.0  0.0  713.5460
      2     1.000 231     1.000 990
2319910 Cu HUMATE   0.0000    0.0000                          0. 0.0  0.0  2063.5450
      2     1.000 231     1.000 991
9501800 ZnCl +      7.7900    0.4300                          1. 4.0  0.0  100.8230
      2     1.000 950     1.000 180
9501801 ZnCl2 AQ    8.5000    0.4500                          0. 0.0  0.0  136.2760
      2     1.000 950     2.000 180
9501802 ZnCl3 -     9.5600    0.5000                         -1. 4.0  0.0  171.7290
      2     1.000 950     3.000 180
9501803 ZnCl4 -2    10.9600   0.1990                         -2. 5.0  0.0  207.1820
      2     1.000 950     4.000 180
9502700 ZnF +       2.2200    1.1500                          1. 0.0  0.0  84.3680
      2     1.000 950     1.000 270
9503300 ZnOH +      13.3990   -8.9600                         1. 0.0  0.0  82.3770
      3     1.000 950     1.000   2    -1.000 330
9503301 Zn(OH)2 AQ  0.0000    -16.8990                        0. 0.0  0.0  99.3840
      3     1.000 950     2.000   2    -2.000 330
9503302 Zn(OH)3 -   0.0000    -28.3990                       -1. 0.0  0.0  116.3920
      3     1.000 950     3.000   2    -3.000 330
9503303 Zn(OH)4 -2  0.0000    -41.1990                       -2. 0.0  0.0  133.3990
      3     1.000 950     4.000   2    -4.000 330
9501804 ZnOHCl AQ   0.0000    -7.4800                         0. 0.0  0.0  117.8300
      4     1.000 950     1.000   2    -1.000 330    1.000 180
9507300 Zn(HS)2 AQ  0.0000    14.9400                         0. 0.0  0.0  131.5130
      2     1.000 950     2.000 730
9507301 Zn(HS)3 -   0.0000    16.1000                        -1. 0.0  0.0  164.5850
      2     1.000 950     3.000 730
9507320 ZnSO4 AQ    1.3600    2.3700                          0. 0.0  0.0  161.4310
      2     1.000 950     1.000 732
9507321 Zn(SO4)2-2  0.0000    3.2800                         -2. 0.0  0.0  257.4930
      2     1.000 950     2.000 732
9501300 ZnBr +      0.0000    -0.5800                         1. 0.0  0.0  145.2740
      2     1.000 950     1.000 130
9501301 ZnBr2 AQ    0.0000    -0.9800                         0. 0.0  0.0  225.1780
      2     1.000 950     2.000 130
9503800 ZnI +       0.0000    -2.9100                         1. 0.0  0.0  192.2740
      2     1.000 950     1.000 380
9503801 ZnI2 AQ     0.0000    -1.6900                         0. 0.0  0.0  319.1780
      2     1.000 950     2.000 380
9501400 ZnHCO3 +    0.0000    12.400                          1. 0.0  0.0  126.3570
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 1.00 3     1.000 950     1.000 140     1.000 330
9501401 ZnCO3 AQ    0.0000    5.3000                      0. 0.0  0.0  125.3790
 2.00 2     1.000 950     1.000 140
9501402 Zn(CO3)2-2  0.0000    9.6300                     -2. 0.0  0.0  185.3580
 4.00 2     1.000 950     2.000 140
1601800 CdCl +      0.5900    1.9800                      1. 0.0  0.0  147.8530
      2     1.000 160     1.000 180
1601801 CdCl2 AQ    1.2400    2.6000                      0. 0.0  0.0  183.3060
      2     1.000 160     2.000 180
1601802 CdCl3 -     3.9000    2.3990                     -1. 0.0  0.0  218.7590
      2     1.000 160     3.000 180
1602700 CdF +       0.0000    1.1000                      1. 0.0  0.0  131.3980
      2     1.000 160     1.000 270
1602701 CdF2 AQ     0.0000    1.5000                      0. 0.0  0.0  150.3960
      2     1.000 160     2.000 270
1601400 Cd(CO3)3-4  0.0000    6.2200                     -4. 0.0  0.0  292.4280
 6.00 2     1.000 160     3.000 140
1603300 CdOH +      13.1000   -10.0800                    1. 0.0  0.0  129.4070
      3     1.000 160     1.000   2    -1.000 330
1603301 Cd(OH)2 AQ  0.0000    -20.3500                    0. 0.0  0.0  146.4140
      3     1.000 160     2.000   2    -2.000 330
1603302 Cd(OH)3 -   0.0000    -33.3000                   -1. 0.0  0.0  163.4220
      3     1.000 160     3.000   2    -3.000 330
1603303 Cd(OH)4 -2  0.0000    -47.3500                   -2. 0.0  0.0  180.4290
      3     1.000 160     4.000   2    -4.000 330
1603304 Cd2OH +3    10.8990   -9.3900                     3. 0.0  0.0  241.8074
      3     2.000 160     1.000   2    -1.000 330
1601803 CdOHCl AQ   4.3550    -7.4040                     0. 0.0  0.0  164.8600
      4     1.000 160     1.000   2    -1.000 330    1.000 180
1604920 CdNO3 +     -5.2000   0.3990                      1. 0.0  0.0  174.4040
      2     1.000 160     1.000 492
1607320 CdSO4 AQ    1.0800    2.4600                      0. 0.0  0.0  208.4610
      2     1.000 160     1.000 732
1607300 CdHS +      0.0000    10.1700                     1. 0.0  0.0  145.4720
      2     1.000 160     1.000 730
1607301 Cd(HS)2 AQ  0.0000    16.5300                     0. 0.0  0.0  178.5430
      2     1.000 160     2.000 730
1607302 Cd(HS)3 -   0.0000    18.7100                    -1. 0.0  0.0  211.6150
      2     1.000 160     3.000 730
1607303 Cd(HS)4 -2  0.0000    20.9000                    -2. 0.0  0.0  244.6870
      2     1.000 160     4.000 730
1601300 CdBr +      -0.8100   2.1700                      1. 0.0  0.0  192.3040
      2     1.000 160     1.000 130
1601301 CdBr2 AQ    0.0000    2.8990                      0. 0.0  0.0  272.2080
      2     1.000 160     2.000 130
1603800 CdI +       -2.3700   2.1500                      1. 0.0  0.0  239.3040
      2     1.000 160     1.000 380
1603801 CdI2 AQ     0.0000    3.5900                      0. 0.0  0.0  366.2080
      2     1.000 160     2.000 380
1601400 CdHCO3 +    0.0000    12.400                      1. 0.0  0.0  173.4170
 1.00 3     1.000 160     1.000 140     1.000 330
1601401 CdCO3 AQ    0.0000    5.3990                      0. 0.0  0.0  172.4090
 2.00 2     1.000 160     1.000 140
1607321 Cd(SO4)2-2  0.0000    3.5000                     -2. 0.0  0.0  208.4610
      2     1.000 160     2.000 732
1609900 Cd FULVATE  0.0000    0.0000                      0. 0.0  0.0  762.3990
      2     1.000 160     1.000 990
1609910 Cd HUMATE   0.0000    0.0000                      0. 0.0  0.0  2112.3990
      2     1.000 160     1.000 991
6001800 PbCl +      4.3800    1.6000                      1. 0.0  0.0  242.6430
      2     1.000 600     1.000 180
6001801 PbCl2 AQ    1.0800    1.8000                      0. 0.0  0.0  278.0960
      2     1.000 600     2.000 180
6001802 PbCl3 -     2.1700    1.6990                     -1. 0.0  0.0  313.5490
      2     1.000 600     3.000 180
6001803 PbCl4 -2    3.5300    1.3800                     -2. 0.0  0.0  349.0020
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      2     1.000 600     4.000 180
6001400 Pb(CO3)2-2  0.0000    10.6400                    -2. 0.0  0.0  327.2080
 4.00 2     1.000 600     2.000 140
6002700 PbF +       0.0000     1.2500                     1. 0.0  0.0  226.1880
      2     1.000 600     1.000 270
6002701 PbF2 AQ     0.0000     2.5600                     0. 0.0  0.0  245.1860
      2     1.000 600     2.000 270
6002702 PbF3 -      0.0000     3.4200                    -1. 0.0  0.0  264.1850
      2     1.000 600     3.000 270
6002703 PbF4 -2     0.0000     3.1000                    -2. 0.0  0.0  283.1830
      2     1.000 600     4.000 270
6003300 PbOH +      0.0000    -7.7100                     1. 0.0  0.0  224.1970
      3     1.000 600     1.000   2    -1.000 330
6003301 Pb(OH)2 AQ  0.0000    -17.1200                    0. 0.0  0.0  241.2040
      3     1.000 600     2.000   2    -2.000 330
6003302 Pb(OH)3 -   0.0000    -28.0600                   -1. 0.0  0.0  258.2120
      3     1.000 600     3.000   2    -3.000 330
6003303 Pb2OH +3    0.0000    -6.3600                     3. 0.0  0.0  431.3870
      3     2.000 600     1.000   2    -1.000 330
6004920 PbNO3 +     0.0000     1.1700                     1. 0.0  0.0  269.1940
      2     1.000 600     1.000 492
6007320 PbSO4 AQ    0.0000     2.7500                     0. 0.0  0.0  303.2510
      2     1.000 600     1.000 732
6007300 Pb(HS)2 AQ  0.0000    15.2700                     0. 0.0  0.0  273.3330
      2     1.000 600     2.000 730
6007301 Pb(HS)3 -   0.0000    16.5700                    -1. 0.0  0.0  306.4050
      2     1.000 600     3.000 730
6003304 Pb3(OH)4+2  26.5000   -23.8800                    2. 0.0  0.0  689.5990
      3     3.000 600     4.000   2    -4.000 330
6001300 PbBr +      2.8800     1.7700                     1. 0.0  0.0  287.0940
      2     1.000 600     1.000 130
6001301 PbBr2 AQ    0.0000     1.4400                     0. 0.0  0.0  366.9980
      2     1.000 600     2.000 130
6003800 PbI +       0.0000     1.9400                     1. 0.0  0.0  334.0940
      2     1.000 600     1.000 380
6003801 PbI2 AQ     0.0000     3.1990                     0. 0.0  0.0  460.9980
      2     1.000 600     2.000 380
6001401 PbCO3 AQ    0.0000     7.2400                     0. 0.0  0.0  267.1990
 2.00 2     1.000 600     1.000 140
6003305 Pb(OH)4 -2  0.0000    -39.6990                   -2. 0.0  0.0  375.2190
      3     1.000 600     4.000   2    -4.000 330
6007321 Pb(SO4)2-2  0.0000     3.4700                    -2. 0.0  0.0  399.3130
      2     1.000 600     2.000 732
6001402 PbHCO3 +    0.0000    13.200                      1. 0.0  0.0  268.2070
 1.00 3     1.000 600     1.000 140     1.000 330
5401300 NiBr +      0.0000     0.5000                     1. 0.0  0.0  138.6140
      2     1.000 540     1.000 130
5401800 NiCl +      0.0000     0.3990                     1. 0.0  0.0  94.1630
      2     1.000 540     1.000 180
5402700 NiF +       0.0000     1.3000                     1. 0.0  0.0  77.7080
      2     1.000 540     1.000 270
5403300 NiOH +     12.4200    -9.8600                     1. 0.0  0.0  75.7170
      3     1.000 540     1.000   2    -1.000 330
5403301 Ni(OH)2 AQ  0.0000    -19.0000                    0. 0.0  0.0  92.7240
      3     1.000 540     2.000   2    -2.000 330
5403302 Ni(OH)3 -   0.0000    -30.0000                   -1. 0.0  0.0  109.7320
      3     1.000 540     3.000   2    -3.000 330
5407320 NiSO4 AQ    1.5200     2.2900                     0. 0.0  0.0  154.7710
      2     1.000 540     1.000 732
5401801 NiCl2 AQ    0.0000     0.9600                     0. 0.0  0.0  129.6160
      2     1.000 540     2.000 180
5401400 NiHCO3 +    0.0000    12.470                      1. 0.0  0.0  119.7270
 1.00 3     1.000 540     1.000 140     1.000 330
5401401 NiCO3 AQ    0.0000     6.8700                     0. 0.0  0.0  118.7190
 2.00 2     1.000 540     1.000 140
5401402 Ni(CO3)2-2  0.0000    10.1100                    -2. 0.0  0.0  178.7280
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 4.00 2     1.000 540     2.000 140
5407321 Ni(SO4)2-2  0.0000    1.0200                    -2. 0.0  0.0  250.8330
      2     1.000 540     2.000 732
5409921 Ni ACETATE  0.0000    1.4300                     1. 0.0  0.0  117.7600
      2     1.000 540     1.000 992
5409941 Ni GLYCINE  0.000     6.1800                     1. 0.0  0.0  132.7800
      2     1.000 540     1.000 994
5409942 Ni GLYCINE  0.000     11.13                      3. 0.0  0.0  191.4900
      2     2.000 540     1.000 994
5409951 Ni SALICYL  0.000     6.95                       0. 0.0  0.0  194.8300
      2     1.000 540     1.000 995
5409952 Ni SALICYL  0.000     11.75                      2. 0.0  0.0  253.5400
      2     2.000 540     1.000 995
5409961 Ni GLUTAMA  0.000     5.90                       0. 0.0  0.0  203.8400
      2     1.000 540     1.000 996
5401572 Ni GLUTAMA  0.000     10.34                      2. 0.0  0.0  262.5500
      2     2.000 540     1.000 996
5409971 Ni PHTHALA  0.000     2.95                       0. 0.0  0.0  222.8400
      2     1.000 540     1.000 997
0201300 AGBr AQ     0.0000    4.2400                     0. 0.0  0.0  187.7720
      2     1.000  20     1.000 130
0201301 AgBr2 -     0.0000    7.2800                    -1. 0.0  0.0  267.6760
      2     1.000  20     2.000 130
0201800 AgCL AQ     -2.6800   3.2700                     0. 0.0  0.0  143.3210
      2     1.000  20     1.000 180
0201801 AgCL2 -     -3.9300   5.2700                    -1. 0.0  0.0  178.7740
      2     1.000  20     2.000 180
0201802 AgCL3 -2    0.0000    5.2900                    -2. 0.0  0.0  214.2270
      2     1.000  20     3.000 180
0201803 AgCL4 -3    0.0000    5.5100                    -3. 0.0  0.0  249.6790
      2     1.000  20     4.000 180
0202700 AgF AQ      -2.8300   0.3600                     0. 0.0  0.0  126.8660
      2     1.000  20     1.000 270
0207300 AgHS AQ     0.0000    14.0500                    0. 0.0  0.0  140.9390
      2     1.000  20     1.000 730
0207301 Ag(HS)2 -   0.0000    18.4500                   -1. 0.0  0.0  174.0110
      2     1.000  20     2.000 730
0203800 AgI AQ      0.0000    6.6000                     0. 0.0  0.0  234.7720
      2     1.000  20     1.000 380
0203801 AgI2 -      0.0000    10.6800                   -1. 0.0  0.0  361.6760
      2     1.000  20     2.000 380
0203300 AgOH AQ     0.0000    -12.0000                   0. 0.0  0.0  124.8750
      3     1.000  20     1.000   2    -1.000 330
0203301 Ag(OH)2 -   0.0000    -24.0000                  -1. 0.0  0.0  141.8820
      3     1.000  20     2.000   2    -2.000 330
0207320 AgSO4 -     1.4900    1.2900                    -1. 0.0  0.0  203.9290
      2     1.000  20     1.000 732
0204920 AgNO3 AQ    0.0000    -0.2900                    0. 0.0  0.0  169.8720
      2     1.000  20     1.000 492
0204910 Ag(NO2)2 -  0.0000    2.2200                    -1. 0.0  0.0  199.8790
      2     1.000  20     2.000 491
0201302 AgBr3 -2    0.0000    8.7100                    -2. 0.0  0.0  347.5800
      2     1.000  20     3.000 130
0203802 AgI3 -2     -27.0300  13.3700                   -2. 0.0  0.0  488.5810
      2     1.000  20     3.000 380
0203803 AgI4 -3     0.0000    14.0800                   -3. 0.0  0.0  615.4850
      2     1.000  20     4.000 380
0207302 Ag(S4)2 -3  0.0000    0.9910                    -3. 22.0 0.0  364.3800
      4     1.000  20     2.000 730    -2.000 330     6.000 731
0207303 AgS4S5 -3   0.0000    0.6800                    -3. 24.0 0.0  396.4440
      4     1.000  20     2.000 730    -2.000 330     7.000 731
0207304 Ag(HS)S4-2  0.0000    10.4310                   -2. 15.0 0.0  269.1960
      4     1.000  20     2.000 730    -1.000 330     3.000 731
0209900 Ag FULVATE  0.0000    0.0000                    -1. 0.0  0.0  757.8680
      2     1.000  20     1.000 990
0209910 Ag HUMATE   0.0000    0.0000                    -1. 0.0  0.0  2107.8670
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      2     1.000  20     1.000 991
3300600 H2AsO3 -    6.5600    -9.2280                    -1. 0.0  0.0  124.9350
      2     1.000  60    -1.000 330
3300601 HAsO3 -2    14.1990   -21.33                     -2. 0.0  0.0  123.9270
      2     1.000  60    -2.000 330
3300602 AsO3 -3     20.2500   -34.7440                   -3. 0.0  0.0  122.9190
      2     1.000  60    -3.000 330
3300610 H4AsO3 +    0.0000    -0.3050                     1. 0.0  0.0  126.9510
      2     1.000  60     1.000 330
3300611 H2AsO4 -    -1.6900   -2.2430                    -1. 0.0  0.0  140.9350
      2     1.000  61    -1.000 330
3300612 HAsO4 -2    -0.9200   -9.0010                    -2. 0.0  0.0  139.9270
      2     1.000  61    -2.000 330
3300613 AsO4 -3     3.4300    -20.5970                   -3. 0.0  0.0  138.9190
      2     1.000  61    -3.000 330
7400021 HSbO2          -0.0150   -0.0073                  0.00 0.00 0.00 154.7567
 0.00 2     1.000 740    -1.000   2
7402700 SbOF (aq)       0.0000    6.1864                  0.00 0.00 0.00 156.7478
 0.00 4     1.000 740     1.000 270     1.000 330    -2.000   2
7402702 Sb(OH)2F aq     0.0000    6.1937                  0.00 0.00 0.00 174.7631
 0.00 4     1.000 740     1.000 270     1.000 330    -1.000   2
7403300 SbO+            1.9700    0.9228                  1.00 0.00 0.00 137.7494
 0.00 3     1.000 740     1.000 330    -2.000   2
7403301 SbO2-          16.7750  -11.8011                  -1.0 0.00 0.00 153.7488
 0.00 3     1.000 740    -1.000   2    -1.000 330
7403302 Sb(OH)2+        0.0000    1.3853                  1.00 0.00 0.00 155.7647
 0.00 3     1.000 740     1.000 330    -1.000   2
7407300 Sb2S4-2       -75.6800   49.3005                  -2.0 0.00 0.00 371.7640
 0.00 4     2.000 740     4.000 730     2.000 330    -6.000   2
7410021 SbO3-           0.0000    2.9319                  -1.0 0.00 0.00 169.7482
 0.00 2     1.000 741    -3.000   2
7413300 SbO2+           0.0000    2.3895                  1.00 0.00 0.00 153.7488
 0.00 3     1.000 741     2.000 330    -4.000   2
7400020 Sb(OH)4-1      16.6950  -12.0429                  -1.0 0.00 0.00 189.7794
 0.00 3     1.000 740     1.000   2    -1.000 330
3301400 HCO3 -       -3.6170   10.3300                    -1. 5.4  0.0  61.0170
 1.00 2     1.000 140     1.000 330
3301401 H2CO3 AQ     -2.2470   16.681                      0. 0.0  0.0  62.0250
      2     1.000 140     2.000 330
3307320 HSO4 -       4.9100    1.9870                     -1. 4.5  0.0  97.0690
      2     1.000 732     1.000 330
3302700 HF AQ        3.4600    3.1690                      0. 0.0  0.0  20.0060
      2     1.000 270     1.000 330
3302701 HF2 -        4.5500    3.7490                     -1. 3.5  0.0  39.0040
      2     2.000 270     1.000 330
3302702 H2F2 AQ      0.0000    6.7680                      0. 0.0  0.0  40.0120
      2     2.000 270     2.000 330
3305800 HPO4 -2      -3.5300   12.3460                    -2. 5.0  0.0  95.9790
      2     1.000 580     1.000 330
3305801 H2PO4 -      -4.5200   19.5530                    -1. 5.4  0.0  96.9870
      2     1.000 580     2.000 330
3305802 H3PO4         0.0000   21.7000                     0. 0.0  0.0  97.9950
      2     1.000 580     3.000 330
3307300 H2S AQ       -5.300     6.9940                     0. 0.0  0.0  34.0790
      2     1.000 730     1.000 330
3307301 S -2         12.1000   -12.9180                   -2. 5.0  0.0  32.0640
      2     1.000 730    -1.000 330
3309900 H FULVATE    0.0000    0.0000                     -1. 0.0  0.0  651.0080
      2     1.000 990     1.000 330
3309910 H HUMATE     0.0000    0.0000                     -1. 0.0  0.0  2001.0070
      2     1.000 991     1.000 330
8913300 UOH +3       11.715    -0.656                      3. 0.0  0.0  255.0364
      3     1.000 891     1.000   2    -1.000 330
8913301 U(OH)2 +2    17.730    -2.270                      2. 0.0  0.0  272.0437
      3    -2.000 330     1.000 891     2.000   2
8913302 U(OH)3 +1    22.645    -4.935                      1. 0.0  0.0  289.0511
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      3     1.000 891     3.000   2    -3.000 330
8913303 U(OH)4 AQ   24.760    -8.498                          0. 0.0  0.0  306.0586
      3     1.000 891     4.000   2    -4.000 330
8913304 U(OH)5 -1   27.575    -13.120                        -1. 0.0  0.0  323.0659
      3     1.000 891     5.000   2    -5.000 330
8913305 U6(OH)15+9            -17.229                         9. 0.0  0.0  1683.2846
      3     6.000 891    15.000   2   -15.000 330
8912700 UF +3       5.050     8.659                          3. 0.0  0.0  257.0274
      2     1.000 891     1.000 270
8912701 UF2 +2      7.200     14.457                         2. 0.0  0.0  276.0258
      2     1.000 891     2.000 270
8912702 UF3 +1      7.150     19.115                         1. 0.0  0.0  295.0242
      2     1.000 891     3.000 270
8912703 UF4 AQ      4.600     23.640                         0. 0.0  0.0  314.0226
      2     1.000 891     4.000 270
8912704 UF5 -1      4.850     25.238                        -1. 0.0  0.0  333.0210
      2     1.000 891     5.000 270
8912705 UF6 -2      3.300     27.718                        -2. 0.0  0.0  352.0194
      2     1.000 891     6.000 270
8911800 UCl +3      9.933     1.338                          3. 0.0  0.0  273.4820
      2     1.000 891     1.000 180
8917320 USO4 +2     3.700     5.461                          2. 0.0  0.0  334.0906
      2     1.000 891     1.000 732
3917321 U(SO4)2 AQ  7.600     9.749                          0. 0.0  0.0  430.1522
      2     1.000 891     2.000 732
8915800 UHPO4 +2    7.500     24.443                         2. 0.0  0.0  334.0084
      3     1.000 891     1.000 580     1.000 330
8915801 U(HPO4)2AQ  1.700     46.833                         0. 0.0  0.0  429.9877
      3     1.000 891     2.000 580     2.000 330
8915802 U(HPO4)3-2  -7.800    67.564                        -2. 0.0  0.0  525.9671
      3     1.000 891     3.000 580     3.000 330
8915803 U(HPO4)4-4  -26.500   88.483                        -4. 0.0  0.0  621.9465
      3     1.000 891     4.000 580     4.000 330
8933300 UO2OH +1    10.216    -5.090                         1. 0.0  0.0  287.0352
      3     1.000 893     1.000   2    -1.000 330
8933301 UO2)2OH2+2  10.230    -5.645                         2. 0.0  0.0  574.0703
      3     2.000 893     2.000   2    -2.000 330
8933302 UO2)3OH5+1  25.075    -15.593                        1. 0.0  0.0  895.1203
      3     3.000 893     5.000   2    -5.000 330
8931400 UO2CO3 AQ   0.840     10.071                         0. 0.0  0.0  330.0372
 2.00 2     1.000 893     1.000 140
8931401 UO2CO3)2-2  3.480     17.008                        -2. 0.0  0.0  390.0465
 4.00 2     1.000 893     2.000 140
8931402 UO2CO3)3-4  -8.780    21.384                        -4. 0.0  0.0  450.0559
 6.00 2     1.000 893     3.000 140
8932700 UO2F +1     -0.450    5.105                          1. 0.0  0.0  289.0262
      2     1.000 893     1.000 270
8932701 UO2F2 AQ    -0.900    8.920                          0. 0.0  0.0  308.0246
      2     1.000 893     2.000 270
8932702 UO2F3 -1    -0.850    11.364                        -1. 0.0  0.0  327.0230
      2     1.000 893     3.000 270
8932703 UO2F4 -2    -1.100    12.607                        -2. 0.0  0.0  346.0214
      2     1.000 893     4.000 270
8931800 UO2Cl +1    1.233     0.220                          1. 0.0  0.0  305.4808
      2     1.000 893     1.000 180
8937320 UO2SO4 AQ   5.100     2.709                          0. 0.0  0.0  366.0894
      2     1.000 893     1.000 732
8937321 UO2SO4)2-2  6.100     4.183                         -2. 0.0  0.0  462.1510
      2     1.000 893     2.000 732
8935800 UO2HPO4 AQ  -2.100    20.814                         0. 0.0  0.0  366.0072
      3     1.000 893     1.000 580     1.000 330
8935801 UO2HPO4)2   -11.399   42.988                        -2. 0.0  0.0  461.9865
      3     1.000 893     2.000 580     2.000 330
8935802 UO2H2PO4+1  -3.700    22.643                         1. 0.0  0.0  367.0151
      3     1.000 893     1.000 580     2.000 330
8935803 UO2H2PO4)2  -16.5     44.70                          0. 0    0    464.002
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      3     1.000 893     2.000 580     4.000 330
8935804 UO2H2PO4)3  -28.6     66.245                          -1. 0    0    560.989
      3     1.000 893     3.000 580     6.000 330
8937700 UO2H3SIO4             -2.4                             1. 0    0    365.135
      3     1.000 893     1.000 770    -1.000 330
7317300 S2 -2       11.4      -14.528                         -2. 0.0  0.0  64.128
      3     1.000 730     1.000 731    -1.000 330
7317301 S3 -2       10.4      -13.282                         -2. 0.0  0.0  96.192
      3     1.000 730     2.000 731    -1.000 330
7317302 S4 -2        9.7       -9.829                         -2. 0.0  0.0  128.236
      3     1.000 730     3.000 731    -1.000 330
7317303 S5 -2        9.3       -9.595                         -2. 0.0  0.0  160.320
      3     1.000 730     4.000 731    -1.000 330
7317304 S6 -2                  -9.881                         -2. 0.0  0.0  192.384
      3     1.000 730     5.000 731    -1.000 330
9003300 VOH +                  -5.64                           1.            67.947
      3     1.000 900     1.000   2    -1.000 330
9013300 VOH +2       9.35      -2.30                           2.            67.947
      3     1.000 901     1.000   2    -1.000 330
9013301 V(OH)2 +1              -5.83                           1.            84.955
      3     1.000 901     2.000   2    -2.000 330
9013302 V(OH)3 AQ              -11.02                          0.            101.962
      3     1.000 901     3.000   2    -3.000 330
9017320 VSO4 +1                1.44                            1.            146.998
      2     1.000 901     1.000 732
9013303 V2(OH)3 +3             -7.50                           3.            152.902
      3     2.000 901     3.000   2    -3.000 330
9013304 V2(OH)2 +4             -3.75                           4.            135.895
      3     2.000 901     2.000   2    -2.000 330
9023300 V(OH)3 +1              -5.67                           1.            101.962
      3     1.000 902     2.000   2    -1.000 330
9023301 H2V2O4 +2              -6.44                           2.            167.894
      3     2.000 902     2.000   2    -2.000 330
9022700 VOF +        1.9       3.34                           1.            85.937
      2     1.000 902     1.000 270
9022701 VOF2 AQ      3.50      5.74                           0.            104.935
      2     1.000 902     2.000 270
9022702 VOF3 -1      4.90      7.30                          -1.            123.933
      2     1.000 902     3.000 270
9022703 VOF4 -2      6.40      8.11                          -2.            142.931
      2     1.000 902     4.000 270
9027320 VOSO4 AQ     3.72      2.45                           0.            162.997
      2     1.000 902     1.000 732
9021800 VOCl +1                0.02                            1.            102.392
      2     1.000 902     1.000 180
9033300 H3VO4 AQ    10.63     -3.30                           0.            117.962
      3     1.000 903     2.000   2    -1.000 330
9033301 H2VO4 -1    11.33     -7.09                          -1.            116.954
      3     1.000 903     2.000   2    -2.000 330
9033302 HVO4 -2     14.93     -15.15                         -2.            115.946
      3     1.000 903     2.000   2    -3.000 330
9033303 VO4 -3      19.53     -28.40                         -3.            114.938
      3     1.000 903     2.000   2    -4.000 330
9030020 V2O7 -4                -29.08                          -4.           213.876
      3     2.000 903     3.000   2    -6.000 330
9030021 HV2O7 -3               -16.32                          -3.           214.884
      3     2.000 903     3.000   2    -5.000 330
9030022 H3V2O7 -1              -3.79                           -1.           216.900
      3     2.000 903     3.000   2    -3.000 330
9030023 V3O9 -3                -15.88                          -3.           296.815
      3     3.000 903     3.000   2    -6.000 330
9030024 V4O12 -4               -20.79                          -4.           395.753
      3     4.000 903     4.000   2    -8.000 330
9030025 V10O28 -6              -17.53                          -6.           957.383
      3    10.000 903     8.000   2   -16.000 330
9030026 HV10O28 -5  21.52      -11.35                         -5.            958.391
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      3    10.000 903      8.000   2   -15.000 330
9030027 H2V10O28 -4           -7.71                          -4.            959.399
      3    10.000 903      8.000   2   -14.000 330
9032700 VO2F AQ               3.12                           0.            101.937
      2     1.000 903      1.000 270
9032701 VO2F2 -1              5.67                           -1.            120.935
      2     1.000 903      2.000 270
9032702 VO2F3 -2              6.97                           -2.            139.933
      2     1.000 903      3.000 270
9032703 VO2F4 -3              7.07                           -3.            158.931
      2     1.000 903      4.000 270
9037320 VO2SO4 -1             1.71                           -1.            178.996
      2     1.000 903      1.000 732
9034920 VO2NO3 AQ            -0.43                           0.             144.944
      2     1.000 903      1.000 492
8703300 TlOH AQ        13.9350  -13.1717                     0.00 0.00 0.00 221.3773
 0.00 3     1.000 870      1.000   2    -1.000 330
8702700 TlF AQ          0.0000   -0.4251                    0.00 0.00 0.00 223.3684
 0.00 2     1.000 870      1.000 270
8701800 TlCl AQ        -1.1470    0.6824                    0.00 0.00 0.00 239.8230
 0.00 2     1.000 870      1.000 180
8701801 TlCl2-1         0.0000    0.2434                    -1.0 0.00 0.00 275.2760
 0.00 2     1.000 870      2.000 180
3701300 TlBr AQ        -2.4610    0.9477                    0.00 0.00 0.00 284.2740
 0.00 2     1.000 870      1.000 130
8701301 TlBr2-1         2.9980    0.9719                    -1.0 0.00 0.00 364.1780
 0.00 2     1.000 870      2.000 130
8701302 TlBrCl-1        0.0000    0.8165                    -1.0 0.00 0.00 319.7270
 0.00 3     1.000 870      1.000 130     1.000 180
8703800 TlI AQ          0.0000    1.4279                    0.00 0.00 0.00 331.2745
 0.00 2     1.000 870      1.000 380
8703801 TlI2-1          0.0000    1.8588                    -1.0 0.00 0.00 458.1790
 0.00 2     1.000 870      2.000 380
8703802 TlIBr-1         0.0000    2.1850                    -1.0 0.00 0.00 411.1785
 0.00 3     1.000 870      1.000 380     1.000 130
8707320 TlSO4-1        -0.2200    1.3853                    -1.0 0.00 0.00 300.4276
 0.00 2     1.000 870      1.000 732
8704920 TlNO3 AQ       -0.6500    0.3665                    0.00 0.00 0.00 266.3749
 0.00 2     1.000 870      1.000 492
8704910 TlNO2 AQ        0.0000    0.9969                    0.00 0.00 0.00 250.3755
 0.00 2     1.000 870      1.000 491
8707300 TlHS AQ         0.0000    1.8178                    0.00 0.00 0.00 237.4379
 0.00 2     1.000 870      1.000 730
8707301 Tl2HS+1         0.0000    7.6979                    1.00 0.00 0.00 441.8079
 0.00 2     2.000 870      1.000 730
8707302 Tl2OH(HS)3-     0.0000    1.0044                    -2.0 0.00 0.00 524.9510
 0.00 4     2.000 870      3.000 730     1.000   2    -1.000 330
8707303 Tl2(OH)2(HS     0.0000  -11.0681                    -2.0 0.00 0.00 508.8904
 0.00 4     2.000 870      2.000 730     2.000   2    -2.000 330
8713300 Tl+3            0.0000    4.7424                    3.00 0.00 0.00 204.3700
 0.00 3     1.000 871      3.000 330    -3.000   2
8713301 TlOH+2          0.0000    3.5770                    2.00 0.00 0.00 221.3773
 0.00 3     1.000 871      2.000 330    -2.000   2
8713302 Tl(OH)2+1       0.0000    2.1183                    1.00 0.00 0.00 238.3846
 0.00 3     1.000 871      1.000 330    -1.000   2
8711800 TlCl+2          0.0000   12.2342                    2.00 0.00 0.00 239.8230
 0.00 4     1.000 871      1.000 180     3.000 330    -3.000   2
8711801 TlCl2+1         0.0000   18.0402                    1.00 0.00 0.00 275.2760
 0.00 4     1.000 871      2.000 180     3.000 330    -3.000   2
8711802 TlCl3 AQ        0.0000   21.4273                    0.00 0.00 0.00 310.7290
 0.00 4     1.000 871      3.000 180     3.000 330    -3.000   2
8711803 TlCl4-1         0.0000   24.2281                    -1.0 0.00 0.00 346.1820
 0.00 4     1.000 871      4.000 180     3.000 330    -3.000   2
8711300 TlBr+2          0.0000   14.2221                    2.00 0.00 0.00 284.2740
 0.00 4     1.000 871      1.000 130     3.000 330    -3.000   2
8711301 TLBr2+1         0.0000   21.5761                    1.00 0.00 0.00 364.1780
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 0.00 4     1.000 871     2.000 130     3.000 330    -3.000   2
8711302 TlBr3 AQ        0.0000   27.0244                   0.00 0.00 0.00 444.0820
 0.00 4     1.000 871     3.000 130     3.000 330    -3.000   2
8711303 TlBr4-1         0.0000   31.1533                  -1.0 0.00 0.00 523.9860
 0.00 4     1.000 871     4.000 130     3.000 330    -3.000   2
8713800 TlI4-1          0.0000   34.7596                  -1.0 0.00 0.00 711.9880
 0.00 4     1.000 871     4.000 380     3.000 330    -3.000   2
8714920 TlNO3+2         0.0000    7.0073                  2.00 0.00 0.00 266.3749
 0.00 4     1.000 871     1.000 492     3.000 330    -3.000   2
8713303 Tl(OH)4-1       0.0000  -10.2545                  -1.0 0.00 0.00 272.3992
 0.00 3     1.000 871     1.000   2    -1.000 330
8711804 TlOHCl+1        0.0000   10.6290                  1.00 0.00 0.00 256.8303
 0.00 4     1.000 871     1.000 180     2.000 330    -2.000   2
3307601 Se-2           11.5000  -14.9529                  -2.0 0.00 0.00  78.9600
 0.00 2     1.000 760    -1.000 330
3307600 H2Se            0.8000    3.8115                  0.00 0.00 0.00  80.9758
 0.00 2     1.000 760     1.000 330
4707600 MnSe            0.0000   -6.7435                  0.00 0.00 0.00 133.8980
 0.00 3     1.000 760     1.000 470    -1.000 330
 207600 Ag2Se           0.0000   34.0677                  0.00 0.00 0.00 294.6960
 0.00 3     1.000 760     2.000  20    -1.000 330
 207601 AgOH(Se)2-4     0.0000  -18.6237                  -4.0 0.00 0.00 282.7953
 0.00 4     2.000 760     1.000  20     1.000   2    -3.000 330
3307611 SeO3-2          1.2800   -7.3005                  -2.0 0.00 0.00 126.9582
 0.00 2     1.000 761    -1.000 330
3307610 H2SeO3          1.6900    2.5728                  0.00 0.00 0.00 128.9740
 0.00 2     1.000 761     1.000 330
2817610 FeHSeO3+2       0.0000    1.8618                  2.00 0.00 0.00 183.8131
 0.00 2     1.000 761     1.000 281
 207610 AgSeO3-1        0.0000   -5.5985                  -1.0 0.00 0.00 234.8262
 0.00 3     1.000 761     1.000  20    -1.000 330
 207611 Ag(SeO3)2-3     0.0000  -10.9933                  -3.0 0.00 0.00 361.7844
 0.00 3     2.000 761     1.000  20    -2.000 330
1607610 Cd(SeO3)2-2     0.0000  -11.1890                  -2.0 0.00 0.00 366.3264
 0.00 3     2.000 761     1.000 160    -2.000 330
3307620 HSeO4-1         4.2000    1.9058                  -1.0 0.00 0.00 143.9655
 0.00 2     1.000 762     1.000 330
4707620 MnSeO4          3.4600    2.4188                  0.00 0.00 0.00 197.8956
 0.00 2     1.000 762     1.000 470
2007620 CoSeO4          2.9100    2.7120                  0.00 0.00 0.00 201.8908
 0.00 2     1.000 762     1.000 200
5407620 NiSeO4          3.5000    2.6387                  0.00 0.00 0.00 201.6576
 0.00 2     1.000 762     1.000 540
1607620 CdSeO4          0.0000    2.2415                  0.00 0.00 0.00 255.3676
 0.00 2     1.000 762     1.000 160
9507620 ZnSeO4          0.0000    2.2019                  0.00 0.00 0.00 208.3376
 0.00 2     1.000 762     1.000 950
9507621 Zn(SeO4)2-2     0.0000   -0.0704                  -2.0 0.00 0.00 351.2952
 0.00 2     2.000 762     1.000 950
3600000 Hg (aq)       -16.6050    6.9316                  0.00 0.00 0.00 200.5900
 0.00 2     0.500 360     1.000   1
3613300 Hg+2          -11.0600    6.0970                  2.00 0.00 0.00 200.5900
 0.00 3     1.000 361     2.000 330    -2.000   2
3611301 HgBr+           0.0000   15.8347                  1.00 0.00 0.00 280.4940
 0.00 4     1.000 361     1.000 130     2.000 330    -2.000   2
3611302 HgBr2 (aq)    -30.8320   23.6065                  0.00 0.00 0.00 360.3980
 0.00 4     1.000 361     2.000 130     2.000 330    -2.000   2
3611303 HgBr3-1         0.0000   25.7857                  -1.0 0.00 0.00 440.3020
 0.00 4     1.000 361     2.000 330     3.000 130    -2.000   2
3611304 HgBr4-2         0.0000   27.0633                  -2.0 0.00 0.00 520.2060
 0.00 4     1.000 361     2.000 330     4.000 130    -2.000   2
3611305 HgBrCl (aq)     0.0000   22.0145                  0.00 0.00 0.00 315.9470
 0.00 5     1.000 361     1.000 130     1.000 180     2.000 330    -2.000   2
3611306 HgBrI (aq)      0.0000   27.1212                  0.00 0.00 0.00 407.3985
 0.00 5     1.000 361     1.000 130     1.000 380     2.000 330    -2.000   2
3611307 HgBrI3-2        0.0000   34.2135                  -2.0 0.00 0.00 661.2075
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 0.00 5     1.000 361     1.000 130     3.000 380     2.000 330    -2.000   2
3611308 HgBr2I2-2       0.0000   32.3994                    -2.0 0.00 0.00 614.2070
 0.00 5     1.000 361     2.000 130     2.000 380     2.000 330    -2.000   2
3611309 HgBr3I-2        0.0000   30.1528                    -2.0 0.00 0.00 567.2065
 0.00 5     1.000 361     3.000 130     1.000 380     2.000 330    -2.000   2
3613301 HgBrOH (aq)     0.0000   11.5980                     0.00 0.00 0.00 297.5013
 0.00 4     1.000 361     1.000 130     1.000 330    -1.000   2
3611800 HgCl+1          0.0000   12.8500                     1.00 0.00 0.00 236.0430
 0.00 4     1.000 361     1.000 180     2.000 330    -2.000   2
3611801 HgCl2 (aq)      0.0000   19.2203                     0.00 0.00 0.00 271.4960
 0.00 4     1.000 361     2.000 180     2.000 330    -2.000   2
3811802 HgCl3-1         0.0000   20.1226                    -1.0 0.00 0.00 306.9490
 0.00 4     1.000 361     3.000 180     2.000 330    -2.000   2
3611803 HgCl4-2         0.0000   20.5338                    -2.0 0.00 0.00 342.4020
 0.00 4     1.000 361     4.000 180     2.000 330    -2.000   2
3611804 HgClI (aq)      0.0000   25.3532                     0.00 0.00 0.00 362.9475
 0.00 5     1.000 361     1.000 180     1.000 380     2.000 330    -2.000   2
3611805 HgClOH (aq)  -12.4820    9.3170                     0.00 0.00 0.00 253.0503
 0.00 4     1.000 361     1.000 180     1.000 330    -1.000   2
3612701 HgF+1           0.0000    8.0848                     1.00 0.00 0.00 219.5884
 0.00 4     1.000 361     1.000 270     2.000 330    -2.000   2
3613801 HGI+1           0.0000   18.8949                     1.00 0.00 0.00 327.4945
 0.00 4     1.000 361     1.000 380     2.000 330    -2.000   2
3613802 HgI2 (aq)    -44.5220   30.1081                     0.00 0.00 0.00 454.3990
 0.00 4     1.000 361     2.000 380     2.000 330    -2.000   2
3613803 HgI3-1       -47.9430   33.7935                    -1.0 0.00 0.00 581.3035
 0.00 4     1.000 361     3.000 380     2.000 330    -2.000   2
3613804 HgI4-2          0.0000   35.7858                    -2.0 0.00 0.00 708.2080
 0.00 4     1.000 361     4.000 380     2.000 330    -2.000   2
3614900 HgNH3+2         0.0000    5.6139                     2.00 0.00 0.00 217.6204
 0.00 4     1.000 361     1.000 490     1.000 330    -2.000   2
3614901 Hg(NH3)2+2      0.0000    5.0341                     2.00 0.00 0.00 234.6508
 0.00 3     1.000 361     2.000 490    -2.000   2
3614902 Hg(NH3)3+2      0.0000   -3.2493                     2.00 0.00 0.00 251.6812
 0.00 4     1.000 361     3.000 490    -1.000 330    -2.000   2
3614903 Hg(NH3)4+2      0.0000  -11.7307                     2.00 0.00 0.00 268.7116
 0.00 4     1.000 361     4.000 490    -2.000 330    -2.000   2
3614920 HgNO3+1         0.0000    6.4503                     1.00 0.00 0.00 262.5949
 0.00 4     1.000 361     1.000 492     2.000 330    -2.000   2
3614921 Hg(NO3)2 (a     0.0000    4.7791                     0.00 0.00 0.00 324.5998
 0.00 4     1.000 361     2.000 492     2.000 330    -2.000   2
3613302 HgOH+1          0.0000    2.6974                     1.00 0.00 0.00 217.5973
 0.00 3     1.000 361     1.000 330    -1.000   2
3613303 Hg(OH)3-1       0.0000  -15.0042                    -1.0 0.00 0.00 251.6119
 0.00 3     1.000 361     1.000   2    -1.000 330
3617300 HgS2-2          0.0000   31.2398                    -2.0 0.00 0.00 264.7100
 0.00 3     1.000 361     2.000 730    -2.000   2
3617301 Hg(HS)2 (aq     0.0000   43.8178                     0.00 0.00 0.00 266.7258
 0.00 4     1.000 361     2.000 730     2.000 330    -2.000   2
3617320 HgSO4 (aq)      0.0000    7.4911                     0.00 0.00 0.00 296.6476
 0.00 4     1.000 361     1.000 732     2.000 330    -2.000   2
2113300 Cr+3         -20.1400    9.62                       3.00 0.00 0.00  51.9960
 0.00 3     1.000 211     2.000 330    -2.000   2
2113301 Cr(OH)+2        0.0000    5.6200                     2.00 0.00 0.00  69.0033
 0.00 3     1.000 211     1.000 330    -1.000   2
2110020 Cr(OH)3 AQ      0.0000   -7.1300                     0.00 0.00 0.00 103.0179
 0.00 3     1.000 211     1.000   2    -1.000 330
2110021 Cr(OH)4-        0.0000  -18.1500                      -1. 0.00 0.00 120.0252
 0.00 3     1.000 211     2.000   2    -2.000 330
2113304 CrO2-           0.0000  -17.7456                      -1. 0.00 0.00  83.9948
 0.00 2     1.000 211    -2.000 330
2111300 CrBr+2       -11.2110    7.5519                     2.00 0.00 0.00 131.9000
 0.00 4     1.000 211     1.000 130     2.000 330    -2.000   2
2111800 CrCl+2       -13.8470    9.3683                     2.00 0.00 0.00  87.4490
 0.00 4     1.000 211     1.000 180     2.000 330    -2.000   2
2111801 CrCl2 +       -9.3740    8.6580                     1.00 0.00 0.00 122.9020
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 0.00 4     1.000 211     2.000 180     2.000 330    -2.000   2
2111802 CrOHCl2 AQ     0.0000    2.9627                   0.00 0.00 0.00 139.9093
 0.00 4     1.000 211     2.000 180     1.000 330    -1.000   2
2112700 CrF+2        -16.7890   14.5424                   2.00 0.00 0.00  70.9944
 0.00 4     1.000 211     1.000 270     2.000 330    -2.000   2
2113800 CrI+2          0.0000    4.8289                   2.00 0.00 0.00 178.9005
 0.00 4     1.000 211     1.000 380     2.000 330    -2.000   2
2114900 Cr(NH3)6+3     0.0000  -32.5709                   3.00 0.00 0.00 154.1784
 0.00 4     1.000 211     6.000 490    -4.000 330    -2.000   2
2114901 CrNH3)5OH+2    0.0000  -30.2759                   2.00 0.00 0.00 154.1553
 0.00 4     1.000 211     5.000 490    -4.000 330    -1.000   2
2114902 CCrNH3)4OH2    0.0000  -29.8574                   1.00 0.00 0.00 154.1322
 0.00 3     1.000 211     4.000 490    -4.000 330
2114903 TCrNH3)4OH2    0.0000  -30.5537                   1.00 0.00 0.00 154.1322
 0.00 3     1.000 211     4.000 490    -4.000 330
2114904 CrNH3)6CL+2    0.0000  -31.7932                   2.00 0.00 0.00 189.6314
 0.00 5     1.000 211     6.000 490     1.000 180    -2.000   2    -4.000 330
2114905 CrNH3)6BR+2    0.0000  -31.8870                   2.00 0.00 0.00 234.0824
 0.00 5     1.000 211     6.000 490     1.000 130    -4.000 330    -2.000   2
2114906 CrNH3)6I +2    0.0000  -32.0080                   2.00 0.00 0.00 281.0829
 0.00 5     1.000 211     6.000 490     1.000 380    -4.000 330    -2.000   2
2114920 CrNO3 +2     -15.6400    8.2094                   2.00 0.00 0.00 114.0009
 0.00 4     1.000 211     1.000 492     2.000 330    -2.000   2
2115800 CrH2PO4 +2     0.0000   31.9068                   2.00 0.00 0.00 148.9832
 0.00 4     1.000 211     4.000 330     1.000 580    -2.000   2
2117320 CrSO4 +      -12.6200   10.9654                   1.00 0.00 0.00 148.0536
 0.00 4     1.000 211     1.000 732     2.000 330    -2.000   2
2117321 CrOHSO4 AQ     0.0000    8.2754                   0.00 0.00 0.00 165.0609
 0.00 4     1.000 211     1.000 732     1.000 330    -1.000   2
2117322 Cr2OH2SO4)S    0.0000   14.5278                   0.00 0.00 0.00 330.1218
 0.00 4     2.000 211     2.000 732     2.000 330    -2.000   2
2117323 Cr2OH2SO4+2    0.0000   16.1550                   2.00 0.00 0.00 234.0642
 0.00 4     2.000 211     1.000 732     2.000 330    -2.000   2
2117324 Cr2OH2SO42     0.0000   17.9288                   0.00 0.00 0.00 330.1218
 0.00 4     2.000 211     2.000 732     2.000 330    -2.000   2
2123300 HCrO4 -        0.9000    6.5089                  -1.0 0.00 0.00 117.0015
 0.00 2     1.000 212     1.000 330
2123301 H2CrO4 AQ      0.0000    5.6513                   0.00 0.00 0.00 118.0094
 0.00 2     1.000 212     2.000 330
2123302 Cr2O7 -2      -2.9950   14.5571                  -2.0 0.00 0.00 215.9878
 0.00 3     2.000 212     2.000 330    -1.000   2
2121800 CrO3Cl -       0.0000    7.3086                  -1.0 0.00 0.00 135.4472
 0.00 4     1.000 212     1.000 180     2.000 330    -1.000   2
2125800 Cr03H2PO4-     0.0000   29.3634                  -1.0 0.00 0.00 196.9814
 0.00 4     1.000 212     4.000 330     1.000 580    -1.000   2
2125801 CrO3HPO4-2     0.0000   26.6806                  -2.0 0.00 0.00 195.9735
 0.00 4     1.000 212     3.000 330     1.000 580    -1.000   2
2127320 CrO3SO4-2      0.0000    8.9937                  -2.0 0.00 0.00 196.0518
 0.00 4     1.000 212     1.000 732     2.000 330    -1.000   2
5002120 NaCrO4-        0.0000    0.6963                  -1.0 0.00 0.00 138.9834
 0.00 2     1.000 212     1.000 500
4102120 KCrO4-         0.0000    0.7990                  -1.0 0.00 0.00 155.0919
 0.00 2     1.000 212     1.000 410
1001431 BaFe(CN)6-1   -69.6800   55.4356                  -1.00 0.00 0.00 349.2804
 0.00 3     1.000 100     1.000 281     6.000 143
1501434 CaHFe(CN)6-2  -82.0000   52.7097                  -2.00 0.00 0.00 253.0394
 0.00 5     1.000 150     1.000 330     1.000 280     6.000 143     1.000   1
4101433 KFe(CN)6-3    -84.0000   48.1204                  -3.00 0.00 0.00 251.0517
 0.00 3     1.000 410     1.000 280     6.000 143
4101434 K2Fe(CN)6-2   -77.3000   48.9780                  -2.00 0.00 0.00 290.1500
 0.00 3     2.000 410     1.000 280     6.000 143
4101435 KHFe(CN)6-2   -78.1000   51.4702                  -2.00 0.00 0.00 252.0597
 0.00 4     1.000 410     1.000 330     1.000 280     6.000 143
4401432 Li2Fe(CN)6-2  -83.4980   48.5338                  -2.00 0.00 0.00 225.8354
 0.00 3     2.000 440     1.000 280     6.000 143
4401433 LiHFe(CN)6-2  -80.9990   51.2188                  -2.00 0.00 0.00 219.9024
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 0.00 4     1.000 440     1.000 330     1.000 280     6.000 143
4901431 NH4Fe(CN)6-3  -84.5000   48.0684                 -3.00 0.00 0.00 314.0324
 0.00 3     1.000 490     1.000 280     6.000 143
4901433 NH5Fe(CN)6-   -83.9000   51.4035                 -2.00 0.00 0.00 315.0403
 0.00 4     1.000 490     1.000 330     1.000 280     6.000 143
5001431 NAFe(CN)6-3   -84.9000   47.9885                 -3.00 0.00 0.00 234.9432
 0.00 3     1.000 500     1.000 280     6.000 143
5001432 Na2Fe(CN)6-2  -85.0000   48.7435                 -2.00 0.00 0.00 257.9330
 0.00 3     2.000 500     1.000 280     6.000 143
5001433 NaHFe(CN)6-2  -85.6000   51.4335                 -2.00 0.00 0.00 235.9512
 0.00 4     1.000 500     1.000 330     1.000 280     6.000 143
4901432 NH4)2FeCN6-2  -83.0000   48.8666                 -2.00 0.00 0.00 332.0709
 0.00 3     2.000 490     1.000 280     6.000 143
 201431 Ag(CN)OH-       0.0000   -0.5600                 -1.00 0.00 0.00 150.8933
 0.00 4     1.000 143     1.000  20     1.000   2    -1.000 330
 201432 Ag(CN)2-      -32.6750   20.3814                 -1.00 0.00 0.00 159.9037
 0.00 2     2.000 143     1.000  20
4101431 K2H2Fe(CN)6   -85.8600   52.3058                  0.00 0.00 0.00 292.1659
 0.00 4     6.000 143     2.000 410     2.000 330     1.000 280
1501431 CaFe(CN)6-    -69.5000   55.4730                 -1.00 0.00 0.00 252.0314
 0.00 3     6.000 143     1.000 150     1.000 281
1501432 CaFe(CN)6-2   -83.1000   49.6898                 -2.00 0.00 0.00 252.0314
 0.00 3     6.000 143     1.000 150     1.000 280
1501433 Ca2Fe(CN)6    -83.7000   50.9952                  0.00 0.00 0.00 292.1094
 0.00 3     6.000 143     2.000 150     1.000 280
1601431 CdCN+          0.0000    5.3200                  1.00 0.00 0.00 138.4287
 0.00 2     1.000 143     1.000 160
1601432 Cd(CN)2 (aq)  -13.0000   10.3703                  0.00 0.00 0.00 164.4465
 0.00 2     2.000 143     1.000 160
1601433 Cd(CN)3-      -21.6000   14.8341                 -1.00 0.00 0.00 190.4642
 0.00 2     3.000 143     1.000 160
1601434 Cd(CN)4-2     -23.5600   18.2938                 -2.00 0.00 0.00 216.4820
 0.00 2     4.000 143     1.000 160
2301431 Cu(CN)4-3     -51.4000   30.3456                 -3.00 0.00 0.00 167.6170
 0.00 2     4.000 143     1.000 230
2301432 Cu(CN)2-      -29.1000   24.0272                 -1.00 0.00 0.00 115.5815
 0.00 2     2.000 143     1.000 230
2301433 Cu(CN)3-2     -40.2000   28.6524                 -2.00 0.00 0.00 141.5992
 0.00 2     3.000 143     1.000 230
2801431 Fe(CN)6-4     -85.8000   45.6063                 -4.00 0.00 0.00 211.9534
 0.00 2     6.000 143     1.000 280
2801432 HFe(CN)6-3    -84.1600   49.9969                 -3.00 0.00 0.00 212.9614
 0.00 3     6.000 143     1.000 280     1.000 330
2801433 H2Fe(CN)6-2   -83.1000   52.4450                 -2.00 0.00 0.00 213.9693
 0.00 3     6.000 143     2.000 330     1.000 280
2811431 Fe(CN)6-3     -70.1000   52.6283                 -3.00 0.00 0.00 211.9534
 0.00 2     6.000 143     1.000 281
3301431 HCN           -10.4000    9.2356                  0.00 0.00 0.00  27.0257
 0.00 2     1.000 143     1.000 330
3301441 HOCN           -2.0000    3.4450                  0.00 0.00 0.00  43.0251
 0.00 2     1.000 144     1.000 330
3611431 HgCN+         -33.8300   24.1738                  1.00 0.00 0.00 226.6077
 0.00 4     1.000 143     1.000 361     2.000 330    -2.000   2
3611432 Hg(CN)2       -57.2400   40.6513                  0.00 0.00 0.00 252.6255
 0.00 4     2.000 143     1.000 361     2.000 330    -2.000   2
3611433 Hg(CN)3-      -64.8300   44.4042                 -1.00 0.00 0.00 278.6432
 0.00 4     3.000 143     1.000 361     2.000 330    -2.000   2
3611434 Hg(CN)4-2     -69.9300   47.4094                 -2.00 0.00 0.00 304.6610
 0.00 4     4.000 143     1.000 361     2.000 330    -2.000   2
3611435 Hg(CN)2Cl-     0.0000   40.3735                 -1.00 0.00 0.00 288.0782
 0.00 5     2.000 143     1.000 180     1.000 361     2.000 330    -2.000   2
3611436 Hg(CN)3Cl-2    0.0000   43.8332                 -2.00 0.00 0.00 314.0959
 0.00 5     3.000 143     1.000 180     1.000 361     2.000 330    -2.000   2
3611437 Hg(CN)3Br-2    0.0000   44.9415                 -2.00 0.00 0.00 358.5472
 0.00 5     3.000 143     1.000 130     1.000 361     2.000 330    -2.000   2
3801432 I2CN-          0.0000  -11.8480                 -1.00 0.00 0.00 279.8267
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 0.00 3     1.000 143     2.000 380    -2.000   1
3801433 I(CN)2-          0.0000  -11.4580                -1.00 0.00 0.00 178.9399
 0.00 3     2.000 143     1.000 380    -2.000   1
4101432 K3HFe(CN)6     -85.9900   50.2241                 0.00 0.00 0.00 330.2563
 0.00 4     6.000 143     3.000 410     1.000 330     1.000 280
4401431 LiFe(CN)6-3    -80.1490   47.6858                -3.00 0.00 0.00 218.8944
 0.00 3     6.000 143     1.000 440     1.000 280
4601431 MgFe(CN)6-     -69.3100   55.3916                -1.00 0.00 0.00 236.2584
 0.00 3     6.000 143     1.000 460     1.000 281
4601432 MgFe(CN)6-2      0.0000   49.4251                -2.00 0.00 0.00 236.2584
 0.00 3     6.000 143     1.000 460     1.000 280
5401431 Ni(CN)4-2      -43.1900   30.1257                -2.00 0.00 0.00 162.7610
 0.00 2     4.000 143     1.000 540
8001431 SrFe(CN)6-     -69.8300   55.6181                -1.00 0.00 0.00 299.5734
 0.00 3     1.000 800     1.000 281     6.000 143
8701431 Tl(CN)4-         0.0000   -8.0189                -1.00 0.00 0.00 308.4543
 0.00 3     4.000 143     1.000 870    -2.000   1
8701432 TlFe(CN)6-3    -84.8800   48.7508                -3.00 0.00 0.00 416.3367
 0.00 3     6.000 143     1.000 870     1.000 280
9501431 Zn(CN)4-2      -25.5390   16.7150                -2.00 0.00 0.00 169.4610
 0.00 2     4.000 143     1.000 950
9501432 Zn(CN)3-       -20.1990   16.0480                -1.00 0.00 0.00 143.4432
 0.00 2     3.000 143     1.000 950
9501430 Zn(CN)2(aq)    -10.9990   11.0710                 0.00 0.00 0.00 117.4255
 0.00 2     2.000 143     1.000 950
5401436 Ni(CN)3-         0.0000   22.6346                -1.00 0.00 0.00 136.7432
 0.00 2     3.000 143     1.000 540
5401432 NiH(CN)4-        0.0000   36.7482                -1.00 0.00 0.00 163.7689
 0.00 3     4.000 143     1.000 540     1.000 330
5401433 NiH2CN4(aq)      0.0000   41.4576                 0.00 0.00 0.00 164.7768
 0.00 3     4.000 143     1.000 540     2.000 330
5401434 NiH3(CN)4+       0.0000   43.9498                 1.00 0.00 0.00 165.7848
 0.00 3     4.000 143     1.000 540     3.000 330
5401435 Ni(CN)2(aq)      0.0000   14.5864                 0.00 0.00 0.00 110.7255
 0.00 2     2.000 143     1.000 540
2811432 Fe2(CN)6(aq)     0.0000   56.9822                 0.00 0.00 0.00 267.8004
 0.00 2     6.000 143     2.000 281
 201440 Ag(OCN)2-        0.0000    5.0034                -1.00 0.00 0.00 191.9025
 0.00 2     2.000 144     1.000  20
 201433 Ag(CN)3-2      -33.4950   21.4002                -2.00 0.00 0.00 185.9214
 0.00 2     3.000 143     1.000  20
1001430 BaFe(CN)6-2      0.0000   49.4032                -2.00 0.00 0.00 349.2804
 0.00 3     6.000 143     1.000 280     1.000 100
3309921 H ACETATE        0.0000    4.7600                 0. 0.0  0.0  60.0600
      2     1.000 992     1.000 330
3309931 H TARTRAT        0.0000    4.1600                -1. 0.0  0.0  149.1000
      2     1.000 993     1.000 330
3309932 H TARTRAT        0.0000    6.6700                 0. 0.0  0.0  150.1100
      2     1.000 993     2.000 330
3309941 H GLYCINE        0.0000    9.7800                 0. 0.0  0.0  75.0800
      2     1.000 994     1.000 330
3309942 H GLYCINE        0.0000   12.1200                 1. 0.0  0.0  76.0900
      2     1.000 994     2.000 330
3309951 H SALICYL        0.0000   13.400                 -1. 0.0  0.0  137.1300
      2     1.000 995     1.000 330
3309952 H SALICYL        0.0000   16.4                    0. 0.0  0.0  138.1400
      2     1.000 995     2.000 330
3309961 H GLUTAMA        0.0000    9.9500                -1. 0.0  0.0  146.1400
      2     1.000 996     1.000 330
3309962 H GLUTAMA        0.0000   14.37                   0. 0.0  0.0  147.1500
      2     1.000 996     2.000 330
3309971 H PHTHALA        0.0000    5.4000                -1. 0.0  0.0  165.1400
      2     1.000 997     1.000 330
3309972 H PHTHALA        0.0000    8.3500                 0. 0.0  0.0  166.1500
      2     1.000 997     2.000 330
1609921 CD ACETATE       0.0000    1.9300                 1. 0.0  0.0  171.4600
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      2     1.000 160     1.000 992
1609931 CD TARTRAT     0.0000    3.9000                  0. 0.0  0.0  260.5000
      2     1.000 160     1.000 993
1609941 CD GLYCINE     0.0000    4.8000                  1. 0.0  0.0  186.4800
      2     1.000 160     1.000 994
1609942 CD GLYCINE     0.0000    8.4000                  0. 0.0  0.0  260.5500
      2     1.000 160     2.000 994
1609961 CD GLUTAMA     0.0000    4.7800                  0. 0.0  0.0  257.5400
      2     1.000 160     1.000 996
1609962 CD GLUTAMA     0.0000    2.7800                 -2. 0.0  0.0  402.6700
      2     1.000 160     2.000 996
1609971 CD PHTHALA     0.0000    2.5000                  0. 0.0  0.0  276.5400
      2     1.000 160     1.000 997
6009931 PB TARTRAT     0.0000    3.7800                  0. 0.0  0.0  355.3000
      2     1.000 600     1.000 993
6009941 PB GLYCINE     0.0000    5.4700                  1. 0.0  0.0  281.2800
      2     1.000 600     1.000 994
6009942 PB GLYCINE     0.0000    8.3200                  0. 0.0  0.0  355.3500
      2     1.000 600     2.000 994
1009921 BA ACETATE     0.0000    1.0700                  1. 0.0  0.0  196.4100
      2     1.000 100     1.000 992
1009931 BA TARTRATE    0.0000    2.5400                  0. 0.0  0.0  285.4500
      2     1.000 100     1.000 993
1009941 BA GLYCINE     0.0000    0.7700                  1. 0.0  0.0  211.4300
      2     1.000 100     1.000 994
1009951 BA SALICYL     0.0000    0.2100                  0. 0.0  0.0  273.4800
      2     1.000 100     1.000 995
1009961 BA GLUTAMA     0.0000    1.2800                  0. 0.0  0.0  282.4900
      2     1.000 100     1.000 996
1009971 BA PHTHALA     0.0000    2.3300                  0. 0.0  0.0  301.4900
      2     1.000 100     1.000 997
0209921 AG ACETATE     0.0000    0.7300                  0. 0.0  0.0  166.9300
      2     1.000  20     1.000 992
0209922 AG ACETATE2    0.0000    0.64                   -1. 0.0  0.0  225.9800
      2     1.000  20     2.000 992
0209941 AG GLYCINE     0.0000    3.5100                  0. 0.0  0.0  181.9500
      2     1.000  20     1.000 994
0209942 AG GLYCINE     0.0000    3.3800                 -1. 0.0  0.0  256.0200
      2     1.000  20     2.000 994
2119921 Cr ACETATE     0.0000   14.2500                  2. 0.0  0.0  111.0600
 0.00 4     1.000 211     1.000 992     2.000 330    -2.000 002
2119922 Cr ACETATE2    0.0000   16.6800                  1. 0.0  0.0  170.1100
 0.00 4     1.000 211     2.000 992     2.000 330    -2.000 002
2119923 Cr ACETATE3    0.0000   19.20                    0. 0.0  0.0  229.0
 0.00 4     1.000 211     3.000 992     2.000 330    -2.000 002
2119941 CR GLYCINE     0.0000    8.4000                  2. 0.0  0.0  126.0800
 0.00 2     1.000 211     1.000 994
2119942 CR GLYCINE     0.0000    6.4000                  0. 0.0  0.0  200.1500
 0.00 2     1.000 211     2.000 994
2119943 CR GLYCINE     0.0000    5.7000                 -1. 0.0  0.0  274.2200
 0.00 2     1.000 211     3.000 994
2119971 CR PHTHALA     0.0000   15.1400                  1. 0.0  0.0  216.1400
 0.00 4     1.000 211     1.000 997     2.000 330    -2.000   2
2119972 CR PHTHALA     0.0000   19.6200                 -1. 0.0  0.0  380.2700
 0.00 4     1.000 211     2.000 997     2.000 330    -2.000   2
2119973 CR PHTHALA     0.0000    22.100                 -3. 0.0  0.0  544.4000
 0.00 4     1.000 211     3.000 997     2.000 330    -2.000   2
8719931 Tl TARTRAT     0.0000    1.39000                -1. 0.0  0.0  352.4800
 0.00 2     1.000 870     1.000 993
3609941 Hg GLYCINE     0.0000   10.800                   1. 0.0  0.0  274.6800
 0.00 2     1.000 360     1.000 994
3609942 Hg GLYCINE     0.0000   20.000                   1. 0.0  0.0  348.7500
 0.00 2     1.000 360     2.000 994
1609721 CdBUTANOATE    0.0000    1.25                    1. 0.0  0.0  199.4
      2     1.000 160     1.000 972
1609671 CdCITRATE      0.0000    5.30                   -1. 0.0  0.0  301.4
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      2     1.000 160     1.000 967
1609673 CdH2CITRATE    0.0000    2.05                          1. 0.0  0.0  303.4
      3     1.000 160     1.000 967     2.000 330
1609672 CdHCITRATE     0.0000    3.37                          0. 0.0  0.0  302.4
      3     1.000 160     1.000 967     1.000 330
1609674 CdCITRATE2     0.0000    5.34                         -4. 0.0  0.0  490.4
      2     1.000 160     2.000 967
1609692 CdHEDTA        0.0000    2.9                          -1. 0.0  0.0  401.4
      3     1.000 160     1.000 969     1.000 330
1609922 CdACETATE2     0.0000    3.15                          0. 0.0  0.0  230.4
      2     1.000 160     2.000 992
1609923 CdACETATE3     0.0000    2.17                         -1. 0.0  0.0  289.4
      2     1.000 160     3.000 992
1609924 CdACETATE4     0.0000    2.04                         -2. 0.0  0.0  394.4
      2     1.000 160     4.000 992
1609551 CdDIETHAM      0.0000    2.62                          2. 0.0  0.0  185.40
      2     1.000 160     1.000 955
1609552 CdDIETHAMIN2   0.0000    4.86                          2. 0.0  0.0  258.41
      2     1.000 160     2.000 955
1609553 CdDIETHAMIN3   0.0000    6.36                          2. 0.0  0.0  331.42
      2     1.000 160     3.000 955
1609554 CdDIETHAMIN4   0.0000    7.31                          2. 0.0  0.0  404.43
      2     1.000 160     4.000 955
1609711 CdPROPANOATE   0.0000    1.19                          1. 0.0  0.0  185.4
      2     1.000 160     1.000 971
1609712 CdPROPANOAT2   0.0000    1.86                          0. 0.0  0.0  285.4
      2     1.000 160     2.000 971
1609713 CdPROPANOAT3   0.0000    2.345                        -1. 0.0  0.0  331.4
      2     1.000 160     3.000 971
1609714 CdPROPANOAT4   0.0000    1.98                         -2. 0.0  0.0  404.527
      2     1.000 160     4.000 971
1609722 CdBUTANOAT2    0.0000    1.98                          0. 0.0  0.0  286.4
      2     1.000 160     2.000 972
1609723 CdBUTANOATE3   0.0000    2.34                         -1. 0.0  0.0  373.4
      2     1.000 160     3.000 972
1609724 CdBUTANOAT4    0.0000    1.98                         -2. 0.0  0.0  460.4
      2     1.000 160     4.000 972
1609641 CdPROPAM       0.0000    2.62                          2. 0.0  0.0  171.41
      2     1.000 160     1.000 964
1609642 CdPROPAM2      0.0000    4.64                          2. 0.0  0.0  230.41
      2     1.000 160     2.000 964
1609643 CdPROPAM3      0.0000    6.03                          2. 0.0  0.0  289.42
      2     1.000 160     3.000 964
1609651 CdISOPROPAM    0.0000    2.55                          2. 0.0  0.0  171.41
      2     1.000 160     1.000 965
1609652 CdISOPROPAM2   0.0000    4.57                          2. 0.0  0.0  230.41
      2     1.000 160     2.000 965
1609653 CdISOPROPAM3   0.0000    6.07                          2. 0.0  0.0  289.40
      2     1.000 160     3.000 965
1609654 CdISOPROPAM4   0.0000    6.90                          2. 0.0  0.0  348.41
      2     1.000 160     4.000 965
3309171 H Benzoat      0.0000    4.2000                        0. 0.0  0.0  122.1300
      2     1.000 917     1.000 330
3309181 H PAcetat      0.0000    4.3100                        0. 0.0  0.0  136.1600
      2     1.000 918     2.000 330
3309201 H IPhthal      0.0000    3.5000                       -1. 0.0  0.0  165.1400
      2     1.000 920     1.000 330
3309202 H IPhthal      0.0000    8.0000                        0. 0.0  0.0  166.1500
      2     1.000 920     2.000 330
2819711 FePrpanot      0.0000    3.4000                        0. 0.0  0.0  128.8700
      2     1.000 971     1.000 281
2819731 FeIsobuty      0.0000    3.6000                        2. 0.0  0.0  142.8800
      2     1.000 973     1.000 281
2819721 FeButanot      0.0000    5.5600                        2. 0.0  0.0  142.8800
      2     1.000 972     1.000 281
2819841 FeIsvaler      0.0000    5.580                         2. 0.0  0.0  156.9700
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      2     1.000 984     1.000 281
2819851 FeValerat      0.0000    5.58                    2. 0.0  0.0  156.9700
      2     1.000 985     1.000 281
2319171 CuBenzoat      0.0000    2.1000                  1. 0.0  0.0  184.6600
      2     1.000 917     1.000 231
2319181 CuPAcetat      0.0000    1.9700                  1. 0.0  0.0  198.6900
      2     1.000 918     1.000 231
1009731 BaIsobuty      0.0000    0.6400                  1. 0.0  0.0  224.3700
      2     1.000 973     1.000 100
1009841 BaIsvaler      0.0000    0.680                   1. 0.0  0.0  238.4600
      2     1.000 984     1.000 100
1009851 BaValerat      0.0000    0.66                    1. 0.0  0.0  238.4600
      2     1.000 985     1.000 100
1009201 BaIPhthal      0.0000    1.5500                  0. 0.0  0.0  301.4700
      2     1.000 920     1.000 100
1609731 CdIsobuty      0.0000    1.1700                  1. 0.0  0.0  199.4300
      2     1.000 973     1.000 160
1609851 CdValerat      0.0000    1.19                    1. 0.0  0.0  199.4300
      2     1.000 985     1.000 160
1609171 CdBenzoat      0.0000    1.9000                  1. 0.0  0.0  233.5200
      2     1.000 917     1.000 160
1609172 CdBenzoat      0.0000    1.6500                  0. 0.0  0.0  354.6400
      2     2.000 917     1.000 160
9509181 ZnPAcetat      0.0000    1.6700                  1. 0.0  0.0  200.5200
      2     1.000 918     1.000 950
1609181 CdPAcetat      0.0000    1.1500                  1. 0.0  0.0  247.5500
      2     1.000 918     1.000 160
1609182 CdPAcetat2     0.0000    1.9200                  0. 0.0  0.0  382.7000
      2     2.000 918     1.000 160
1609201 CdIPhthal      0.0000    1.3300                  0. 0.0  0.0  276.5300
      2     1.000 920     1.000 160
1609202 CdIPhthal2     0.0000    2.1700                 -2. 0.0  0.0  440.6700
      2     2.000 920     1.000 160
1609203 CdIPhthalH     0.0000    5.3200                  1. 0.0  0.0  277.5400
      3     2.000 920     1.000 160     1.000 330
2119731 CrIsobuty      0.0000   12.7300                  2. 0.0  0.0  139.0300
      4     2.000 330    -2.000   2     1.000 973     1.000 211
2119721 CrButanot      0.0000   12.7400                  2. 0.0  0.0  139.030
      4     2.000 330    -2.000   2     1.000 972     1.000 211
2119841 CrIsvaler      0.0000   12.760                   2. 0.0  0.0  153.1200
      4     2.000 330    -2.000   2     1.000 984     1.000 211
2119851 CrValerat      0.0000   12.75                    2. 0.0  0.0  153.1200
      4     2.000 330    -2.000   2     1.000 985     1.000 211
6009731 PbIsobuty      0.0000    2.6700                  1. 0.0  0.0  308.3100
      2     1.000 973     1.000 600
6009841 PbIsvaler      0.0000    2.050                   1. 0.0  0.0  308.3100
      2     1.000 984     1.000 600
6009851 PbValerat      0.0000    2.06                    1. 0.0  0.0  308.3100
      2     1.000 985     1.000 600
6009171 PbBenzoat      0.0000    2.5000                  1. 0.0  0.0  328.3100
      2     1.000 917     1.000 600
4609171 MgBenzoat      0.0000    0.1000                  1. 0.0  0.0  145.4300
      2     1.000 917     1.000 460
1509171 CaBenzoat      0.0000    0.2000                  1. 0.0  0.0  161.2000
      2     1.000 917     1.000 150
9509171 ZnBenzoat      0.0000    1.4000                  1. 0.0  0.0  186.4900
      2     1.000 917     1.000 950
6009201 PbIPhthal      0.0000    2.1700                  0. 0.0  0.0  371.3200
      2     1.000 920     1.000 600
6009202 PbIPhthal2     0.0000    3.3600                 -2. 0.0  0.0  535.4600
      2     2.000 920     1.000 600
6009203 PbIPhthalH     0.0000    6.2800                  1. 0.0  0.0  372.3300
      3     1.000 920     1.000 600     1.000 330
3619731 HgIsobuty      0.0000   10.6870                  1. 0.0  0.0  287.6200
      4     2.000 330    -2.000   2     1.000 973     1.000 361
3619721 HgButanot      0.0000   10.0970                  1. 0.0  0.0  287.6200
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      4     2.000 330    -2.000   2     1.000 972     1.000 361
3619841 HgIsvaler       0.0000   10.7170                  1. 0.0  0.0  301.7100
      4     2.000 330    -2.000   2     1.000 984     1.000 361
3619851 HgValerat       0.0000   10.727                   1. 0.0  0.0  301.7100
      4     2.000 330    -2.000   2     1.000 985     1.000 361
3619971 HgPhthala       0.0000   10.9970                  0. 0.0  0.0  364.7200
      4     2.000 330    -2.000   2     1.000 997     1.000 361
5409731 NiIsobuty       0.0000    1.2300                  1. 0.0  0.0  145.7400
      2     1.000 973     1.000 540
5409841 NiIsvaler       0.0000    1.270                   1. 0.0  0.0  159.8300
      2     1.000 984     1.000 540
5409851 NiValerat       0.0000    1.26                    1. 0.0  0.0  159.8300
      2     1.000 985     1.000 540
5409171 NiBenzoat       0.0000    1.400                   1. 0.0  0.0  179.8300
      2     1.000 917     1.000 540
5409181 NiPAcetat       0.0000    0.65000                 1. 0.0  0.0  193.8600
      2     1.000 918     1.000 540
5409182 NiPAcetat       0.0000    0.99000                 0. 0.0  0.0  342.3400
      2     2.000 918     1.000 540
5409972 NiPhthalaH      0.0000    6.1000                  1. 0.0  0.0  223.8500
      3     1.000 997     1.000 540     1.000 330
2109692 CrHEDTA         0.0000    6.1                     0. 0.0  0.0  341.0
      3     1.000 210     1.000 969     1.000 330
2119711 CrPROPANAT      0.0000  14.32                     2. 0.0  0.0  125.0
      4     1.000 211     1.000 971     2.000 330    -2.000   2
2119712 CrPROPANAT2     0.0000  16.66                     1. 0.0  0.0  198.0
      4     1.000 211     2.000 971     2.000 330    -2.000   2
2119713 CrPROPANAT3     0.0000  19.32                     0. 0.0  0.0  270.996
      4     1.000 211     3.000 971     2.000 330    -2.000   2
2109921 CrAcetate     0.0000    1.80                    2. 0.0  0.0  111.05
      2     1.000 210     1.000 992
2109922 CrAcetate2    0.0000    2.92                    1. 0.0  0.0  170.10
      2     1.000 210     2.000 992
2319691 CuEDTA          0.0000   18.785                  -2. 0.0  0.0  339.54
      2     1.000 231     1.000 969
2319692 CuHEDTA         0.0000   11.195                  -1. 0.0  0.0  340.54
      3     1.000 231     1.000 969     1.000 330
2319922 CuACETATE2      0.0000    3.63                    0. 0.0  0.0  181.582
      2     1.000 231     2.000 992
2319923 CuACETATE3      0.0000    3.10                   -1. 0.0  0.0  240.603
      2     1.000 231     3.000 992
2319924 CuACETATE4      0.0000    2.90                   -2. 0.0  0.0  299.624
      2     1.000 231     4.000 992
2319711 CuPROPANOAT     0.0000    2.22                    1. 0.0  0.0  136.57
      2     1.000 231     1.000 971
2319712 CuPROPANAT2     0.0000    2.62                    0. 0.0  0.0  209.60
      2     1.000 231     2.000 971
2319713 CuPROANAT3      0.0000    2.30                   -1. 0.0  0.0  282.64
      2     1.000 231     3.000 971
2319714 CuPROPANAT4     0.0000    2.70                   -2. 0.0  0.0  355.67
      2     1.000 231     4.000 971
2319582 CuMETHAM2       0.0000    7.51                    2. 0.0  0.0  94.558
      2     1.000 231     2.000 958
2319591 CuDIMETHAM      0.0000    3.21                    2. 0.0  0.0  108.57
      2     1.000 231     1.000 959
2319592 CUDIMETHAM2     0.0000    5.66                    2. 0.0  0.0  153.598
      2     1.000 231     2.000 959
2319593 CuDIMETHAM3     0.0000    7.26                    2. 0.0  0.0  198.628
      2     1.000 231     3.000 959
2319721 CuBUTANOAT      0.0000    2.14                    1. 0.0  0.0  150.583
      2     1.000 231     1.000 972
2319722 CuBUTANOAT2     0.0000    2.6                     0. 0.0  0.0  237.626
      2     1.000 231     2.000 972
2319723 CuBUTANOAT3     0.0000    2.30                   -1. 0.0  0.0  342.67
      2     1.000 231     3.000 972
2319724 CuBUTANOAT4     0.0000    2.95                   -2. 0.0  0.0  411.712
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      2     1.000 231     4.000 972
2319731 CuISBUTRAT     0.0000    2.170                    1. 0.0  0.0  150.583
      2     1.000 231     1.000 973
2319732 CuISOBUTYRT2   0.0000    2.7                      0. 0.0  0.0  237.626
      2     1.000 231     2.000 973
6009671 PB CITRATE     0.0000    4.34                    -1. 0.0  0.0  396.252
      2     1.000 600     1.000 967
6009672 PBCITRATE2     0.0000    6.08                    -4. 0.0  0.0  585.315
      2     1.000 600     2.000 967
6009673 PBCITRATE3     0.0000    6.97                    -7. 0.0  0.0  774.378
      2     1.000 600     3.000 967
6009681 PBNTA          0.0000   11.6233                  -1. 0.0  0.0  395.254
      2     1.000 600     1.000 968
6009682 PBHNTA         0.0000    3.795                    0. 0.0  0.0  396.254
      3     1.000 600     1.000 968     1.000 330
6009692 PBHEDTA        0.0000    9.68                    -1. 0.0  0.0  497.4
      3     1.000 600     1.000 969     1.000 330
6009693 PBH2EDTA       0.0000    6.22                     0. 0.0  0.0  498.4
      3     1.000 600     1.000 969     2.000 330
6009921 PBACETATE      0.0000    2.87                     1. 0.0  0.0  266.24
      2     1.000 600     1.000 992
6009922 PBACETATE2     0.0000    4.08                     0. 0.0  0.0  325.232
      2     1.000 600     2.000 992
6009923 PBACETATE3     0.0000    3.59                    -1. 0.0  0.0  384.25
      2     1.000 600     3.000 992
6009711 PBPROPANAT     0.0000    2.64                     1. 0.0  0.0  280.222
      2     1.000 600     1.000 971
6009712 PBPROPANOAT2   0.0000    4.15                     0. 0.0  0.0  353.25
      2     1.000 600     2.000 971
6009713 PBPROPANOAT3   0.0000    2.99                    -1. 0.0  0.0  426.286
      2     1.000 600     3.000 971
6009714 PBPROPANOAT4   0.0000    4.18                    -2. 0.0  0.0  499.318
      2     1.000 600     4.000 971
6009721 PB BUTANOAT    0.0000    2.125                    1. 0.0  0.0  294.23
      2     1.000 600     1.000 972
6009722 PBBUTANOATE2   0.0000    3.735                    0. 0.0  0.0  381.28
      2     1.000 600     2.000 972
6009723 PBBUTANOAT3    0.0000    4.125                   -1. 0.0  0.0  468.32
      2     1.000 600     3.000 972
6009724 PBBUTANOAT4    0.0000    4.43                    -2. 0.0  0.0  555.36
      2     1.000 600     4.000 972
5409671 NICITRATE      0.0000    6.62                    -1. 0.0  0.0  247.77
      2     1.000 540     1.000 967
5409672 NICITRATEH     0.0000    4.09                     0. 0.0  0.0  248.77
      3     1.000 540     1.000 967     1.000 330
5409673 NICITRATEH2    0.0000    2.13                     1. 0.0  0.0  249.77
      3     1.000 540     1.000 967     2.000 330
5409691 NIEDTA         0.0000   20.33                    -2. 0.0  0.0  347.92
      2     1.000 540     1.000 969
5409692 NIHEDTA        0.0000   11.56                    -1. 0.0  0.0  348.92
      3     1.000 540     1.000 969     1.000 330
5409711 NIPROPANOAT    0.0000     .73                     1. 0.0  0.0  131.73
      2     1.000 540     1.000 971
5409712 NIPROPANOAT2   0.0000    0.8000                   0. 0.0  0.0  204.76
      2     1.000 540     2.000 971
5409713 NIPROPANOAT3   0.0000     .97                    -1. 0.0  0.0  277.795
      2     1.000 540     3.000 971
5409721 NI BUTANOAT    0.0000     .77                     1. 0.0  0.0  145.75
      2     1.000 540     1.000 972
5409722 NIBUTANOAT2    0.0000     .85                     0. 0.0  0.0  218.785
      2     1.000 540     2.000 972
5409723 NIBUTAOAT3     0.0000    1.34                    -1. 0.0  0.0  291.82
      2     1.000 540     3.000 972
5409641 NINPROPYLAM    0.0000    2.81                     2. 0.0  0.0  117.75
      2     1.000 540     1.000 964
5409642 NINPROPYLAM2   0.0000    5.02                     2. 0.0  0.0  176.79
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      2     1.000 540     2.000 964
5409643 NINPROPYLAM3   0.0000    6.79                    2. 0.0  0.0  235.83
      2     1.000 540     3.000 964
5409644 NINPROPYLAM4   0.0000    8.31                    2. 0.0  0.0  294.87
      2     1.000 540     4.000 964
5409651 NIIPROYLAM     0.0000    2.71                    2. 0.0  0.0  117.75
      2     1.000 540     1.000 965
5409652 NIIPROPYLAM2   0.0000    4.86                    2. 0.0  0.0  176.79
      2     1.000 540     2.000 965
5409653 NIIPROPYLAM3   0.0000    6.57                    2. 0.0  0.0  235.83
      2     1.000 540     3.000 965
5409654 NIIPROPYLAM4   0.0000    7.83                    2. 0.0  0.0  294.87
      2     1.000 540     4.000 965
5409655 NIIPROPYLAM5   0.0000    8.43                    2. 0.0  0.0  353.91
      2     1.000 540     5.000 965
0209551 AGDIETHAM      0.0000    3.965                   1. 0.0  0.0  152.897
      2     1.000 020     1.000 955
0209552 AGDIETHAM2     0.0000    7.02                    1. 0.0  0.0  197.926
      2     1.000 020     2.000 955
0209581 AGMETHAM       0.0000    3.18                    1. 0.0  0.0  138.928
      2     1.000 020     1.000 958
0209582 AGMETHAM2      0.0000    7.14                    1. 0.0  0.0  169.99
      2     1.000 020     2.000 958
0209611 AGHEXYLAM      0.0000    3.66                    1. 0.0  0.0  208.868
      2     1.000 020     1.000 961
0209612 AGHEXYLAM2     0.0000    7.35                    1. 0.0  0.0  309.868
      2     1.000 020     2.000 961
0209651 AGIPROPAM      0.0000    3.19                    1. 0.0  0.0  166.91
      2     1.000 020     1.000 965
0209652 AGIPROPYLAM2   0.0000    6.85                    1. 0.0  0.0  225.948
      2     1.000 020     2.000 965
0209561 AGNBUTYLAM     0.0000    3.55                    1. 0.0  0.0  181.01
      2     1.000 020     1.000 956
0209562 AGNBUTYLAM2    0.0000    7.77                    1. 0.0  0.0  254.148
      2     1.000 020     2.000 956
0209961 AGGLUTAM       0.0000    3.79                    0. 0.0  0.0  252.998
      2     1.000 020     1.000 996
0209962 AGGLUTAM2      0.0000    6.55                   -1. 0.0  0.0  398.128
      2     1.000 020     2.000 996
0209681 AGNTA          0.0000    5.36                   -2. 0.0  0.0  295.928
      2     1.000 020     1.000 968
0209691 AGEDTA         0.0000    7.355                  -3. 0.0  0.0  383.868
      2     1.000 020     1.000 969
0209692 AGEDTA2        0.0000   11.355                  -7. 0.0  0.0  659.868
      2     1.000 020     2.000 969
0209693 AGHEDTA        0.0000    3.36                   -2. 0.0  0.0  384.868
      3     1.000 020     1.000 969     1.000 330
0209801 AG2METPYR      0.0000    2.32                    1. 0.0  0.0  201.868
      2     1.000 020     1.000 980
0209802 AG2METPYR2     0.0000    4.68                    1. 0.0  0.0  295.868
      2     1.000 020     2.000 980
0209811 AG3METPYR      0.0000    2.20                    1. 0.0  0.0  201.868
      2     1.000 020     1.000 981
0209812 AG3METPYR2     0.0000    4.46                    1. 0.0  0.0  295.868
      2     1.000 020     2.000 981
0209821 AG4METPYR      0.0000    2.21                    1. 0.0  0.0  201.868
      2     1.000 020     1.000 982
0209822 AG4METPYR2     0.0000    4.67                    1. 0.0  0.0  295.868
      2     1.000 020     2.000 982
0209641 AGNPROPYLAM    0.0000    3.47                    1. 0.0  0.0  166.908
      2     1.000 020     1.000 964
0209642 AGNPROPYLAM2   0.0000    7.51                    1. 0.0  0.0  225.948
      2     1.000 020     2.000 964
9509961 ZNGLUTAM       0.0000    3.79                    0. 0.0  0.0  210.5
      2     1.000 950     1.000 996
9509962 ZNGLUTAM2      0.0000    8.25                   -2. 0.0  0.0  355.63
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      2     1.000 950     2.000 996
9509963 ZNGLUTAM3      0.0000    9.8                          -4. 0.0  0.0  500.76
      2     1.000 950     3.000 996
9509811 ZN3METPYR      0.0000    1.00                          2. 0.0  0.0  159.37
      2     1.000 950     1.000 981
9509812 ZN3METPYR2     0.0000    2.1                           2. 0.0  0.0  224.74
      2     1.000 950     2.000 981
9509813 ZN3METPYR3     0.0000    2.6                           2. 0.0  0.0  290.11
      2     1.000 950     3.000 981
9509814 ZN3METPYR4     0.0000    3.7                           2. 0.0  0.0  355.48
      2     1.000 950     4.000 981
9509941 ZNGLYCERIN     0.0000    5.38                          1. 0.0  0.0  139.44
      2     1.000 950     1.000 994
9509942 ZNGLYCERIN2    0.0000    9.81                          0. 0.0  0.0  213.51
      2     1.000 950     2.000 994
9509943 ZNGLYCERN3     0.0000   12.3                          -1. 0.0  0.0  287.58
      2     1.000 950     3.000 994
9509671 ZNCITRATE      0.0000    6.10                         -1. 0.0  0.0  254.43
      2     1.000 950     1.000 967
9509672 ZNCITRATE2     0.0000    6.70                         -4. 0.0  0.0  443.49
      2     1.000 950     2.000 967
9509673 ZNCITRATEH     0.0000    3.78                          0. 0.0  0.0  255.43
      3     1.000 950     1.000 967     1.000 330
9509674 ZNCITRATEH2    0.0000    1.68                          1. 0.0  0.0  256.43
      3     1.000 950     1.000 967     2.000 330
9509971 ZNPHTHLATE     0.0000    2.91                          0. 0.0  0.0  229.50
      2     1.000 950     1.000 997
9509972 ZNPHTHALATE2   0.0000    4.2                          -2. 0.0  0.0  393.64
      2     1.000 950     2.000 997
6009961 PBGLUTAM       0.0000    4.70                          0. 0.0  0.0  352.32
      2     1.000 600     1.000 996
6009962 PBGLUTAM2      0.0000    7.55                         -2. 0.0  0.0  497.45
      2     1.000 600     2.000 996
6009691 PBEDTA         0.0000   17.88                         -2. 0.0  0.0  483.19
      2     1.000 600     1.000 969
6009971 PBPHTHALAT     0.0000    2.78                          0. 0.0  0.0  371.32
      2     1.000 600     1.000 997
6009972 PBPHTHALA2     0.0000    4.01                         -2. 0.0  0.0  535.45
      2     1.000 600     2.000 997
6009973 PBPHTHALAH     0.0000    6.56                          1. 0.0  0.0  536.46
      3     1.000 600     1.000 997     1.000 330
6009924 PBACETATE4     0.0000    3.4                          -2. 0.0  0.0  443.39
      2     1.000 600     4.000 992
2319681 CUNTA          0.0000   13.1                          -1. 0.0  0.0  251.61
      2     1.000 231     1.000 968
2319682 CUNTA2         0.0000   17.5                          -4. 0.0  0.0  439.67
      2     1.000 231     2.000 968
2319581 CUMETHAM       0.0000    4.11                          2. 0.0  0.0  94.474
      2     1.000 231     1.000 958
2319583 CUMETHAM3      0.0000   10.21                          2. 0.0  0.0  156.51
      2     1.000 231     3.000 958
2319584 CUMETHAM4      0.0000   12.08                          2. 0.0  0.0  187.528
      2     1.000 231     4.000 958
2319811 CU3METPYR      0.0000    2.74                          2. 0.0  0.0  157.546
      2     1.000 231     1.000 981
2319812 CU3METPYR2     0.0000    4.8                           2. 0.0  0.0  251.546
      2     1.000 231     2.000 981
2319813 CU3METPYR3     0.0000    6.3                           2. 0.0  0.0  345.546
      2     1.000 231     3.000 981
2319814 CU3METPYR4     0.0000    7.2                           2. 0.0  0.0  439.546
      2     1.000 231     4.000 981
2319821 CU4METPYR      0.0000    2.88                          2. 0.0  0.0  157.546
      2     1.000 231     1.000 982
2319822 CU4METPYR2     0.0000    5.16                          2. 0.0  0.0  251.546
      2     1.000 231     2.000 982
2319823 CU4METPYR3     0.0000    6.77                          2. 0.0  0.0  345.546
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      2     1.000 231     3.000 982
2319824 CU4METPYR4     0.0000    8.08                          2. 0.0  0.0  439.546
      2     1.000 231     4.000 982
2319825 CU4METPYR5     0.0000    8.3                           2. 0.0  0.0  533.546
      2     1.000 231     5.000 982
2319961 CUGLUTAM       0.0000    8.33                          0. 0.0  0.0  208.676
      2     1.000 231     1.000 996
2319671 CUCITRATE      0.0000    7.26                         -1. 0.0  0.0  252.606
      2     1.000 231     1.000 967
2319672 CUCITRATE2     0.0000    8.72                         -4. 0.0  0.0  441.666
      2     1.000 231     2.000 967
2319673 CUHCITRATE     0.0000    4.27                          0. 0.0  0.0  253.60
      3     1.000 231     1.000 967     1.000 330
2319674 CUH2CITRATE    0.0000    2.2                           1. 0.0  0.0  254.60
      3     1.000 231     1.000 967     2.000 330
2319841 CUISVALER      0.0000    2.08                          1. 0.0  0.0  164.676
      2     1.000 231     1.000 984
2319971 CUPHTHALAT     0.0000    4.04                          0. 0.0  0.0  227.676
      2     1.000 231     1.000 997
2319970 CuPhthalaH     0.0000    6.74                          1. 4.0  0.0  228.68
      3     1.000 231     1.000 997     1.000 330
2319851 CUVALERAT      0.0000    2.12                          1. 0.0  0.0  164.676
      2     1.000 231     1.000 985
2319852 CUVALERAT2     0.0000    3.0                           0. 0.0  0.0  265.806
      2     1.000 231     2.000 985
1009691 BAEDTA         0.0000    8.00                         -2. 0.0  0.0  413.34
      2     1.000 100     1.000 969
1009671 BACITRATE      0.0000    4.06                         -1. 0.0  0.0  326.4
      2     1.000 100     1.000 967
1009672 BACITRATEH     0.0000    2.70                          0. 0.0  0.0  327.4
      3     1.000 100     1.000 967     1.000 330
1009673 BACITRATEH2    0.0000    1.27                          1. 0.0  0.0  328.4
      3     1.000 100     1.000 967     2.000 330
1009711 BAPROPANOAT    0.0000     .34                          1. 0.0  0.0  210.372
      2     1.000 100     1.000 971
1009721 BABUTANOAT     0.0000     .94                          1. 0.0  0.0  224.413
      2     1.000 100     1.000 972
2109691 CR EDTA        0.0000   13.61                         -2. 0.0  0.0  327.996
      2     1.000 210     1.000 969
5409801 NI2METPYR      0.0000     .4                           2. 0.0  0.0  152.71
      2     1.000 540     1.000 980
5409811 NI3METPYR      0.0000    2.02                          2. 0.0  0.0  152.71
      2     1.000 540     1.000 981
5409812 NI3METPYR2     0.0000    3.3                           2. 0.0  0.0  246.71
      2     1.000 540     2.000 981
5409813 NI3METPYR3     0.0000    4.1                           2. 0.0  0.0  340.71
      2     0.000 540     3.000 981
5409814 NI3METPYR4     0.0000    4.6                           2. 0.0  0.0  434.71
      2     1.000 540     4.000 981
5409821 NI4METPYR      0.0000    2.11                          2. 0.0  0.0  152.71
      2     1.000 540     1.000 982
5409822 NI4METPYR2     0.0000    3.59                          2. 0.0  0.0  246.71
      2     1.000 540     2.000 982
5409823 NI4METPYR3     0.0000    4.34                          2. 0.0  0.0  340.71
      2     1.000 540     3.000 982
5409824 NI4METPYR4     0.0000    4.70                          2. 0.0  0.0 434.71
      2     1.000 540     4.000 982
5409551 NIDIETHAM1     0.0000    2.78                          2. 0.0  0.0  152.71
      2     1.000 540     1.000 955
5409552 NIDIETHAM2     0.0000    4.97                          2. 0.0  0.0  246.71
      2     1.000 540     2.000 955
5409553 NIDIEHTAM3     0.0000    6.72                          2. 0.0  0.0  340.71
      2     1.000 540     3.000 955
5409554 NIDIETHAM4     0.0000    7.93                          2. 0.0  0.0  434.71
      2     1.000 540     4.000 955
5409555 NIDIETHAM5     0.0000    8.87                          2. 0.0  0.0  529
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      2     1.000 540     5.000 955
5409943 NIGLYCINE3     0.0000   14.2                      -1. 0.0  0.0  280.92
      2     1.000 540     3.000 994
1609811 CD3METPYR      0.0000    1.62                      2. 0.0  0.0  206.4
      2     1.000 160     1.000 981
1609812 CD3METPYR2     0.0000    2.8                       2. 0.0  0.0  300.4
      2     1.000 160     2.000 981
1609813 CD3METPYR3     0.0000    3.6                       2. 0.0  0.0  394.4
      2     1.000 160     3.000 981
1609814 CD3METPYR4     0.0000    4.0                       2. 0.0  0.0  488.4
      2     1.000 160     4.000 981
1609821 CD4METPYR      0.0000    1.51                      2. 0.0  0.0  206.4
      2     1.000 160     1.000 982
1609822 CD4METPYR2     0.0000    2.5                       2. 0.0  0.0  300.4
      2     1.000 160     2.000 982
1609823 CD4METPYR3     0.0000    2.9                       2. 0.0  0.0  394.4
      2     1.000 160     3.000 982
1609824 CD4METPYR4     0.0000    4.0                       2. 0.0  0.0  488.4
      2     1.000 160     4.000 982
1609943 CDGLYCINE      0.0000   10.7                       1. 0.0  0.0  186.47
      2     1.000 160     3.000 994
1609972 CDPHTHALA2     0.0000    2.88                     -2. 0.0  0.0  440.67
      2     1.000 160     2.000 997
1609973 CDPHTHALAH     0.0000    5.88                      1. 0.0  0.0  277.54
      3     1.000 160     1.000 997     1.000 330
1609841 CDISVALERAT    0.0000    1.34                      1. 0.0  0.0  215.53
      2     1.000 160     1.000 984
1609842 CDISVALERAT2   0.0000    2.30                      0. 0.0  0.0  314.6
      2     1.000 160     2.000 984
1609843 CDISVALERAT3   0.0000    2.50                     -1. 0.0  0.0  415.79
      2     1.000 160     3.000 984
1609844 CDISVALERAT4   0.0000    2.0                      -2. 0.0  0.0  516.92
      2     1.000 160     4.000 984
3609831 HGFORMATE      0.0000    2.94                      0. 0.0  0.0  245.61
      2      .500 360     1.000 983
3609832 HGFORMATE2     0.0000    5.45                     -1. 0.0  0.0  290.63
      2      .500 360     2.000 983
3609921 HgAcetate      0.0000    7.14                      0. 0.0  0.0  259.64
      2      .500 360     1.000 992
3609922 HgAcetate2     0.0000   13.26                     -1. 0.0  0.0  318.69
      2      .500 360     2.000 992
3609711 HGPROPANOAT    0.0000    3.72                      0. 0.0  0.0  273.62
      2      .500 360     1.000 971
3609712 HGPROPANOT2    0.0000    6.99                     -1. 0.0  0.0  346.654
      2      .500 360     2.000 971
3619711 HGPROPANOAT    0.0000    9.417                      0. 0.0  0.0  273.62
      4      .500 361     1.000 971     2.000 330   -2.000 002
3619712 HGPROPANOT2    0.0000   13.107                     -1. 0.0  0.0  346.654
      4      .500 361     2.000 971     2.000 330   -2.000 002
8709671 TL CITRATE     0.0000    1.61                     -2. 0.0  0.0  393.43
      2     1.000 870     1.000 967
8709681 TL NTA         0.0000    4.71                     -2. 0.0  0.0  392.434
      2     1.000 870     1.000 968
8709691 TL EDTA        0.0000    6.41                     -3. 0.0  0.0  480.37
      2     1.000 870     1.000 969
8709921 TL ACETATE     0.0000    -.11                      0. 0.0  0.0  263.42
      2     1.000 870     1.000 992
9509691 ZN EDTA        0.0000   16.44                     -2. 0.0  0.0  354.58
      2     1.000 950     1.000 969
9509692 ZN HEDTA       0.0000    9.00                     -1. 0.0  0.0  355.58
      3     1.000 950     1.000 969     1.000 330
9509921 ZN ACETATE     0.0000    1.57                      1. 0.0  0.0  124.392
      2     1.000 950     1.000 992
9509922 ZN ACETATE2    0.0000    1.90                      0. 0.0  0.0  183.412
      2     1.000 950     2.000 992
9509923 ZNACETATE3     0.0000    1.57                     -1. 0.0  0.0  242.433
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      2     1.000 950     3.000 992
9509924 ZN ACETATE4    0.0000    1.36                    -2. 0.0  0.0  301.454
      2     1.000 950     4.000 992
9509551 ZN DIETHYLAM   0.0000    2.51                     2. 0.0  0.0  110.399
      2     1.000 950     1.000 955
9509552 ZN DIETHYLAM2  0.0000    4.96                     2. 0.0  0.0  155.428
      2     1.000 950     2.000 955
9509553 ZN DIETHAM3    0.0000    7.49                     2. 0.0  0.0  200.457
      2     1.000 950     3.000 955
9509554 ZN DIETHAM4    0.0000    9.83                     2. 0.0  0.0  245.486
      2     1.000 950     4.000 955
9509711 ZNPROPANOT     0.0000     .72                     1. 0.0  0.0  138.399
      2     1.000 950     1.000 971
9509712 ZNPROPANOT2    0.0000    1.230                    0. 0.0  0.0  211.434
      2     1.000 950     2.000 971
9509713 ZNPROPANOT3    0.0000    1.82                    -1. 0.0  0.0  284.47
      2     1.000 950     3.000 971
9509714 ZNPROPANOT4    0.0000    1.36                    -2. 0.0  0.0  357.5
      2     1.000 950     4.000 971
9509721 ZNBUTANOAT     0.0000     .983                    1. 0.0  0.0  152.413
      2     1.000 950     1.000 972
9509722 ZNBUTANOT2     0.0000    1.65                     0. 0.0  0.0  239.46
      2     1.000 950     2.000 972
9509723 ZNBUTANOT3     0.0000    1.69                    -1. 0.0  0.0  326.5
      2     1.000 950     3.000 972
9509724 ZNBUTANOAT4    0.0000    2.05                    -2. 0.0  0.0  413.54
      2     1.000 950     4.000 972
9509641 ZNNPRPYLAM     0.0000    2.42                     2. 0.0  0.0  124.41
      2     1.000 950     1.000 964
9509642 ZNNPRPYLAM2    0.0000    4.85                     2. 0.0  0.0  183.45
      2     1.000 950     2.000 964
9509643 ZNNPRPYLAM3    0.0000    7.38                     2. 0.0  0.0  242.29
      2     1.000 950     3.000 964
9509644 ZNNPRPYLAM4    0.0000    9.49                     2. 0.0  0.0  301.53
      2     1.000 950     4.000 964
9509651 ZNIPRPYLAM1    0.0000    2.37                     2. 0.0  0.0  124.41
      2     1.000 950     1.000 965
9509652 ZNIPRPYLAM2    0.0000    4.67                     2. 0.0  0.0  183.45
      2     1.000 950     2.000 965
9509653 ZNIPRPYLAM3    0.0000    7.14                     2. 0.0  0.0  242.49
      2     1.000 950     3.000 965
9509654 ZNIPRPYLAM4    0.0000    9.44                     2. 0.0  0.0  301.53
      2     1.000 950     4.000 965
3309671 CITRATEH       0.0000    6.33                    -2. 0.0  0.0  190.062
      2     1.000 330     1.000 967
3309672 CITRATEH2      0.0000   11.05                    -1. 0.0  0.0  191.062
      2     2.000 330     1.000 967
3309673 CITRATEH3      0.0000   14.18                     0. 0.0  0.0  192.062
      2     3.000 330     1.000 967
1509671 CACITRATE      0.0000    4.73                    -1. 0.0  0.0  229.143
      2     1.000 150     1.000 967
1509672 CACITRATEH     0.0000    3.02                     0. 0.0  0.0  230.143
      3     1.000 150     1.000 967     1.000 330
1509673 CACITRATEH2    0.0000    1.29                     1. 0.0  0.0  231.143
      3     1.000 150     1.000 967     2.000 330
4709671 MNCITRATE      0.0000    5.28                    -1. 0.0  0.0  244.001
      2     1.000 470     1.000 967
4709672 MNCITRATEH     0.0000    3.02                     0. 0.0  0.0  245.001
      3     1.000 470     1.000 967     1.000 330
2809671 FECITRATE      0.0000    5.7                     -1. 0.0  0.0  244.910
      2     1.000 280     1.000 967
2809672 FECITRATEH     0.0000    3.5                      0. 0.0  0.0  245.910
      3     1.000 280     1.000 967     1.000 330
2819671 FECITRATE      0.0000   12.55                     0. 0.0  0.0  244.910
      2     1.000 281     1.000 967
2819672 FECITRATEH     0.0000   19.8                      1. 0.0  0.0  245.910
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      3     1.000 281     1.000 967     1.000 330
3309631 HEN             0.0000    9.96                    1. 0.0  0.0  61.12
      2     1.000 330     1.000 963
3309632 H2EN            0.0000   16.85                    2. 0.0  0.0  62.12
      2     2.000 330     1.000 963
2319631 CUEN            0.0000   10.49                    2. 0.0  0.0  123.666
      2     1.000 231     1.000 963
2319632 CUEN2           0.0000   19.62                    2. 0.0  0.0  183.786
      2     1.000 231     2.000 963
1609631 CDEN            0.0000    5.61                    2. 0.0  0.0  172.591
      2     1.000 160     1.000 963
1609632 CDEN2           0.0000   10.34                    2. 0.0  0.0  232.639
      2     1.000 160     2.000 963
1609633 CDEN3           0.0000   12.26                    2. 0.0  0.0  292.759
      2     1.000 160     3.000 963
0209631 AGEN            0.0000    4.7                     1. 0.0  0.0  167.988
      2     1.000 020     1.000 963
0209632 AGEN2           0.0000    7.70                    1. 0.0  0.0  228.108
      2     1.000 020     2.000 963
0209633 AGENH           0.0000    7.31                    2. 0.0  0.0  168.988
      3     1.000 020     1.000 963     1.000 330
0209634 AG2EN           0.0000    1.43                    2. 0.0  0.0  275.856
      2     2.000 020     1.000 963
0209635 AG2EN2          0.0000   12.73                    2. 0.0  0.0  335.976
      2     2.000 020     2.000 963
5409631 NIEN            0.0000    7.24                    2. 0.0  0.0  118.83
      2     1.000 540     1.000 963
5409632 NIEN2           0.0000   13.36                    2. 0.0  0.0  178.95
      2     1.000 540     2.000 963
5409633 NIEN3           0.0000   17.54                    2. 0.0  0.0  239.07
      2     1.000 540     3.000 963
6009631 PBEN            0.0000    7.00                    2. 0.0  0.0  267.31
      2     1.000 600     1.000 963
6009632 PBEN2           0.0000    8.45                    2. 0.0  0.0  326.43
      2     1.000 600     2.000 963
9509631 ZNEN            0.0000    5.65                    2. 0.0  0.0  125.49
      2     1.000 950     1.000 963
9509632 ZNEN2           0.0000   10.62                    2. 0.0  0.0  185.61
      2     1.000 950     2.000 963
9509633 ZNEN3           0.0000   13.83                    2. 0.0  0.0  245.73
      2     1.000 950     3.000 963
4709631 MNEN            0.0000    2.67                    2. 0.0  0.0  115.058
      2     1.000 470     1.000 963
4709632 MNEN2           0.0000    4.2                     2. 0.0  0.0  175.178
      2     1.000 470     2.000 963
2809631 FEEN            0.0000    4.36                    2. 0.0  0.0  115.967
      2     1.000 280     1.000 963
2809632 FEEN2           0.0000    7.65                    2. 0.0  0.0  176.087
      2     1.000 280     2.000 963
2809633 FEEN3           0.0000    9.68                    2. 0.0  0.0  236.207
      2     1.000 280     3.000 963
3309681 NTAH            0.0000   10.334                  -2. 0.0  0.0  189.06
      2     1.000 330     1.000 968
3309682 NTAH2           0.0000   13.27                   -1. 0.0  0.0  190.06
      2     2.000 330     1.000 968
3309683 NTAH3           0.0000   14.12                    0. 0.0  0.0  191.06
      2     3.000 330     1.000 968
3309691 EDTAH           0.0000    9.96                   -3. 0.0  0.0  290.21
      2     1.000 330     1.000 969
3309692 EDTAH2          0.0000   16.21                   -2. 0.0  0.0  291.21
      2     2.000 330     1.000 969
3309693 EDTAH3          0.0000   18.86                   -1. 0.0  0.0  292.21
      2     3.000 330     1.000 969
3309694 EDTAH4          0.0000   20.93                    0. 0.0  0.0  293.21
      2     4.000 330     1.000 969
3309711 PROPANOTH       0.0000    4.874                   0. 0.0  0.0  74.03
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      2     1.000 330     1.000 971
3309581 METHYLAM H     0.0000   10.72                    1. 0.0  0.0  32.06
      2     1.000 330     1.000 958
3309611 HEXYLAM H      0.0000   10.63                    1. 0.0  0.0  101.17
      2     1.000 330     1.000 961
3309721 BUTANOAT H     0.0000    4.73                    0. 0.0  0.0  88.04
      2     1.000 330     1.000 972
3309684 NTAH4          0.0000   16.224                   1. 0.0  0.0  192.06
      2     4.000 330     1.000 968
3309695 EDTA H5        0.0000   23.464                   1. 0.0  0.0  297.24
      2     5.000 330     1.000 969
3309551 DIETHYLAM H    0.0000   10.774                   1. 0.0  0.0  74.14
      2     1.000 330     1.000 955
3309661 TMETHAM H      0.0000    9.80                    1. 0.0  0.0  60.04
      2     1.000 330     1.000 966
3309801 2METPYR H      0.0000    5.95                    1. 0.0  0.0  94.12
      2     1.000 330     1.000 980
3309811 3METPYR H      0.0000    5.70                    1. 0.0  0.0  94.12
      2     1.000 330     1.000 981
3309821 4METPYR H      0.0000    6.00                    1. 0.0  0.0  94.12
      2     1.000 330     1.000 982
3309641 NPROPYLAMH     0.0000   10.8                     1. 0.0  0.0  60.44
      2     1.000 330     1.000 964
3309963 GLUTAM H3      0.0000   16.60                    1. 0.0  0.0  148.13
      2     3.000 330     1.000 996
3309831 FORMATE H      0.0000    3.745                   0. 0.0  0.0  46.02
      2     1.000 330     1.000 983
3309841 ISOVALERIC H   0.0000    4.781                   0. 0.0  0.0  102.13
      2     1.000 330     1.000 984
3309731 ISOBUTRYIC H   0.0000    4.849                   0. 0.0  0.0  88.043
      2     1.000 330     1.000 973
3309851 VALERIC H      0.0000    4.843                   0. 0.0  0.0  102.13
      2     1.000 330     1.000 985
1609691 CDEDTA         0.0000   16.275                  -2. 0.0  0.0  401.61
      2     1.000 160     1.000 969
1609681 CDNTA          0.0000    9.4                    -1. 0.0  0.0  300.46
      2     1.000 160     1.000 968
1609682 CDNTA2         0.0000   14.3                    -4. 0.0  0.0  488.52
      2     1.000 160     2.000 968
4609631 MGEN           0.0000     .37                    2. 0.0  0.0  84.43
      2     1.000 460     1.000 963
1509631 CAEN           0.0000     .1                     2. 0.0  0.0  100.20
      2     1.000 150     1.000 963
4609671 MGCITRATE      0.0000    3.37                   -1. 0.0  0.0  223.37
      2     1.000 460     1.000 967
4609672 MGCITRATEH     0.0000    8.17                    0. 0.0  0.0  224.37
      3     1.000 460     1.000 967     1.000 330
4609673 MGCITRATEH2    0.0000   11.59                    1. 0.0  0.0  225.37
      3     1.000 460     1.000 967     2.000 330
5009920 NaACETATE      0.0000   -0.18                    0. 0.0  0.0   82.0398
      2     1.000 500     1.000 992
5009970 NaPhthala      0.0000    0.70                   -1. 0.0  0.0  187.12
      2     1.000 500     1.000 997
4609920 MgACETATE      0.0000    1.27                    1. 0.0  0.0   83.3620
      2     1.000 460     1.000 992
4609710 MgPropana      0.0000    0.54                    1. 0.0  0.0   97.330
      2     1.000 460     1.000 971
4609720 MgButyrat      0.0000    0.53                    1. 0.0  0.0  111.340
      2     1.000 460     1.000 972
1509920 CaACETATE      0.0000    1.18                    1. 0.0  0.0   99.13
      2     1.000 150     1.000 992
1509200 CaIPhthal      0.0000    2.00                    0. 0.0  0.0   99.13
      2     1.000 150     1.000 920
1509710 CaPropana      0.0000    0.50                    1. 0.0  0.0  113.10
      2     1.000 150     1.000 971
1509720 CaButyrat      0.0000    0.51                    1. 0.0  0.0  127.11
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      2     1.000 150     1.000 972
1509970 CaPhthala       0.0000    2.42                      0. 0.0  0.0  204.21
      2     1.000 150     1.000 997
4709920 MnACETATE       0.0000    1.40                      1. 0.0  0.0   93.312
      2     1.000 470     1.000 992
2809920 FeACETATE       0.0000    1.40                      1. 0.0  0.0  114.8970
      2     1.000 280     1.000 992
3619920 HgACETATE       0.0000   9.417                      1. 0.0  0.0  259.66
      4     1.000 361     1.000 992     2.000 330    -2.000   2
3619921 HgACETATE2      0.0000   13.11                      0. 0.0  0.0  318.71
      4     1.000 361     2.000 992     2.000 330    -2.000   2
3619922 HgACETATE3      0.0000   19.38                     -1. 0.0  0.0  377.76
      4     1.000 361     3.000 992     2.000 330    -2.000   2
3619923 HgACETATE4      0.0000   23.16                     -2. 0.0  0.0  436.81
      4     1.000 361     4.000 992     2.000 330    -2.000   2
2819920 FeACETATE       0.0000    3.21                      2. 0.0  0.0  114.897
      2     1.000 281     1.000 992
2819921 FeACETATE2      0.0000    6.50                      1. 0.0  0.0  174.3971
      2     1.000 281     2.000 992
2819922 FeACETATE3      0.0000    8.30                      0. 0.0  0.0  233.447
      2     1.000 281     3.000 992
1509690 Ca EDTA         0.0000   12.4                      -2. 0.0  0.0  316.1000
      2     1.000 150     1.000 969
1509691 CaHEDTA         0.0000   16.0                      -1. 0.0  0.0  317.0000
      3     1.000 150     1.000 969     1.000 330
4609690 Mg EDTA         0.0000   10.6                      -2. 0.0  0.0  300.3000
      2     1.000 460     1.000 969
4609691 MgHEDTA         0.0000   15.1                      -1. 0.0  0.0  301.3000
      3     1.000 460     1.000 969     1.000 330
4109690 K EDTA          0.0000    1.7                      -3. 0.0  0.0  315.1000
      2     1.000 410     1.000 969
5009690 Na EDTA         0.0000    2.5                      -3. 0.0  0.0  299.0000
      2     1.000 500     1.000 969

      0

      0

      0
2089100 URANINITE        18.630     4.700    .000    .000                 270.0278
      3    -4.000 330     1.000 891     2.000   2
2089101 UO2  (AM)        26.230     -.934    .000    .000                 270.0278
      3    -4.000 330     1.000 891     2.000   2
3089100 U4O9 (C)        101.235     3.384    .000  -3.080                1096.1106
      4   -18.000 330    -2.000   1     4.000 891     9.000   2
3089101 U3O8 (C)        116.020   -21.107    .000 -34.589                 842.0822
      4   -16.000 330    -4.000   1     3.000 891     8.000   2
8089100 USIO4 (C)        14.548     7.620    .000    .000                 330.1121
      3    -4.000 330     1.000 891     1.000 770
4289100 UF4  (C)         18.900    18.606    .000    .000                 314.0226
      2     1.000 891     4.000 270
4289101 UF4.2.5H2O         .588    27.570    .000    .000                 359.0606
      3     1.000 891     4.000 270     2.500   2
7089100 UHPO4)2,4H2O     -3.840    51.584    .000    .000                 502.0486
      4     1.000 891     2.000 580     2.000 330     4.000   2
7015000 NINGYOITE         2.270    53.906    .000    .000                 504.0822
      4     1.000 891     1.000 150     2.000 580     2.000   2
2089300 UO3 (C)          19.315    -7.719    .000    .000                 286.0272
      3    -2.000 330     1.000 893     1.000   2
2089301 GUMMITE          23.015   -10.403    .000    .000                 286.0272
      3    -2.000 330     1.000 893     1.000   2
2089302 B-UO2(OH)2       13.730    -5.544    .000    .000                 304.0424
      3    -2.000 330     1.000 893     2.000   2
2089303 SCHOEPITE        12.045    -5.404    .000    .000                 322.0576
      3    -2.000 330     1.000 893     3.000   2
5089300 RUTHERFORDIN      1.440    14.439    .000    .000                 330.0370
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      2     1.000 893     1.000 140
7089300 (UO2)3(PO4)2   -94.900    49.037 129.134    .000              1000.0262
      2     3.000 893     2.000 580
7089301 H-AUTUNITE       3.600    47.931    .000    .000               732.0144
      3     2.000 330     2.000 893     2.000 580
7050000 NA-AUTUNITE       .460    47.409    .000    .000               775.9780
      3     2.000 500     2.000 893     2.000 580
7041000 K-AUTUNITE       -5.860    48.244    .000    .000               808.2024
      3     2.000 410     2.000 893     2.000 580
7049000 URAMPHITE        -9.700    51.749    .000    .000               766.0756
      3     2.000 893     2.000 490     2.000 580
7046000 SALEEITE         20.180    43.646    .000    .000               754.3104
      3     2.000 893     1.000 460     2.000 580
7015001 AUTUNITE         14.340    43.927    .000    .000               770.0784
      3     2.000 893     1.000 150     2.000 580
7080000 SR-AUTUNITE      13.050    44.457    .000    .000               817.6184
      3     2.000 893     1.000 800     2.000 580
7010000 URANOCIRCITE     10.100    44.631    .000    .000               867.3384
      3     2.000 893     1.000 100     2.000 580
7028000 BASSETITE        19.900    44.485    .000    .000               785.8454
      3     2.000 893     1.000 280     2.000 580
7023102 TORBERNITE       15.900    45.279    .000    .000               793.5444
      3     2.000 893     1.000 231     2.000 580
7060000 PRZHEVALSKIT     11.000    44.365    .000    .000               937.1883
      3     2.000 893     1.000 600     2.000 580
8015000 URANOPHANE         .000   -17.490    .000    .000               766.5176
      4    -6.000 330     2.000 893     1.000 150     2.000 770
5189300 UO2NO3)2         20.140   -12.369    .000    .000               394.0380
      2     1.000 893     2.000 492
5189301 UO2NO3.2H2O       6.060    -4.851    .000    .000               430.0690
      3     1.000 893     2.000 492     2.000   2
5189302 UO2NO3.3H2O       2.405    -3.642    .000    .000               448.0840
      3     1.000 893     2.000 492     3.000   2
5189303 UO2NO3.6H2O      -4.770    -2.300    .000    .000               502.1300
      3     1.000 893     2.000 492     6.000   2
2003000 ALOH3(A)         27.045   -10.380  -9.690    .000                78.0073
      3     1.000  30     3.000   2    -3.000 330
6003000 ALOHSO4            .000     3.230   3.390   3.070               140.0505
      4    -1.000 330     1.000  30     1.000 732     1.000   2
6003001 AL4(OH)10SO4       .000   -22.700    .000    .000               374.0616
      4   -10.000 330     4.000  30     1.000 732    10.000   2
6041000 ALUM K           -7.220     5.170    .000    .000               438.3597
      4     1.000 410     1.000  30     2.000 732    12.000   2
6041001 ALUNITE          -3.918     1.346    .000    .000               414.2141
      5     1.000 410     3.000  30     2.000 732     6.000   2    -6.000 330
6015000 ANHYDRITE         3.769     4.637    .000    .000               136.1416
      2     1.000 150     1.000 732
5015000 ARAGONITE         2.615     8.360    .000    .000               100.0894
      2     1.000 150     1.000 140
5046000 ARTINITE         28.742    -9.600    .000    .000               196.6941
      4    -2.000 330     2.000 460     1.000 140     5.000   2
4210000 BAF2             -1.000     5.760   6.740   4.650               175.3368
      2     1.000 100     2.000 270
6010000 BARITE           -6.280     9.976    .000   9.773               233.4016
      2     1.000 100     1.000 732
2003001 BOEHMITE         28.130    -8.578  -8.065    .000                59.9884
      3    -3.000 330     1.000  30     2.000   2
2046000 BRUCITE          25.840   -16.792    .000    .000                58.3268
      3     1.000 460     2.000   2    -2.000 330
5015001 CALCITE           2.585     8.475   8.560    .000               100.0894
      2     1.000 150     1.000 140
6080000 CELESTITE          .470     6.465    .000   6.349               183.6816
      2     1.000 800     1.000 732
2077000 CHALCEDONY       -4.615     3.523    .000    .000                60.0848
      2    -2.000   2     1.000 770
8646000 CHRYSOTILE       52.485   -32.188    .000    .000               277.1349
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      4    -6.000 330     3.000 460     2.000 770     1.000   2
8246000 CLINOENSTITE    20.015   -11.338 -10.972 -11.632                100.3964
      4    -1.000   2     1.000 460     1.000 770    -2.000 330
2077001 CRISTOBALITE    -5.500     3.587    .000    .000                 60.0848
      2    -2.000   2     1.000 770
2003002 DIASPORE        24.630    -6.873    .000    .000                 59.9884
      3    -3.000 330     1.000  30     2.000   2
8215000 DIOPSIDE        32.280   -19.886    .000    .000                216.5608
      5    -2.000   2     1.000 150     1.000 460     2.000 770    -4.000 330
5015002 DOLOMITE         8.290    17.000    .000    .000                184.4108
      3     1.000 150     1.000 460     2.000 140
6046000 EPSOMITE        -2.820     2.140    .000    .000                246.4807
      3     1.000 460     1.000 732     7.000   2
8646003 SEPIOLITE(C)    27.268   -15.913    .000    .000                323.9313
      4     -.500   2     2.000 460     3.000 770    -4.000 330
2028100 FERRIHYDRITE      .000    -4.891  -1.557  -4.996                104.8692
      3    -3.000 330     1.000 281     3.000   2
2028101 FE3(OH)8          .000   -20.222 -17.112 -24.105                297.6002
      4    -8.000 330     2.000 281     1.000 280     8.000   2
4128100 FEOH)2.7CL.3      .000     3.040    .000    .000                110.4029
      4    -2.700 330     1.000 281     2.700   2      .300 180
1028000 FES PPT           .000     3.915    .000    .000                 85.9110
      3    -1.000 330     1.000 280     1.000 730
6028100 FE2(SO4)3       59.120    -3.580    .650    .000                395.8788
      2     2.000 281     3.000 732
7015003 HYDRAPATITE   0.00000    44.199    .000    .000                502.3200
      4     5.000 150     3.000 580     1.000 002    -1.000 330
7015002 FCO3APATITE   -39.390   114.400    .000    .000                967.3670
      6     9.496 150      .360 500      .144 460     4.800 580     1.200 140
  2.480 270
4215000 FLUORITE        -4.710    10.960    .000    .000                 78.0768
      2     1.000 150     2.000 270
8046000 FORSTERITE      48.510   -28.298    .000    .000                236.8234
      3    -4.000 330     2.000 460     1.000 770
2003003 GIBBSITE (C)    22.800    -8.770  -8.487  -9.440                 78.0037
      3    -3.000 330     1.000  30     3.000   2
3003000 Al2O3           0.0000   -22.980   0.000   0.000 0.00 0.00 0.00 101.9504
 0.00 3     2.000  30     3.000   2    -6.000 330
2028102 GOETHITE        14.480     -.500    .000    .000                 86.8536
      3    -3.000 330     1.000 281     2.000   2
8628000 GREENALITE        .000   -20.810    .000    .000                365.7393
      4    -6.000 330     3.000 280     2.000 770     1.000   2
1028001 GREIGITE          .000    45.035    .000    .000                289.7970
      4    -4.000 330     2.000 281     1.000 280     4.000 730
6015001 GYPSUM           -.261     4.848    .000    .000                172.1722
      3     1.000 150     1.000 732     2.000   2
4150000 HALITE           -.918    -1.582    .000    .000                 58.4428
      2     1.000 500     1.000 180
3028100 HEMATITE        30.845     4.008    .000    .000                155.6919
      3    -6.000 330     2.000 281     3.000   2
5015003 HUNTITE         25.760    29.968    .000    .000                353.0536
      3     3.000 460     1.000 150     4.000 140
5046001 HYDRMAGNESIT    52.210     8.766    .000    .000                467.6736
      4     5.000 460     4.000 140    -2.000 330     6.000   2
6050000 JAROSITE NA     36.180    11.200    .000    .000                478.6978
      5    -6.000 330     1.000 500     3.000 281     2.000 732     6.000   2
6041002 JAROSITE K      31.280    14.800    .000    .000                494.8100
      5    -6.000 330     1.000 410     3.000 281     2.000 732     6.000   2
6028101 JAROSITE H      55.150    12.100    .000    .000                480.7320
      4    -5.000 330     3.000 281     2.000 732     7.000   2
1028002 MACKINAWITE       .000     4.648    .000    .000                 87.9110
      3    -1.000 330     1.000 280     1.000 730
8450000 MAGADIITE         .000    14.300    .000    .000                532.6521
      4    -1.000 330    -9.000   2     1.000 500     7.000 770
3028101 MAGHEMITE         .000    -6.386    .000    .000                159.6922
      3    -6.000 330     2.000 281     3.000   2
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5046002 MAGNESITE        6.169     8.029   8.279   7.779                 84.3214
      2     1.000 460     1.000 140
3028000 MAGNETITE       50.460    -3.737  -3.367  -6.595                231.5386
      4    -8.000 330     2.000 281     1.000 280     4.000   2
6028000 MELANTERITE     -2.860     2.470    .000    .000                 278.0157
      3     1.000 280     1.000 732     7.000   2
6050001 MIRABILITE     -18.987     1.114    .000    .000                 322.1942
      3     2.000 500     1.000 732    10.000   2
3050000 NATRON         -15.745     1.311    .000    .000                 286.1420
      3     2.000 500     1.000 140    10.000   2
5046003 NESQUEHONITE     5.789     5.621   5.133   4.546                 138.3673
      3     1.000 460     1.000 140     3.000   2
8646001 PHLOGOPITE      86.360   -66.300    .000    .000                 417.2863
      5   -10.000 330     1.000 410     3.000 460     1.000  30     3.000 770
1028003 PYRITE         -11.300    18.479    .000    .000                 119.9750
      4    -2.000 330    -2.000   1     1.000 280     2.000 730
2077002 QUARTZ          -6.220     4.006    .000    .000                  60.0848
      2    -2.000   2     1.000 770
8646004 SEPIOLITE(A)      .000   -18.780    .000    .000                 323.9308
      4     -.500   2     2.000 460     3.000 770    -4.000 330
5028000 SIDERITE         5.328    10.550  12.104    .000                 115.8564
      2     1.000 280     1.000 140
2077003 SIO2(A,GL)      -4.440     3.018    .000    .000                  60.0848
      2    -2.000   2     1.000 770
2077004 SIO2(A,PT)      -3.910     2.710    .000    .000                  60.0848
      2    -2.000   2     1.000 770
4280000 SRF2            -1.250     8.540   9.120    .000                 125.6168
      2     1.000 800     2.000 270
7028100 STRENGITE        2.030    26.400  29.123  26.235                 186.8490
      3     1.000 281     1.000 580     2.000   2
5080000 STRONTIANITE      .690     9.250  11.789    .000                 147.6294
      2     1.000 800     1.000 140
8646002 TALC            35.005   -23.055 -18.988 -23.088                 379.2888
      4    -4.000   2     3.000 460     4.000 770    -6.000 330
6050002 THENARDITE        .572      .179    .000    .000                 142.0412
      2     2.000 500     1.000 732
5050001 THERMONATR       2.802     -.125    .000    .000                 124.0043
      3     2.000 500     1.000 140     1.000   2
8215001 TREMOLITE       96.615   -56.546    .000    .000                 812.4096
      5    -8.000   2     2.000 150     5.000 460     8.000 770   -14.000 330
7028001 VIVIANITE         .000    36.000    .000    .000                 501.6062
      3     3.000 280     2.000 580     8.000   2
5010000 WITHERITE        -.360     8.585  13.335    .000                 197.3494
      2     1.000 100     1.000 140
2047000 PYROLUSITE      29.180   -15.861    .000 -16.038                  86.9368
      4    -4.000 330    -1.000   1     1.000 471     2.000   2
2047001 BIRNESSITE        .000   -18.091    .000    .000                  86.9368
      4    -4.000 330    -1.000   1     1.000 471     2.000   2
2047002 NSUTITE           .000   -17.504    .000    .000                  86.9368
      4    -4.000 330    -1.000   1     1.000 471     2.000   2
3047100 BIXBYITE        15.245      .611   2.226    .430                 157.8742
      3    -6.000 330     2.000 471     3.000   2
3047000 HAUSMANNITE     80.140   -61.540    .000    .000                 228.8116
      4    -8.000 330    -2.000   1     3.000 470     4.000   2
2047003 PYROCROITE      22.590   -15.088    .000 -15.381                  88.9528
      3    -2.000 330     1.000 470     2.000   2
2047100 MANGANITE         .000      .238    .000    .000                  87.9448
      3    -3.000 330     1.000 471     2.000   2
5047000 RHODOCHROSIT     2.079    10.410  11.019   9.993                 114.9474
      2     1.000 470     1.000 140
4147000 MNCL2, 4H2O    -17.380    -2.710    .000    .000                 197.9052
      3     1.000 470     2.000 180     4.000   2
1047000 MNS GREEN        5.790    -3.800    .000    .000                  87.0020
      3    -1.000 330     1.000 470     1.000 730
6047000 MNSO4           15.480    -2.669    .000    .000                 150.9996
      2     1.000 470     1.000 732
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6047100 MN2(SO4)3        39.060     5.711     .000     .000                398.0608
      2     2.000 471     3.000 732
7047000 MN3(PO4)2        -2.120    23.827     .000     .000                354.7568
      2     3.000 470     2.000 580
3041000 A-CRYPTOMELN       .000      .000     .000     .000                775.7382
      5   -34.000 330    16.000 471      .800 410    17.000   2    -7.400 470
3010000 HOLLANDITE         .000      .000     .000     .000                817.4214
      6   -32.000 330    14.000 471      .820 100      .570 280    16.000   2
 -6.410 470
3015000 TODOROKITE         .000      .000     .000     .000                592.4641
      6   -24.000 330     .393 150      .473 460    10.000 471    14.000   2
 -3.866 470
3044000 LITHIOPHORIT       .000      .000     .000     .000               1953.3934
      6   -70.000 330     2.000 440     8.000  30    20.000 471    49.000   2
 -8.000 470
3015001 RANCIEITE          .000      .000     .000     .000                466.1930
      5   -18.000 330     .440 150     8.000 471    12.000   2    -3.440 470
0023000 CU METAL I      -17.130     8.760     .000   8.800                  63.5460
      2     1.000 230     1.000   1
4123000 NANTOKITE        -9.980     6.760     .000   6.630                  98.9990
      2     1.000 230     1.000 180
4223000 CUF              12.370    -7.080     .000     .000                 82.5444
      2     1.000 230     1.000 270
2023000 CUPRITE          -6.245     1.550    1.870     .700                143.0914
      3    -2.000 330     2.000 230     1.000   2
1023000 CHALCOCITE      -49.350    34.619   34.920  30.900                 159.1560
      3    -1.000 330     2.000 230     1.000 730
1023001 DJURLEITE       -47.881    33.920     .000     .000                154.9620
      4    -1.000 330      .066 231     1.868 230     1.000 730
1023002 ANILITE         -43.535    31.878     .000     .000                143.2695
      4    -1.000 330      .250 231     1.500 230     1.000 730
1023003 BLAUBLEI II        .000    27.279     .000     .000                121.0284
      4    -1.000 330      .600 231      .800 230     1.000 730
1023100 BLAUBLEI I         .000    24.162     .000     .000                101.9646
      4    -1.000 330      .900 231      .200 230     1.000 730
1023101 COVELLITE       -24.010    23.038     .000  22.170                  95.6100
      3    -1.000 330     1.000 231     1.000 730
6023000 CU2SO4            4.560     1.950     .000     .000                223.1536
      2     2.000 230     1.000 732
3023000 CUPROUSFERIT      3.800     8.920     .000   6.880                 151.3918
      4    -4.000 330     1.000 230     1.000 281     2.000   2
4123100 MELANOTHALLI     12.320    -3.730     .000  -4.450                 134.4520
      2     1.000 231     2.000 180
5023100 CUCO3              .000     9.630    9.650   9.610                 123.5552
      2     1.000 231     1.000 140
4223100 CUF2             13.320      .620     .000     .000                101.5428
      2     1.000 231     2.000 270
4223101 CUF2, 2H2O        3.650     4.550     .000     .000                137.5732
      3     1.000 231     2.000 270     2.000   2
2023100 CU(OH)2          15.250    -8.640     .000  -9.200                  97.5606
      3    -2.000 330     1.000 231     2.000   2
4123101 ATACAMITE        18.690    -7.340   -7.240  -7.490                 213.5669
      4    -3.000 330     2.000 231     3.000   2     1.000 180
5123100 CU2(OH)3NO3      17.350    -9.240     .000  -9.310                 240.1188
      4    -3.000 330     2.000 231     3.000   2     1.000 492
6023100 ANTLERITE          .000    -8.290     .000  -8.900                 354.7248
      4    -4.000 330     3.000 231     4.000   2     1.000 732
6023101 BROCHANTITE        .000   -15.340  -15.150 -15.500                 452.2854
      4    -6.000 330     4.000 231     6.000   2     1.000 732
6023102 LANGITE          39.610   -16.790     .000 -17.400                 470.3006
      4    -6.000 330     4.000 231     7.000   2     1.000 732
2023101 TENORITE         15.240    -7.620   -7.350  -7.890                  79.5454
      3    -2.000 330     1.000 231     1.000   2
6023103 CUOCUSO4         35.575   -11.530     .000     .000                239.1490
      4    -2.000 330     2.000 231     1.000   2     1.000 732
7023100 CU3(PO4)2          .000    36.850     .000  36.900                 380.5808
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      2     3.000 231     2.000 580
7023101 CU3(PO4)2,3W       .000    35.120    .000    .000              434.6264
      3     3.000 231     2.000 580     3.000   2
6023104 CUSO4             18.140    -3.010  -2.630  -3.420              159.6036
      2     1.000 231     1.000 732
6023105 CHALCANTHITE      -1.440     2.640   2.960   2.135              249.6796
      3     1.000 231     1.000 732     5.000   2
2023102 DIOPTASE           8.960    -6.500    .000    .000              157.6449
      3    -2.000 330     1.000 231     1.000 770
3023100 CUPRICFERIT       38.690    -5.880  -5.350    .000              239.2376
      4    -8.000 330     1.000 231     2.000 281     4.000   2
1023102 CHALCOPYRITE     -35.480    35.270    .000  30.790              183.5130
      4    -2.000 330     1.000 231     1.000 280     2.000 730
4023000 CUBR             -13.080     8.210    .000    .000              143.4500
      2     1.000 230     1.000 130
4323000 CUI              -20.140    11.890    .000    .000              190.4505
      2     1.000 230     1.000 380
0095000 ZN METAL          36.780   -25.757    .000 -25.790               65.3800
      2     1.000 950     2.000   1
4195000 ZNCL2             17.480    -7.030    .000  -7.060              136.2860
      2     1.000 950     2.000 180
5095000 SMITHSONITE        4.360    10.000  10.810   9.820              125.3892
      2     1.000 950     1.000 140
5095001 ZNCO3, 1H2O         .000    10.260    .000    .000              143.4044
      3     1.000 950     1.000 140     1.000   2
4295000 ZNF2              13.080     1.520    .000   1.080              103.3768
      2     1.000 950     2.000 270
2095000 ZN(OH)2 (A)         .000   -12.450 -12.260 -12.480               99.3946
      3    -2.000 330     1.000 950     2.000   2
2095001 ZN(OH)2 (C)         .000   -12.200    .000    .000               99.3946
      3    -2.000 330     1.000 950     2.000   2
2095002 ZN(OH)2 (B)         .000   -11.750 -11.320 -11.890               99.3946
      3    -2.000 330     1.000 950     2.000   2
2095003 ZN(OH)2 (G)         .000   -11.710 -11.190 -11.840               99.3946
      3    -2.000 330     1.000 950     2.000   2
2095004 ZN(OH)2 (E)         .000   -11.500 -10.950 -11.620               99.3946
      3    -2.000 330     1.000 950     2.000   2
4195001 ZN2(OH)3CL          .000   -15.200    .000    .000              217.2349
      4    -3.000 330     2.000 950     3.000   2     1.000 180
4195002 ZN5(OH)8CL2         .000   -38.500    .000    .000              533.8644
      4    -8.000 330     5.000 950     8.000   2     2.000 180
6095000 ZN2(OH)2SO4         .000    -7.500    .000    .000              260.8322
      4    -2.000 330     2.000 950     2.000   2     1.000 732
6095001 ZN4(OH)6SO4         .000   -28.400    .000    .000              459.6214
      4    -6.000 330     4.000 950     6.000   2     1.000 732
5195000 ZNNO3)2,6H2O      -5.510    -3.440    .000    .000              297.4810
      3     1.000 950     2.000 492     6.000   2
2095005 ZNO(ACTIVE)         .000   -11.310 -11.570 -11.860               81.3794
      3    -2.000 330     1.000 950     1.000   2
2095006 ZINCITE           21.860   -11.140 -10.990 -11.540               81.3794
      3    -2.000 330     1.000 950     1.000   2
6095002 ZN3O(SO4)2        62.000   -19.020    .000    .000              404.2546
      4    -2.000 330     3.000 950     2.000 732     1.000   2
7095000 ZN3(PO4),4W         .000    32.040    .000    .000              458.1436
      3     3.000 950     2.000 580     4.000   2
1095000 ZNS (A)           -3.670     9.052    .000    .000               97.4400
      3    -1.000 330     1.000 950     1.000 730
1095001 SPHALERITE        -8.250    11.618  13.212   5.952               97.4400
      3    -1.000 330     1.000 950     1.000 730
1095002 WURTZITE          -5.060     9.682  10.182   8.552               97.4400
      3    -1.000 330     1.000 950     1.000 730
8295000 ZNSIO3            18.270    -2.930    .000    .000              141.4637
      4    -2.000 330    -1.000   2     1.000 950     1.000 770
8095000 WILLEMITE         33.370   -15.330 -13.350    .000              220.8431
      3    -4.000 330     2.000 950     1.000 770
6095003 ZINCOSITE         19.200    -3.010    .000  -3.930              161.4376
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      2     1.000 950     1.000 732
6095004 ZNSO4, 1H2O     10.640      .570    .000    .500                179.4528
      3     1.000 950     1.000 732     1.000   2
6095005 BIANCHITE         .160     1.765    .000   1.020                269.5288
      3     1.000 950     1.000 732     6.000   2
6095006 GOSLARITE       -3.300     1.960    .000   1.870                287.5440
      3     1.000 950     1.000 732     7.000   2
4095000 ZNBR2, 2H2O      7.510    -5.210    .000    .000                261.2184
      3     1.000 950     2.000 130     2.000   2
4395000 ZNI2            13.440    -7.230    .000    .000                319.1890
      2     1.000 950     2.000 380
0016000 CD METAL        18.000   -13.490    .000 -13.640                112.4100
      2     1.000 160     2.000   1
0016001 GAMMA CD        18.140   -13.590    .000    .000                112.4100
      2     1.000 160     2.000   1
5016000 OTAVITE           .580    13.740  13.810  11.210                172.4192
      2     1.000 160     1.000 140
4116000 CDCL2            4.470      .680    .000    .470                183.3160
      2     1.000 160     2.000 180
4116001 CDCL2, 1H2O      1.820     1.710    .000    .000                201.3312
      3     1.000 160     2.000 180     1.000   2
4116002 CDCL2,2.5H2O    -1.710     1.940    .000    .000                228.3536
      3     1.000 160     2.000 180     2.500   2
4216000 CDF2             9.720     2.980    .000    .000                150.4068
      2     1.000 160     2.000 270
2016000 CD(OH)2 (A)     20.770   -13.730 -13.610 -14.300                146.4246
      3    -2.000 330     1.000 160     2.000   2
2016001 CD(OH)2 (C)       .000   -13.650    .000    .000                146.4246
      3    -2.000 330     1.000 160     2.000   2
4116003 CDOHCL           7.407    -3.520  -3.300    .000                164.8703
      4    -1.000 330     1.000 160     1.000   2     1.000 180
6016000 CD3(OH)4SO4       .000   -22.560    .000    .000                501.3168
      4    -4.000 330     3.000 160     4.000   2     1.000 732
6016001 CD3OH2(SO4)2      .000    -6.710    .000    .000                563.3598
      4    -2.000 330     3.000 160     2.000   2     2.000 732
6016002 CD4(OH)6SO4       .000   -28.400    .000    .000                647.7414
      4    -6.000 330     4.000 160     6.000   2     1.000 732
2016002 MONTEPONITE     24.760   -15.120    .000 -15.740                128.4094
      3    -2.000 330     1.000 160     1.000   2
7016000 CD3(PO4)2         .000    32.600    .000    .000                527.1728
      2     3.000 160     2.000 580
8216000 CDSIO3          16.630    -9.060  -7.960    .000                188.4937
      4    -1.000   2     1.000 160     1.000 770    -2.000 330
6016003 CDSO4           14.740      .100    .130    .050                208.4676
      2     1.000 160     1.000 732
6016004 CDSO4, 1H2O      7.520     1.657   1.680   1.630                226.4828
      3     1.000 160     1.000 732     1.000   2
6016005 CDSO4,2.7H2O     4.300     1.873   1.890   1.860                256.3879
      3     1.000 160     1.000 732     2.670   2
1016000 GREENOCKITE    -16.360    15.930    .000  13.112                144.4700
      3    -1.000 330     1.000 160     1.000 730
4016000 CDBR2, 4H2O     -7.230     2.420    .000    .000                344.2788
      3     1.000 160     2.000 130     4.000   2
4316000 CDI2            -4.080     3.610    .000    .000                366.2190
      2     1.000 160     2.000 380
0060000 PB METAL          -.400    -4.270  -4.070  -4.310                207.2000
      2     1.000 600     2.000   1
4160000 COTUNNITE       -5.600     4.770   4.976   4.670                278.1060
      2     1.000 600     2.000 180
4160001 MATLOCKITE      -7.950     9.430    .000   8.600                261.6514
      3     1.000 600     1.000 180     1.000 270
4160002 PHOSGENITE        .000    19.810  19.940    .000                545.3152
      3     2.000 600     2.000 180     1.000 140
5060000 CERRUSITE       -4.860    13.130  13.440  12.830                267.2092
      2     1.000 600     1.000 140
4260000 PBF2              .700     7.440   7.570    .000                245.1968
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      2     1.000 600     2.000 270
2060000 MASSICOT         16.780   -12.910 -12.790    .000              223.1994
      3    -2.000 330     1.000 600     1.000   2
2060001 LITHARGE         16.380   -12.720 -12.640 -13.070              223.1994
      3    -2.000 330     1.000 600     1.000   2
2060002 PBO, .3H2O         .000   -12.980    .000    .000              229.1444
      3    -2.000 330     1.000 600     1.330   2
5060001 PB2OCO3          11.460     .500    .780    .000              490.4086
      4    -2.000 330     2.000 600     1.000   2     1.000 140
6060000 LARNAKITE         6.440     .280   6.300    .000              526.4570
      4    -2.000 330     2.000 600     1.000 732     1.000   2
6060001 PB3O2SO4         20.750   -10.400    .000    .000              749.6564
      4    -4.000 330     3.000 600     1.000 732     2.000   2
6060002 PB4O3SO4         35.070   -22.100    .000    .000              972.8558
      4    -6.000 330     4.000 600     1.000 732     3.000   2
7060001 CLPYROMORPH        .000    84.430    .000  34.510             1356.3672
      3     5.000 600     3.000 580     1.000 180
7060002 HXYPYROMORPH       .000    62.790    .000    .000              1337.9215
      4    -1.000 330     5.000 600     3.000 580     1.000   2
5060002 PB3O2CO3         26.430   -11.020    .000    .000              713.6080
      4    -4.000 330     3.000 600     1.000 140     2.000   2
7060003 PLUMBGUMMITE       .000    32.790    .000    .000              581.1391
      5    -5.000 330     1.000 600     3.000  30     2.000 580     6.000   2
7060004 HINSDALITE         .000     2.500    .000    .000              581.2174
      6    -6.000 330     1.000 600     3.000  30     1.000 580     1.000 732
  6.000 002
7060005 TSUMEBITE          .000     9.790    .000    .000              677.9849
      5    -3.000 330     2.000 600     1.000 231     1.000 580     6.000   2
8260000 PBSIO3            9.260    -7.320  -6.120  -7.640              283.2837
      4    -1.000   2    -2.000 330     1.000 600     1.000 770
8060000 PB2SIO4          26.000   -19.760 -19.220 -20.050              506.4831
      3    -4.000 330     2.000 600     1.000 770
6060003 ANGLESITE        -2.150     7.790   7.870    .000              303.2576
      2     1.000 600     1.000 732
1060001 GALENA          -19.400    15.132  16.452  13.682              239.2600
      3    -1.000 330     1.000 600     1.000 730
2060003 PLATTNERITE      70.730   -49.300 -49.000    .000              239.1988
      4    -4.000 330    -2.000   1     1.000 600     2.000   2
3060000 PB2O3              .000   -61.040    .000    .000              462.3982
      4    -6.000 330    -2.000   1     2.000 600     3.000   2
3060001 MINIUM           102.760   -73.690 -70.800    .000              685.5976
      4    -8.000 330    -2.000   1     3.000 600     4.000   2
2060004 PB(OH)2 (C)      13.990    -8.150    .000 -13.630              241.2146
      3    -2.000 330     1.000 600     2.000   2
4160003 LAURIONITE         .000     -.623   -.175    .000              259.6603
      4    -1.000 330     1.000 600     1.000 180     1.000   2
4160004 PB2(OH)3CL         .000    -8.793    .000    .000              500.8749
      4    -3.000 330     2.000 600     3.000   2     1.000 180
5060003 HYDCERRUSITE       .000    17.460    .000    .000              775.6330
      4    -2.000 330     3.000 600     2.000 140     2.000   2
2060005 PB2O(OH)2          .000   -26.200    .000 -27.100              464.4140
      3    -4.000 330     2.000 600     3.000   2
4060000 PBBR2            -8.100     5.180   5.340   4.410              367.0080
      2     1.000 600     2.000 130
4060001 PBBRF              .000     8.490    .000    .000              306.1024
      3     1.000 600     1.000 130     1.000 270
4360000 PBI2             -15.160     8.070    .000    .000              461.0090
      2     1.000 600     2.000 380
6060004 PB4(OH)6SO4        .000   -21.100    .000    .000             1026.9014
      4    -6.000 330     4.000 600     1.000 732     6.000   2
5054000 NICO3              9.940     6.840    .000    .000              118.7092
      2     1.000 540     1.000 140
2054000 NI(OH)2          -30.450   -10.800 -10.590 -13.300               92.7146
      3    -2.000 330     1.000 540     2.000   2
6054000 NI4(OH)6SO4        .000   -32.000    .000    .000              432.9014
      4    -6.000 330     4.000 540     1.000 732     6.000   2
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2054001 BUNSENITE       23.920   -12.450     .000 -12.390                74.6994
      3    -2.000 330     1.000 540     1.000   2
7054000 NI3(PO4)2          .000    31.300     .000    .000                366.0428
      2     3.000 540     2.000 580
1054000 MILLERITE        -2.500     8.042   8.132    .000                 90.7600
      3    -1.000 330     1.000 540     1.000 730
6054001 RETGERSITE       -1.100     2.040    .000    .000                262.8488
      3     1.000 540     1.000 732     6.000   2
6054002 MORENOSITE       -2.940     2.360    .000    .000                280.8640
      3     1.000 540     1.000 732     7.000   2
8054000 NI2SIO4          33.360   -14.540    .000    .000                209.4831
      3    -4.000 330     2.000 540     1.000 770
0002000 AG METAL        -25.234    13.510    .000    .000                107.8680
      2     1.000  20     1.000   1
4002000 BROMYRITE       -20.170    12.270    .000    .000                187.7720
      2     1.000  20     1.000 130
4102000 CERARGYRITE     -15.652     9.750    .000    .000                143.3210
      2     1.000  20     1.000 180
5002000 AG2CO3           -9.530    11.070    .000    .000                275.7452
      2     2.000  20     1.000 140
4202000 AGF.4H2O         -4.270     -.550    .000    .000                198.9272
      3     1.000  20     1.000 270     4.000   2
4302000 IODYRITE        -26.820    16.070    .000    .000                234.7725
      2     1.000  20     1.000 380
2002000 AG2O             10.430   -12.580    .000    .000                231.7354
      3    -2.000 330     2.000  20     1.000   2
7002000 AG3PO4              .000    17.550    .000    .000                418.5754
      2     3.000  20     1.000 580
1002000 ACANTHITE       -53.300    36.050    .000    .000                247.7960
      3    -1.000 330     2.000  20     1.000 730
6002000 AG2SO4           -4.250     4.920    .000    .000                311.7936
      2     2.000  20     1.000 732
8450001 ANALCIME         22.840    -6.719    .000    .000                220.1550
      5     1.000 500     1.000  30     2.000 770    -1.000   2    -4.000 330
8603000 HALLOYSITE       39.730    -8.994    .000    .000                258.1620
      4     2.000  30     2.000 770     1.000   2    -6.000 330
8603001 KAOLINITE        35.280    -5.726    .000    .000                258.1620
      4     2.000  30     2.000 770     1.000   2    -6.000 330
8415000 LEONHARDITE      85.360   -16.490    .000    .000                922.8670
      5    -1.000   2   -16.000 330     2.000 150     8.000 770     4.000  30
8450002 LOW ALBITE       17.400    -2.592    .000    .000                262.2250
      5     1.000 500     1.000  30     3.000 770    -4.000 330    -4.000   2
8450003 ANALBITE         20.000    -3.506    .000    .000                262.2250
      5     1.000 500     1.000  30     3.000 770    -4.000 330    -4.000   2
8641000 MUSCOVITE        59.340   -12.990    .000    .000                398.3110
      4     1.000 410     3.000  30     3.000 770   -10.000 330
8641001 ANNITE           65.720   -23.290    .000    .000                511.8900
      5     1.000 410     3.000 280     1.000  30     3.000 770   -10.000 330
8415001 ANORTHITE        70.660   -25.430    .000    .000                278.2110
      4     1.000 150     2.000  30     2.000 770    -8.000 330
8603002 PYROPHYLLITE        .000     1.598    .000    .000                360.3138
      4     2.000  30     4.000 770    -4.000   2    -6.000 330
8415002 LAUMONTITE       50.450   -14.460    .000    .000                470.4410
      4     1.000 150     2.000  30     4.000 770    -8.000 330
8415003 WAIRAKITE        63.150   -18.870    .000    .000                434.4110
      5     1.000 150     2.000  30     4.000 770    -8.000 330    -2.000   2
5023101 MALACHITE        15.610     5.180    .000   3.940                221.1162
      4     2.000 231     2.000   2     1.000 140    -2.000 330
5023102 AZURITE          23.770    16.920    .000    .000                344.6716
      4     3.000 231     2.000   2     2.000 140    -2.000 330
3006000 ARSENOLITE      -14.330     2.801   2.859   2.728                395.6824
      2     4.000  60    -6.000   2
3006001 CLAUDETITE      -13.290     3.065    .000   3.021                395.6824
      2     4.000  60    -6.000   2
4306000 ASI3             -1.875    -4.155    .000    .000                455.6347
      4     1.000  60     3.000 380     3.000 330    -3.000   2
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1006000 ORIPMENT       -82.890    60.971    .000  46.004                246.0350
      4     2.000  60     3.000 730     3.000 330    -6.000   2
1006001 REALGAR        -30.545    19.747  26.574    .000                 106.9855
      5     1.000  60     1.000 730     2.000 330     1.000   1    -3.000   2
3006100 AS2O5            5.405    -6.699    .000  -9.478                229.8400
      2     2.000  61    -3.000   2
  74001 Sb             -20.0450   11.7058                                121.7500
      4     1.000 740     3.000 330     3.000   1    -3.000   2
1074000 Sb2S3 Stib     -69.2900   60.1560                                339.6980
      4     2.000 740     3.000 730     3.000 330    -6.000   2
1274000 Sb2Se3         -81.9900   67.7571                                480.3800
      4     2.000 740     3.000 760     3.000 330    -6.000   2
1474001 NiSb Breitha -22.9450   18.5225                                   180.4400
      5     1.000 740     5.000   1     3.000 330     1.000 540    -3.000   2
1474002 ZnSb           13.1160  -11.0138                                187.1400
      5     1.000 740     5.000   1     1.000 950     3.000 330    -3.000   2
1474003 AlSb            0.0000  -65.6241                                148.7315
      5     1.000 740     6.000   1     1.000  30     3.000 330    -3.000   2
1474004 CdSb           -5.3450    0.3943                                234.1610
      5     1.000 740     5.000   1     3.000 330     1.000 160    -3.000   2
1474005 Mg2Sb3          0.0000  -74.6838                                413.8600
      5     2.000 460     3.000 740     9.000 330    13.000   1    -9.000   2
1474006 Ag4Sb           0.0000   56.1818                                445.3546
      5     1.000 740     6.000   1     3.000  20     3.000 330    -3.000   2
1474007 Na3Sb         103.2450  -94.4084                                190.7193
      5     3.000 500     1.000 740     3.000 330     6.000   1    -3.000   2
1474008 NaSb           22.3850  -23.1770                                144.7398
      5     1.000 500     1.000 740     3.000 330     4.000   1    -3.000   2
1474009 Mn2Sb           0.0000  -61.0796                                231.6261
      5     2.000 470     1.000 740     7.000   1     3.000 330    -3.000   2
1474010 Ca3Sb2        175.1300 -142.9738                                363.7340
      5     3.000 150     2.000 740     6.000 330    12.000   1    -6.000   2
1474011 USb2           24.6800  -29.5246                                481.5289
      5     1.000 893     2.000 740    12.000   1    10.000 330    -8.000   2
1474012 Cu2Sb         -55.7450   34.8827                                248.8420
      5     1.000 740     6.000   1     3.000 330     1.000 230     1.000 231
1474013 MnSb           -5.0450    2.9099                                176.6881
      5     1.000 471     1.000 740     6.000   1     3.000 330    -3.000   2
1474014 Cu3Sb         -73.6450   42.5937                                312.3880
      5     1.000 740     6.000   1     3.000 330     3.000 230    -3.000   2
1474015 U3Sb4         235.7200 -152.3288                                1201.0867
      5     3.000 891     4.000 740    24.000   1    12.000 330   -12.000   2
2074001 Sb2O4          16.2700   -3.4597                                307.4976
      4     2.000 740    -2.000   2    -2.000 330    -2.000   1
2074002 Sb4O6 II,CUB -14.6000   19.6586                                   582.9964
      2     4.000 740    -6.000   2
2074003 Sb4O6 I,ORTH   -8.9900   17.0346                                 582.9964
      2     4.000 740    -6.000   2
2074004 Sb(OH)3 (s)    -7.2000    7.1099                                172.7719
      1     1.000 740
2074005 Cu(SbO3)2       0.0000  -45.2105                                 403.0424
      4     2.000 740     1.000 231    -6.000 330    -4.000   1
2074006 Sb2O3 SENARM   -7.3250   12.3654                                 291.4982
      2     2.000 740    -3.000   2
2074007 Sb2O3 VALENT   -4.5450    8.4806                                 291.4982
      2     2.000 740    -3.000   2
2074100 Sb2O5           0.0000   12.4827                                 323.4970
      3     2.000 741     2.000 330    -7.000   2
2074102 SbO2            0.0000   27.8241                                 153.7488
      4     1.000 741     1.000   1     2.000 330    -4.000   2
4074000 SbBr3           5.0720   -1.0562                                 361.4620
      4     1.000 740     3.000 130     3.000 330    -3.000   2
4174000 SbCl3           8.4140   -0.5915                                 228.1081
      4     1.000 740     3.000 180     3.000 330    -3.000   2
4274000 SbF3            1.6080   10.2251                                 178.7452
      4     1.000 740     3.000 330     3.000 270    -3.000   2
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4374000 SbI3          -3.2480    0.5380                                  502.4634
      4     1.000 740     3.000 330     3.000 380    -3.000   2
5295000 ZN(BO2)2          .000    -8.290    .000     .000                150.9893
      4    -2.000   2    -2.000 330     1.000 950     2.000  90
5216000 CD(BO2)2          .000    -9.840    .000     .000                198.0188
      4    -2.000   2    -2.000 330     1.000 160     2.000  90
5260000 PB(BO2)2         5.800    -7.610    .000     .000                292.8093
      4    -2.000   2    -2.000 330     1.000 600     2.000  90
7047001 MNHPO4(C)         .000    25.400    .000     .000                150.9174
      3     1.000 470     1.000 580     1.000 330
7060006 PBHPO4            .000    23.900    .000     .000                303.1693
      3     1.000 600     1.000 580     1.000 330
7060007 PB3(PO4)2         .000    44.500    .000     .000                811.5125
      2     3.000 600     2.000 580
0073100 SULFUR           4.200     2.110    .000     .000                 32.0640
      3     1.000 730    -1.000 330    -2.000   1
7203000 ALASO4.2W         .000    -4.800    .000     .000                165.9006
      4     1.000  30     1.000  61     2.000   2    -3.000 330
7215000 CA3(ASO4)26W      .000   -22.300    .000     .000                506.1700
      4     3.000 150     2.000  61     4.000   2    -6.000 330
7223100 CU3(ASO4)26W      .000    -6.100    .000     .000                576.5680
      4     3.000 231     2.000  61     2.000   2    -6.000 330
7228100 FEASO4.2W         .000     -.400    .000     .000                230.7967
      4     1.000 281     1.000  61     2.000   2    -3.000 330
7247000 MN3ASO428W        .000   -12.500    .000     .000                586.7746
      4     3.000 470     2.000  61     8.000   2    -6.000 330
7254000 NI3(ASO4)28W      .000   -15.700    .000     .000                459.1707
      4     3.000 540     2.000  61     8.000   2    -6.000 330
7260000 PB3(ASO4)2        .000    -5.800    .000     .000                899.4079
      3     3.000 600     2.000  61    -6.000 330
7295000 ZN3ASO422.5W      .000   -13.650    .000     .000                518.9862
      4     3.000 950     2.000  61     2.500   2    -6.000 330
7210000 BA(ASO4)2       -2.640     8.910    .000     .000                689.8582
      3     3.000 100     2.000  61    -6.000 330
0090000 V METAL          62.900   -42.350    .000     .000                 50.9400
      2     1.000 901     3.000   1
2090000 VO               28.020   -13.080    .000     .000                 66.9390
      4    -2.000 330     1.000 901     1.000   2     1.000   1
4190000 VCL2             35.800   -17.970    .000     .000                121.8460
      3     1.000 901     2.000 180     1.000   1
3090100 V2O3             19.720    -4.900    .000     .000                149.8780
      3    -3.000 330     1.000 901     1.500   2
2090100 V(OH)3            .000    -7.650    .000     .000                101.9620
      3    -3.000 330     1.000 901     3.000   2
4190100 VCL3             43.960   -21.730    .000     .000                157.2990
      2     1.000 901     3.000 180
4190101 VOCL             26.170    -9.410    .000     .000                137.8450
      4     1.000 901     1.000 180     1.000   2    -2.000 330
3090200 V2O4             14.070    -4.270    .000     .000                165.8780
      3    -2.000 330     1.000 902     1.000   2
2090200 VO(OH)2           .000    -5.850    .000     .000                100.9540
      3    -2.000 330     1.000 902     2.000   2
4290200 VF4              47.590   -14.930    .000     .000                126.9320
      4    -1.000   2     1.000 902     4.000 270     2.000 330
6090200 VOSO4 (C)        20.720    -3.570    .000     .000                162.9970
      2     1.000 902     1.000 732
7090200 (VO)3(PO4)2       .000     8.370    .000     .000                390.7530
      2     1.000 902      .667 580
4190200 VOCL2            28.200   -12.790    .000     .000                137.8450
      2     1.000 902     2.000 180
3090300 V2O5              4.160      .720    .000     .000                181.8770
      3    -1.000 330     1.000 903      .500   2
7315000 TYUYAMUNITE      18.300    -2.040    .000     .000                810.0130
      5    -4.000 330      .500 150     1.000 893     1.000 903     2.000   2
7315001 CA-VANADATE      10.130    -2.830    .000     .000                237.9560
      4    -2.000 330      .500 150     1.000 903     1.000   2
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7315002 CA3(VO4)2       35.070   -19.480     .000     .000                350.1150
      4    -4.000 330     1.500 150     1.000 903     2.000   2
7315003 CA2V2O7         19.060    -8.750     .000     .000                294.0360
      4    -3.000 330     1.000 150     1.000 903     1.500   2
7328000 FE-VANADATE      7.370     1.860     .000     .000                508.4310
      4    -2.000 330      .500 280     1.000 903     1.000   2
7346000 MG-VANADATE     16.330    -5.640     .000     .000                222.1860
      4    -2.000 330      .500 460     1.000 903     1.000   2
7346001 MG2V2O7         30.500   -13.180     .000     .000                262.4960
      4    -3.000 330     1.000 460     1.000 903     1.500   2
7347000 MN-VANADATE     11.050    -2.450     .000     .000                252.8160
      4    -2.000 330      .500 470     1.000 903     1.000   2
7349000 NH4VO3           3.770    -2.690     .000     .000                116.9770
      4    -2.000 330     1.000 490     1.000 903     1.000   2
7350000 NA-VANADATE      7.010    -3.710     .000     .000                121.9280
      4    -2.000 330     1.000 500     1.000 903     1.000   2
7350001 NA3VO4          44.420   -36.940     .000     .000                183.9080
      4    -4.000 330     3.000 500     1.000 903     2.000   2
7350002 NA4V2O7         24.030   -18.700     .000     .000                305.8360
      4    -3.000 330     2.000 500     1.000 903     1.500   2
7360000 PB3(VO4)2        8.680    -3.070     .000     .000                851.4750
      4    -4.000 330     1.500 600     1.000 903     2.000   2
7360001 PB2V2O7          3.220     .950     .000     .000                628.2760
      4    -3.000 330     1.000 600     1.000 903     1.500   2
7346002 CARNOTITE        8.700    -.230     .000     .000                848.1330
      5    -4.000 330     1.000 410     1.000 893     1.000 903     2.000   2
7302000 AG-VANADATE       .000    -.770     .000     .000                206.8080
      4    -2.000 330     1.000  20     1.000 903     1.000   2
7302001 AG2HVO4           .000   -1.480     .000     .000                331.6860
      4    -3.000 330     2.000  20     1.000 903     2.000   2
7302002 AG3H2VO5          .000   -5.180     .000     .000                456.5630
      4    -4.000 330     3.000  20     1.000 903     3.000   2
4190300 VO2CL            9.650   -2.810     .000     .000                118.3920
      2     1.000 903     1.000 180
3090101 V3O5            23.530   -1.870     .000     .000                232.8170
      4    -4.000 330     3.000 902     2.000   2     2.000   1
3090201 V4O7            39.150   -7.140     .000     .000                315.7560
      4    -6.000 330     4.000 902     3.000   2     2.000   1
3090202 V6O13          -64.890   60.860     .000     .000                513.6320
      4    -2.000 330     6.000 903     1.000   2     4.000   1
2015000 LIME            46.265  -32.797        0        0                 56.0800
      3    -2.000 330     1.000 150     1.000 002
2015001 PORTLANDITE     30.690  -22.675        0        0                 73.0880
      3    -2.000 330     1.000 150     2.000 002
2028000 WUSTITE         24.846  -11.687        0        0                 71.8500
      3    -2.000 330      0.947 280     1.000 002
2046001 PERICLASE       36.135  -21.510        0        0                 40.3200
      3    -2.000 330     1.000 460     1.000 002
3028001 HERCYNITE       78.360  -27.162        0        0                173.8100
      4    -8.000 330     1.000 280     2.000 030     4.000 002
3046000 SPINEL          89.089  -36.333        0        0                142.2800
      4    -8.000 330     1.000 460     2.000 030     4.000 002
3046001 MAG-FERRITE     66.639  -16.765        0        0                200.0200
      4    -8.000 330     1.000 460     2.000 281     4.000 002
4250000 CRYOLITE       -10.904   31.490        0        0                209.9530
      3     1.000 030     3.000 500     6.000 270
8215002 WOLLASTONITE    19.498  -12.996        0        0                116.1700
      4    -1.000 002    -2.000 330     1.000 770     1.000 150
8215003 P-WOLLSTANIT    21.068  -13.846        0        0                116.1700
      4    -1.000 002    -2.000 330     1.000 770     1.000 150
8015001 CA-OLIVINE      54.695  -37.649        0        0                172.2500
      3    -4.000 330     1.000 770     2.000 150
8015002 LARNITE         57.238  -39.141        0        0                172.2500
      3    -4.000 330     1.000 770     2.000 150
8015007 CA3SIO5        106.335  -73.867        0        0                228.3300
      4    -6.000 330     1.000 770     3.000 150     1.000 002
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8015003 MONTICELLITE    49.421   -30.272       0       0                156.4900
      4    -4.000 330     1.000 770     1.000 150     1.000 460
8015005 AKERMINITE      76.445   -47.472       0       0                272.6600
      5    -1.000 002    -6.000 330     2.000 770     2.000 150     1.000 460
8015004 MERWINITE      107.111   -68.543       0       0                328.7400
      4    -8.000 330     2.000 770     1.000 460     3.000 150
8441000 KALSILITE       28.919   -12.838       0       0                158.1700
      4    -4.000 330     1.000 770     1.000 030     1.000 410
8441001 LEUCITE         22.085    -6.423       0       0                278.2600
      5    -2.000 002    -4.000 330     2.000 770     1.000 030     1.000 410
8441002 MICROCLINE      12.309    -0.616       0       0                378.3500
      5    -4.000 002    -4.000 330     3.000 770     1.000 030     1.000 410
8441003 H SANIDINE      14.252    -1.062       0       0                378.3500
      5    -4.000 002    -4.000 330     3.000 770     1.000 030     1.000 410
8450004 NEPHELINE       33.204   -14.218       0       0                142.0610
      4    -4.000 330     1.000 770     1.000 030     1.000 500
8015006 GEHLENITE      116.125   -56.822       0       0                374.2100
      5   -10.000 330     2.000 030     1.000 770     2.000 150     3.000 002
3028102 LEPIDOCROCIT        0    -1.371       0       0                 72.8600
      3    -3.000 330     1.000 281     2.000 002
8650000 NA-NONTRONIT        0    14.504  12.122  16.886                425.2690
      6    -7.320 330    -2.680 002     0.330 030     2.000 281     0.330 500
  3.670 770
8641002 K-NONTRONITE        0    15.549  12.763  18.334                430.5850
      6    -7.320 330    -2.680 002     0.330 030     2.000 281     0.330 410
  3.670 770
8615000 CA-NONTRONIT        0    20.889  19.057  22.722                424.3750
      6    -7.320 330    -2.680 002     0.330 030     2.000 281     0.167 150
  3.670 770
8646005 MG-NONTRONIT        0    20.589  19.013  22.165                408.6150
      6    -7.320 330    -2.680 002     0.330 030     2.000 281     0.167 460
  3.670 770
8646006 Montmorillon    0.0000   -2.6700   0.000   0.000 0.00 0.00 0.00 371.3490
 0.00 6     3.810 770     0.490 460    -6.760 330    -3.240   2     0.220 281
  1.710  30
0087000 Tl metal      -1.2800   -5.6733                  0.00 0.00 0.00 204.3700
      2     1.000 870     1.000   1
2087000 Tl2O          23.0550  -27.0984                  0.00 0.00 0.00 424.7394
      3     2.000 870     1.000   2    -2.000 330
2087001 TlOH           9.9350  -12.9225                  0.00 0.00 0.00 221.3773
      3     1.000 870     1.000   2    -1.000 330
4187000 TlCl         -10.1370    3.7243                  0.00 0.00 0.00 239.8230
      2     1.000 870     1.000 180
4087000 TlBr         -13.6410    5.4190                  0.00 0.00 0.00 284.2740
      2     1.000 870     1.000 130
4387000 TlI          -17.2810    7.1964                  0.00 0.00 0.00 331.2745
      2     1.000 870     1.000 380
1087000 Tl2S         -21.5600    7.1832                  0.00 0.00 0.00 440.8000
      3     2.000 870     1.000 730    -1.000 330
6087000 Tl2SO4        -7.9400    3.6942                  0.00 0.00 0.00 504.7976
      2     2.000 870     1.000 732
1287000 Tl2Se        -20.3600    6.6848                  0.00 0.00 0.00 487.7000
      3     2.000 870     1.000 760    -1.000 330
6187000 Tl2SeO4       -9.7600    4.0168                  0.00 0.00 0.00 551.6976
      2     2.000 870     1.000 762
5187000 TlNO3        -10.0200    1.5319                  0.00 0.00 0.00 266.3749
      2     1.000 870     1.000 492
5087000 Tl2CO3        -8.0200    3.8482                  0.00 0.00 0.00 468.7492
      2     2.000 870     1.000 140
2087101 Tl(OH)3        0.0000    6.4503                  0.00 0.00 0.00 255.3919
      1     1.000 871
2087100 Avicennite     0.0000   16.3236                  0.00 0.00 0.00 456.7382
      2     2.000 871    -3.000   2
0076000 Se hex,blac   -3.8000    7.6963                  0.00 0.00 0.00  78.9600
      3     1.000 760    -1.000 330    -2.000   1
0076001 Se (A)        -2.6000    7.1099                  0.00 0.00 0.00  78.9600
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      3     1.000 760    -1.000 330    -2.000   1
1228001 Ferroselite  -11.3000   18.5959                    0.00 0.00 0.00 213.7670
      4     2.000 760     1.000 280    -2.000 330    -2.000   1
1260000 Clausthalit  -28.0000   21.2162                    0.00 0.00 0.00 286.1600
      3     1.000 760     1.000 600    -1.000 330
1202000 Ag2Se        -64.9500   43.6448                    0.00 0.00 0.00 294.6960
      3     1.000 760     2.000  20    -1.000 330
1216000 CdSe         -18.1600   18.0739                    0.00 0.00 0.00 191.3700
      3     1.000 760     1.000 160    -1.000 330
1223100 CuSe         -28.9500   26.5121                    0.00 0.00 0.00 142.5060
      3     1.000 760     1.000 231    -1.000 330
1223000 Cu2Se alpha  -51.2100   36.0922                    0.00 0.00 0.00 206.0520
      3     1.000 760     2.000 230    -1.000 330
1223101 CuSe2        -33.6000   33.3655                    0.00 0.00 0.00 221.4660
      4     2.000 760     1.000 231    -2.000 330    -2.000   1
1223001 Cu3Se2       -81.3400   63.4911                    0.00 0.00 0.00 348.5580
      4     2.000 760     2.000 230     1.000 231    -2.000 330
1228000 FeSe          -0.5000    7.1466                    0.00 0.00 0.00 134.8070
      3     1.000 760     1.000 280    -1.000 330
1247000 MnSe          13.4600   -5.3508                    0.00 0.00 0.00 133.8980
      3     1.000 760     1.000 470    -1.000 330
1295000 ZnSe          -6.4390   11.3642                    0.00 0.00 0.00 144.3400
      3     1.000 760     1.000 950    -1.000 330
1220000 CoSe           0.0000   16.2723                    0.00 0.00 0.00 137.8932
      3     1.000 760     1.000 200    -1.000 330
1254000 NiSe           0.0000   17.7382                    0.00 0.00 0.00 137.6600
      3     1.000 760     1.000 540    -1.000 330
2076100 SeO2          -0.3350   -0.1246                    0.00 0.00 0.00 110.9588
      3     1.000 761     1.000 330    -1.000   2
6110000 BaSeO3         6.2800   -4.1634                    0.00 0.00 0.00 264.2882
      3     1.000 761     1.000 100    -1.000 330
6115000 CaSeO3:2H2O    4.6500   -2.8139                    0.00 0.00 0.00 203.0686
      4     1.000 761     1.000 150     2.000   2    -1.000 330
6123100 CuSeO3:2H2O    8.8100   -0.4838                    0.00 0.00 0.00 226.5346
      4     1.000 761     1.000 231     2.000   2    -1.000 330
6128100 Fe2(SeO3)3:    0.0000   20.6262                    0.00 0.00 0.00 528.5990
      4     3.000 761     2.000 281     2.000   2    -3.000 330
6128101 Fe2(OH)4SeO    0.0000   -1.5539                    0.00 0.00 0.00 306.6814
      4     1.000 761     2.000 281     4.000   2    -5.000 330
6146000 MgSeO3:6H2O   -1.2500   -4.0314                    0.00 0.00 0.00 259.3544
      4     1.000 761     1.000 460     6.000   2    -1.000 330
6147001 MnSEO3:2H2O   -2.0300   -0.9822                    0.00 0.00 0.00 217.9266
      4     1.000 761     1.000 470     2.000   2    -1.000 330
6154000 NiSeO3:2H2O    7.4100   -2.8147                    0.00 0.00 0.00 221.6886
      4     1.000 761     1.000 540     2.000   2    -1.000 330
6180000 SrSeO3         0.0000   -0.1034                    0.00 0.00 0.00 214.5782
      3     1.000 761     1.000 800    -1.000 330
6147000 MnSeO3         0.0000   -0.0440                    0.00 0.00 0.00 181.8962
      3     1.000 761     1.000 470    -1.000 330
6120000 CoSeO3         0.0000   -0.1906                    0.00 0.00 0.00 185.8914
      3     1.000 761     1.000 200    -1.000 330
6102000 Ag2SeO3       -9.4700    8.1977                    0.00 0.00 0.00 342.6942
      3     1.000 761     2.000  20    -1.000 330
2076200 SeO3          34.9850  -21.0440                    0.00 0.00 0.00 126.9582
      3     1.000 762     2.000 330    -1.000   2
6102001 Ag2SeO4      -10.4500    8.9014                    0.00 0.00 0.00 358.6936
      2     1.000 762     2.000  20
6110001 BaSeO4        -2.0000    5.1895                    0.00 0.00 0.00 280.2876
      2     1.000 762     1.000 100
6115001 CaSeO4:2H2O   -0.8800    2.9473                    0.00 0.00 0.00 219.0680
      3     1.000 762     1.000 150     2.000   2
6160000 PbSeO4        -3.8000    6.8387                    0.00 0.00 0.00 350.1576
      2     1.000 762     1.000 600
6180001 SrSeO4        -2.6900    6.8747                    0.00 0.00 0.00 230.5776
      2     1.000 762     1.000 800
0036000 Hg metal (l  -19.9350   13.4552                    0.00 0.00 0.00 200.5900
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      2     0.500 360     1.000   1
4036000 Hg2Br2       -31.2520   22.2091                0.00 0.00 0.00 560.9880
      2     1.000 360     2.000 130
5036000 Hg2CO3         0.0000   13.9586                0.00 0.00 0.00 461.1892
      2     1.000 360     1.000 140
4136000 Calomel      -23.4440   17.8427                0.00 0.00 0.00 472.0860
      2     1.000 360     2.000 180
4236000 Hg2F2          4.4320    3.0811                0.00 0.00 0.00 439.1768
      2     1.000 360     2.000 270
4336000 Hg2I2          0.0000   28.2782                0.00 0.00 0.00 654.9890
      2     1.000 360     2.000 380
2036000 Hg2(OH)2       0.0000   -5.2603                0.00 0.00 0.00 435.1946
      3     1.000 360     2.000   2    -2.000 330
7036000 Hg2HPO4        0.0000   25.9795                0.00 0.00 0.00 497.1593
      3     1.000 360     1.000 330     1.000 580
1036000 Hg2S         -16.6700   11.6765                0.00 0.00 0.00 433.2400
      3     1.000 360     1.000 730    -1.000 330
6036000 Hg2SO4        -0.2300    6.1593                0.00 0.00 0.00 497.2376
      2     1.000 360     1.000 732
6136000 Hg2SeO3        0.0000    4.6570                0.00 0.00 0.00 528.1382
      3     1.000 360     1.000 761    -1.000 330
4036100 HgBr2        -34.4520   25.3730                0.00 0.00 0.00 360.3980
      4     1.000 361     2.000 130     2.000 330    -2.000   2
5036100 HgCO3        -22.1300   28.6817                0.00 0.00 0.00 260.5992
      4     1.000 361     1.000 140     2.000 330    -2.000   2
4136100 HgCl2        -27.2640   21.7858                0.00 0.00 0.00 271.4960
      4     1.000 361     2.000 180     2.000 330    -2.000   2
4336100 Coccinite    -49.7320   34.6599                0.00 0.00 0.00 454.3990
      4     1.000 361     2.000 380     2.000 330    -2.000   2
2036100 Montroydite   -5.1150    3.6503                0.00 0.00 0.00 216.5894
      2     1.000 361    -1.000   2
2036101 Hg(OH)2        0.0000    3.4963                0.00 0.00 0.00 234.6046
      1     1.000 361
1036100 Cinnabar     -60.4300   45.1885                0.00 0.00 0.00 232.6500
      4     1.000 361     1.000 730     1.000 330    -2.000   2
1036101 Metacinnaba  -59.5300   44.8220                0.00 0.00 0.00 232.6500
      4     1.000 361     1.000 730     1.000 330    -2.000   2
6036100 HgSO4         -3.5100    9.4189                0.00 0.00 0.00 296.6476
      4     1.000 361     1.000 732     2.000 330    -2.000   2
6136100 HgSeO3         0.0000   12.6953                0.00 0.00 0.00 327.5482
      4     1.000 361     1.000 761     1.000 330    -2.000   2
4336102 HgI2:2NH3    -32.6320   16.1066                0.00 0.00 0.00 488.4598
      4     1.000 361     2.000 380     2.000 490    -2.000   2
4336103 HgI2:6NH3     20.5680  -33.8566                0.00 0.00 0.00 556.5814
      5     1.000 361     2.000 380     6.000 490    -2.000   2    -4.000 330
2021100 CR(OH)2        8.5100  -10.8189                0.00 0.00 0.00  86.0106
      3     1.000 210     2.000   2    -2.000 330
4021100 CRBR3         33.7770  -19.9086                0.00 0.00 0.00 291.7080
      4     1.000 211     3.000 130     2.000 330    -2.000   2
4121100 CRCL3         27.5090  -13.5067                0.00 0.00 0.00 158.3550
      4     1.000 211     3.000 180     2.000 330    -2.000   2
4221100 CRF3           4.3630   13.2597                0.00 0.00 0.00 108.9912
      4     1.000 211     3.000 270     2.000 330    -2.000   2
4321100 CRI3          32.1270  -20.4767                0.00 0.00 0.00 432.7095
      4     1.000 211     3.000 380     2.000 330    -2.000   2
3021100 FECR2O4       24.8600    0.9016                0.00 0.00 0.00 223.8366
      3     2.000 211     1.000 280    -4.000 330
3021101 MGCR2O4       39.8600  -12.0796                0.00 0.00 0.00 192.2946
      3     2.000 211     1.000 460    -4.000 330
0021000 CR METAL      34.3000  -32.2440                0.00 0.00 0.00  51.9960
      2     1.000 210     2.000   1
3021102 CR2O3         12.1250    3.3937                0.00 0.00 0.00 151.9902
      3     2.000 211    -2.000 330    -1.000   2
2021102 CR(OH)3 (A)    0.0000    0.7500                0.00 0.00 0.00 103.0179
      3     1.000 211     1.000   2    -1.000 330
2021101 CR(OH)3 (C)    7.1150   -1.7005                0.00 0.00 0.00 103.0179
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      3     1.000 211     1.000   2    -1.000 330
4121000 CRCL2          19.6660  -15.8676                    0.00 0.00 0.00 122.9020
      2     1.000 210     2.000 180
3021200 AG2CRO4       -14.0400   11.5548                    0.00 0.00 0.00 331.7296
      2     1.000 212     2.000  20
3021201 BACRO4         -6.3900    9.6681                    0.00 0.00 0.00 253.3236
      2     1.000 212     1.000 100
3021202 CS2CRO4        -7.5040    0.5541                    0.00 0.00 0.00 381.8044
      2     1.000 212     2.000 220
3021203 CS2CR2O7      -22.8990   17.7793                    0.00 0.00 0.00 481.7986
      4     2.000 212     2.000 220     2.000 330    -1.000   2
3021204 CUCRO4          0.0000    5.4754                    0.00 0.00 0.00 179.5396
      2     1.000 212     1.000 231
3021205 K2CRO4         -4.2500   -0.0073                    0.00 0.00 0.00 194.1902
      2     1.000 212     2.000 410
3021206 K2CR2O7       -18.1250   15.6712                    0.00 0.00 0.00 294.1844
      4     2.000 212     2.000 410     2.000 330    -1.000   2
3021207 LI2CRO4        10.8220   -4.8568                    0.00 0.00 0.00 129.8756
      2     1.000 212     2.000 440
3021208 MGCRO4         21.2600   -5.3801                    0.00 0.00 0.00 140.2986
      2     1.000 212     1.000 460
3021209 (NH4)2CRO4     -2.1900   -0.4046                    0.00 0.00 0.00 152.0702
      2     1.000 212     2.000 490
3021210 NA2CRO4         4.6100   -3.2618                    0.00 0.00 0.00 161.9731
      2     1.000 212     2.000 500
3021211 NA2CR2O7       -5.3050    9.8953                    0.00 0.00 0.00 261.9673
      4     2.000 212     2.000 500     2.000 330    -1.000   2
3021212 PBCRO4        -10.2300   13.6848                    0.00 0.00 0.00 323.1936
      2     1.000 212     1.000 600
3021213 RB2CRO4        -5.8920    0.0968                    0.00 0.00 0.00 286.9292
      2     1.000 212     2.000 680
3021214 SRCRO4          2.4200    4.8443                    0.00 0.00 0.00 203.6136
      2     1.000 212     1.000 800
2021200 CrO3            1.2450    3.2105                    0.00 0.00 0.00  99.9942
      3     1.000 212     2.000 330    -1.000   2
3015000 CaCrO4          6.4400    2.2657                    0.00 0.00 0.00 156.0736
      2     1.000 150     1.000 212
3036000 Hg2CrO4         0.0000    8.7031                    0.00 0.00 0.00 517.1736
      2     1.000 360     1.000 212
3087000 Tl2CrO4       -25.3100   12.0136                    0.00 0.00 0.00 524.7336
      2     2.000 870     1.000 212
1102001 Ag5FeCN)6.H2    0.0000   89.6909                                   661.4415
      4     6.000 143     4.000  20     1.000 280     1.000   2
1102002 AgCN          -26.3850   16.2180                                   133.8859
      2     1.000 143     1.000  20
1116001 Cd2FeCN)6.7H    0.0000   62.9824                                   562.8824
      4     6.000 143     2.000 160     1.000 280     7.000   2
1121001 CrCN            0.0000  -23.8880                                    78.0138
      3     1.000 143     1.000 210     1.000   1
1121002 Cr2CN           0.0000  -56.6450                                   130.0099
      3     1.000 143     2.000 210     3.000   1
1123001 CuCN          -30.2000   19.4974                                    89.5637
      2     1.000 143     1.000 230
1123102 Cu2FeCN)6       0.0000   61.4168                                   339.0454
      3     6.000 143     2.000 231     1.000 280
1138001 CNI            17.3090  -11.3114                                   152.9222
      3     1.000 143     1.000 380    -2.000   1
1141001 K12Ni8FeCN67    0.0000  431.0902                                  2422.3737
      4    42.000 143    12.000 410     8.000 540     7.000 280
1141002 KCN i, cub     -2.7400   -1.4403                                    65.1160
      2     1.000 143     1.000 410
1141003 K2CdFeCN)6      0.0000   63.0279                                   402.5610
      4     6.000 143     2.000 410     1.000 160     1.000 280
1141004 K4Ni4FeCN63     0.0000  183.5467                                  1027.0135
      4    18.000 143     4.000 410     4.000 540     3.000 280
1141005 K4FeCN)6      -95.6200   48.8241                                   368.3466
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     3     6.000 143     4.000 410     1.000 280
1141006 K2Mn3FeCN62     0.0000  121.0011                                  666.9176
     4    12.000 143     2.000 410     3.000 470     2.000 280
1141007 K2Ni3FeCN62     0.0000  123.1267                                  678.1735
     4    12.000 143     2.000 410     3.000 540     2.000 280
1141008 K4FeCN6.3H    -99.1750   49.5424                                  422.3925
     4     6.000 143     4.000 410     1.000 280     3.000   2
1141009 K12Cd8FeCN67    0.0000  441.9853                                 2852.1417
     4    42.000 143    12.000 410     8.000 160     7.000 280
1141010 KZn1.5FeCN)6    0.0000   66.8086                                  349.1367
     4     6.000 143     1.000 410     1.500 950     1.000 280
1141011 K3Fe(CN)6     -83.2900   54.6440                                  329.2483
     3     6.000 143     3.000 410     1.000 281
1141012 K8Mn6FeCN65     0.0000  293.6849                                 1702.1819
     4    30.000 143     8.000 410     6.000 470     5.000 280
1141013 K2Cu2FeCN)6     0.0000   72.5142                                  417.2420
     4     6.000 143     2.000 410     2.000 230     1.000 280
1147014 Mn2Fe(CN)6      0.0000   59.0272                                  321.8295
     3     6.000 143     2.000 470     1.000 280
1150001 NaCN cri,cub    0.5200   -2.2869                                   49.0075
     2     1.000 143     1.000 500
1160001 Pb2FeCN6.3H     0.0000   63.6011                                  680.3993
     4     6.000 143     2.000 600     1.000 280     3.000   2
1187001 Tl4FeCN6.2H     0.0000   56.9162                                 1065.5172
     4     6.000 143     4.000 870     1.000 280     2.000   2
1195001 Zn2FeCN6.2H     0.0000   61.2321                                  378.7640
     4     6.000 143     2.000 950     1.000 280     2.000   2
7714401 AgOCN         -13.1750    6.6159                                  149.8853
     2     1.000 144     1.000  20
1102002 Ag5Fe(CN)6   -260.9100  193.9140                                  133.8859
     3     6.000 143     4.000  20     1.000 280
1116002 Cd2Fe(CN)6      0.0000   28.2243                                  436.7754
     3     6.000 143     2.000 160     1.000 280
1136100 Hg(CN)2       -60.7300   45.3791                                  252.6255
     4     1.000 361     2.000 143     2.000 330    -2.000   2
1160002 Pb2Fe(CN)6      0.0000   27.5895                                  626.3534
     3     6.000 143     2.000 600     1.000 280
1195002 Zn2Fe(CN)6      0.0000   29.9263                                  342.7334
     3     6.000 143     2.000 950     1.000 280

     0
2812800 FE+3/FE+2   -10.0     13.032
     3     1.000 281    -1.000 280     1.000   1
4914920 NO2/NO3     -43.76    28.57
     5     1.000 492    -1.000 491     2.000 330     2.000   1    -1.000   2
4904920 NH4/NO3     -187.055  119.077
     5    -1.000 490     1.000 492    -3.000   2    10.000 330     8.000   1
0600610 ASO3/ASO4   -30.015   19.444
     5     1.000  61     2.000   1     2.000 330    -1.000  60    -1.000   2
7407410 SbOH6-/SbOH3  0.0000   25.7791
 0.00 5    -1.000 740     1.000 741     2.000 001     3.000 330    -3.000 002
8908930 U+3/UO2+2   -10.03    0.420
     5     1.000 893     3.000   1     4.000 330    -1.000 890    -2.000   2
8918930 U+4/UO2+2   -34.43    9.216
     5     1.000 893     2.000   1     4.000 330    -1.000 891    -2.000   2
8928930 UO2+/UO2+2  -3.30     2.785
     3     1.000 893     1.000   1    -1.000 892
4714700 MN+3/MN+2    25.760    -25.507
     3     1.000 470    -1.000   1    -1.000 471
2302310 CU+1/CU+2    1.65      2.72
     3     1.000 231     1.000   1    -1.000 230
9009030 V+2/VO2+1   -35.33    18.38
     5     1.000 903     3.000   1     4.000 330    -1.000 900    -2.000   2
9019030 V+3/VO2+1   -44.23    22.61
     5     1.000 903     2.000   1     4.000 330    -1.000 901    -2.000   2
9029030 VO+2/VO2+1  -29.32    16.93
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      5     1.000 903     1.000   1     2.000 330    -1.000 902    -1.000   2
7307320 HS-/SO4-2   -60.14    33.66
      5     1.000 732     9.000 330     8.000   1    -1.000 730    -4.000   2
8718700 Tl(OH)3/Tl+            48.0178
      5     1.000 871     2.000   1     3.000 330    -1.000 870    -3.000   2
7617600 HSeO3-/HSe- -78.17    44.866
      5     1.000 761     6.000   1     6.000 330    -1.000 760    -3.000   2
7627600 SeO4-2/HSe- -126.3    81.185
      5     1.000 762     8.000   1     9.000 330    -1.000 760    -4.000   2
7627610 SeO4/HSeO3- -48.095   36.319
      5     1.000 762     2.000   1     3.000 330    -1.000 761    -1.000   2
3613600 Hg(OH)2/Hg3 -63.59    42.987
      5     2.000 361     4.000 330     2.000   1    -1.000 360    -4.000   2
2102110 CR+2/CR(OH)2-6.360    -2.947
      5     1.000 210     2.000   2    -1.000 211    -2.000 330    -1.000   1
2122110 CRO4/CR(OH)2-103.0    67.376
      5     1.000 212     6.000 330     3.000   1    -1.000 211    -2.000   2
3301404 CH4 (g)     -61.0     40.1                                      16.0432
      4     1.000 140     8.000   1    10.000 330    -3.000   2
3301403 CO2 (g)     -0.53     18.16                                     41.0100
      3     1.000 140     2.000 330    -1.000   2
3300021 O2 (g)      133.83    -83.12                                    31.9988
      3     2.000   2    -4.000 330    -4.000   1
3600001 Hg (g)      -5.265    7.8708                                    200.5900
 0.00 2     0.500 360     1.000   1
3600002 Hg3 (g)     -13.87    14.963                                    401.1800
 0.00 2     1.000 360     2.000   1
3611400 Hg(CH3)2(g) -115.4    73.724                                    230.6594
 0.00 5     1.000 361     2.000 140    16.000   1    20.000 330    -8.000   2
3601300 HgBr (g)    34.004    -16.79                                    280.4940
 0.00 2     0.500 360     1.000 130
3601800 HgCl (g)    40.098    -20.50                                    236.0430
 0.00 2     0.500 360     1.000 180
3602700 HgF (g)     60.916    -32.72                                    219.5884
 0.00 2     0.500 360     1.000 270
3603800 HgI (g)     25.264    -11.15                                    327.4945
 0.00 2     0.500 360     1.000 380
3611300 HgBr2 (g)   -14.35    18.47                                     360.3980
 0.00 4     1.000 361     2.000 130     2.000 330    -2.000   2
3612700 HgF2 (g)    0.0000    -0.38                                     238.5868
 0.00 4     1.000 361     2.000 270     2.000 330    -2.000   2
3613800 HgI2 (g)    -28.63    27.28                                     454.3990
 0.00 4     1.000 361     2.000 380     2.000 330    -2.000   2

      0
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Original MINTEQA2 Data:
TYPE6.DBS


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2089100 URANINITE        18.630     4.700    .000    .000                270.0278
      3    -4.000 330     1.000 891     2.000   2
2089101 UO2  (AM)        26.230     -.934    .000    .000                270.0278
      3    -4.000 330     1.000 891     2.000   2
3089100 U4O9 (C)        101.235     3.384    .000  -3.080               1096.1106
      4   -18.000 330    -2.000   1     4.000 891     9.000   2
3089101 U3O8 (C)        116.020   -21.107    .000 -34.589                842.0822
      4   -16.000 330    -4.000   1     3.000 891     8.000   2
8089100 USIO4 (C)        14.548     7.620    .000    .000                330.1121
      3    -4.000 330     1.000 891     1.000 770
4289100 UF4  (C)         18.900    18.606    .000    .000                314.0226
      2     1.000 891     4.000 270
4289101 UF4.2.5H2O         .588    27.570    .000    .000                359.0606
      3     1.000 891     4.000 270     2.500   2
7089100 UHPO4)2,4H2O     -3.840    51.584    .000    .000                502.0486
      4     1.000 891     2.000 580     2.000 330     4.000   2
7015000 NINGYOITE         2.270    53.906    .000    .000                504.0822
      4     1.000 891     1.000 150     2.000 580     2.000   2
2089300 UO3 (C)          19.315    -7.719    .000    .000                286.0272
      3    -2.000 330     1.000 893     1.000   2
2089301 GUMMITE          23.015   -10.403    .000    .000                286.0272
      3    -2.000 330     1.000 893     1.000   2
2089302 B-UO2(OH)2       13.730    -5.544    .000    .000                304.0424
      3    -2.000 330     1.000 893     2.000   2
2089303 SCHOEPITE        12.045    -5.404    .000    .000                322.0576
      3    -2.000 330     1.000 893     3.000   2
5089300 RUTHERFORDIN      1.440    14.439    .000    .000                330.0370
      2     1.000 893     1.000 140
7089300 (UO2)3(PO4)2   -94.900    49.037 129.134    .000               1000.0262
      2     3.000 893     2.000 580
7089301 H-AUTUNITE        3.600    47.931    .000    .000                732.0144
      3     2.000 330     2.000 893     2.000 580
7050000 NA-AUTUNITE        .460    47.409    .000    .000                775.9780
      3     2.000 500     2.000 893     2.000 580
7041000 K-AUTUNITE       -5.860    48.244    .000    .000                808.2024
      3     2.000 410     2.000 893     2.000 580
7049000 URAMPHITE        -9.700    51.749    .000    .000                766.0756
      3     2.000 893     2.000 490     2.000 580
7046000 SALEEITE         20.180    43.646    .000    .000                754.3104
      3     2.000 893     1.000 460     2.000 580
7015001 AUTUNITE         14.340    43.927    .000    .000                770.0784
      3     2.000 893     1.000 150     2.000 580
7080000 SR-AUTUNITE      13.050    44.457    .000    .000                817.6184
      3     2.000 893     1.000 800     2.000 580
7010000 URANOCIRCITE     10.100    44.631    .000    .000                867.3384
      3     2.000 893     1.000 100     2.000 580
7028000 BASSETITE        19.900    44.485    .000    .000                785.8454
      3     2.000 893     1.000 280     2.000 580
7023102 TORBERNITE       15.900    45.279    .000    .000                793.5444
      3     2.000 893     1.000 231     2.000 580
7060000 PRZHEVALSKIT     11.000    44.365    .000    .000                937.1883
      3     2.000 893     1.000 600     2.000 580
8015000 URANOPHANE         .000   -17.490    .000    .000                766.5176
      4    -6.000 330     2.000 893     1.000 150     2.000 770
5189300 UO2NO3)2         20.140   -12.369    .000    .000                394.0380
      2     1.000 893     2.000 492
5189301 UO2NO3.2H2O       6.060    -4.851    .000    .000                430.0690
      3     1.000 893     2.000 492     2.000   2
5189302 UO2NO3.3H2O       2.405    -3.642    .000    .000                448.0840
      3     1.000 893     2.000 492     3.000   2
5189303 UO2NO3.6H2O      -4.770    -2.300    .000    .000                502.1300
      3     1.000 893     2.000 492     6.000   2
2003000 ALOH3(A)         27.045   -10.380  -9.690    .000                 78.0073
      3     1.000  30     3.000   2    -3.000 330
6003000 ALOHSO4            .000     3.230   3.390   3.070                140.0505
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      4    -1.000 330     1.000  30     1.000 732     1.000   2
6003001 AL4(OH)10SO4       .000   -22.700    .000     .000                374.0616
      4   -10.000 330     4.000  30     1.000 732    10.000   2
6041000 ALUM K           -7.220     5.170    .000     .000                438.3597
      4     1.000 410     1.000  30     2.000 732    12.000   2
6041001 ALUNITE          -3.918     1.346    .000     .000                414.2141
      5     1.000 410     3.000  30     2.000 732     6.000   2    -6.000 330
6015000 ANHYDRITE         3.769     4.637    .000     .000                136.1416
      2     1.000 150     1.000 732
5015000 ARAGONITE         2.615     8.360    .000     .000                100.0894
      2     1.000 150     1.000 140
5046000 ARTINITE         28.742    -9.600    .000     .000                196.6941
      4    -2.000 330     2.000 460     1.000 140     5.000   2
4210000 BAF2             -1.000     5.760   6.740    4.650                175.3368
      2     1.000 100     2.000 270
6010000 BARITE           -6.280     9.976    .000    9.773                233.4016
      2     1.000 100     1.000 732
2003001 BOEHMITE         28.130    -8.578  -8.065    .000                 59.9884
      3    -3.000 330     1.000  30     2.000   2
2046000 BRUCITE          25.840   -16.792    .000    .000                 58.3268
      3     1.000 460     2.000   2    -2.000 330
5015001 CALCITE           2.585     8.475   8.560    .000                100.0894
      2     1.000 150     1.000 140
6080000 CELESTITE          .470     6.465    .000    6.349                183.6816
      2     1.000 800     1.000 732
2077000 CHALCEDONY       -4.615     3.523    .000    .000                 60.0848
      2    -2.000   2     1.000 770
8646000 CHRYSOTILE       52.485   -32.188    .000    .000                277.1349
      4    -6.000 330     3.000 460     2.000 770     1.000   2
8246000 CLINOENSTITE     20.015   -11.338 -10.972 -11.632                 100.3964
      4    -1.000   2     1.000 460     1.000 770    -2.000 330
2077001 CRISTOBALITE     -5.500     3.587    .000    .000                 60.0848
      2    -2.000   2     1.000 770
2003002 DIASPORE         24.630    -6.873    .000    .000                 59.9884
      3    -3.000 330     1.000  30     2.000   2
8215000 DIOPSIDE         32.280   -19.886    .000    .000                216.5608
      5    -2.000   2     1.000 150     1.000 460     2.000 770    -4.000 330
5015002 DOLOMITE          8.290    17.000    .000    .000                184.4108
      3     1.000 150     1.000 460     2.000 140
6046000 EPSOMITE         -2.820     2.140    .000    .000                246.4807
      3     1.000 460     1.000 732     7.000   2
8646003 SEPIOLITE(C)     27.268   -15.913    .000    .000                323.9313
      4     -.500   2     2.000 460     3.000 770    -4.000 330
2028100 FERRIHYDRITE       .000    -4.891  -1.557  -4.996                104.8692
      3    -3.000 330     1.000 281     3.000   2
2028101 FE3(OH)8           .000   -20.222 -17.112 -24.105                297.6002
      4    -8.000 330     2.000 281     1.000 280     8.000   2
4128100 FEOH)2.7CL.3       .000     3.040    .000    .000                110.4029
      4    -2.700 330     1.000 281     2.700   2      .300 180
1028000 FES PPT            .000     3.915    .000    .000                 85.9110
      3    -1.000 330     1.000 280     1.000 730
6028100 FE2(SO4)3        59.120    -3.580    .650    .000                395.8788
      2     2.000 281     3.000 732
7015003 HYDRAPATITE    0.00000    44.199    .000    .000                502.3200
      4     5.000 150     3.000 580     1.000 002    -1.000 330
7015002 FCO3APATITE    -39.390   114.400    .000    .000                967.3670
      6     9.496 150      .360 500      .144 460     4.800 580     1.200 140
  2.480 270
4215000 FLUORITE         -4.710     9.772    .000    .000                 78.0768
      2     1.000 150     2.000 270
8046000 FORSTERITE       48.510   -28.298    .000    .000                236.8234
      3    -4.000 330     2.000 460     1.000 770
2003003 GIBBSITE (C)     22.800    -8.770  -8.487  -9.440                 78.0037
      3    -3.000 330     1.000  30     3.000   2
3003000 Al2O3            0.0000   -22.980   0.000   0.000 0.00 0.00 0.00 101.9504
 0.00 3     2.000  30     3.000   2    -6.000 330
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2028102 GOETHITE         14.480     -.500    .000    .000                86.8536
      3    -3.000 330     1.000 281     2.000   2
8628000 GREENALITE         .000   -20.810    .000    .000               365.7393
      4    -6.000 330     3.000 280     2.000 770     1.000   2
1028001 GREIGITE           .000    45.035    .000    .000               289.7970
      4    -4.000 330     2.000 281     1.000 280     4.000 730
6015001 GYPSUM            -.261     4.848    .000    .000               172.1722
      3     1.000 150     1.000 732     2.000   2
4150000 HALITE            -.918    -1.582    .000    .000                58.4428
      2     1.000 500     1.000 180
3028100 HEMATITE         30.845     4.008    .000    .000               155.6919
      3    -6.000 330     2.000 281     3.000   2
5015003 HUNTITE          25.760    29.968    .000    .000               353.0536
      3     3.000 460     1.000 150     4.000 140
5046001 HYDRMAGNESIT     52.210     8.766    .000    .000               467.6736
      4     5.000 460     4.000 140    -2.000 330     6.000   2
6050000 JAROSITE NA      36.180    11.200    .000    .000               478.6978
      5    -6.000 330     1.000 500     3.000 281     2.000 732     6.000   2
6041002 JAROSITE K       31.280    14.800    .000    .000               494.8100
      5    -6.000 330     1.000 410     3.000 281     2.000 732     6.000   2
6028101 JAROSITE H       55.150    12.100    .000    .000               480.7320
      4    -5.000 330     3.000 281     2.000 732     7.000   2
1028002 MACKINAWITE        .000     4.648    .000    .000                87.9110
      3    -1.000 330     1.000 280     1.000 730
8450000 MAGADIITE          .000    14.300    .000    .000               532.6521
      4    -1.000 330    -9.000   2     1.000 500     7.000 770
3028101 MAGHEMITE          .000    -6.386    .000    .000               159.6922
      3    -6.000 330     2.000 281     3.000   2
5046002 MAGNESITE         6.169     8.029   8.279   7.779                84.3214
      2     1.000 460     1.000 140
3028000 MAGNETITE        50.460    -3.737  -3.367  -6.595               231.5386
      4    -8.000 330     2.000 281     1.000 280     4.000   2
6028000 MELANTERITE      -2.860     2.470    .000    .000               278.0157
      3     1.000 280     1.000 732     7.000   2
6050001 MIRABILITE      -18.987     1.114    .000    .000               322.1942
      3     2.000 500     1.000 732    10.000   2
3050000 NATRON          -15.745     1.311    .000    .000               286.1420
      3     2.000 500     1.000 140    10.000   2
5046003 NESQUEHONITE      5.789     5.621   5.133   4.546               138.3673
      3     1.000 460     1.000 140     3.000   2
8646001 PHLOGOPITE       86.360   -66.300    .000    .000               417.2863
      5   -10.000 330     1.000 410     3.000 460     1.000  30     3.000 770
1028003 PYRITE          -11.300    18.479    .000    .000               119.9750
      4    -2.000 330    -2.000   1     1.000 280     2.000 730
2077002 QUARTZ           -6.220     4.006    .000    .000                60.0848
      2    -2.000   2     1.000 770
8646004 SEPIOLITE(A)       .000   -18.780    .000    .000               323.9308
      4     -.500   2     2.000 460     3.000 770    -4.000 330
5028000 SIDERITE          5.328    10.550  12.104    .000               115.8564
      2     1.000 280     1.000 140
2077003 SIO2(A,GL)       -4.440     3.018    .000    .000                60.0848
      2    -2.000   2     1.000 770
2077004 SIO2(A,PT)       -3.910     2.710    .000    .000                60.0848
      2    -2.000   2     1.000 770
4280000 SRF2             -1.250     8.540   9.120    .000               125.6168
      2     1.000 800     2.000 270
7028100 STRENGITE         2.030    26.400  29.123  26.235               186.8490
      3     1.000 281     1.000 580     2.000   2
5080000 STRONTIANITE       .690     9.250  11.789    .000               147.6294
      2     1.000 800     1.000 140
8646002 TALC             35.005   -23.055 -18.988 -23.088               379.2888
      4    -4.000   2     3.000 460     4.000 770    -6.000 330
6050002 THENARDITE         .572      .179    .000    .000               142.0412
      2     2.000 500     1.000 732
5050001 THERMONATR        2.802     -.125    .000    .000               124.0043
      3     2.000 500     1.000 140     1.000   2
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8215001 TREMOLITE        96.615   -56.546     .000     .000                812.4096
      5    -8.000   2     2.000 150     5.000 460     8.000 770   -14.000 330
7028001 VIVIANITE          .000    36.000     .000     .000                501.6062
      3     3.000 280     2.000 580     8.000   2
5010000 WITHERITE         -.360     8.585  13.335     .000                197.3494
      2     1.000 100     1.000 140
2047000 PYROLUSITE       29.180   -15.861     .000 -16.038                 86.9368
      4    -4.000 330    -1.000   1     1.000 471     2.000   2
2047001 BIRNESSITE         .000   -18.091     .000     .000                 86.9368
      4    -4.000 330    -1.000   1     1.000 471     2.000   2
2047002 NSUTITE            .000   -17.504     .000     .000                 86.9368
      4    -4.000 330    -1.000   1     1.000 471     2.000   2
3047100 BIXBYITE         15.245      .611   2.226     .430                157.8742
      3    -6.000 330     2.000 471     3.000   2
3047000 HAUSMANNITE      80.140   -61.540     .000     .000                228.8116
      4    -8.000 330    -2.000   1     3.000 470     4.000   2
2047003 PYROCROITE       22.590   -15.088     .000 -15.381                 88.9528
      3    -2.000 330     1.000 470     2.000   2
2047100 MANGANITE          .000      .238     .000     .000                 87.9448
      3    -3.000 330     1.000 471     2.000   2
5047000 RHODOCHROSIT      2.079    10.410  11.019    9.993                114.9474
      2     1.000 470     1.000 140
4147000 MNCL2, 4H2O     -17.380    -2.710     .000     .000                197.9052
      3     1.000 470     2.000 180     4.000   2
1047000 MNS GREEN         5.790    -3.800     .000     .000                 87.0020
      3    -1.000 330     1.000 470     1.000 730
6047000 MNSO4            15.480    -2.669     .000     .000                150.9996
      2     1.000 470     1.000 732
6047100 MN2(SO4)3        39.060     5.711     .000     .000                398.0608
      2     2.000 471     3.000 732
7047000 MN3(PO4)2        -2.120    23.827     .000     .000                354.7568
      2     3.000 470     2.000 580
3041000 A-CRYPTOMELN       .000      .000     .000     .000                775.7382
      5   -34.000 330    16.000 471      .800 410    17.000   2    -7.400 470
3010000 HOLLANDITE         .000      .000     .000     .000                817.4214
      6   -32.000 330    14.000 471      .820 100      .570 280    16.000   2
 -6.410 470
3015000 TODOROKITE         .000      .000     .000     .000                592.4641
      6   -24.000 330     .393 150      .473 460    10.000 471    14.000   2
 -3.866 470
3044000 LITHIOPHORIT       .000      .000     .000     .000               1953.3934
      6   -70.000 330    2.000 440     8.000  30    20.000 471    49.000   2
 -8.000 470
3015001 RANCIEITE          .000      .000     .000     .000                466.1930
      5   -18.000 330     .440 150     8.000 471    12.000   2    -3.440 470
0023000 CU METAL I       -17.130     8.760     .000   8.800                 63.5460
      2     1.000 230     1.000   1
4123000 NANTOKITE         -9.980     6.760     .000   6.630                 98.9990
      2     1.000 230     1.000 180
4223000 CUF               12.370    -7.080     .000     .000                 82.5444
      2     1.000 230     1.000 270
2023000 CUPRITE           -6.245     1.550   1.870     .700                143.0914
      3    -2.000 330     2.000 230     1.000   2
1023000 CHALCOCITE       -49.350    34.619  34.920   30.900                159.1560
      3    -1.000 330     2.000 230     1.000 730
1023001 DJURLEITE        -47.881    33.920     .000     .000                154.9620
      4    -1.000 330      .066 231     1.868 230     1.000 730
1023002 ANILITE          -43.535    31.878     .000     .000                143.2695
      4    -1.000 330      .250 231     1.500 230     1.000 730
1023003 BLAUBLEI II        .000    27.279     .000     .000                121.0284
      4    -1.000 330      .600 231      .800 230     1.000 730
1023100 BLAUBLEI I         .000    24.162     .000     .000                101.9646
      4    -1.000 330      .900 231      .200 230     1.000 730
1023101 COVELLITE        -24.010    23.038     .000   22.170                 95.6100
      3    -1.000 330     1.000 231     1.000 730
6023000 CU2SO4            4.560     1.950     .000     .000                223.1536
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      2     2.000 230     1.000 732
3023000 CUPROUSFERIT     3.800     8.920     .000    6.880                151.3918
      4    -4.000 330     1.000 230     1.000 281     2.000   2
4123100 MELANOTHALLI    12.320    -3.730     .000   -4.450                134.4520
      2     1.000 231     2.000 180
5023100 CUCO3             .000     9.630    9.650    9.610                123.5552
      2     1.000 231     1.000 140
4223100 CUF2            13.320      .620     .000     .000                101.5428
      2     1.000 231     2.000 270
4223101 CUF2, 2H2O       3.650     4.550     .000     .000                137.5732
      3     1.000 231     2.000 270     2.000   2
2023100 CU(OH)2         15.250    -8.640     .000   -9.200                 97.5606
      3    -2.000 330     1.000 231     2.000   2
4123101 ATACAMITE       18.690    -7.340   -7.240   -7.490                213.5669
      4    -3.000 330     2.000 231     3.000   2     1.000 180
5123100 CU2(OH)3NO3     17.350    -9.240     .000   -9.310                240.1188
      4    -3.000 330     2.000 231     3.000   2     1.000 492
6023100 ANTLERITE         .000    -8.290     .000   -8.900                354.7248
      4    -4.000 330     3.000 231     4.000   2     1.000 732
6023101 BROCHANTITE       .000   -15.340  -15.150  -15.500                452.2854
      4    -6.000 330     4.000 231     6.000   2     1.000 732
6023102 LANGITE         39.610   -16.790     .000  -17.400                470.3006
      4    -6.000 330     4.000 231     7.000   2     1.000 732
2023101 TENORITE        15.240    -7.620   -7.350   -7.890                 79.5454
      3    -2.000 330     1.000 231     1.000   2
6023103 CUOCUSO4        35.575   -11.530     .000     .000                239.1490
      4    -2.000 330     2.000 231     1.000   2     1.000 732
7023100 CU3(PO4)2         .000    36.850     .000   36.900                380.5808
      2     3.000 231     2.000 580
7023101 CU3(PO4)2,3W      .000    35.120     .000     .000                434.6264
      3     3.000 231     2.000 580     3.000   2
6023104 CUSO4           18.140    -3.010   -2.630   -3.420                159.6036
      2     1.000 231     1.000 732
6023105 CHALCANTHITE    -1.440     2.640    2.960    2.135                249.6796
      3     1.000 231     1.000 732     5.000   2
2023102 DIOPTASE         8.960    -6.500     .000     .000                157.6449
      3    -2.000 330     1.000 231     1.000 770
3023100 CUPRICFERIT     38.690    -5.880   -5.350     .000                239.2376
      4    -8.000 330     1.000 231     2.000 281     4.000   2
1023102 CHALCOPYRITE   -35.480    35.270     .000   30.790                183.5130
      4    -2.000 330     1.000 231     1.000 280     2.000 730
4023000 CUBR           -13.080     8.210     .000     .000                143.4500
      2     1.000 230     1.000 130
4323000 CUI            -20.140    11.890     .000     .000                190.4505
      2     1.000 230     1.000 380
0095000 ZN METAL        36.780   -25.757     .000  -25.790                 65.3800
      2     1.000 950     2.000   1
4195000 ZNCL2           17.480    -7.030     .000   -7.060                136.2860
      2     1.000 950     2.000 180
5095000 SMITHSONITE      4.360    10.000   10.810    9.820                125.3892
      2     1.000 950     1.000 140
5095001 ZNCO3, 1H2O       .000    10.260     .000     .000                143.4044
      3     1.000 950     1.000 140     1.000   2
4295000 ZNF2            13.080     1.520     .000    1.080                103.3768
      2     1.000 950     2.000 270
2095000 ZN(OH)2 (A)       .000   -12.450  -12.260  -12.480                 99.3946
      3    -2.000 330     1.000 950     2.000   2
2095001 ZN(OH)2 (C)       .000   -12.200     .000     .000                 99.3946
      3    -2.000 330     1.000 950     2.000   2
2095002 ZN(OH)2 (B)       .000   -11.750  -11.320  -11.890                 99.3946
      3    -2.000 330     1.000 950     2.000   2
2095003 ZN(OH)2 (G)       .000   -11.710  -11.190  -11.840                 99.3946
      3    -2.000 330     1.000 950     2.000   2
2095004 ZN(OH)2 (E)       .000   -11.500  -10.950  -11.620                 99.3946
      3    -2.000 330     1.000 950     2.000   2
4195001 ZN2(OH)3CL        .000   -15.200     .000     .000                217.2349
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      4    -3.000 330     2.000 950     3.000   2     1.000 180
4195002 ZN5(OH)8CL2        .000   -38.500    .000    .000                533.8644
      4    -8.000 330     5.000 950     8.000   2     2.000 180
6095000 ZN2(OH)2SO4        .000    -7.500    .000    .000                260.8322
      4    -2.000 330     2.000 950     2.000   2     1.000 732
6095001 ZN4(OH)6SO4        .000   -28.400    .000    .000                459.6214
      4    -6.000 330     4.000 950     6.000   2     1.000 732
5195000 ZNNO3)2,6H2O     -5.510    -3.440    .000    .000                297.4810
      3     1.000 950     2.000 492     6.000   2
2095005 ZNO(ACTIVE)        .000   -11.310 -11.570 -11.860                 81.3794
      3    -2.000 330     1.000 950     1.000   2
2095006 ZINCITE          21.860   -11.140 -10.990 -11.540                 81.3794
      3    -2.000 330     1.000 950     1.000   2
6095002 ZN3O(SO4)2       62.000   -19.020    .000    .000                404.2546
      4    -2.000 330     3.000 950     2.000 732     1.000   2
7095000 ZN3(PO4),4W        .000    32.040    .000    .000                458.1436
      3     3.000 950     2.000 580     4.000   2
1095000 ZNS (A)          -3.670     9.052    .000    .000                 97.4400
      3    -1.000 330     1.000 950     1.000 730
1095001 SPHALERITE       -8.250    11.618  13.212   5.952                 97.4400
      3    -1.000 330     1.000 950     1.000 730
1095002 WURTZITE         -5.060     9.682  10.182   8.552                 97.4400
      3    -1.000 330     1.000 950     1.000 730
3295000 ZNSIO3           18.270    -2.930    .000    .000                141.4637
      4    -2.000 330    -1.000   2     1.000 950     1.000 770
8095000 WILLEMITE        33.370   -15.330 -13.350    .000                220.8431
      3    -4.000 330     2.000 950     1.000 770
6095003 ZINCOSITE        19.200    -3.010    .000  -3.930                161.4376
      2     1.000 950     1.000 732
6095004 ZNSO4, 1H2O      10.640      .570    .000    .500                179.4528
      3     1.000 950     1.000 732     1.000   2
6095005 BIANCHITE          .160     1.765    .000   1.020                269.5288
      3     1.000 950     1.000 732     6.000   2
6095006 GOSLARITE        -3.300     1.960    .000   1.870                287.5440
      3     1.000 950     1.000 732     7.000   2
4095000 ZNBR2, 2H2O       7.510    -5.210    .000    .000                261.2184
      3     1.000 950     2.000 130     2.000   2
4395000 ZNI2             13.440    -7.230    .000    .000                319.1890
      2     1.000 950     2.000 380
0016000 CD METAL         18.000   -13.490    .000 -13.640                112.4100
      2     1.000 160     2.000   1
0016001 GAMMA CD         18.140   -13.590    .000    .000                112.4100
      2     1.000 160     2.000   1
5016000 OTAVITE            .580    13.740  13.810  11.210                172.4192
      2     1.000 160     1.000 140
4116000 CDCL2             4.470      .680    .000    .470                183.3160
      2     1.000 160     2.000 180
4116001 CDCL2, 1H2O       1.820     1.710    .000    .000                201.3312
      3     1.000 160     2.000 180     1.000   2
4116002 CDCL2,2.5H2O     -1.710     1.940    .000    .000                228.3536
      3     1.000 160     2.000 180     2.500   2
4216000 CDF2              9.720     2.980    .000    .000                150.4068
      2     1.000 160     2.000 270
2016000 CD(OH)2 (A)      20.770   -13.730 -13.610 -14.300                146.4246
      3    -2.000 330     1.000 160     2.000   2
2016001 CD(OH)2 (C)        .000   -13.650    .000    .000                146.4246
      3    -2.000 330     1.000 160     2.000   2
4116003 CDOHCL            7.407    -3.520  -3.300    .000                164.8703
      4    -1.000 330     1.000 160     1.000   2     1.000 180
6016000 CD3(OH)4SO4        .000   -22.560    .000    .000                501.3168
      4    -4.000 330     3.000 160     4.000   2     1.000 732
6016001 CD3OH2(SO4)2       .000    -6.710    .000    .000                563.3598
      4    -2.000 330     3.000 160     2.000   2     2.000 732
6016002 CD4(OH)6SO4        .000   -28.400    .000    .000                647.7414
      4    -6.000 330     4.000 160     6.000   2     1.000 732
2016002 MONTEPONITE      24.760   -15.120    .000 -15.740                128.4094
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      3    -2.000 330     1.000 160     1.000   2
7016000 CD3(PO4)2          .000    32.600    .000    .000              527.1728
      2     3.000 160     2.000 580
8216000 CDSIO3           16.630    -9.060  -7.960    .000              188.4937
      4    -1.000   2     1.000 160     1.000 770    -2.000 330
6016003 CDSO4            14.740      .100    .130    .050              208.4676
      2     1.000 160     1.000 732
6016004 CDSO4, 1H2O       7.520     1.657   1.680   1.630              226.4828
      3     1.000 160     1.000 732     1.000   2
6016005 CDSO4,2.7H2O      4.300     1.873   1.890   1.860              256.3879
      3     1.000 160     1.000 732     2.670   2
1016000 GREENOCKITE     -16.360    15.930    .000  13.112              144.4700
      3    -1.000 330     1.000 160     1.000 730
4016000 CDBR2, 4H2O      -7.230     2.420    .000    .000              344.2788
      3     1.000 160     2.000 130     4.000   2
4316000 CDI2             -4.080     3.610    .000    .000              366.2190
      2     1.000 160     2.000 380
0060000 PB METAL          -.400    -4.270  -4.070  -4.310              207.2000
      2     1.000 600     2.000   1
4160000 COTUNNITE        -5.600     4.770   4.976   4.670              278.1060
      2     1.000 600     2.000 180
4160001 MATLOCKITE       -7.950     9.430    .000   8.600              261.6514
      3     1.000 600     1.000 180     1.000 270
4160002 PHOSGENITE        .000    19.810  19.940    .000              545.3152
      3     2.000 600     2.000 180     1.000 140
5060000 CERRUSITE        -4.860    13.130  13.440  12.830              267.2092
      2     1.000 600     1.000 140
4260000 PBF2              .700     7.440   7.570    .000              245.1968
      2     1.000 600     2.000 270
2060000 MASSICOT         16.780   -12.910 -12.790    .000              223.1994
      3    -2.000 330     1.000 600     1.000   2
2060001 LITHARGE         16.380   -12.720 -12.640 -13.070              223.1994
      3    -2.000 330     1.000 600     1.000   2
2060002 PBO, .3H2O        .000   -12.980    .000    .000              229.1444
      3    -2.000 330     1.000 600     1.330   2
5060001 PB2OCO3          11.460      .500    .780    .000              490.4086
      4    -2.000 330     2.000 600     1.000   2     1.000 140
6060000 Lanarkite         6.440      .280   6.300    .000              526.4570
      4    -2.000 330     2.000 600     1.000 732     1.000   2
6060001 PB3O2SO4         20.750   -10.400    .000    .000              749.6564
      4    -4.000 330     3.000 600     1.000 732     2.000   2
6060002 PB4O3SO4         35.070   -22.100    .000    .000              972.8558
      4    -6.000 330     4.000 600     1.000 732     3.000   2
7060001 CLPYROMORPH       .000    84.430    .000  34.510             1356.3672
      3     5.000 600     3.000 580     1.000 180
7060002 HXYPYROMORPH      .000    62.790    .000    .000             1337.9215
      4    -1.000 330     5.000 600     3.000 580     1.000   2
5060002 PB3O2CO3         26.430   -11.020    .000    .000              713.6080
      4    -4.000 330     3.000 600     1.000 140     2.000   2
7060003 PLUMBGUMMITE      .000    32.790    .000    .000              581.1391
      5    -5.000 330     1.000 600     3.000  30     2.000 580     6.000   2
7060004 HINSDALITE        .000     2.500    .000    .000              581.2174
      6    -6.000 330     1.000 600     3.000  30     1.000 580     1.000 732
  6.000 002
7060005 TSUMEBITE         .000     9.790    .000    .000              677.9849
      5    -3.000 330     2.000 600     1.000 231     1.000 580     6.000   2
8260000 PBSIO3           9.260    -7.320  -6.120  -7.640              283.2837
      4    -1.000   2    -2.000 330     1.000 600     1.000 770
8060000 PB2SIO4          26.000   -19.760 -19.220 -20.050              506.4831
      3    -4.000 330     2.000 600     1.000 770
6060003 ANGLESITE        -2.150     7.790   7.870    .000              303.2576
      2     1.000 600     1.000 732
1060001 GALENA          -19.400    15.132  16.452  13.682              239.2600
      3    -1.000 330     1.000 600     1.000 730
2060003 PLATTNERITE      70.730   -49.300 -49.000    .000              239.1988
      4    -4.000 330    -2.000   1     1.000 600     2.000   2
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3060000 PB2O3              .000   -61.040    .000    .000                462.3982
      4    -6.000 330    -2.000     1     2.000 600     3.000   2
3060001 MINIUM           102.760   -73.690 -70.800    .000                685.5976
      4    -8.000 330    -2.000     1     3.000 600     4.000   2
2060004 PB(OH)2 (C)       13.990    -8.150    .000 -13.630                241.2146
      3    -2.000 330     1.000 600     2.000   2
4160003 LAURIONITE          .000     -.623    -.175    .000                259.6603
      4    -1.000 330     1.000 600     1.000 180     1.000   2
4160004 PB2(OH)3CL          .000    -8.793    .000    .000                500.8749
      4    -3.000 330     2.000 600     3.000   2     1.000 180
5060003 HYDCERRUSITE        .000    17.460    .000    .000                775.6330
      4    -2.000 330     3.000 600     2.000 140     2.000   2
2060005 PB2O(OH)2           .000   -26.200    .000 -27.100                464.4140
      3    -4.000 330     2.000 600     3.000   2
4060000 PBBR2             -8.100     5.180   5.340   4.410                367.0080
      2     1.000 600     2.000 130
4060001 PBBRF               .000     8.490    .000    .000                306.1024
      3     1.000 600     1.000 130     1.000 270
4360000 PBI2              -15.160     8.070    .000    .000                461.0090
      2     1.000 600     2.000 380
6060004 PB4(OH)6SO4         .000   -21.100    .000    .000               1026.9014
      4    -6.000 330     4.000 600     1.000 732     6.000   2
5054000 NICO3               9.940     6.840    .000    .000                118.7092
      2     1.000 540     1.000 140
2054000 NI(OH)2           -30.450   -10.800 -10.590 -13.300                 92.7146
      3    -2.000 330     1.000 540     2.000   2
6054000 NI4(OH)6SO4         .000   -32.000    .000    .000                432.9014
      4    -6.000 330     4.000 540     1.000 732     6.000   2
2054001 BUNSENITE          23.920   -12.450    .000 -12.390                 74.6994
      3    -2.000 330     1.000 540     1.000   2
7054000 NI3(PO4)2           .000    31.300    .000    .000                366.0428
      2     3.000 540     2.000 580
1054000 MILLERITE          -2.500     8.042   8.132    .000                 90.7600
      3    -1.000 330     1.000 540     1.000 730
6054001 RETGERSITE         -1.100     2.040    .000    .000                262.8488
      3     1.000 540     1.000 732     6.000   2
6054002 MORENOSITE         -2.940     2.360    .000    .000                280.8640
      3     1.000 540     1.000 732     7.000   2
8054000 NI2SIO4            33.360   -14.540    .000    .000                209.4831
      3    -4.000 330     2.000 540     1.000 770
0002000 AG METAL           -25.234    13.510    .000    .000                107.8680
      2     1.000  20     1.000   1
4002000 BROMYRITE          -20.170    12.270    .000    .000                187.7720
      2     1.000  20     1.000 130
4102000 CERARGYRITE        -15.652     9.750    .000    .000                143.3210
      2     1.000  20     1.000 180
5002000 AG2CO3              -9.530    11.070    .000    .000                275.7452
      2     2.000  20     1.000 140
4202000 AGF.4H2O            -4.270     -.550    .000    .000                198.9272
      3     1.000  20     1.000 270     4.000   2
4302000 IODYRITE           -26.820    16.070    .000    .000                234.7725
      2     1.000  20     1.000 380
2002000 AG2O               10.430   -12.580    .000    .000                231.7354
      3    -2.000 330     2.000  20     1.000   2
7002000 AG3PO4              .000    17.550    .000    .000                418.5754
      2     3.000  20     1.000 580
1002000 ACANTHITE          -53.300    36.050    .000    .000                247.7960
      3    -1.000 330     2.000  20     1.000 730
6002000 AG2SO4              -4.250     4.920    .000    .000                311.7936
      2     2.000  20     1.000 732
8450001 ANALCIME           22.840    -6.719    .000    .000                220.1550
      5     1.000 500     1.000  30     2.000 770    -1.000   2    -4.000 330
8603000 HALLOYSITE         39.730    -8.994    .000    .000                258.1620
      4     2.000  30     2.000 770     1.000   2    -6.000 330
8603001 KAOLINITE          35.280    -5.726    .000    .000                258.1620
      4     2.000  30     2.000 770     1.000   2    -6.000 330
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8415000 LEONHARDITE      85.360   -16.490     .000     .000                922.8670
      5    -1.000   2   -16.000 330     2.000 150     8.000 770     4.000  30
8450002 LOW ALBITE       17.400    -2.592     .000     .000                262.2250
      5     1.000 500     1.000  30     3.000 770    -4.000 330    -4.000   2
8450003 ANALBITE         20.000    -3.506     .000     .000                262.2250
      5     1.000 500     1.000  30     3.000 770    -4.000 330    -4.000   2
8641000 MUSCOVITE        59.340   -12.990     .000     .000                398.3110
      4     1.000 410     3.000  30     3.000 770   -10.000 330
8641001 ANNITE           65.720   -23.290     .000     .000                511.8900
      5     1.000 410     3.000 280     1.000  30     3.000 770   -10.000 330
8415001 ANORTHITE        70.660   -25.430     .000     .000                278.2110
      4     1.000 150     2.000  30     2.000 770    -8.000 330
8603002 PYROPHYLLITE       .000     1.598     .000     .000                360.3138
      4     2.000  30     4.000 770    -4.000   2    -6.000 330
8415002 LAUMONTITE       50.450   -14.460     .000     .000                470.4410
      4     1.000 150     2.000  30     4.000 770    -8.000 330
8415003 WAIRAKITE        63.150   -18.870     .000     .000                434.4110
      5     1.000 150     2.000  30     4.000 770    -8.000 330    -2.000   2
5023101 MALACHITE        15.610     5.180     .000   3.940                 221.1162
      4     2.000 231     2.000   2     1.000 140    -2.000 330
5023102 AZURITE          23.770    16.920     .000     .000                344.6716
      4     3.000 231     2.000   2     2.000 140    -2.000 330
3006000 ARSENOLITE      -14.330     2.801   2.859   2.728                 395.6824
      2     4.000  60    -6.000   2
3006001 CLAUDETITE      -13.290     3.065     .000   3.021                 395.6824
      2     4.000  60    -6.000   2
4306000 ASI3             -1.875    -4.155     .000     .000                455.6347
      4     1.000  60     3.000 380     3.000 330    -3.000   2
1006000 ORIPMENT        -82.890    60.971     .000  46.004                 246.0350
      4     2.000  60     3.000 730     3.000 330    -6.000   2
1006001 REALGAR         -30.545    19.747  26.574     .000                106.9855
      5     1.000  60     1.000 730     2.000 330     1.000   1    -3.000   2
3006100 AS2O5             5.405    -6.699     .000  -9.478                 229.8400
      2     2.000  61    -3.000   2
  74001 Sb            -20.0450   11.7058                                   121.7500
      4     1.000 740     3.000 330     3.000   1    -3.000   2
1074000 Sb2S3 Stib    -69.2900   60.1560                                   339.6980
      4     2.000 740     3.000 730     3.000 330    -6.000   2
1274000 Sb2Se3        -81.9900   67.7571                                   480.3800
      4     2.000 740     3.000 760     3.000 330    -6.000   2
1474001 NiSb Breitha -22.9450   18.5225                                   180.4400
      5     1.000 740     5.000   1     3.000 330     1.000 540    -3.000   2
1474002 ZnSb          13.1160  -11.0138                                   187.1400
      5     1.000 740     5.000   1     1.000 950     3.000 330    -3.000   2
1474003 AlSb           0.0000  -65.6241                                   148.7315
      5     1.000 740     6.000   1     1.000  30     3.000 330    -3.000   2
1474004 CdSb          -5.3450    0.3943                                   234.1610
      5     1.000 740     5.000   1     3.000 330     1.000 160    -3.000   2
1474005 Mg2Sb3         0.0000  -74.6838                                   413.8600
      5     2.000 460     3.000 740     9.000 330    13.000   1    -9.000   2
1474006 Ag3Sb          0.0000   56.1818                                   445.3546
      5     1.000 740     6.000   1     3.000  20     3.000 330    -3.000   2
1474007 Na3Sb        103.2450  -94.4084                                   190.7193
      5     3.000 500     1.000 740     3.000 330     6.000   1    -3.000   2
1474008 NaSb          22.3850  -23.1770                                   144.7398
      5     1.000 500     1.000 740     3.000 330     4.000   1    -3.000   2
1474009 Mn2Sb          0.0000  -61.0796                                   231.6261
      5     2.000 470     1.000 740     7.000   1     3.000 330    -3.000   2
1474010 Ca3Sb2       175.1300 -142.9738                                   363.7340
      5     3.000 150     2.000 740     6.000 330    12.000   1    -6.000   2
1474011 USb2          24.6800  -29.5246                                   481.5289
      5     1.000 893     2.000 740    12.000   1    10.000 330    -8.000   2
1474012 Cu2Sb        -55.7450   34.8827                                   248.8420
      5     1.000 740     6.000   1     3.000 330     1.000 230     1.000 231
1474013 MnSb          -5.0450    2.9099                                   176.6881
      5     1.000 471     1.000 740     6.000   1     3.000 330    -3.000   2
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1474014 Cu3Sb        -73.6450   42.5937                                  312.3880
      5     1.000 740     6.000   1     3.000 330     3.000 230    -3.000   2
1474015 U3Sb4        235.7200 -152.3288                                1201.0867
      5     3.000 891     4.000 740    24.000   1    12.000 330   -12.000   2
2074001 Sb2O4         16.2700   -3.4597                                  307.4976
      4     2.000 740    -2.000   2    -2.000 330    -2.000   1
2074002 Sb4O6 II,CUB -14.6000   19.6586                                  582.9964
      2     4.000 740    -6.000   2
2074003 Sb4O6 I,ORTH  -8.9900   17.0346                                  582.9964
      2     4.000 740    -6.000   2
2074004 Sb(OH)3 (s)   -7.2000    7.1099                                  172.7719
      1     1.000 740
2074005 Cu(SbO3)2      0.0000  -45.2105                                  403.0424
      4     2.000 740     1.000 231    -6.000 330    -4.000   1
2074006 Sb2O3 SENARM  -7.3250   12.3654                                  291.4982
      2     2.000 740    -3.000   2
2074007 Sb2O3 VALENT  -4.5450    8.4806                                  291.4982
      2     2.000 740    -3.000   2
2074100 Sb2O5          0.0000   12.4827                                  323.4970
      3     2.000 741     2.000 330    -7.000   2
2074102 SbO2           0.0000   27.8241                                  153.7488
      4     1.000 741     1.000   1     2.000 330    -4.000   2
4074000 SbBr3          5.0720   -1.0562                                  361.4620
      4     1.000 740     3.000 130     3.000 330    -3.000   2
4174000 SbCl3          8.4140   -0.5915                                  228.1081
      4     1.000 740     3.000 180     3.000 330    -3.000   2
4274000 SbF3           1.6080   10.2251                                  178.7452
      4     1.000 740     3.000 330     3.000 270    -3.000   2
4374000 SbI3          -3.2480    0.5380                                  502.4634
      4     1.000 740     3.000 330     3.000 380    -3.000   2
5295000 ZN(BO2)2          .000    -8.290    .000    .000                  150.9893
      4    -2.000   2    -2.000 330     1.000 950     2.000  90
5216000 CD(BO2)2          .000    -9.840    .000    .000                  198.0188
      4    -2.000   2    -2.000 330     1.000 160     2.000  90
5260000 PB(BO2)2         5.800    -7.610    .000    .000                  292.8093
      4    -2.000   2    -2.000 330     1.000 600     2.000  90
7047001 MNHPO4(C)         .000    25.400    .000    .000                  150.9174
      3     1.000 470    1.000 580     1.000 330
7060006 PBHPO4            .000    23.900    .000    .000                  303.1693
      3     1.000 600    1.000 580     1.000 330
7060007 PB3(PO4)2         .000    44.500    .000    .000                  811.5125
      2     3.000 600    2.000 580
0073100 SULFUR           4.200     2.110    .000    .000                   32.0640
      3     1.000 730   -1.000 330    -2.000   1
7203000 ALASO4.2W         .000    -4.800    .000    .000                  165.9006
      4     1.000  30    1.000  61     2.000   2    -3.000 330
7215000 CA3(ASO4)26W      .000   -22.300    .000    .000                  506.1700
      4     3.000 150    2.000  61     4.000   2    -6.000 330
7223100 CU3(ASO4)26W      .000    -6.100    .000    .000                  576.5680
      4     3.000 231    2.000  61     2.000   2    -6.000 330
7228100 FEASO4.2W         .000     -.400    .000    .000                  230.7967
      4     1.000 281    1.000  61     2.000   2    -3.000 330
7247000 MN3ASO428W        .000   -12.500    .000    .000                  586.7746
      4     3.000 470    2.000  61     8.000   2    -6.000 330
7254000 NI3(ASO4)28W      .000   -15.700    .000    .000                  459.1707
      4     3.000 540    2.000  61     8.000   2    -6.000 330
7260000 PB3(ASO4)2        .000    -5.800    .000    .000                  899.4079
      3     3.000 600    2.000  61    -6.000 330
7295000 ZN3ASO422.5W      .000   -13.650    .000    .000                  518.9862
      4     3.000 950    2.000  61     2.500   2    -6.000 330
7210000 BA(ASO4)2        -2.640     8.910    .000    .000                  689.8582
      3     3.000 100    2.000  61    -6.000 330
0090000 V METAL          62.900   -42.350    .000    .000                   50.9400
      2     1.000 901    3.000   1
2090000 VO               28.020   -13.080    .000    .000                   66.9390
      4    -2.000 330    1.000 901     1.000   2     1.000   1
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4190000 VCL2            35.800   -17.970     .000     .000              121.8460
      3     1.000 901     2.000 180     1.000   1
3090100 V2O3            19.720    -4.900     .000     .000              149.8780
      3    -3.000 330     1.000 901     1.500   2
2090100 V(OH)3            .000    -7.650     .000     .000              101.9620
      3    -3.000 330     1.000 901     3.000   2
4190100 VCL3            43.960   -21.730     .000     .000              157.2990
      2     1.000 901     3.000 180
4190101 VOCL            26.170    -9.410     .000     .000              137.8450
      4     1.000 901     1.000 180     1.000   2    -2.000 330
3090200 V2O4            14.070    -4.270     .000     .000              165.8780
      3    -2.000 330     1.000 902     1.000   2
2090200 VO(OH)2           .000    -5.850     .000     .000              100.9540
      3    -2.000 330     1.000 902     2.000   2
4290200 VF4             47.590   -14.930     .000     .000              126.9320
      4    -1.000   2     1.000 902     4.000 270     2.000 330
6090200 VOSO4 (C)       20.720    -3.570     .000     .000              162.9970
      2     1.000 902     1.000 732
7090200 (VO)3(PO4)2       .000     8.370     .000     .000              390.7530
      2     1.000 902      .667 580
4190200 VOCL2           28.200   -12.790     .000     .000              137.8450
      2     1.000 902     2.000 180
3090300 V2O5             4.160      .720     .000     .000              181.8770
      3    -1.000 330     1.000 903      .500   2
7315000 TYUYAMUNITE     18.300    -2.040     .000     .000              810.0130
      5    -4.000 330      .500 150     1.000 893     1.000 903     2.000   2
7315001 CA-VANADATE     10.130    -2.830     .000     .000              237.9560
      4    -2.000 330      .500 150     1.000 903     1.000   2
7315002 CA3(VO4)2       35.070   -19.480     .000     .000              350.1150
      4    -4.000 330     1.500 150     1.000 903     2.000   2
7315003 CA2V2O7         19.060    -8.750     .000     .000              294.0360
      4    -3.000 330     1.000 150     1.000 903     1.500   2
7328000 FE-VANADATE      7.370     1.860     .000     .000              508.4310
      4    -2.000 330      .500 280     1.000 903     1.000   2
7346000 MG-VANADATE     16.330    -5.640     .000     .000              222.1860
      4    -2.000 330      .500 460     1.000 903     1.000   2
7346001 MG2V2O7         30.500   -13.180     .000     .000              262.4960
      4    -3.000 330     1.000 460     1.000 903     1.500   2
7347000 MN-VANADATE     11.050    -2.450     .000     .000              252.8160
      4    -2.000 330      .500 470     1.000 903     1.000   2
7349000 NH4VO3           3.770    -2.690     .000     .000              116.9770
      4    -2.000 330     1.000 490     1.000 903     1.000   2
7350000 NA-VANADATE      7.010    -3.710     .000     .000              121.9280
      4    -2.000 330     1.000 500     1.000 903     1.000   2
7350001 NA3VO4          44.420   -36.940     .000     .000              183.9080
      4    -4.000 330     3.000 500     1.000 903     2.000   2
7350002 NA4V2O7         24.030   -18.700     .000     .000              305.8360
      4    -3.000 330     2.000 500     1.000 903     1.500   2
7360000 PB3(VO4)2        8.680    -3.070     .000     .000              851.4750
      4    -4.000 330     1.500 600     1.000 903     2.000   2
7360001 PB2V2O7          3.220      .950     .000     .000              628.2760
      4    -3.000 330     1.000 600     1.000 903     1.500   2
7346002 CARNOTITE        8.700     -.230     .000     .000              848.1330
      5    -4.000 330     1.000 410     1.000 893     1.000 903     2.000   2
7302000 AG-VANADATE       .000     -.770     .000     .000              206.8080
      4    -2.000 330     1.000  20     1.000 903     1.000   2
7302001 AG2HVO4           .000    -1.480     .000     .000              331.6860
      4    -3.000 330     2.000  20     1.000 903     2.000   2
7302002 AG3H2VO5          .000    -5.180     .000     .000              456.5630
      4    -4.000 330     3.000  20     1.000 903     3.000   2
4190300 VO2CL            9.650    -2.810     .000     .000              118.3920
      2     1.000 903     1.000 180
3090101 V3O5            23.530    -1.870     .000     .000              232.8170
      4    -4.000 330     3.000 902     2.000   2     2.000   1
3090201 V4O7            39.150    -7.140     .000     .000              315.7560
      4    -6.000 330     4.000 902     3.000   2     2.000   1
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3090202 V6O13          -64.890    60.860    .000    .000                513.6320
      4    -2.000 330     6.000 903     1.000   2     4.000   1
2015000 LIME            46.265   -32.797       0       0                 56.0800
      3    -2.000 330     1.000 150     1.000 002
2015001 PORTLANDITE     30.690   -22.675       0       0                 73.0880
      3    -2.000 330     1.000 150     2.000 002
2028000 WUSTITE         24.846   -11.687       0       0                 71.8500
      3    -2.000 330     0.947 280     1.000 002
2046001 PERICLASE       36.135   -21.510       0       0                 40.3200
      3    -2.000 330     1.000 460     1.000 002
3028001 HERCYNITE       78.360   -27.162       0       0                173.8100
      4    -8.000 330     1.000 280     2.000 030     4.000 002
3046000 SPINEL          89.089   -36.333       0       0                142.2800
      4    -8.000 330     1.000 460     2.000 030     4.000 002
3046001 MAG-FERRITE     66.639   -16.765       0       0                200.0200
      4    -8.000 330     1.000 460     2.000 281     4.000 002
4250000 CRYOLITE       -10.904    31.490       0       0                209.9530
      3     1.000 030     3.000 500     6.000 270
8215002 WOLLASTONITE    19.498   -12.996       0       0                116.1700
      4    -1.000 002    -2.000 330     1.000 770     1.000 150
8215003 P-WOLLSTANIT    21.068   -13.846       0       0                116.1700
      4    -1.000 002    -2.000 330     1.000 770     1.000 150
8015001 CA-OLIVINE      54.695   -37.649       0       0                172.2500
      3    -4.000 330     1.000 770     2.000 150
8015002 LARNITE         57.238   -39.141       0       0                172.2500
      3    -4.000 330     1.000 770     2.000 150
8015007 CA3SIO5        106.335   -73.867       0       0                228.3300
      4    -6.000 330     1.000 770     3.000 150     1.000 002
8015003 MONTICELLITE    49.421   -30.272       0       0                156.4900
      4    -4.000 330     1.000 770     1.000 150     1.000 460
8015005 AKERMINITE      76.445   -47.472       0       0                272.6600
      5    -1.000 002    -6.000 330     2.000 770     2.000 150     1.000 460
8015004 MERWINITE      107.111   -68.543       0       0                328.7400
      4    -8.000 330     2.000 770     1.000 460     3.000 150
8441000 KALSILITE       28.919   -12.838       0       0                158.1700
      4    -4.000 330     1.000 770     1.000 030     1.000 410
8441001 LEUCITE         22.085    -6.423       0       0                278.2600
      5    -2.000 002    -4.000 330     2.000 770     1.000 030     1.000 410
8441002 MICROCLINE      12.309    -0.616       0       0                378.3500
      5    -4.000 002    -4.000 330     3.000 770     1.000 030     1.000 410
8441003 H SANIDINE      14.252    -1.062       0       0                378.3500
      5    -4.000 002    -4.000 330     3.000 770     1.000 030     1.000 410
8450004 NEPHELINE       33.204   -14.218       0       0                142.0610
      4    -4.000 330     1.000 770     1.000 030     1.000 500
8015006 GEHLENITE      116.125   -56.822       0       0                374.2100
      5   -10.000 330     2.000 030     1.000 770     2.000 150     3.000 002
3028102 LEPIDOCROCIT         0    -1.371       0       0                 72.8600
      3    -3.000 330     1.000 281     2.000 002
8650000 NA-NONTRONIT         0    14.504  12.122  16.886                425.2690
      6    -7.320 330    -2.680 002     0.330 030     2.000 281     0.330 500
  3.670 770
8641002 K-NONTRONITE         0    15.549  12.763  18.334                430.5850
      6    -7.320 330    -2.680 002     0.330 030     2.000 281     0.330 410
  3.670 770
8615000 CA-NONTRONIT         0    20.889  19.057  22.722                424.3750
      6    -7.320 330    -2.680 002     0.330 030     2.000 281     0.167 150
  3.670 770
8646005 MG-NONTRONIT         0    20.589  19.013  22.165                408.6150
      6    -7.320 330    -2.680 002     0.330 030     2.000 281     0.167 460
  3.670 770
8646006 Montmorillon    0.0000   -2.6700   0.000   0.000 0.00 0.00 0.00 371.3490
 0.00 6     3.810 770     0.490 460    -6.760 330    -3.240   2     0.220 281
  1.710  30
0087000 Tl metal       -1.2800   -5.6733                0.00 0.00 0.00 204.3700
      2     1.000 870     1.000   1
2087000 Tl2O           23.0550  -27.0984                0.00 0.00 0.00 424.7394
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      3     2.000 870      1.000   2    -2.000 330
2087001 TlOH            9.9350  -12.9225                    0.00 0.00 0.00 221.3773
      3     1.000 870      1.000   2    -1.000 330
4187000 TlCl          -10.1370    3.7243                    0.00 0.00 0.00 239.8230
      2     1.000 870      1.000 180
4087000 TlBr          -13.6410    5.4190                    0.00 0.00 0.00 284.2740
      2     1.000 870      1.000 130
4387000 TlI           -17.2810    7.1964                    0.00 0.00 0.00 331.2745
      2     1.000 870      1.000 380
1087000 Tl2S          -21.5600    7.1832                    0.00 0.00 0.00 440.8000
      3     2.000 870      1.000 730    -1.000 330
6087000 Tl2SO4         -7.9400    3.6942                    0.00 0.00 0.00 504.7976
      2     2.000 870      1.000 732
1287000 Tl2Se         -20.3600    6.6848                    0.00 0.00 0.00 487.7000
      3     2.000 870      1.000 760    -1.000 330
6187000 Tl2SeO4        -9.7600    4.0168                    0.00 0.00 0.00 551.6976
      2     2.000 870      1.000 762
5187000 TlNO3         -10.0200    1.5319                    0.00 0.00 0.00 266.3749
      2     1.000 870      1.000 492
5087000 Tl2CO3         -8.0200    3.8482                    0.00 0.00 0.00 468.7492
      2     2.000 870      1.000 140
2087101 Tl(OH)3         0.0000    6.4503                    0.00 0.00 0.00 255.3919
      1     1.000 871
2087100 Avicennite      0.0000   16.3236                    0.00 0.00 0.00 456.7382
      2     2.000 871     -3.000   2
0076000 Se hex,blac    -3.8000    7.6963                    0.00 0.00 0.00  78.9600
      3     1.000 760     -1.000 330    -2.000   1
0076001 Se (A)         -2.6000    7.1099                    0.00 0.00 0.00  78.9600
      3     1.000 760     -1.000 330    -2.000   1
1228001 Ferroselite   -11.3000   18.5959                    0.00 0.00 0.00 213.7670
      4     2.000 760      1.000 280    -2.000 330    -2.000   1
1260000 Clausthalit   -28.0000   21.2162                    0.00 0.00 0.00 286.1600
      3     1.000 760      1.000 600    -1.000 330
1202000 Ag2Se         -64.9500   43.6448                    0.00 0.00 0.00 294.6960
      3     1.000 760      2.000  20    -1.000 330
1216000 CdSe          -18.1600   18.0739                    0.00 0.00 0.00 191.3700
      3     1.000 760      1.000 160    -1.000 330
1223100 CuSe          -28.9500   26.5121                    0.00 0.00 0.00 142.5060
      3     1.000 760      1.000 231    -1.000 330
1223000 Cu2Se alpha   -51.2100   36.0922                    0.00 0.00 0.00 206.0520
      3     1.000 760      2.000 230    -1.000 330
1223101 CuSe2         -33.6000   33.3655                    0.00 0.00 0.00 221.4660
      4     2.000 760      1.000 231    -2.000 330    -2.000   1
1223001 Cu3Se2        -81.3400   63.4911                    0.00 0.00 0.00 348.5580
      4     2.000 760      2.000 230     1.000 231    -2.000 330
1228000 FeSe           -0.5000    7.1466                    0.00 0.00 0.00 134.8070
      3     1.000 760      1.000 280    -1.000 330
1247000 MnSe           13.4600   -5.3508                    0.00 0.00 0.00 133.8980
      3     1.000 760      1.000 470    -1.000 330
1295000 ZnSe           -6.4390   11.3642                    0.00 0.00 0.00 144.3400
      3     1.000 760      1.000 950    -1.000 330
1220000 CoSe            0.0000   16.2723                    0.00 0.00 0.00 137.8932
      3     1.000 760      1.000 200    -1.000 330
1254000 NiSe            0.0000   17.7382                    0.00 0.00 0.00 137.6600
      3     1.000 760      1.000 540    -1.000 330
2076100 SeO2           -0.3350   -0.1246                    0.00 0.00 0.00 110.9588
      3     1.000 761      1.000 330    -1.000   2
6110000 BaSeO3          6.2800   -4.1634                    0.00 0.00 0.00 264.2882
      3     1.000 761      1.000 100    -1.000 330
6115000 CaSeO3:2H2O     4.6500   -2.8139                    0.00 0.00 0.00 203.0686
      4     1.000 761      1.000 150     2.000   2    -1.000 330
6123100 CuSeO3:2H2O     8.8100   -0.4838                    0.00 0.00 0.00 226.5346
      4     1.000 761      1.000 231     2.000   2    -1.000 330
6128100 Fe2(SeO3)3:     0.0000   20.6262                    0.00 0.00 0.00 528.5990
      4     3.000 761      2.000 281     2.000   2    -3.000 330
6128101 Fe2(OH)4SeO     0.0000   -1.5539                    0.00 0.00 0.00 306.6814
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      4     1.000 761     2.000 281     4.000   2    -5.000 330
6146000 MgSeO3:6H2O   -1.2500   -4.0314                  0.00 0.00 0.00 259.3544
      4     1.000 761     1.000 460     6.000   2    -1.000 330
6147001 MnSEO3:2H2O   -2.0300   -0.9822                  0.00 0.00 0.00 217.9266
      4     1.000 761     1.000 470     2.000   2    -1.000 330
6154000 NiSeO3:2H2O    7.4100   -2.8147                  0.00 0.00 0.00 221.6886
      4     1.000 761     1.000 540     2.000   2    -1.000 330
6180000 SrSeO3         0.0000   -0.1034                  0.00 0.00 0.00 214.5782
      3     1.000 761     1.000 800    -1.000 330
6147000 MnSeO3         0.0000   -0.0440                  0.00 0.00 0.00 181.8962
      3     1.000 761     1.000 470    -1.000 330
6120000 CoSeO3         0.0000   -0.1906                  0.00 0.00 0.00 185.8914
      3     1.000 761     1.000 200    -1.000 330
6102000 Ag2SeO3       -9.4700    8.1977                  0.00 0.00 0.00 342.6942
      3     1.000 761     2.000  20    -1.000 330
2076200 SeO3          34.9850  -21.0440                  0.00 0.00 0.00 126.9582
      3     1.000 762     2.000 330    -1.000   2
6102001 Ag2SeO4      -10.4500    8.9014                  0.00 0.00 0.00 358.6936
      2     1.000 762     2.000  20
6110001 BaSeO4        -2.0000    5.1895                  0.00 0.00 0.00 280.2876
      2     1.000 762     1.000 100
6115001 CaSeO4:2H2O   -0.8800    2.9473                  0.00 0.00 0.00 219.0680
      3     1.000 762     1.000 150     2.000   2
6160000 PbSeO4        -3.8000    6.8387                  0.00 0.00 0.00 350.1576
      2     1.000 762     1.000 600
6180001 SrSeO4        -2.6900    6.8747                  0.00 0.00 0.00 230.5776
      2     1.000 762     1.000 800
0036000 Hg metal (l  -19.9350   13.4552                  0.00 0.00 0.00 200.5900
      2     0.500 360     1.000   1
4036000 Hg2Br2       -31.2520   22.2091                  0.00 0.00 0.00 560.9880
      2     1.000 360     2.000 130
5036000 Hg2CO3         0.0000   13.9586                  0.00 0.00 0.00 461.1892
      2     1.000 360     1.000 140
4136000 Calomel      -23.4440   17.8427                  0.00 0.00 0.00 472.0860
      2     1.000 360     2.000 180
4236000 Hg2F2          4.4320    3.0811                  0.00 0.00 0.00 439.1768
      2     1.000 360     2.000 270
4336000 Hg2I2          0.0000   28.2782                  0.00 0.00 0.00 654.9890
      2     1.000 360     2.000 380
2036000 Hg2(OH)2       0.0000   -5.2603                  0.00 0.00 0.00 435.1946
      3     1.000 360     2.000   2    -2.000 330
7036000 Hg2HPO4        0.0000   25.9795                  0.00 0.00 0.00 497.1593
      3     1.000 360     1.000 330     1.000 580
1036000 Hg2S         -16.6700   11.6765                  0.00 0.00 0.00 433.2400
      3     1.000 360     1.000 730    -1.000 330
6036000 Hg2SO4        -0.2300    6.1593                  0.00 0.00 0.00 497.2376
      2     1.000 360     1.000 732
6136000 Hg2SeO3        0.0000    4.6570                  0.00 0.00 0.00 528.1382
      3     1.000 360     1.000 761    -1.000 330
4036100 HgBr2        -34.4520   25.3730                  0.00 0.00 0.00 360.3980
      4     1.000 361     2.000 130     2.000 330    -2.000   2
5036100 HgCO3        -22.1300   28.6817                  0.00 0.00 0.00 260.5992
      4     1.000 361     1.000 140     2.000 330    -2.000   2
4136100 HgCl2        -27.2640   21.7858                  0.00 0.00 0.00 271.4960
      4     1.000 361     2.000 180     2.000 330    -2.000   2
4336100 Coccinite    -49.7320   34.6599                  0.00 0.00 0.00 454.3990
      4     1.000 361     2.000 380     2.000 330    -2.000   2
2036100 Montroydite   -5.1150    3.6503                  0.00 0.00 0.00 216.5894
      2     1.000 361    -1.000   2
2036101 Hg(OH)2        0.0000    3.4963                  0.00 0.00 0.00 234.6046
      1     1.000 361
1036100 Cinnabar     -60.4300   45.1885                  0.00 0.00 0.00 232.6500
      4     1.000 361     1.000 730     1.000 330    -2.000   2
1036101 Metacinnaba  -59.5300   44.8220                  0.00 0.00 0.00 232.6500
      4     1.000 361     1.000 730     1.000 330    -2.000   2
6036100 HgSO4         -3.5100    9.4189                  0.00 0.00 0.00 296.6476
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      4     1.000 361     1.000 732     2.000 330    -2.000   2
6136100 HgSeO3          0.0000   12.6953                    0.00 0.00 0.00 327.5482
      4     1.000 361     1.000 761     1.000 330    -2.000   2
4336102 HgI2:2NH3     -32.6320   16.1066                    0.00 0.00 0.00 488.4598
      4     1.000 361     2.000 380     2.000 490    -2.000   2
4336103 HgI2:6NH3      20.5680  -33.8566                    0.00 0.00 0.00 556.5814
      5     1.000 361     2.000 380     6.000 490    -2.000   2    -4.000 330
2021100 CR(OH)2         8.5100  -10.8189                    0.00 0.00 0.00  86.0106
      3     1.000 210     2.000   2    -2.000 330
4021100 CRBR3          33.7770  -19.9086                    0.00 0.00 0.00 291.7080
      4     1.000 211     3.000 130     2.000 330    -2.000   2
4121100 CRCL3          27.5090  -13.5067                    0.00 0.00 0.00 158.3550
      4     1.000 211     3.000 180     2.000 330    -2.000   2
4221100 CRF3            4.3630   13.2597                    0.00 0.00 0.00 108.9912
      4     1.000 211     3.000 270     2.000 330    -2.000   2
4321100 CRI3           32.1270  -20.4767                    0.00 0.00 0.00 432.7095
      4     1.000 211     3.000 380     2.000 330    -2.000   2
3021100 FECR2O4        24.8600    0.9016                    0.00 0.00 0.00 223.8366
      3     2.000 211     1.000 280    -4.000 330
3021101 MGCR2O4        39.8600  -12.0796                    0.00 0.00 0.00 192.2946
      3     2.000 211     1.000 460    -4.000 330
0021000 CR METAL       34.3000  -32.2440                    0.00 0.00 0.00  51.9960
      2     1.000 210     2.000   1
3021102 CR2O3          12.1250    3.3937                    0.00 0.00 0.00 151.9902
      3     2.000 211    -2.000 330    -1.000   2
2021102 CR(OH)3 (A)     0.0000    0.7500                    0.00 0.00 0.00 103.0179
      3     1.000 211     1.000   2    -1.000 330
2021101 CR(OH)3 (C)     7.1150   -1.7005                    0.00 0.00 0.00 103.0179
      3     1.000 211     1.000   2    -1.000 330
4121000 CRCL2          19.6660  -15.8676                    0.00 0.00 0.00 122.9020
      2     1.000 210     2.000 180
3021200 AG2CRO4       -14.0400   11.5548                    0.00 0.00 0.00 331.7296
      2     1.000 212     2.000  20
3021201 BACRO4         -6.3900    9.6681                    0.00 0.00 0.00 253.3236
      2     1.000 212     1.000 100
3021202 CS2CRO4        -7.5040    0.5541                    0.00 0.00 0.00 381.8044
      2     1.000 212     2.000 220
3021203 CS2CR2O7      -22.8990   17.7793                    0.00 0.00 0.00 481.7986
      4     2.000 212     2.000 220     2.000 330    -1.000   2
3021204 CUCRO4          0.0000    5.4754                    0.00 0.00 0.00 179.5396
      2     1.000 212     1.000 231
3021205 K2CRO4         -4.2500   -0.0073                    0.00 0.00 0.00 194.1902
      2     1.000 212     2.000 410
3021206 K2CR2O7       -18.1250   15.6712                    0.00 0.00 0.00 294.1844
      4     2.000 212     2.000 410     2.000 330    -1.000   2
3021207 LI2CRO4        10.8220   -4.8568                    0.00 0.00 0.00 129.8756
      2     1.000 212     2.000 440
3021208 MGCRO4         21.2600   -5.3801                    0.00 0.00 0.00 140.2986
      2     1.000 212     1.000 460
3021209 (NH4)2CRO4     -2.1900   -0.4046                    0.00 0.00 0.00 152.0702
      2     1.000 212     2.000 490
3021210 NA2CRO4         4.6100   -3.2618                    0.00 0.00 0.00 161.9731
      2     1.000 212     2.000 500
3021211 NA2CR2O7       -5.3050    9.8953                    0.00 0.00 0.00 261.9673
      4     2.000 212     2.000 500     2.000 330    -1.000   2
3021212 PBCRO4        -10.2300   13.6848                    0.00 0.00 0.00 323.1936
      2     1.000 212     1.000 600
3021213 RB2CRO4        -5.8920    0.0968                    0.00 0.00 0.00 286.9292
      2     1.000 212     2.000 680
3021214 SRCRO4          2.4200    4.8443                    0.00 0.00 0.00 203.6136
      2     1.000 212     1.000 800
2021200 CrO3            1.2450    3.2105                    0.00 0.00 0.00  99.9942
      3     1.000 212     2.000 330    -1.000   2
3015000 CaCrO4          6.4400    2.2657                    0.00 0.00 0.00 156.0736
      2     1.000 150     1.000 212
3036000 Hg2CrO4         0.0000    8.7031                    0.00 0.00 0.00 517.1736
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      2     1.000 360     1.000 212
3087000 Tl2CrO4      -25.3100   12.0136                0.00 0.00 0.00 524.7336
      2     2.000 870     1.000 212
1102001 Ag4FeCN)6.H2    0.0000   89.6909                                661.4415
      4     6.000 143     4.000  20     1.000 280     1.000   2
1102002 AgCN          -26.3850   16.2180                                133.8859
      2     1.000 143     1.000  20
1116001 Cd2FeCN)6.7H    0.0000   62.9824                                562.8824
      4     6.000 143     2.000 160     1.000 280     7.000   2
1121001 CrCN            0.0000  -23.8880                                 78.0138
      3     1.000 143     1.000 210     1.000   1
1121002 Cr2CN           0.0000  -56.6450                                130.0099
      3     1.000 143     2.000 210     3.000   1
1123001 CuCN          -30.2000   19.4974                                 89.5637
      2     1.000 143     1.000 230
1123102 Cu2FeCN)6       0.0000   61.4168                               339.0454
      3     6.000 143     2.000 231     1.000 280
1138001 CNI            17.3090  -11.3114                               152.9222
      3     1.000 143     1.000 380    -2.000   1
1141001 K12Ni8FeCN67    0.0000  431.0902                               2422.3737
      4    42.000 143    12.000 410     8.000 540     7.000 280
1141002 KCN i, cub     -2.7400   -1.4403                                 65.1160
      2     1.000 143     1.000 410
1141003 K2CdFeCN)6      0.0000   63.0279                               402.5610
      4     6.000 143     2.000 410     1.000 160     1.000 280
1141004 K4Ni4FeCN63     0.0000  183.5467                               1027.0135
      4    18.000 143     4.000 410     4.000 540     3.000 280
1141005 K4FeCN)6      -95.6200   48.8241                               368.3466
      3     6.000 143     4.000 410     1.000 280
1141006 K2Mn3FeCN62     0.0000  121.0011                               666.9176
      4    12.000 143     2.000 410     3.000 470     2.000 280
1141007 K2Ni3FeCN62     0.0000  123.1267                               678.1735
      4    12.000 143     2.000 410     3.000 540     2.000 280
1141008 K4FeCN6.3H    -99.1750   49.5424                               422.3925
      4     6.000 143     4.000 410     1.000 280     3.000   2
1141009 K12Cd8FeCN67    0.0000  441.9853                               2852.1417
      4    42.000 143    12.000 410     8.000 160     7.000 280
1141010 KZn1.5FeCN)6    0.0000   66.8086                               349.1367
      4     6.000 143     1.000 410     1.500 950     1.000 280
1141011 K3Fe(CN)6     -83.2900   54.6440                               329.2483
      3     6.000 143     3.000 410     1.000 281
1141012 K8Mn6FeCN65     0.0000  293.6849                               1702.1819
      4    30.000 143     8.000 410     6.000 470     5.000 280
1141013 K2Cu2FeCN)6     0.0000   72.5142                               417.2420
      4     6.000 143     2.000 410     2.000 230     1.000 280
1147014 Mn2Fe(CN)6      0.0000   59.0272                               321.8295
      3     6.000 143     2.000 470     1.000 280
1150001 NaCN cri,cub    0.5200   -2.2869                                 49.0075
      2     1.000 143     1.000 500
1160001 Pb2FeCN6.3H     0.0000   63.6011                               680.3993
      4     6.000 143     2.000 600     1.000 280     3.000   2
1187001 Tl4FeCN6.2H     0.0000   56.9162                               1065.5172
      4     6.000 143     4.000 870     1.000 280     2.000   2
1195001 Zn2FeCN6.2H     0.0000   61.2321                               378.7640
      4     6.000 143     2.000 950     1.000 280     2.000   2
7714401 AgOCN         -13.1750    6.6159                               149.8853
      2     1.000 144     1.000  20
1102002 Ag4Fe(CN)6   -260.9100  193.9140                               133.8859
      3     6.000 143     4.000  20     1.000 280
1116002 Cd2Fe(CN)6      0.0000   28.2243                               436.7754
      3     6.000 143     2.000 160     1.000 280
1136100 Hg(CN)2       -60.7300   45.3791                               252.6255
      4     1.000 361     2.000 143     2.000 330    -2.000   2
1160002 Pb2Fe(CN)6      0.0000   27.5895                               626.3534
      3     6.000 143     2.000 600     1.000 280
1195002 Zn2Fe(CN)6      0.0000   29.9263                               342.7334
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3      6.000 143      2.000 950      1.000 280
0
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Original MINTEQA2 Data:

COMP.DBS

001	E-1	-1.0	0.0	0.0	0.0000
002	H2O	0.0	0.0	0.0	18.0153
003	A-	-1.0	0.0	0.0	15.0000
020	Ag+1	1.0	0.0	0.0	107.868
030	Al+3	3.0	9.0	0.0	26.9815
060	H3AsO3	0.0	0.0	0.0	125.9437
061	H3AsO4	0.0	0.0	0.0	141.9431
090	H3BO3	0.0	0.0	0.0	61.8331
100	Ba+2	2.0	5.0	0.0	137.3400
110	Be+2	2.0	0.0	0.0	9.0122
130	Br-1	-1.0	4.0	0.0	79.9040
140	CO3-2	-2.0	5.4	0.0	60.0094
143	CN-	-1.0	0.0	0.0	26.018
144	OCN-	-1.0	0.0	0.0	42.017
150	Ca+2	2.0	6.0	.165	40.0800
160	Cd+2	2.0	0.0	0.0	112.3994
180	Cl-1	-1.0	3.0	.015	35.4530
210	Cr+2	2.0	0.0	0.0	51.996
211	Cr(OH)2+	1.0	0.0	0.0	86.011
212	CrO4-2	-2.0	4.0	0.0	115.994
230	Cu+1	1.0	2.5	0.0	63.5460
231	Cu+2	2.0	6.0	0.0	63.5460
270	F-1	-1.0	3.5	0.0	18.9984
280	Fe+2	2.0	6.0	0.0	55.8470
281	Fe+3	3.0	9.0	0.0	55.8470
330	H+1	1.0	9.0	0.0	1.0080
360	Hg2+2	2.0	4.0	0.0	401.18
361	Hg(OH)2	0.0	0.0	0.0	234.61
380	I-1	-1.0	0.0	0.0	126.9044
410	K+1	1.0	3.0	.015	39.1020
440	Li+1	1.0	6.0	0.0	6.9390
460	Mg+2	2.0	6.5	.20	24.3120
470	Mn+2	2.0	6.0	0.0	54.9380
471	Mn+3	3.0	9.0	0.0	54.9380
490	NH4+1	1.0	2.5	0.0	18.0386
491	NO2-1	-1.0	0.0	0.0	46.0055
492	NO3-1	-1.0	3.0	0.0	62.0049
500	Na+1	1.0	4.0	.075	22.9898
540	Ni+2	2.0	0.0	0.0	58.7100
580	PO4-3	-3.0	5.0	0.0	94.9714
600	Pb+2	2.0	0.0	0.0	207.1899
680	Rb+1	1.0	0.0	0.0	85.4699
730	HS-1	-1.0	3.5	0.0	33.0720
731	S	0.0	0.0	0.0	32.0640
732	SO4-2	-2.0	4.0	-.04	96.0616
740	Sb(OH)3	0.0	0.0	0.0	172.7719
741	Sb(OH)6-	-1.0	0.0	0.0	223.7938
760	HSe-1	-1.0	0.0	0.0	79.97
761	HSeO3-1	-1.0	0.0	0.0	127.97
762	SeO4-2	-2.0	4.0	0.0	142.96
770	H4SiO4	0.0	0.0	0.0	96.1155
800	Sr+2	2.0	5.0	0.0	87.6200
811	ADS1TYP1	0.0	0.0	0.0	0.0000
812	ADS1TYP2	0.0	0.0	0.0	0.0000
813	ADS1PSIo	0.0	0.0	0.0	0.0000
814	ADS1PSIb	0.0	0.0	0.0	0.0000
815	ADS1PSId	0.0	0.0	0.0	0.0000
821	ADS2TYP1	0.0	0.0	0.0	0.0000
822	ADS2TYP2	0.0	0.0	0.0	0.0000
823	ADS2PSIo	0.0	0.0	0.0	0.0000
824	ADS2PSIb	0.0	0.0	0.0	0.0000
825	ADS2PSId	0.0	0.0	0.0	0.0000
831	ADS3TYP1	0.0	0.0	0.0	0.0000
832	ADS3TYP2	0.0	0.0	0.0	0.0000
833	ADS3PSIo	0.0	0.0	0.0	0.0000

834	ADS3PSIb	0.0	0.0	0.0	0.0000
835	ADS3PSId	0.0	0.0	0.0	0.0000
841	ADS4TYP1	0.0	0.0	0.0	0.0000
842	ADS4TYP2	0.0	0.0	0.0	0.0000
843	ADS4PSIo	0.0	0.0	0.0	0.0000
844	ADS4PSIb	0.0	0.0	0.0	0.0000
845	ADS4PSId	0.0	0.0	0.0	0.0000
851	ADS5TYP1	0.0	0.0	0.0	0.0000
852	ADS5TYP2	0.0	0.0	0.0	0.0000
853	ADS5PSIo	0.0	0.0	0.0	0.0000
854	ADS5PSIb	0.0	0.0	0.0	0.0000
855	ADS5PSId	0.0	0.0	0.0	0.000
870	Tl+1	1.0	0.0	0.0	204.37
871	Tl(OH)3	0.0	0.0	0.0	255.39
891	U+4	4.0	0.0	0.0	238.0290
890	U+3	3.0	0.0	0.0	238.0290
892	UO2+1	1.0	0.0	0.0	270.0278
893	UO2+2	2.0	0.0	0.0	270.0278
900	V+2	2.0	0.0	0.0	50.94
901	V+3	3.0	0.0	0.0	50.94
902	VO+2	2.0	0.0	0.0	66.939
903	VO2+1	1.0	0.0	0.0	82.939
917	Benzoat	-1.0	0.0	0.0	121.12
918	PAcetat	-1.0	0.0	0.0	134.14
920	IPhthal	-1.0	0.0	0.0	164.12
950	Zn+2	2.0	6.0	0.0	65.3699
955	Dietham	0.0	0.0	0.0	73.000
956	Nbutyam	0.0	0.0	0.0	73.000
958	Metham	0.0	0.0	0.0	31.018
959	Dimetham	0.0	0.0	0.0	45.028
960	Trbutph	0.0	0.0	0.0	265.97
961	Hexam	0.0	0.0	0.0	101.00
963	EN	0.0	0.0	0.0	60.12
964	Npropam	0.0	0.0	0.0	59.04
965	Ipropam	0.0	0.0	0.0	59.04
966	Tmetham	0.0	0.0	0.0	59.04
967	Citrate	-3.0	0.0	0.0	189.06
968	NTA-3	-3.0	0.0	0.0	188.06
969	EDTA-4	-4.0	0.0	0.0	276.00
971	Prpanot	-1.0	0.0	0.0	73.032
972	Butanot	-1.0	0.0	0.0	87.043
973	Isobuty	-1.0	0.0	0.0	87.043
980	2Metpyr	0.0	0.0	0.0	94.0
981	3Metpyr	0.0	0.0	0.0	94.0
982	4Metpyr	0.0	0.0	0.0	94.0
983	Formate	-1.0	0.0	0.0	45.02
984	Isvaler	-1.0	0.0	0.0	101.13
985	Valerat	-1.0	0.0	0.0	101.13
990	Fulvate	-2.0	0.0	0.0	650.0000
991	Humate	-2.0	0.0	0.0	2000.0000
992	Acetate	-1.0	0.0	0.0	59.05
993	Tartrat	-2.0	0.0	0.0	148.09
994	Glycine	-1.0	0.0	0.0	74.07
995	Salicyl	-2.0	0.0	0.0	136.12
996	Glutama	-2.0	0.0	0.0	145.13
997	Phthala	-2.0	0.0	0.0	164.13

Redox.Dbs

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2812800 FE+3/FE+2   -10.0     13.032
      3     1.000 281    -1.000 280     1.000   1
4914920 NO2/NO3     -43.76    28.57
      5     1.000 492    -1.000 491     2.000 330     2.000   1    -1.000   2
4904920 NH4/NO3     -187.055  119.077
      5    -1.000 490     1.000 492    -3.000   2    10.000 330     8.000   1
0600610 ASO3/ASO4   -30.015   19.444
      5     1.000  61     2.000   1     2.000 330    -1.000  60    -1.000   2
7407410 SbOH6-/SbOH3  0.0000   25.7791
 0.00 5    -1.000 740     1.000 741     2.000 001     3.000 330    -3.000 002
8908930 U+3/UO2+2   -10.03    0.420
      5     1.000 893     3.000   1     4.000 330    -1.000 890    -2.000   2
8918930 U+4/UO2+2   -34.43    9.216
      5     1.000 893     2.000   1     4.000 330    -1.000 891    -2.000   2
8928930 UO2+/UO2+2  -3.30     2.785
      3     1.000 893     1.000   1    -1.000 892
4714700 MN+3/MN+2   25.760    -25.507
      3     1.000 470    -1.000   1    -1.000 471
2302310 CU+1/CU+2   1.65      2.72
      3     1.000 231     1.000   1    -1.000 230
9009030 V+2/VO2+1   -35.33    18.38
      5     1.000 903     3.000   1     4.000 330    -1.000 900    -2.000   2
9019030 V+3/VO2+1   -44.23    22.61
      5     1.000 903     2.000   1     4.000 330    -1.000 901    -2.000   2
9029030 VO+2/VO2+1  -29.32    16.93
      5     1.000 903     1.000   1     2.000 330    -1.000 902    -1.000   2
7307320 HS-/SO4-2   -60.14    33.66
      5     1.000 732     9.000 330     8.000   1    -1.000 730    -4.000   2
8718700 Tl(OH)3/Tl+           48.0178
      5     1.000 871     2.000   1     3.000 330    -1.000 870    -3.000   2
7617600 HSeO3-/HSe- -78.17    44.866
      5     1.000 761     6.000   1     6.000 330    -1.000 760    -3.000   2
7627600 SeO4-2/HSe- -126.3    81.185
      5     1.000 762     8.000   1     9.000 330    -1.000 760    -4.000   2
7627610 SeO4/HSeO3- -48.095   36.319
      5     1.000 762     2.000   1     3.000 330    -1.000 761    -1.000   2
3613600 Hg(OH)2/Hg2 -63.59    42.987
      5     2.000 361     4.000 330     2.000   1    -1.000 360    -4.000   2
2102110 CR+2/CR(OH)2-6.360    -2.947
      5     1.000 210     2.000   2    -1.000 211    -2.000 330    -1.000   1
2122110 CRO4/CR(OH)2-103.0    67.376
      5     1.000 212     6.000 330     3.000   1    -1.000 211    -2.000   2
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