2782

WATEQF - A FORTRAN IV VERSION OF WATEQ, A COMPUTER PROGRAM FOR CALCULATING CHEMICAL EQUILIBRIUM OF NATURAL WATERS

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U. S. GEOLOGICAL SURVEY

Water-Resources Investigations 76-13

September 1976

Revised and Reprinted

December 1978
January 1984

UNITED STATES DEPARTMENT OF THE INTERIOR
Thomas S. Kleppe, Secretary
GEOLOGICAL SURVEY
V. E. McKelvey, Director

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Tape copies, at cost, of the source code and data table of Attachment B may be obtained from: U.S. Geological Survey, Office of Program Support Services, 802 National Center, Reston, VA 22092.

CONTENTS

TABLES AND ATTACHMENTS

ABSTRACT

WATEQF is a FORTRAN IV computer program that models the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The original version (WATEQ) was written in 1973 by A. H. Truesdell and B. F. Jones in Programming Language/one (PL/1). With but a few exceptions, the thermochemical data, speciation, activity coefficients, and general calculation procedure of WATEQF is identical to the PL/1 version. This report notes the differences between WATEQF and WATEQ, demonstrates how to set up the input data to execute WATEQF, provides a test case for comparison, and makes available a listing of WATEQF.

INTRODUCTION

WATEQF is a FORTRAN IV computer program that models the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The original version (WATEQ) was written by Truesdell and Jones (1973) in Programming Language/one (PL/1). With but a few exceptions, the thermochemical data, speciation, activity coefficients, and general calculation procedure of WATEQF is identical to the PL/1 version. For discussion of the program theory and original source of most of the thermochemical data, see Truesdell and Jones (1974). It is the purpose of this report to note the differences between WATEQF and WATEQ, demonstrate how to set up the input data to execute WATEQF, provide a test case for comparison (Attachment A), and make available a listing of WATEQF (Attachment B). This report also provides a list of all equilibrium reactions that are considered (Attachment C). The current version of WATEQF is written in FORTRAN 77.

DIFFERENCES BETWEEN WATEQF AND WATEQ

1. In addition to the 100 aqueous species used in the WATEQ aqueous model, WATEQF includes 14 species of manganese and computes saturation data for 21 manganese minerals. See Table 1 for the thermochemical data used.

2. All reference to maximum and minimum estimates of log K used by WATEQ have been omitted in WATEQF.

3. In addition to calculating pe from dissolved oxygen and Eh, pe can also be set by the dissolved oxygen relation of Sato (1960) and by the $SO_4^{=}$ / $S^{=}$ ratio.

4. The carbon-bearing species are computed from either titration alkalinity, carbonate alkalinity, or total carbon in solution.

5. An option has been added that allows calculation of activity coefficients of charged ion pairs from either the Debye-Hückle equation or the Davies equation.

6. Thermodynamic data used in the program can be changed through the use of optional input cards.

7. Various print options are provided to limit the amount of printed output.

8. WATEQF now consists of a main program and 5 subroutines, PREP, SET, MODEL, PRINT, and SAT. PREP reads the water data, converts the units of concentration to molality, and calculates all temperature dependent data at the temperature of the water

sample. SET initalizes values of individual species for the iterative Mass Action - Mass Balance loop. MODEL calculates activity coefficients and solves Mass Action and Mass Balance equations for the species considered. PRINT prints the results calculated from the aqueous model, and SAT calculates and prints the thermodynamic saturation state of the water with respect to the various minerals considered by the program.

9. The method of convergence on Mass Balance for anions has been changed to a more accurate and rapid convergence method, essentially identical to the method used by Truesdell and Jones (1974) for Mass Balance on cations.

10. The aqueous model will not be solved on analyses if pH is outside the interval 3.0 - 11.0, or if there is greater than 30 percent error in charge balance. This procedure is useful in screening data for punching and/or errors in the analysis. The procedure can be ignored, however, with the appropriate option specified in the input.

11. There are several changes in the aqueous model over those of Truesdell and Jones (1973) as shown in Table 1 and Attachment B, although none results in major differences between the calculations of WATEQ and WATEQF for most natural waters. The choice of speciation, thermodynamic data, and activity coefficients used by WATEQF are in a continuous process of revision, as better data become available. The responsibility for final selection of constants used in WATEQF rests with the user.

INPUT

The data matrix of species considered and thermochemical constants is read initially, either from disk or cards. The format of the data matrix is summarized as follows:

Variables	Format
(NSPEC(I), Z(I), GFW(I), DHA(I), I=1,115)	(5X, A8, 2X, I2, 3X, F10.4, 1X, F4.1)
(NREACT(I), DH(I), LOGKTO(I), I=1,193)	(5X, A8, 2X, 2F10.4)

Following input of the data matrix, data cards for one or more water analyses are read. Each water analysis requires 5 cards (4 data cards followed by a blank card). WATEQF can receive additional data on option cards that fit into the data stream between card 4 and the blank card (5).

The required input for each water analysis is summarized as follows:

Card	Variables	Format	Comments
1	TITL	20A4	Title
2	TEMP, PH, EHM, EHMC, EMFZ, DENS, DOX, FLAG, CORALK, PECALC, IGO, (PRT(I), I=1,4) IDAV, ISPEC, IMIN	(5(F6.0,1X), 2F5.0, 1X, 9I1, 2I3)	See description below
3	CUNITS(I) (I=1,2,3,4, 5,6)	(6E12.5,8X)	Ca,Mg,Na,K,Cl,SO_4 (in order)
4	CUNITS(I) (I=7,35,8,45, 88,62)	(6E12.5,8X)	HCO_3^-,SiO_2,Fe,PO_4, SR, F (in order)
----------Optional input appears here-----			
5	Blank card		Required to note end of data for a particular analysis

DESCRIPTION OF INPUT VARIABLES

NSPEC(I)	Names of the species
Z(I)	Charge of the species
GFW(I)	Gram formula wt. of ith species
DHA(I)	Debye-Hückel $\mathring{a}$ parameter for ith species
NREACT(I)	Name of ith reaction
DH(I)	ΔH_r^o for ith reaction (Kcal/mole)
LOGKTO(I)	Log K for the ith reaction at 25°C
TITL	General description, identifying information, etc.
TEMP	Temperature in degrees C.
pH	Negative log of the activity of hydrogen ion.
EHM	"True" Eh of solution to which no temperature correction will be made (volts)

EHMC — Electrical potential (volts) of the Eh cell with a calomel reference electrode.

EMFZ — Electrical potential (volts) of the Eh cell with calomel reference in Zobell's solution.

DENS — Solution density (g/cm^3). If not known, read 1.0.

DOX — Dissolved oxygen content (mg/l).

FLAG — Signal for units of input concentrations (CUNITS). 0=mmoles/l, 1=meq/l, 2=mg/l, 3=ppm, 4=molality.

CORALK — Carbon signal. Set to zero (or blank) if the alkalinity has not been corrected for silica, boron, etc. CORALK=1 if this correction has been made. Normally, one would report alkalinity as HCO_3 (and CO_3 if detected) and set CORALK to zero. To input total carbon rather than alkalinity, set CORALK to 2. Total CO_2 can then be input as HCO_3, or; if desired, as the individual species of HCO_3^-, $CO_3^=$ and $H_2CO_3^*$. $H_2CO_3^*$ and $CO_3^=$ are read on an optional "CONC" card. ($H_2CO_3^*$ denotes $H_2CO_3^0 + CO_{2aq}$).

PECALC — Signal for pe calculation. If PECALC = 0, pe is set to 100 and oxidation-reduction is ignored. =1 computes pe from Eh, =2 computes pe from dissolved oxygen, =3 computes pe from dissolved oxygen using the Sato (1960) relation, =4 computes pe from $SO_4^= / S^=$.

IGO — =0 or blank, if desired to have the data checked for possible input error or analytical error. pH must be greater than 3 and less than 11 and the analysis must have less than 30% error in charge balance. =1 if this check is not desired.

PRT(I), I=1,4 — Signals which when set to some non-zero value (say 1) omit print of: I=1, thermochemical data table; I=2, mass balance convergence iterations; I=3, ion ratios; I=4, mineral saturation calculations. Set PRT(4) = 9 for a limited print of saturation indices including calcite, dolomite, siderite, rhodocrosite, gypsum, celestite, barite, hydroxyapatite, vivianite, fluorite, amorph. FeOOH, goethite, hematite, gibbsite, birnessite, manganite, silica gel, silica glass, chalcedony, quartz, kaolinite, sepiolite (ppt.), sepiolite, FeS (amorph.) and Mackinawite. To obtain the above printout, leave the appropriate value of PRT(I) blank or zero.

IDAVES Signal used to indicate desired method of calculation of activity coefficients, γ_i, of charged ion pairs. If 1, the Davies equation,

$$\log \gamma_i = -A z_i^2 \left(\frac{\sqrt{I}}{1 + \sqrt{I}} - .3I \right)$$

is used. If zero, or blank, the Debye-Hückel equation,

$$\log \gamma_i = \frac{-A z_i^2 \sqrt{I}}{1 + Ba_i \sqrt{I}}$$

is used. A and B are constants that depend on the dielectric constant, density and temperature of the solvent, Z_i is the charge on the ion, I is ionic strength ($I = 1/2 \Sigma_i m_i z_i^2$, where m_i is the molality of the ith ion), and a_i is the "ion size" parameter. As a general rule, the Davies equation is probably accurate to ionic strengths less than 0.5 and the Debye-Hückel equation is more accurate at ionic strength less than 0.1 (Stumm and Morgan, 1970). Activity coefficients of Ca^{++}, Mg^{++}, Na^+, K^+, Cl^-, $SO_4^=$, $CO_3^=$, and HCO_3^- are always calculated from the extended Debye-Hückel equations of Truesdell and Jones (1974).

ISPEC Number of species desired in output (if less than total number possible for the given water analysis). Leave ISPEC blank or zero to obtain output for all possible species for the defined system. If ISPEC is greater than zero, ISPEC values of KSPEC (species index numbers) must be read (Type 1 optional input; see below).

IMIN Number of minerals for which saturation data are required (if less than the total possible). Leave IMIN blank (or zero) to obtain saturation data on all possible minerals for the defined system. If IMIN is greater than zero, IMIN values of KMIN (mineral reaction index numbers) must be read (Type 1 optional input; see below).

Total concentration (units of FLAG) of Calcium (1), Magnesium (2), Sodium (3), Potassium (4), Chloride (5), Sulfate (6), Carbon, as HCO_3^-, (7), Silica, as SiO_2, (35) Iron (8), Phosphate, as PO_4^{3-} (45), Strontium (88), and Fluoride (62), where the numbers in parentheses are the appropriate species index numbers in the program. To enter other species, use Type 2 optional input cards (see below).

DESCRIPTION OF OPTIONAL INPUT

Additional input is optional and must appear between cards 4 and 5. Two types of optional input cards are used, Type 1 and Type 2. If used, Type 1 optional input cards must precede Type 2 optional input cards.

Type 1 Optional Input

These cards are used to limit the number of species or minerals in the output. Omit these cards to obtain the complete calculated results for the given water analysis. To specify individual species for which output is desired, read ISPEC values of KSPEC(I),

Variable	Format
(KSPEC(I), I=1, ISPEC)	(16I5)

where KSPEC(I) is the index number of the ith species for which output is desired. Species index numbers are listed in the data tables of Attachment A. To specify individual minerals for which saturation data is desired, read IMIN values of KMIN(I),

Variable	Format
(KMIN(I), I=1, IMIN)	(16I5)

where KMIN(I) is the index number of the ith mineral reaction for which saturation output is desired. Mineral index numbers are listed in the data tables of Attachment A. If values of both KSPEC(I) and KMIN(I) are entered, KSPEC(I) must be read before KMIN(I).

Type 2 Optional Input

Type 2 optional input cards are used to (1) enter the total concentrations of species not included on cards 3 and 4 ("CONC" card(s)); (2) change the convergence tests on mass balance for anion species ("EROR" card); (3) change ΔH_r° ("DELH" card(s)); (4) change log K at 25°C ("TABL" card(s)); or, (5) change existing analytical expressions for logK(T), or enter new analytical expressions for reactions previously defined by the Van't Hoff equation ("LOGK" card(s)). It is possible to use none, 1,2,3, 4, or all 5 cases of type 2 optional input in a single data set, providing the sequencing is 1., "CONC", 2., "EROR", 3., "DELH", 4., "TABL", 5., "LOGK". The form of type 2 optional input cards is

Variable	Format
(WORD,(INT(I),VAL(I), I=1,5))	(A4,1X,5(I3,E12.5))

where WORD is "CONC", "EROR", "DELH", "TABL", or "LOGK". The meaning of INT(I) and VAL(I) is described below for each value of WORD.

"CONC" enters concentration (units of FLAG) of constituents not on card 3 and 4. INT(I) = 17 (H_2S), 18 (CO_3), 39 (NH_4), 51 (Al), 81(Li), 85 (NO_3), 86 (H_2CO_3), 87 (B), 90 (Ba), 98 (Br), and 101 (Mn). VAL (I) is the concentration of the INT(I) constituent.

"EROR" overrides pre-set mass balance convergence constraints on anions. Pre-set values of EROR1-EROR5 are 0.001 (0.1 percent error in mass balance). EROR1-EROR5 are entered on the "EROR" card as VAL (1) - VAL (5). In the order 1=carbon, 2=sulfate, 3=fluoride, 4=phosphate, 5=chloride. Values of INT(I) are not used.

"DELH" overrides values of the standard delta enthalpy of reaction (25 degrees C) used in computing the temperature dependence of equilibrium constants from the Van't Hoff equation. INT(I) is the index number of the ith reaction (see Attachment A) for which DH(I) is to be changed and VAL(I) is the appropriate new value of DH(INT(I)).

"TABL" overrides values of LOGKTO(INT(I)) (log K of reaction at 25 degrees C used in computing the temperature dependence of equilibrium constants from the Van't Hoff equation). INT(I) is the index number of the ith reaction (see Attachment B) for which LOGKTO is to be changed and VAL(I) is the appropriate new value of LOGKTO(I).

"LOGK" overrides existing analytical expressions for log K as a function of T (degree K), or enters as many as 35 new, previously undefined analytical expressions for log K (T degrees K).The form of the analytical expression must be

$$\text{Log KT(INT(I))} = A + BT + C/T + DT^2 + E/T^2,$$

where T is temperature in degree K and A,B,C,D, and E are fit parameters (may be zero or blank). INT(1) is the index number of reaction (see Attachment A) and INT(2)-INT(5) are ignored. VAL(1)=A, VAL(2)=B, VAL(3)=C, VAL(4)=D, VAL(5)=E.

Values of A,B,C,D, and E for analytical expressions pre-set in the program are listed in the data tables of Attachment A. Note that the analytical expression for reaction (26) is further modified in the program (see card B1600 of Attachment B). If any of the cards, "EROR", "DELH", "TABL", "LOGK", are used in a particular water data set, calculations for that data set and all subsequent data sets will use the new input values. The last card in each water analysis data set must be blank, whether option cards are used or not.

OXIDATION-REDUCTION OPTIONS

There are several possible options that result from choosing appropriate values of EHM, EHMC, DOX, EMFZ, and PECALC. To specify Eh directly, the desired value should be read as EHM (in volts). This value of Eh will not be corrected for temperature. If the redox potential with Calomel reference was measured in the field and it is desired to correct that measurement for temperature, the measured value should be read as EHMC (in volts). EHM must then be greater than 9.0. Any value of EHMC less than 9.0 is then considered real and a temperature-corrected Eh (EHM) is computed. If no Eh was measured, EHMC and EHM should be greater than 9.0. If the Eh-Calomel of a standard Zobell's solution was measured in the field, read the value as EMFZ (in volts) and EHMC will be corrected. If EMFZ is greater than 9.0, EHMC will be corrected for temperature only (provided EHMC is less than 9.0).

Oxidation-reduction equations used in calculating the distribution of species are written in terms of pe. pe can be computed from Eh, dissolved oxygen, or $SO_4^=$ / $S^=$. If PECALC = 1, pe is calculated from Eh. If PECALC = 2, pe is computed from dissolved oxygen. If PECALC = 3, pe is computed from dissolved oxygen using the relation of Sato (1960). If PECALC = 4, pe is computed from $SO_4^=$ / $S^=$ (provided $SO_4^=$ and total H_2S are entered). If PECALC = 0, redox relations are ignored. If pe is to be computed from dissolved oxygen, a real value of DOX must be read, and to calculate pe from Eh requires either a real value of EHM or EHMC to be read.

Six possible examples of redox options are tabulated and discussed below:

	EHM	EHMC	EMFZ	DOX	PECALC
1)	< 9	> 9	> 9	blank	1
2)	< 9	> 9	> 9	> 0.0	2
3)	> 9	< 9	> 9	blank	1
4)	> 9	< 9	> 9	> 0.0	2
5)	> 9	< 9	< 9	blank	1
6)	blank or >9	blank or >9	blank or >9	blank	0

1) Eh is to be used without correction and pe is to be computed from Eh.

2) Same as 1) but pe is computed from dissolved oxygen.

3) Eh was measured in the field and it is desired to correct that measurement for temperature. The Eh of standard Zobell's solution was not measured. pe is to be computed from Eh.

4) Same as 3) but pe is to be computed from dissolved oxygen.

5) Eh was measured in the field as well as the Eh of standard Zobell's solution. pe is to be computed from Eh.

6) No information on oxidation-reduction is available, and redox relations are to be ignored. Note: For this case the iron and manganese concentrations are automatically set to zero.

Other possible options should be obvious from these examples.

OUTPUT

The output of WATEQF consists of a table of data constants used in the calculations (printed once). The output for each water analysis lists the title card and tabulates most of the input data. At the end of each iteration through the equilibria equations, the difference between the computed and analytical anion species is tabulated so that convergence progress can be followed. When convergence on the aqueous model has been obtained, various parameters that describe the solution are printed. Some of these are ionic strength, activity of water, comparison of computed and analytical charge balance, pH, pe, temperature, P_{CO_2}, P_{O_2}, total dissolved solids, and others. The concentration of each aqueous species (value greater than zero) is printed as ppm, molality, and activity, and log values, as well as ionic activity coefficients and their logs. Mole ratios and log activity ratios are computed and tabulated. The activity product of 101 minerals and their saturation index, ΔG_r and logK are printed. Saturation output for minerals in which the activity of an ith species in the reaction is zero are omitted from the tabulation. Parts of the output can be deleted with appropriate values of PRT(I), as described above, and by use of the ISPEC and IMIN options.

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Table 1: Revised Thermochemical Data[1/], [2/]

I	NREACT	Source	ΔH^{o}_{T}	LogK 25°C	Analytical Expression for log K($T^{o}K$)[3/]
10	SIDERITE	1	-6.14	-10.57	
12	DOLOMITE	2	-9.436	-17.09	
13	CALCITE	3			-171.9065 - 0.077993T + 2839.319/T + 71.595 log T
18	ANHYDRITE	4	-4.3	-4.384	
19	GYPSUM	5			82.090 - 3853.936/T - 29.8115 log T
22	ARAGONIT	3			-171.9773 - 0.077993T + 2903.293/T + 71.595 log T
25	KMGOH	6			0.684 + 0.0051T
31	KNAHPO	7	0.0	0.29	
33	KKHPO	7	0.0	0.29	
36	KH2CO3	3[4/]			+356.3094 + 0.06091964T - 21834.37/T - 126.8339 log T + 1684915./T^2
63	FLUOR	8		-10.50	
69	KHCO3	3[4/]			+107.8871 + 0.03252849T - 5151.79/T - 38.92561 log T + 563713.9/T^2
74	KMGCO3	9			0.991 + 0.00667T
75	KMGHCO3	10			2.319 -.011056T + 2.29812x$10^{-5}T^2$
78	KCAHCO3	3			1209.120 + 0.31294T - 34765.06/T -478.782 log T
79	KCACO3	3			-1228.732 - 0.299444T + 35512.75/T + 485.818 log T
80	KCAF+	11	4.12	0.94	
138	KCO2	3			108.3865 + 0.01985076T - 6919.53/T - 40.45154 log T + 669365./T^2
143	STRONT	12			155.0305 - 7239.594/T - 56.58638 log T
144	CELEST	13			73.415 - 3603.341/T - 29.8115 log T
145	BARITE	14	6.141	-9.978	
149	KSRHCO3+	12			-3.248 - 0.014867 T
158	KMN 3+	15	25.760	-25.507	
159	KMNCL+	16	0.0	0.607	
160	KMNCL2	16	0.0	0.041	
161	KMNCL3-	16	0.0	-0.305	
162	KMNOH+	16	0.0	3.449	
163	KMN(OH)3	16	0.0	7.782	
164	KMNF+	16	0.0	0.850	
165	KMNSO4	17	3.700	1.708	
166	KMNNO3,2	16	-0.396	0.059	
167	KMNHCO3+	18	0.0	1.716	

Table 1: Revised Thermochemical Data (continued)

I	NREACT	Source	ΔH°_r	LogK 25°C	Analytical Expression for log K($T^{\circ}K$)
168	KMNO4-	16	176.620	-127.824	
169	KMNO4--	16	150.020	-118.440	
170	KSRCO3	12			-1.019 + 0.012826 T
171	KHMNO2--	19	0.0	-34.440	
172	MANGANO	20	-24.025	17.938	
173	PYROLUST	20	-29.180	15.861	
174	BIRNSITE	21	0.0	18.091	
175	NUSTITE	21	0.0	17.504	
176	BIXBYITE	20	-15.245	-0.611	
177	HAUSMITE	20	-80.140	61.540	
178	MNOH2	21	4.100	-12.912	
179	MNOH3	19	20.090	-35.644	
180	MANGANIT	21	0.0	-0.238	
181	RHODOCHR	20	-2.079	-10.539	
182	KSRSO4	22	1.6	2.55	
183	MNCL2	20	-17.622	8.760	
184	MNCL2,1W	16	-7.175	5.522	
185	MNCL2,2W	16	1.710	3.974	
186	MNCL2,4W	16	17.380	2.710	
187	TEPHRITE	20	-40.060	23.122	
188	RHODONIT	20	-21.885	9.522	
189	MNS GRN	19	-5.790	3.800	
190	MNSO4	16	-15.480	2.669	
191	MN2SO4,3	19	-39.060	-5.711	
192	MN3PO4,2	19	2.120	-23.827	
193	MNHPO4	16	0.0	-12.947	

$(T^{\circ}K)$

Data Sources for Table 1

1. Log K of Smith (1918) recalculated using the WATEQF aqueous model at 30°C.
2. Robie, Hemingway and Fisher (1978).
3. Plummer and Busenberg (1982).
4. Log K of Harvie and Weare (1980) adjusted to be consistent with log K gypsum. ΔH_r° from Parker and others (1976).
5. Calculated from the data of Marshall and Slusher (1966) using the aqueous model of WATEQF.
6. McGee and Hostetler (1975).
7. Estimated using the pH and composition of NBS buffers (6.86 and 7.41), and charge balance.
8. E. A. Jenne (1975), oral communication to B. F. Jones.
9. Siebert (1974).
10. Fit to the data of Siebert (1974).
11. Nordstrom and Jenne (1976).
12. Busenberg, Plummer and Parker (in prep.).
13. Calculated from the data of Gallo (1935) for $SrSO_4$ precipitated as given by Linke and Seidell (1965) and consistent with the $SrCO_3^{\circ}$ ion pair of Smith and Martell (1976).
14. Parker, Wagman and Evans (1976).
15. ΔG_f°, ΔH_f° Mn^{++}, Wagman, et al, (1969). ΔG_f°, ΔH_f° Mn^{3+}, Latimer (1952).
16. Wagman, et al, (1969)
17. ΔG_f°, Hem (1963), ΔH_f° Wagman, et al, (1969).
18. Hem (1963).
19. Latimer (1952).
20. Robie and Waldbaum (1968).
21. Garrels and Christ (1965).
22. Smith and Martell (1976)

Footnotes to Table 1

1/ No attempt has been made for internal consistency of thermodynamic data in WATEQF. Responsibility for selection of thermodynamic data rests with the user.

2/ The ion pairs $Na_2CO_3^{\circ}$ and $Na_2SO_4^{\circ}$ are no longer used in WATEQF. The CaF^+, $SrHCO_3^+$, $SrCO_3^{\circ}$ and $SrSO_4^{\circ}$ ion pairs has been added to the model.

3/ Reactions are written as in Attachment C.

4/ Reactions 36 and 63 have been changed from dissociation (in WATEQ) to association in WATEQF. For the most part, all ion pair reactions are written as association in WATEQF, that is, most ion pair equilibria show the pair as a product. All mineral equilibria are written with the solid as reactant. See Attachment C for details of all reactions in WATEQF.

List of data cards for test case

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  SEA WATER TEST CASE  FROM NORDSTROM, ET AL. PAPER IN ACS SYMPOSIUM.
25.0    8.22    0.500  9.9     9.9     1.023 6.6  301000001  0  0
412.3          1291.8         10768.          399.1          19353.          2712.
141.682        4.28           0.002           0.06           8.14            1.39
CONC  98 67.3          87  4.45          90  0.02          85 0.29          39 0.03
CONC  51 0.002         81  0.181         101 0.0002
```

OUTPUT OF TEST CASE

DATA

I	NREACT	DH	LOGKTO	I	NSPEC	Z	DHA	GFW
1	KFE +3	9.7000	-13.0380	1	CA	2	6.0	40.0800
2	KFEH+2	20.1150	-15.2280	2	MG	2	6.5	24.3120
3	KFEOH+	13.2180	-9.5000	3	NA	1	4.0	22.9898
4	KFEOH3	30.3000	-31.0000	4	K	1	3.0	39.1020
5	KFESO4	13.6100	-9.1180	5	CL	-1	3.0	35.4530
6	KFECL	18.1520	-11.6000	6	SO4	-2	4.0	96.0616
7	KFECL2	0.0000	-10.9190	7	HCO3	-1	5.4	61.0173
8	KFECL3	0.0000	-11.9250	8	FE	2	6.0	55.8470
9	KFESO	3.2300	2.2500	9	FE	3	9.0	55.8470
10	SIDERITE	-6.1400	-10.5700	10	FEOH	2	5.0	72.8544
11	MAGNESIT	-6.1690	-8.2400	11	FEOH	1	5.0	72.8549
12	DOLOMITE	-9.4360	-17.0900	12	FE(OH)3	-1	5.0	106.8690
13	CALCITE	-2.2970	-8.4800*	13	FEHPO4	1	5.4	151.8200
14	KH3SIO4	8.9350	-9.9290*	14	H2S AQ	0	0.0	34.0799
15	KH2SIO4	29.7170	-21.6170*	15	FESO4	1	5.0	151.9086
16	KHPO4	-3.5300	12.3460	16	FECL	2	5.0	91.3000
17	KH2PO4	-4.5200	19.5530	17	ANAL H2S	0	0.0	34.0799
18	ANHYDRIT	-4.3000	-4.3840	18	CO3	-2	5.4	60.0094
19	GYPSUM	-0.0280	-4.6020*	19	MGOH	1	6.5	41.3194
20	BRUCITE	0.8500	-11.4100	20	MGF	1	4.5	43.3104
21	CHRYSOTL	27.5850	-51. :00	21	MGCO3 AQ	0	0.0	84.3214
22	ARAGONIT	-2.5890	-8.3360*	22	MGHCO3	1	4.0	85.3293
23	KMGF	4.6740	1.8200	23	MGSO4 AQ	0	0.0	120.3736
24	KCASO4	1.5000	2.3090	24	H4SIO4AQ	0	0.0	96.1155
25	KMGOH	2.0900	2.2100*	25	H3SIO4	-1	4.0	95.1075
26	KH3BO3	3.2190	-9.2350*	26	H2SIO4	-2	5.4	94.0995
27	KNH3	12.4770	-9.2440*	27	OH	-1	3.5	17.0074
28	FORSTRIT	4.8700	-28.1100	28	FECL2	1	5.0	126.7530
29	DIOPSIDE	21.1000	-36.2200	29	CAOH	1	6.0	57.0874
30	CLENSTIT	6.6750	-16.8700	30	CAHCO3	1	6.0	101.0973
31	KNAHPO	0.0000	0.2900	31	CACO3 AQ	0	0.0	100.0890
32	TREMOLIT	90.2150	-140.3000	32	CASO4 AQ	0	0.0	136.1416
33	KKHPO4	0.0000	0.2900	33	FECL3	0	0.0	162.2060
34	KMGHPO4	3.3000	2.8700	34	FESO4	0	0.0	151.9086
35	KCAHPO4	3.3000	2.7390	35	SIO2 TOT	0	0.0	60.0848
36	KH2CO3	-2.1770	6.3520*	36	H3BO3 AQ	0	0.0	61.8331
37	SEPIOLIT	26.5320	-40.1000	37	H2BO3	-1	2.5	60.8251
38	TALC	45.0650	-62.2900	38	NH3 AQ	0	0.0	17.0306
39	HYDMAG	-25.5200	-37.8200	39	NH4	1	2.5	18.0386
40	ADULAR	30.8200	-20.5700	40	MGPO4	-1	5.4	119.2834
41	ALBITE	25.8960	-18.0000	41	MGH2PO4	1	5.4	121.2993
42	ANORTH	17.5300	-19.3300	42	NACO3	-1	5.4	82.9992
43	ANALCM	18.2060	-12.7000	43	NAHCO3	0	0.0	83.9909
44	KMICA	67.8600	-49.0900	44	NASO4	-1	5.4	119.0514
45	PHLOG	0.0000	-63.5300	45	PO4	-3	5.0	94.9714
46	ILLITE	54.6840	-40.3100	46	KSO4	-1	5.4	135.1636
47	KAOLIN	49.1500	-36.9100	47	HPO4	-2	5.0	95.9794
48	HALLOY	44.6800	-32.8200	48	H2PO4	-1	5.4	96.9873
49	BEIDEL	60.3550	-45.2600	49	CAF+	1	5.0	59.0784

50	CHLOR	54.7600	-90.6100	50	NAHPO4	-1	5.4	118.9692
51	ALUNIT	29.8200	-85.3200	51	AL	3	9.0	26.9815
52	GIBCRS	14.4700	-32.7700	52	ALOH	2	5.4	43.9889
53	BOEHM	11.9050	-33.4100	53	AL(OH)2	1	5.4	60.9962
54	PYROPH	0.0000	-42.4300	54	AL(OH)4	-1	4.5	95.0110
55	PHILIP	0.0000	-19.8600	55	ALF	2	5.4	45.9799
56	ERION	0.0000	0.0000	56	ALF2	1	5.4	64.9783
57	CLINOP	0.0000	0.0000	57	ALF3	0	0.0	83.9767
58	MORDEN	0.0000	0.0000	58	ALF4	-1	4.5	102.9751
59	NAHCOL	3.7200	-0.5480	59	ALSO4	1	4.5	123.0431
60	TRONA	-18.0000	-0.7950	60	AL(SO4)2	-1	4.5	219.1047
61	NATRON	15.7450	-1.3110	61	KHPO4	-1	5.4	135.0814
62	THENAT	-2.8020	0.1250	62	F	-1	3.5	18.9984
63	FLUOR	4.7100	-10.9600	63	HSO4	-1	4.5	97.0696
64	MONTCA	58.3730	-45.0000	64	H	1	9.0	1.0080
65	HALITE	0.9180	1.5820	65	FEH2PO4	1	5.4	152.8340
66	THENAR	-0.5720	-0.1790	66	H2S CALC	0	0.0	34.0799
67	MIRABI	18.9870	-1.1130	67	HS	-1	3.5	33.0720
68	MACKIT	0.0000	-4.6310	68	S	-2	5.0	32.0640
69	KHCO3	-3.5610	10.3290*	69	SRHCO3	1	5.4	148.6373
70	KNACO3	8.9110	1.2680	70	PO2	0	0.0	31.9988
71	KNAHCO3	0.0000	-0.2500	71	PCH4	0	0.0	16.0430
72	KNASO4	1.1200	0.7200	72	AH2O	0	0.0	18.0153
73	KKSO4	2.2500	0.8470*	73	MGHPO4	0	0.0	120.2914
74	KMGCO3	2.7100	2.9800*	74	CAHPO4	0	0.0	136.0594
75	KMGHCO3	1.0770	1.0660*	75	CAPO4	-1	5.4	135.0514
76	KMGSO4	4.6000	2.2380	76	CAH2PO4	1	5.4	137.0673
77	KCACH	1.1900	1.4000	77	FE(OH)2	1	5.4	89.8616
78	KCAHCO3	4.1100	1.0950*	78	FE(OH)3	0	0.0	106.8689
79	KCACO3	3.5560	3.2240*	79	FE(OH)4	-1	5.4	123.8762
80	KCAF+	4.1200	0.9400	80	FE(OH)2	0	0.0	89.8616
81	KALOH	1.4300	9.0300	81	LI	1	6.0	6.9390
82	KALOH2	0.0000	18.7000	82	LIOH	0	0.0	23.9464
83	KALOH4	-11.1600	33.0000	83	LISO4	-1	5.0	103.0006
84	KALF	0.0000	7.0100	84	NH4CALC	1	2.5	18.0386
85	KALF2	20.0000	12.7500	85	NO3	-1	3.0	62.0049
86	KALF3	2.5000	17.0200	86	H2CO3	0	0.0	62.0253
87	KALF4	0.0000	19.7200	87	B TOT	0	0.0	10.8100
88	KALSO4	2.1500	3.0200	88	SR	2	5.0	87.6200
89	KASO42	2.8400	4.9200	89	SROH	1	5.0	104.6274
90	KHSO4	4.9100	1.9870*	90	BA	2	5.0	137.3400
91	KH2SC	-65.4400	40.6440	91	BAOH	1	5.0	154.3474
92	KH2S	5.2990	-6.9420*	92	NH4SO4	-1	5.0	114.1002
93	KHS	12.1000	-12.9180	93	HCL	0	0.0	36.4610
94	KOH	34.1570	-20.7800	94	NACL	0	0.0	58.4428
95	KCH4	-57.4350	30.7410	95	KCL	0	0.0	74.5550
96	HYDAPT	17.2250	-59.3500	96	H2SO4	0	0.0	98.0775
97	FLUAPT	19.6950	-66.7900	97	SRCO3	0	0.0	147.6294
98	CHALC	4.6150	-3.5230	98	BR	-1	4.0	79.9090
99	MAGADI	0.0000	-14.3000	99	FEH2PO4	2	5.4	152.8340
100	SILGEL	5.5000	-2.7000	100	FEHPO4	0	0.0	151.8200
101	SILGLAS	4.4400	-3.0170	101	MN	2	6.0	54.9400
102	QUARTZ	6.2200	-4.0050	102	MN	3	9.0	54.9400
103	KFECH2	0.0000	-18.7080	103	MNCL	1	5.0	90.3970
104	KFECH3	0.0000	-28.6380	104	MNCL2	0	0.0	125.8540
105	KFECH4	0.0000	-34.6380	105	MNCL3	-1	5.0	161.3110
106	KFECH2	28.5650	-20.5700	106	MNOH	1	5.0	71.8480
107	VIVIAN	0.0000	-36.0000	107	MN(OH)3	-1	5.0	105.9640
108	MAGNET	-40.6600	-9.5650	108	MNF	1	5.0	73.9400
109	HEMATI	-30.8450	-4.0070	109	MNSO4	0	0.0	151.0060

110	MAGHEM	0.0000	6.3700
111	GOETH	25.5550	-44.1970
112	GREENA	0.0000	-63.1900
113	FECH3A	0.0000	4.8850
114	ANNITE	62.4800	-84.2400
115	PYRITE	11.3000	-18.4800
116	MONTEF	0.0000	-34.9700
117	MONTAB	0.0000	-29.7800
118	HUNTITE	-25.7600	-30.5100
119	GREGITE	0.0000	-17.9700
120	FESPPT	0.0000	-3.9150
121	KFEH2P	0.0000	2.7000
122	KCAPO4	3.1000	6.4590
123	KCAH2P	3.4000	1.4080
124	KMGPO4	3.1000	6.5890
125	KMGH2P	3.4000	1.5130
126	KLIOH	4.8320	0.2000
127	KLISO4	0.0000	0.6400
128	KNH4R	-187.0550	119.0770
129	LAUMON	39.6100	-30.9600
130	KSROH	1.1500	0.8200
131	KBACH	1.7500	0.6400
132	KNH4SO	0.0000	1.1100
133	KHCL	0.0000	-30.0000
134	KNACL	0.0000	-30.0000
135	KKCL	0.0000	-30.0000
136	KH2SO4	0.0000	-30.0000
137	KO2 SATO	0.0000	-11.3850
138	KCO2	-4.7760	-1.4680
139	KFEHPO	0.0000	3.6000
140	KFEHP+	0.0000	-7.6130
141	ALCH3A	12.9900	-31.6100
142	PREHNT	10.3900	-11.5200
143	STRONT	-0.4000	-9.2710*
144	CELEST	0.2280	-6.5780*
145	BARITE	6.1410	-9.9780
146	WITHERIT	6.9500	-8.5850
147	STRENGIT	-2.0300	-26.4000
148	LEON	90.0700	-69.5700
149	KSRHCO3	6.0500	1.1800*
150	NESQUE	-5.7890	-5.2110
151	ARTIN	-1.8420	-18.4000
152	K O2AQ	33.4570	-21.4950
153	KW	13.3410	-13.9920*
154	SEP PT	0.0000	-37.2120
155	DIASP	-15.4050	-35.0600
156	WAIRKT	26.1400	-26.6200
157	KFEHP2	0.0000	-7.5830
158	KMN 3+	25.7600	-25.5070
159	KMNCL+	0.0000	0.6070
160	KMNCL2	0.0000	0.0410
161	KMNCL3-	0.0000	-0.3050
162	KMNOH+	0.0000	3.4490
163	KMN(OH)3	0.0000	7.7820
164	KMNF+	0.0000	0.8500
165	KMNSO4	3.7000	1.7080
166	KMNNO3,2	-0.3960	0.0590
167	KMNHCO3+	0.0000	1.7160
168	KMNO4-	176.6200	-127.8240
169	KMNO4--	150.0200	-118.4400

110	MN(NO3)2	0	0.0	178.9560
111	MNHCO3	1	5.0	115.9590
112	MNO4	-1	3.0	118.9400
113	MNO4	-2	5.0	118.9400
114	SRSO4	0	0.0	183.6800
115	HMNO2	-1	5.0	87.9480

170	KSRCO3	5.2200	2.8100*
171	KHMNO2--	0.0000	-34.4400
172	MANGANO	-24.0250	17.9380
173	PYROLUST	-29.1800	15.8610
174	BIRNSITE	0.0000	18.0910
175	NUSTITE	0.0000	17.5040
176	BIXBYITE	-15.2450	-0.6110
177	HAUSMITE	-80.1400	61.5400
178	MNOH2	4.1000	-12.9120
179	MNOH3	20.0900	-35.6440
180	MANGANIT	0.0000	-0.2380
181	RHODOCHR	-2.0790	-10.5390
182	KSRSO4	1.6000	2.5500
183	MNCL2	-17.6220	8.7600
184	MNCL2,1W	-7.1750	5.5220
185	MNCL2,2W	1.7100	3.9740
186	MNCL2,4W	17.3800	2.7100
187	TEPHRITE	-40.0600	23.1220
188	RHODONIT	-21.8850	9.5220
189	MNS GRN	-5.7900	3.8000
190	MNSO4	-15.4800	2.6690
191	MN2SO4,3	-39.0600	-5.7110
192	MN3PO4,2	2.1200	-23.8270
193	MNHPO4	0.0000	-12.9470

"*" DENOTES THAT AN ANALYTICAL EXPRESSION FOR KT HAS BEEN USED

SUMMARY OF ANALYTICAL EXPRESSIONS OF THE FORM
LOG K = A+B*T+C/T+D*T**2+E/T**2+F*LOG T

I	NREACT	A	B	C	D	E	F
13	CALCITE	-171.9065	-0.077993000	2839.3190	0.0000E-01	0.000000E-01	7.1595000E+01
14	KH3SIO4	6.3680	-0.016346000	-3405.9000	0.0000E-01	0.000000E-01	0.0000000E-01
15	KH2SIO4	39.4780	-0.065927000	-12355.1000	0.0000E-01	0.000000E-01	0.0000000E-01
19	GYPSUM	82.0904	0.000000000	-3853.9360	0.0000E-01	0.000000E-01	-2.9811480E+01
22	ARAGONIT	-171.9773	-0.077993000	2903.2930	0.0000E-01	0.000000E-01	7.1595000E+01
25	KMGOH	0.6840	0.005129500	0.0000	0.0000E-01	0.000000E-01	0.0000000E-01
26	KH3BO3	28.6059	0.012078000	1573.2100	0.0000E-01	0.000000E-01	-1.3225800E+01
27	KNH3	0.6322	-0.001225000	-2835.7600	0.0000E-01	0.000000E-01	0.0000000E-01
36	KH2CO3	356.3094	0.060919640	-21834.3700	0.0000E-01	1.684915E+06	-1.2683390E+02
69	KHCO3	107.8871	0.032528490	-5151.7900	0.0000E-01	5.637139E+05	-3.8925610E+01
73	KKSO4	3.1060	0.000000000	-673.6000	0.0000E-01	0.000000E-01	0.0000000E-01
74	KMGCO3	0.9910	0.006670000	0.0000	0.0000E-01	0.000000E-01	0.0000000E-01
75	KMGHCO3	2.3190	-0.011056000	0.0000	2.2981E-05	0.000000E-01	0.0000000E-01
78	KCAHCO3	1209.1200	0.312940000	-34765.0500	0.0000E-01	0.000000E-01	-4.7878200E+02
79	KCACO3	-1228.7320	-0.299440000	35512.7500	0.0000E-01	0.000000E-01	4.8581800E+02
90	KHSO4	-3.3505	0.018341200	557.2461	0.0000E-01	0.000000E-01	0.0000000E-01
92	KHZS	11.1700	-0.023860000	-3279.0000	0.0000E-01	0.000000E-01	0.0000000E-01
143	STRONT	155.0305	0.000000000	-7239.5940	0.0000E-01	0.000000E-01	-5.6586380E+01
144	CELEST	73.4150	0.000000000	-3603.3410	0.0000E-01	0.000000E-01	-2.7443700E+01
149	KSRHCO3	-3.2480	0.014867000	0.0000	0.0000E-01	0.000000E-01	0.0000000E-01
153	KW	-606.5220	-0.097611000	31286.0000	0.0000E-01	-2.170870E+06	2.1868434E+02
170	KSRCO3	-1.0190	0.012826000	0.0000	0.0000E-01	0.000000E-01	0.0000000E-01

1 SEA WATER TEST CASE FROM NORDSTROM, ET AL. PAPER IN ACS SYMPOSIUM.

INITIAL SOLUTION

TEMPERATURE = 25.00 DEGREES C PH = 8.220
ANALYTICAL EPMCAT = 605.645 ANALYTICAL EPMAN = 605.585

***** OXIDATION - REDUCTION *****

DISSOLVED OXYGEN = 6.600 MG/L
EH MEASURED WITH CALOMEL = 9.9000 VOLTS
MEASURED EH OF ZOBELL SOLUTION = 9.9000 VOLTS
CORRECTED EH = 0.5000 VOLTS
PE COMPUTED FROM CORRECTED EH = 8.452

FLAG	CORALK	PECALC	IDAVES
3	0	1	1

*** TOTAL CONCENTRATIONS OF INPUT SPECIES ***

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL MG/LITRE
CA	2	1.06618E-02	-1.9722	4.21783E+02
MG	2	5.50708E-02	-1.2591	1.32151E+03
NA	1	4.85452E-01	-0.3139	1.10157E+04
K	1	1.05786E-02	-1.9756	4.08279E+02
CL	-1	5.65772E-01	-0.2474	1.97981E+04
SO4	-2	2.92608E-02	-1.5337	2.77438E+03
HCO3	-1	2.40662E-03	-2.6186	1.44941E+02
SIO2 TOT	0	7.38288E-05	-4.1318	4.37844E+00
FE	2	3.71173E-08	-7.4304	2.04600E-03
PO4	-3	6.54794E-07	-6.1839	6.13800E-02
SR	2	9.62870E-05	-4.0164	8.32722E+00
F	-1	7.58306E-05	-4.1202	1.42197E+00
NH4	1	1.72371E-06	-5.7635	3.06900E-02
AL	3	7.68264E-08	-7.1145	2.04600E-03
LI	1	2.70351E-05	-4.5681	1.85163E-01
NO3	-1	4.84751E-06	-5.3145	2.96670E-01
B TOT	0	4.26659E-04	-3.3699	4.55235E+00
BA	2	1.50931E-07	-6.8212	2.04600E-02
BR	-1	8.72903E-04	-3.0590	6.88479E+01
MN	2	3.77301E-09	-8.4233	2.04600E-04

*** CONVERGENCE ITERATIONS ***

ITERATION	S1-ANALCO3	S2-SO4TOT	S3-PTOT	S4-PTOT	S5-CLTOT
1	1.357E-03	9.883E-02	4.799E-05	5.276E-06	1.507E-09
2	3.457E-04	5.120E-03	2.438E-05	4.487E-07	-1.809E-10
3	9.805E-06	-8.828E-05	1.805E-07	-7.034E-10	2.773E-11
4	1.577E-06	1.189E-05	7.886E-08	9.951E-10	-3.830E-12
5	1.064E-07	2.805E-07	4.176E-09	4.410E-11	-7.816E-14

SEA WATER TEST CASE FROM NORDSTROM, ET AL. PAPER IN ACS SYMPOSIUM.

****DESCRIPTION OF SOLUTION ****

	ANAL.	COMP.	PH	ACTIVITY H2O = 0.9805
EPMCAT	605.64	584.79	8.220	PCO2= 3.844557E-04
EPMAN	605.59	584.74		LOG PCO2 = -3.4152
			TEMPERATURE	PO2 = 3.546381E-17
EH = 0.5000	PE = 8.452		25.00 DEG C	PCH4 = 0.000000E-01
PE CALC S =	100.000			CO2 TOT = 2.106494E-03
PE CALC DOX=	12.358		IONIC STRENGTH	DENSITY = 1.0230
PE SATO DOX=	2.248		6.799422E-01	TDS = 35972.8MG/L
TOT ALK =	2.414E+00 MEQ			CARB ALK = 2.346E+00 MEQ
ELECT =	5.359E-02 MEQ			

IN COMPUTING THE DISTRIBUTION OF SPECIES,
PE = 8.452 EQUIVALENT EH = 0.500VOLTS

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	ACTIVITY	LOG ACT	GAMMA
1	CA	2	3.6391E+02	9.4104E-03	2.3458E-03	-2.630	2.4928E-01
2	MG	2	1.1471E+03	4.8904E-02	1.4085E-02	-1.851	2.8802E-01
3	NA	1	1.0616E+04	4.7859E-01	3.3793E-01	-0.471	7.0609E-01
4	K	1	3.9267E+02	1.0408E-02	6.4772E-03	-2.189	6.2231E-01
64	H	1	7.8448E-06	8.0662E-09	6.0256E-09	-8.220	7.4702E-01
5	CL	-1	1.9353E+04	5.6577E-01	3.5209E-01	-0.453	6.2231E-01
6	SO4	-2	1.4332E+03	1.5463E-02	2.7964E-03	-2.553	1.8084E-01
7	HCO3	-1	8.4326E+01	1.4324E-03	9.6616E-04	-3.015	6.7452E-01
18	CO3	-2	2.1032E+00	3.6326E-05	7.5196E-06	-5.124	2.0701E-01
86	H2CO3	0	6.6763E-01	1.1156E-05	1.3089E-05	-4.883	1.1733E+00
27	OH	-1	3.6421E-02	2.2195E-06	1.6580E-06	-5.780	7.4702E-01
62	F	-1	7.1244E-01	3.8867E-05	2.9034E-05	-4.537	7.4702E-01
98	BR	-1	6.7300E+01	8.7290E-04	6.5208E-04	-3.186	7.4702E-01
19	MGOH	1	2.0370E-01	5.1096E-06	3.8170E-06	-5.418	7.4702E-01

23	MGSO4 AQ	0	6.7662E+02	5.8259E-03	6.8132E-03	-2.167	1.1695E+00
22	MGHCO3	1	1.7440E+01	2.1183E-04	1.5824E-04	-3.801	7.4702E-01
21	MGCO3 AQ	0	7.0310E+00	8.6422E-05	1.0107E-04	-3.995	1.1695E+00
20	MGF	1	1.5114E+00	3.6169E-05	2.7019E-05	-4.568	7.4702E-01
29	CAOH	1	7.2038E-03	1.3079E-07	9.7701E-08	-7.010	7.4702E-01
32	CASO4 AQ	0	1.5009E+02	1.1426E-03	1.3363E-03	-2.874	1.1695E+00
30	CAHCO3	1	4.1803E+00	4.2857E-05	2.8908E-05	-4.539	6.7452E-01
31	CACO3 AQ	0	6.2602E+00	6.4826E-05	2.9633E-05	-4.528	4.5712E-01
49	CAF+	1	4.5265E-02	7.9411E-07	5.9321E-07	-6.227	7.4702E-01
44	NASO4	-1	7.6256E+02	6.6387E-03	4.9593E-03	-2.305	7.4702E-01
43	NAHCO3	0	1.2722E+01	1.5699E-04	1.8360E-04	-3.736	1.1695E+00
42	NACO3	-1	5.0491E+00	6.3051E-05	4.7100E-05	-4.327	7.4702E-01
94	NACL	0	5.7367E-27	1.0174E-31	1.1898E-31	-30.925	1.1695E+00
46	KSO4	-1	2.2217E+01	1.7036E-04	1.2727E-04	-3.895	7.4702E-01
95	KCL	0	1.4027E-28	1.9500E-33	2.2805E-33	-32.642	1.1695E+00
63	HSO4	-1	2.0499E-04	2.1888E-09	1.6351E-09	-8.786	7.4702E-01
24	H4SIO4AQ	0	6.6431E+00	7.1635E-05	8.3776E-05	-4.077	1.1695E+00
25	H3SIO4	-1	2.0112E-01	2.1917E-06	1.6373E-06	-5.786	7.4702E-01
26	H2SIO4	-2	1.6236E-04	1.7883E-09	5.5690E-10	-9.254	3.1141E-01
8	FE	2	6.1303E-10	1.1377E-14	3.5429E-15	-14.451	3.1141E-01
9	FE	3	6.8319E-14	1.2679E-18	9.1850E-20	-19.037	7.2442E-02
10	FEOH	2	2.1783E-08	3.0989E-13	9.6502E-14	-13.015	3.1141E-01
11	FEOH	1	1.7155E-11	2.4405E-16	1.8231E-16	-15.739	7.4702E-01
12	FE(OH)3	-1	2.1072E-16	2.0436E-21	1.5266E-21	-20.816	7.4702E-01
77	FE(OH)2	1	6.0351E-04	6.9608E-09	5.1998E-09	-8.284	7.4702E-01
78	FE(OH)3	0	8.7651E-04	8.5007E-09	9.9414E-09	-8.003	1.1695E+00
79	FE(OH)4	-1	2.5883E-03	2.1656E-08	1.6177E-08	-7.791	7.4702E-01
80	FE(OH)2	0	1.8720E-14	2.1591E-19	2.5251E-19	-18.598	1.1695E+00
13	FEHPO4	1	1.5315E-16	1.0456E-21	7.8105E-22	-21.107	7.4702E-01
100	FEHPO4	0	5.6461E-14	3.8545E-19	4.5078E-19	-18.346	1.1695E+00
65	FEH2PO4	1	1.0872E-15	7.3728E-21	5.5076E-21	-20.259	7.4702E-01
99	FEH2PO4	2	3.8461E-17	2.6083E-22	8.1223E-23	-22.090	3.1141E-01
15	FESO4	1	4.1916E-13	2.8598E-18	2.1363E-18	-17.670	7.4702E-01
16	FECL	2	2.5080E-13	2.8471E-18	8.8660E-19	-18.052	3.1141E-01
28	FECL2	1	2.4518E-13	2.0048E-18	1.4976E-18	-17.825	7.4702E-01
33	FECL3	0	6.9599E-15	4.4472E-20	5.2009E-20	-19.284	1.1695E+00
34	FESO4	0	2.2080E-10	1.5065E-15	1.7618E-15	-14.754	1.1695E+00
101	MN	2	1.1764E-04	2.2193E-09	6.9111E-10	-9.160	3.1141E-01
102	MN	3	4.4526E-21	8.3999E-26	6.0851E-27	-26.216	7.2442E-02
106	MNOH	1	2.9902E-07	4.3136E-12	3.2223E-12	-11.492	7.4702E-01
107	MN(OH)3	-1	2.6103E-14	2.5532E-19	1.9073E-19	-18.720	7.4702E-01
111	MNHCO3	1	5.2003E-06	4.6480E-11	3.4722E-11	-10.459	7.47 2E-01
109	MNSO4	0	1.2291E-05	8.4362E-11	9.8660E-11	-10.006	1.1695E+00
110	MN(NO3)2	0	1.5327E-15	8.8768E-21	1.0381E-20	-19.984	1.1695E+00
103	MNCL	1	1.1494E-04	1.3178E-09	9.8446E-10	-9.007	7.4702E-01
104	MNCL2	0	9.7768E-06	8.0515E-11	9.4161E-11	-10.026	1.1695E+00
105	MNCL3	-1	3.1141E-06	2.0008E-11	1.4947E-11	-10.825	7.4702E-01
108	MNF	1	1.3566E-08	1.9016E-13	1.4206E-13	-12.848	7.4702E-01
112	MNO4	-1	1.5361E-24	1.3385E-29	9.9991E-30	-29.000	7.4702E-01
113	MNO4	-2	3.1528E-23	2.7474E-28	8.5555E-29	-28.068	3.1141E-01
115	HMNO2	-1	1.2526E-14	1.4761E-19	1.1027E-19	-18.958	7.4702E-01
51	AL	3	2.7238E-12	1.0463E-16	7.5797E-18	-17.120	7.2442E-02
52	ALOH	2	1.8354E-09	4.3244E-14	1.3466E-14	-13.871	3.1141E-01
53	AL(OH)2	1	8.2277E-06	1.3980E-10	1.0444E-10	9.981	7.4702E-01
54	AL(OH)4	-1	7.0299E-03	7.6686E-08	5.7286E-08	-7.242	7.4702E-01
55	ALF	2	3.2082E-10	7.2316E-15	2.2520E-15	-14.647	3.1141E-01
56	ALF2	1	3.0156E-09	4.8102E-14	3.5933E-14	-13.445	7.4702E-01
57	ALF3	0	1.3460E-09	1.6612E-14	1.9427E-14	-13.712	1.1695E+00
58	ALF4	-1	3.7601E-11	3.7845E-16	2.8271E-16	-15.549	7.4702E-01
59	ALSO4	1	3.5272E-12	2.9711E-17	2.2195E-17	-16.654	7.4702E-01

60	AL(SO4)2	-1	1.3953E-12	6.6003E-18	4.9306E-18	-17.307	7.4702E-01
45	PO4	-3	3.0245E-06	3.3007E-11	2.3911E-12	-11.621	7.2442E-02
47	HPO4	-2	9.5039E-03	1.0263E-07	3.1960E-08	-7.495	3.1141E-01
48	H2PO4	-1	3.8854E-04	4.1521E-09	3.1017E-09	-8.508	7.4702E-01
40	MGPO4	-1	2.0140E-02	1.7500E-07	1.3073E-07	-6.884	7.4702E-01
73	MGHPO4	0	3.3117E-02	2.8534E-07	3.3371E-07	-6.477	1.1695E+00
41	MGH2PO4	1	2.2302E-04	1.9056E-09	1.4235E-09	-8.847	7.4702E-01
75	CAPO4	-1	2.8153E-03	2.1606E-08	1.6140E-08	-7.792	7.4702E-01
74	CAHPO4	0	4.6141E-03	3.5148E-08	4.1105E-08	-7.386	1.1695E+00
76	CAH2PO4	1	3.2958E-05	2.4921E-10	1.8617E-10	-9.730	7.4702E-01
61	KHPO4	-1	7.0421E-05	5.4032E-10	4.0363E-10	-9.394	7.4702E-01
50	NAHPO4	-1	3.2358E-03	2.8190E-08	2.1058E-08	-7.677	7.4702E-01
36	H3BO3 AQ	0	2.2109E+01	3.7059E-04	4.3340E-04	-3.363	1.1695E+00
37	H2BO3	-1	3.2903E+00	5.6067E-05	4.1883E-05	-4.378	7.4702E-01
85	NO3	-1	2.9000E-01	4.8475E-06	3.6212E-06	-5.441	7.4702E-01
38	NH3 AQ	0	1.5606E-03	9.4973E-08	1.1107E-07	-6.954	1.1695E+00
39	NH4	1	2.7361E-02	1.5721E-06	1.1744E-06	-5.930	7.4702E-01
92	NH4SO4	-1	6.2346E-03	5.6633E-08	4.2306E-08	-7.374	7.4702E-01
81	LI	1	1.7882E-01	2.6709E-05	1.9952E-05	-4.700	7.4702E-01
82	LIOH	0	1.0358E-06	4.4833E-11	5.2431E-11	-10.280	1.1695E+00
83	LISO4	-1	3.2400E-02	3.2602E-07	2.4355E-07	-6.613	7.4702E-01
88	SR	2	6.4010E+00	7.5717E-05	2.3579E-05	-4.627	3.1141E-01
69	SRHCO3	1	6.6899E-02	4.6648E-07	3.4847E-07	-6.458	7.4702E-01
97	SRCO3	0	1.3785E-02	9.6782E-08	1.1319E-07	-6.946	1.1695E+00
89	SROH	1	3.4905E-05	3.4577E-10	2.5830E-10	-9.588	7.4702E-01

MOLE RATIOS FROM ANALYTICAL MOLALITY		MOLE RATIOS FROM COMPUTED MOLALITY		LOG ACTIVITY RATIOS	
CL/CA	= 5.3065E+01	CL/CA	= 6.0122E+01	LOG CA/H2	= 13.8103
CL/MG	= 1.0274E+01	CL/MG	= 1.1569E+01	LOG MG/H2	= 14.5888
CL/NA	= 1.1655E+00	CL/NA	= 1.1822E+00	LOG NA/H1	= 7.7488
CL/K	= 5.3483E+01	CL/K	= 5.4358E+01	LOG K/H1	= 6.0314
CL/AL	= 7.3643E+06	CL/AL	= 5.4073E+15	LOG AL/H3	= 7.5397
CL/FE	= 1.5243E+07	CL/FE	= 4.9729E+13	LOG FE/H2	= 1.9894
CL/SO4	= 1.9336E+01	CL/SO4	= 3.6589E+01	LOG CA/MG	= -0.7785
CL/HCO3	= 2.3509E+02	CL/HCO3	= 3.9499E+02	LOG NA/K	= 1.7174
CA/MG	= 1.9360E-01	CA/MG	= 1.9243E-01		
NA/K	= 4.5890E+01	NA/K	= 4.5982E+01		

SEA WATER TEST CASE FROM NORDSTROM, ET AL. PAPER IN ACS SYMPOSIUM.

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
40	ADULAR	2.554E-22	2.692E-21	-21.593	-20.570	9.488E-02	-1.023
41	ALBITE	1.332E-20	1.000E-18	-19.875	-18.000	1.332E-02	-1.875
141	ALCHSA	3.455E-35	2.455E-32	-34.462	-31.610	1.407E-03	-2.852
51	ALUNIT			-93.339	-85.320		-8.019
43	ANALCM	1.499E-16	1.995E-13	-15.824	-12.700	7.513E-04	-3.124
18	ANHYDRIT	6.560E-06	4.130E-05	-5.183	-4.384	1.588E-01	-0.799
114	ANNITE			-99.610	-84.240		-15.370
42	ANORTH	6.324E-26	4.677E-20	-25.199	-19.330	1.352E-06	-5.869

22	ARAGONIT	1.764E-08	4.613E-09	-7.754	-8.336	3.824E+00	0.583
151	ARTIN	1.072E-22	3.981E-19	-21.970	-18.400	2.694E-04	-3.570
145	BARITE	1.314E-10	1.052E-10	-9.881	-9.978	1.249E+00	0.097
53	BOEHM	3.524E-35	3.890E-34	-34.453	-33.410	9.057E-02	1.043
20	BRUCITE	3.872E-14	3.890E-12	-13.412	-11.410	9.953E-03	-2.002
13	CALCITE	1.764E-08	3.313E-09	-7.754	-8.480	5.325E+00	0.726
144	CELEST	6.593E-08	2.641E-07	-7.181	-6.578	2.497E-01	-0.603
98	CHALC	8.714E-05	2.993E-04	-4.060	-3.523	2.905E-01	-0.537
50	CHLOR			-82.129	-90.610		8.481
21	CHRYSOTL			-48.347	-51.800		3.453
30	CLENSTIT	3.441E-18	1.349E-17	-17.463	-16.870	2.551E-01	-0.593
57	CLINOP	1.640E-28	1.000E+00	-27.785	0.000	1.640E-28	-27.785
100	SILGEL	8.714E-05	1.995E-03	-4.060	-2.700	4.367E-02	-1.360
29	DIOPSIDE	1.972E-36	6.026E-37	-35.705	-36.220	3.273E+00	0.515
12	DOLOMITE	1.868E-15	8.128E-18	-14.729	-17.090	2.299E+02	2.361
56	ERION	1.172E-22	1.000E+00	-21.931	0.000	1.172E-22	-21.931
113	FECH3A	3.958E+05	7.674E+04	5.597	4.885	5.158E+00	0.712
97	FLUAPT			-57.487	-66.790		9.303
63	FLUOR	1.978E-12	1.096E-11	-11.704	-10.960	1.804E-01	0.744
28	FORSTRIT	1.359E-31	7.762E-23	-30.867	-28.110	1.751E-03	-2.757
52	GIBCRS	3.455E-35	1.698E-33	-34.462	-32.770	2.034E-02	-1.692
111	GOETH			-36.370	-44.197		7.827
112	GREENA			-86.145	-63.190		-22.955
19	GYPSUM	6.307E-06	2.498E-05	-5.200	-4.602	2.524E-01	-0.598
65	HALITE	1.190E-01	3.819E+01	-0.925	1.582	3.115E-03	-2.507
48	HALLOY			-39.018	-32.820		-6.198
109	HEMATI	1.662E+11	9.840E-05	11.221	-4.007	1.689E+15	15.228
118	HUNTITE	2.096E-29	3.090E-31	-28.679	-30.510	6.782E+01	1.831
39	HYDMAG			-41.346	-37.820		-3.526
96	HYDAPT			-58.731	-59.350		0.619
46	ILLITE			-42.470	-40.310		-2.160
47	KAOLIN			-39.018	-36.910		-2.108
44	KMICA			-52.483	-49.090		-3.393
129	LAUMON	4.439E-34	1.096E-31	-33.353	-30.960	4.048E-03	-2.393
148	LEON			-66.697	-69.570		2.873
99	MAGADI	3.716E-23	5.012E-15	-22.430	-14.300	7.415E-09	-8.130
110	MAGHEM	1.662E+11	2.344E+06	11.221	6.370	7.088E+04	4.851
11	MAGNESIT	1.059E-07	5.754E-09	-6.975	-8.240	1.841E+01	1.265
108	MAGNET	1.457E+00	2.723E-10	0.163	-9.565	5.350E+09	9.728
64	MONTCA			-48.613	-45.000		-3.613
116	MONTBF	5.078E-33	1.072E-35	-32.294	-34.970	4.739E+02	2.676
117	MONTAB	6.322E-28	1.660E-30	-27.199	-29.780	3.809E+02	2.581
58	MORDEN	1.774E-26	1.000E+00	-25.751	0.000	1.774E-26	-25.751
67	MIRABI	2.623E-04	7.709E-02	-3.581	-1.113	3.403E-03	-2.468
59	NAHCOL	3.265E-04	2.831E-01	-3.486	-0.548	1.153E-03	-2.938
61	NATRON	7.053E-07	4.887E-02	-6.152	-1.311	1.443E-05	-4.841
150	NESQUE	9.984E-08	6.152E-06	-7.001	-5.211	1.623E-02	-1.790
55	PHILIP	1.809E-21	1.380E-20	-20.743	-19.860	1.310E-01	-0.883
45	PHLOG			-61.812	-63.530		1.718
142	PREHNT	3.423E-16	3.020E-12	-15.466	-11.520	1.133E-04	-3.946
54	PYROPH			-47.129	-42.430		-4.699
102	QUARTZ	8.714E-05	9.886E-05	-4.060	-4.005	8.815E-01	-0.055
37	SEPIOLIT			-39.016	-40.100		1.084
10	SIDERITE	2.664E-20	2.692E-11	19.574	-10.570	9.898E-10	-9.004
101	SILGLAS	8.714E-05	9.616E-04	-4.060	-3.017	9.062E-02	-1.043
147	STRENGIT	2.112E-31	3.981E-27	-30.675	-26.400	5.304E-05	-4.275
143	STRONT	1.773E-10	5.364E-10	-9.751	-9.271	3.306E-01	-0.481
38	TALC			-56.458	-62.290		5.832
66	THENAR	3.193E-04	6.622E-01	-3.496	-0.179	4.822E-04	-3.317
62	THENAT	8.420E-07	1.334E+00	-6.075	0.125	6.314E-07	-6.200

32	TREMOLIT			-127.868	-140.300		12.432
60	TRONA	2.695E-10	1.603E-01	-9.569	-0.795	1.681E-09	-8.774
107	VIVIAN			-66.663	-36.000		-30.663
146	WITHERIT	3.534E-13	2.600E-09	-12.452	-8.585	1.359E-04	-3.867
154	SEP PT			-39.016	-37.212		-1.804
155	DIASP	3.524E-35	8.710E-36	-34.453	-35.060	4.046E+00	0.607
156	WAIRKT	4.617E-34	2.399E-27	-33.336	-26.620	1.925E-07	-6.716
172	MANGANO	1.866E+07	8.670E+17	7.271	17.938	2.153E-11	-10.667
173	PYROLUST	1.256E+1	7.261E+15	15.099	15.861	1.729E-01	-0.762
174	BIRNSITE	1.256E+15	1.233E+18	15.099	18.091	1.018E-03	-2.992
175	NUSTITE	1.256E+15	3.192E+17	15.099	17.504	3.935E-03	-2.405
176	BIXBYITE	7.293E-04	2.449E-01	-3.137	-0.611	2.978E-03	-2.526
177	HAUSMITE			55.148	61.540		-6.392
178	MNOH2	1.900E-21	1.225E-13	-20.721	-12.912	1.551E-08	-7.809
179	MNOH3			-43.557	-35.644		-7.913
180	MANGANIT	2.674E-02	5.781E-01	-1.573	-0.238	4.626E-02	-1.335
181	RHODOCHR	5.197E-15	2.891E-11	-14.284	-10.539	1.798E-04	-3.745
183	MNCL2	8.567E-11	5.754E+08	-10.067	8.760	1.489E-19	-18.827
184	MNCL2,1W	8.400E-11	3.327E+05	-10.076	5.522	2.525E-16	-15.598
185	MNCL2,2W	8.237E-11	9.419E+03	-10.084	3.974	8.745E-15	-14.058
186	MNCL2,4W	7.919E-11	5.129E+02	-10.101	2.710	1.544E-13	-12.811
187	TEPHRITE	3.035E+10	1.324E+23	10.482	23.122	2.292E-13	-12.640
188	RHODONIT	1.124E-06	3.327E+09	-5.949	9.522	3.379E-16	-15.471
190	MNSO4	1.933E-12	4.667E+02	-11.714	2.669	4.141E-15	-14.383
191	MN2SO4,3			-60.092	-5.711		-54.381
192	MN3PO4,2			-50.724	-23.827		-26.897
193	MNHPO4	2.209E-17	1.130E-13	-16.656	-12.947	1.955E-04	-3.709

SOURCE CODE

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C     **** PROGRAM WATEQF **** A FORTRAN IV VERSION OF WATEQ                A 10
C                                                                           A 20
C     REVISED FROM PL1 VERSION OF TRUESDELL AND JONES.                      A 30
C     NIEL PLUMMER, SUMMER 1972.                                            A 40
C     LATEST REVISION JANUARY, 1984                                         A 50
C                                                                           A 60
C                                                                           A 70
C     **** DESCRIPTION OF INPUT - 5 CARDS ARE REQUIRED ****                 A 80
C     CARD 1   TITLE, JOB DESCRIPTION.  (A80)                               A 90
C     CARD 2     TEMP,PH,EHM,EHMC,EHMZ,DENS,DOX,FLAG,CORALK,PECALC,IGO,     A 100
C                (PRT(I),I=1,4),IDAVES,ISPEC,IMIN                           A 110
C                (5(F6.0,1X),2F5.0,1X,9I1,2I3)                              A 120
C       TEMP....TEMPERATURE IN DEGREES C                                    A 130
C       PH......NEGATIVE LOG ACTIVITY H+                                    A 140
C       EHM.....PREFERRED EH ...SEE OPTIONS                                 A 150
C       EHMC....MEASURED EH ... SEE OPTIONS                                 A 160
C       EMFZ....MEASURED EH OF ZOBELL SOLUTION                              A 170
C       DENS....DENSITY OF SOLUTION   (G/CC)                                A 180
C       DOX.....DISSOLVED OXYGEN (MG/L)                                     A 190
C       FLAG....SIGNAL FOR UNITS OF INPUT CONCENTRATION.                    A 200
C         0 (OR BLANK) = MMOLE/L, 1=MEQ/L, 2=MG/L, 3=PPM, 4=MOLALITY.       A 210
C       CORALK..=0 IF ALKALINITY HAS NOT BEEN CORRECTED FOR BORON ETC.      A 220
C         AND THE ORIGINAL EXPRESSION OF WATEQ IS TO BE USED.  =1 IF        A 230
C         CARBONATE ALKALINITY (CORRECTED FOR NON-CARBONATE ALKALINITY      A 240
C         SPECIES) HAS BEEN INPUT. =2 IF TOTAL INORGANIC CARBON IS          A 250
C         INPUT RATHER THAN ALKALINITY.  =3 IF ALKALINITY HAS NOT BEEN      A 260
C         CORRECTED FRO BORON ETC. - SIMILAR TO CORALK=0, EXCEPT THAT       A 270
C         ALL POSSIBLE NON-CARBONATE ALKALINITY SPECIES ARE CONSIDERED.     A 280
C       PECALC..=0 WILL SET PE TO 100,  =1 COMPUTES PE FROM EH,             A 290
C         =2 COMPUTES PE FROM DOX(THEORETICAL).  = 3 COMPUTES PE FROM       A 300
C         THE SATO RELATION,  = 4 COMPUTES PE FROM S--- - SO4--.            A 310
C       IGO..=0,OR BLANK, IF DESIRED TO HAVE DATA CHECKED FOR INPUT         A 320
C         ERROR. PH MUST BE GREATER THAN 3 AND LESS THAN 11, AND THE        A 330
C         ANALYSIS MUST HAVE LESS THAN 30% ERROR IN CHARGE BALANCE.  =1     A 340
C         IF THIS CHECK IS NOT TO BE MADE.                                  A 350
C       (PRT(I),I=1,4), CAN BE SET TO 1 TO DELETE PRINT OF                  A 360
C          THERMOCHEMICAL DATA,MASS BALANCE CONVERGENCE ITERATIONS,         A 370
C         RATIOS OF IONS, AND MINERAL SATURATION, RESPECTIVELY.  PRT(I)     A 380
C         SHOULD BE SET TO ZERO OR BLANK TO OBTAIN THE RESPECTIVE PRINT.    A 390
C       IDAVES..=1, ACTIVITY COEFFICIENTS OF CHARGED ION PAIRS ARE          A 400
C         CALCULATED FROM THE DAVIES EQUATION.  =0 (OR BLANK), ACTIVITY     A 410
C         COEFFICIENTS OF CHARGED ION PAIRS ARE CALCULATED FROM THE         A 420
C         DEBYE-HUCKEL EQUATION.  IDAVES HAS NO EFFECT ON GAMMA(1)-         A 430
C         GAMMA(7), AND GAMMA(18).                                          A 440
C       ISPEC.. = NUMBER OF SPECIES DESIRED IN OUTPUT(IF LESS THAN TOTAL    A 450
C         POSSIBLE). TO OBTAIN OUTPUT OF MOLALITY, ACTIVITY, ETC. OF        A 460
C         ALL POSSIBLE SPECIES FOR THE DEFINED SYSTEM, LEAVE ISPEC          A 470
C         BLANK (OR ZERO).  IF ISPEC GT. ZERO, ISPEC VALUES OF KSPEC        A 480
C         (SPECIES INDEX NUMBER) MUST BE READ (SEE BELOW).  IF ISPEC =      A 490
C         BLANK (ZERO), OMIT KS.3C CARD(S).                                 A 500
C       IMIN.. = NUMBER OF MINERALS FOR WHICH SATURATION OUTPUT IS          A 510
C         DESIRED (IF LESS THAN TOTAL POSSIBLE).  TO OBTAIN SATURATION      A 520
C         DATA ON ALL POSSIBLE MINERALS FOR THE DEFINED SYSTEM, LEAVE       A 530
C         IMIN BLANK (OR ZERO).  IF IMIN GT. ZERO, IMIN VALUES OF KMIN      A 540
C         (MINERAL INDEX NUMBER) MUST BE READ (SEE BELOW).  IF IMIN =       A 550
C         BLANK (OR ZERO), OMIT KMIN CARDS(S).                              A 560
C     CARD 3     CA MG NA K CL SO4    (6(E12.5),8X)                         A 570
C     CARD 4     HCO3 SIO2 FE PO4 SR F     (6(E12.5),8X)                   A 580
C             ... OPTIONAL CARDS OF TYPE 1 APPEAR HERE ...                  A 590
C             ... OPTIONAL CARDS OF TYPE 2 APPEAR HERE ..                   A 600
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C     CARD 5    BLANK CARD     (DENOTES END OF DATA FOR A PARTICULAR      A 610
C        WATER ANALYSIS.)                                                A 620
C                                                                        A 630
C     ....DESCRIPTION OF OPTIONAL INPUT....                              A 640
C        ALL OPTIONAL INPUT MUST APPEAR BETWEEN CARDS 4 AND 5,           A 650
C        TYPE 1 CARDS MUST PRECEED TYPE 2 CARDS.                         A 660
C                                                                        A 670
C     ****************************                                       A 680
C     TYPE 1 OPTIONAL INPUT CARDS                                        A 690
C     ****************************                                       A 700
C     (KSPEC(I),I=1,ISPEC)  (16I5)  KSPEC(I) IS THE INDEX NUMBER OF THE  A 710
C        ITH SELECTED SPECIES FOR WHICH OUTPUT IS DESIRED.  OMIT CARD    A 720
C        IF ISPEC = BLANK (OR ZERO).                                     A 730
C     (KMIN(I),I=1,IMIN)  (16I5)  KMIN(I) IS THE INDEX NUMBER OF THE     A 740
C        ITH SELECTED MINERAL FOR WHICH SATURATION OUTPUT IS DESIRED.    A 750
C        OMIT CARD IF IMIN = BLANK (OR ZERO).                            A 760
C     NOTE THAT IF BOTH KSPEC AND KMIN ARE READ, KSPEC(I) MUST BE READ   A 770
C     BEFORE KMIN(I).                                                    A 780
C                                                                        A 790
C     ****************************                                       A 800
C     TYPE 2 OPTIONAL INPUT CARDS                                        A 810
C     ****************************                                       A 820
C     WORD,(INT(I),VAL(I),I=1,5)  (A4,1X,5(I3,E12.5))                    A 830
C     WORD = 'CONC', 'EROR', 'DELH', 'TABL', OR'LOGK'.                   A 840
C                                                                        A 850
C       'CONC'..ENTERS CONCENTRATION (UNITS OF FLAG) OF CONSTITUENTS     A 860
C       NOT ON CARDS 3 AND 4.  INT(I) = 17(H2S),18(CO3),39(NH4),51(AL),  A 870
C       81(LI),85(NO3),86(H2CO3),87(B),90(BA),98(BR),AND 101(MN).        A 880
C       VAL(I) IS THE CONCENTRATION OF THE INT(I) CONSTITUENT.           A 890
C                                                                        A 900
C       'EROR'..OVERRIDES PRE-SET MASS BALANCE CONVERGENCE CONSTRAINTS   A 910
C       ON ANIONS.  PER-SET VALUES OF EROR1-ERORS ARE 0.001(0.1% ERROR   A 920
C       IN MASS BALANCE).  EROR1-ERORS ARE ENTERED ON THE 'EROR' CARD    A 930
C       AS VAL(1)-VAL(5), IN THE ORDER 1=CARBON, 2=SULFATE, 3=FLUORIDE,  A 940
C       4=PHOSPHATE, 5=CHLORIDE.  VALUES OF INT(I) ARE NOT USED.         A 950
C                                                                        A 960
C       'DELH'..OVERRIDES VALUES OF THE STANDARD DELTA ENTHALPY OF       A 970
C       REACTION (25 DEG. C) USED IN COMPUTING THE TEMPERATURE           A 980
C       DEPENDENCE OF EQUILIBRIUM CONSTANTS FROM THE VANT HOFF EQUATION. A 990
C       INT(I) IS THE INDEX NUMBER OF THE ITH REACTION FOR WHICH DH(I)   A1000
C       IS TO BE CHANGED AND VAL(I) IS THE APPPRIATE NEW VALUE OF        A1010
C       DH(INT(I)).                                                      A1020
C                                                                        A1030
C       'TABL'..OVERRIDES VALUES OF LOGKTO(INT(I)) (LOG K OF REACTION AT A1040
C       25 DEG. C USED IN COMPUTING THE TEMPERATURE DEPENDENCE OF        A1050
C       EQUILIBRIUM CONSTANTS FROM THE VANT HOFF EQUATION).  INT(I) IS   A1060
C       THE INDEX NUMBER OF THE ITH REACTION FOR WHICH LOGKTO IS TO BE   A1070
C       CHANGED AND VAL(I) IS THE APPROPRIATE NEW VALUE OF LOGKTO(I).    A1080
C                                                                        A1090
C       'LOGK'..OVERRIDES EXISTING ANALYTICAL EXPRESSIONS FOR LOG K AS A A1100
C       FUNCTION OF T(DEG.K), OR ENTERS NEW, PREVIOUSLY UNDEFINED        A1110
C       ANALYTICAL EXPRESSIONS FOR LOG K(T DEG.K).  SIX VALUES ARE       A1120
C       READ, INSTEAD OF THE NORMAL FIVE.  THE FORM OF THE               A1130
C       ANALYTICAL EXPRESSION MUST BE                                    A1140
C            LOG KT(INT(I))=A+B*T+C/T+D*T**2+E/T**2+F*LOG(T)             A1150
C       WHERE T IS TEMPERATURE IN DEG. K, AND A,B,C,D,E AND F ARE FIT    A1160
C       PARAMETERS (MAY BE ZERO OR BLANK).  INT(1) IS THE INDEX NUMBER   A1170
C       OF REACTION AND INT(2)-INT(5) ARE IGNORED.  VAL(1)=A,VAL(2)=B,   A1180
C       VAL(3)=C,VAL(4)=D,VAL(5)=E,VAL(6)=F.                             A1190
C                                                                        A1200
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C                                                                       A1210
C     IF ANY OF THE CARDS, 'EROR','DELH','TABL','LOGK', ARE USED IN A   A1220
C     PARTICULAR WATER DATA SET, CALCULATIONS FOR THAT DATA SET AND ALL  A1230
C     SUBSEQUENT DATA SETS WILL USE THE NEW INPUT VALUES.  DELH AND TABL A1240
C     CARDS CAN BE USED TO OVERRIDE PRE-EXISTING ANALYTICAL EXPRESSIONS. A1250
C     THE ORDER OF TYPE 2 OPTIONAL INPUT CARDS IS 'CONC','EROR','DELH',  A1260
C     'TABL',AND 'LOGK', IF ALL 5 ARE USED.  THE LAST CARD IN EACH WATER A1270
C     ANALYSIS DATA SET MUST BE BLANK.                                   A1280
C                                                                       A1290
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                               A1300
      INTEGER D,E,DD,RBIT,CORALK,Z(120),PRT(4)                          A1310
      INTEGER PECALC,PECK                                               A1320
      DOUBLE PRECISION MI(120),KT(200),LOGKT(200),LOGKTO(200),MTOT,LH2O A1330
     1,MU,NATOT,KTOT,MGTOT,LITOT,NH4TOT,KW                              A1340
      CHARACTER *8 NSPEC(120),NREACT(200)                               A1350
      CHARACTER *80 TITL                                                A1360
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDO,P A1370
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA A1380
     2LFA(120),Z,CUNITS(120),ANALMI(120),GFW(120),DHA(120),NSPEC,NREACT, A1390
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DCK,XLMI( A1400
     4120),ITER,RBIT,CLSAVE,CORALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT A1410
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT A1420
     6,SRTOT,BATOT,CLTOT,MTOT,ICK,PRT,TITL,EPMCAT,EPMAN,NEQU,ISPEC,     A1430
     7KSPEC(120),IMIN,KMIN(200),TDS,IDAVES,IPRT,JJ,JK                   A1440
      JJ=0                                                              A1450
      JK=0                                                              A1460
      D=115                                                             A1470
      E=193                                                             A1480
      IPRT=0                                                            A1490
      NEQU=22                                                           A1500
      OPEN (UNIT=9,FILE='WATEQF.DATA',STATUS='OLD')                     A1510
      DO 11 I=1,D                                                       A1520
   11 READ (9,*) NSPEC(I),Z(I),GFW(I),DHA(I)                            A1530
      DO 12 I=1,E                                                       A1540
   12 READ (9,*) NREACT(I),DH(I),LOGKTO(I)                              A1550
   10 CONTINUE                                                          A1560
      READ (5,70,END=40) TITL                                           A1570
      ICK=0                                                             A1580
      CALL PREP                                                         A1590
      IF (ICK.EQ.1) GO TO 10                                            A1600
      CALL SET                                                          A1610
   20 CONTINUE                                                          A1620
      CALL MODEL                                                        A1630
      IF (ITER.EQ.25) GO TO 30                                          A1640
      IF (RBIT.EQ.1) GO TO 20                                           A1650
      IF (ITER.LT.2) GO TO 20                                           A1660
      CALL PRINT                                                        A1670
      IF (PRT(4).NE.0.AND.PRT(4).NE.9) GO TO 10                         A1680
      CALL SAT                                                          A1690
      GO TO 10                                                          A1700
   30 WRITE (6,80)                                                      A1710
      GO TO 10                                                          A1720
   40 CLOSE (UNIT=9)                                                    A1730
      ENDFILE (UNIT=6)                                                  A1740
      STOP                                                              A1750
C                                                                       A1760
C                                                                       A1770
   50 FORMAT (5X,A8,2X,I2,3X,F10.4,1X,F4.1)                             A1780
   60 FORMAT (5X,A8,2X,2F10.4)                                          A1790
   70 FORMAT (A80)                                                      A1800
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80 FORMAT (4X,'CONVERGENCE DID NOT OCCUR WITHIN 25  ITERATIONS,'/4X      A1810
  1,'CALCULATION TERMINATED',///)                                        A1820
   END                                                                   A1830
   SUBROUTINE PREP                                                       B  10
   IMPLICIT DOUBLE PRECISION (A-H,O-Z)                                   B  20
   INTEGER D,E,DD,RBIT,CORALK,Z(120),FLAG,PRT(4),SIGN(2),PECALC,PECK     B  30
   DIMENSION INT(6), VAL(6), INPT(22), GRAMS(120), IEQU(50), COEF(6,2    B  40
  100), V(120), IDH(50), INTT(50)                                        B  50
   DOUBLE PRECISION MI(120),XT(200),LOGXT(200),LOGXTO(200),MNTOT,LH2O    B  60
  1,MU,NATOT,KTOT,MGTOT,LITOT,NH4TOT,KW                                  B  70
   CHARACTER *8 NSPEC(120),NREACT(200),WORD,CARD(6)                      B  80
   CHARACTER *80 TITL                                                    B  90
   COMMON MI,XT,LOGXT,LOGXTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDO,P    B 100
  1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA    B 110
  2LFA(120),Z,CUNITS(120),ANALMI(120),GFW(120),DHA(120),NSPEC,NREACT,    B 120
  3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XLMI(    B 130
  4120),ITER,RBIT,CISAVE,CORALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT    B 140
  5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT    B 150
  6,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL,EPMCAT,EPMAN,NEQU,ISPEC,        B 160
  7KSPEC(120),KMIN,KMIN(200),TDS,IDAVES,IPRT,JJ,JK                      B 170
   DATA CARD/'CONC','EROR','DELH','TABL','LOGK','    '/,SIGN/' ','*'/    B 180
   DATA IEQU/13,14,15,19,22,25,26,27,36,69,73,74,75,78,79,90,92,143      B 190
  1,144,149,153,170,28*0/                                                B 200
   DATA COEF/72*0.0,-171.9065,-0.077993,2839.319,2*0.0,71.595,6.368      B 210
  1,-0.016346,-3405.9,2*0.0,39.478,-0.065927,-12355.1,21*0.0,            B 220
  882.0904,0.0,-3853.936,2*0.0,-29.81148,12*0.0,                         B 230
  2-171.9773,-.077993,2903.293,2*.0,71.595,12*.0,.684,.0051295,4*.0,     B 240
  328.6059,0.012078,1573.21,2*0.0,-13.2258,0.6322,-0.001225,-2835.76,    B 250
  451*0.0,356.3094,0.06091964,-21834.37,0.0,1684915.0,-126.8339,         B 260
  5192*0.0,107.8871,0.03252849,-5151.79,0.0,563713.9,-38.92561,          B 270
  618*0.0,3.106,0.0,-673.6,3*0.0,0.991,0.00667,4*0.0,2.319,-0.011056,    B 280
  70.0,0.000022981,14*0.0,1209.12,.31294,-34765.05,2*0.0,-478.782,       B 290
  %-1228.732,-0.29944,35512.75,2*0.0,485.818,60*0.0,-5.3505,0.0183412    B 300
  9,557.2461,9*0.0,11.17,-0.02386,-3279.0,303*0.0,155.0305,0.0           B 310
  0,-7239.594,2*0.0,-56.58638,73.415,0.0,-3603.341,2*0.0,-27.4437        B 320
  $,24*0.0,-3.248,0.014867,22*0.0,-606.522,-0.097611,31286.0,0.0,        B 330
  &-2170870.0,218.68434,96*0.0,-1.019,0.012826,184*0.0/                  B 340
   DATA INPT/1,2,3,4,5,6,7,35,8,45,88,62,17,18,39,51,81,85,87,90,98,1    B 350
  101/                                                                   B 360
   C=2.302585092                                                         B 370
   F=23.0603                                                             B 380
   R=1.98719E-03                                                         B 390
   EROR1=.001                                                            B 400
   EROR2=.001                                                            B 410
   EROR3=.001                                                            B 420
   EROR4=.001                                                            B 430
   EROR5=.001                                                            B 440
   ICK=0                                                                 B 450
   PEDO=100.0                                                            B 460
   PESATO=100.                                                           B 470
   PES=100.0                                                             B 480
   DO 10 I=1,D                                                           B 490
   CUNITS(I)=0.0                                                         B 500
   ALFA(I)=0.0                                                           B 510
   MI(I)=0.0                                                             B 520
   XLMI(I)=0.0                                                           B 530
   IF (Z(I).EQ.0) V(I)=1.0                                               B 540
   IF (Z(I).EQ.0) GO TO 10                                               B 550
   IF (Z(I).LT.0) V(I)=-1.0*Z(I)                                         B 560
   IF (Z(I).GT.0) V(I)=1.0*Z(I)                                          B 570
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 10 CONTINUE                                                            B 580
    PECK=0                                                              B 590
    WRITE (6,620)                                                       B 600
    READ (5,630) TEMP,PH,EHM,EHMC,EMFZ,DENS,DOX,FLAG,CORALK,PECALC,IGO  B 610
   1,(PRT(I),I=1,4),IDAVES,ISPEC,IMIN                                   B 620
    IFLAG=FLAG                                                          B 630
    IF (IPRT.EQ.1) PRT(1)=1                                             B 640
    IF (PRT(1).NE.0) GO TO 70                                           B 650
    WRITE (6,640)                                                       B 660
    DO 30 I=1,D                                                         B 670
    ISIG=SIGN(1)                                                        B 680
    DO 20 J=1,NEQU                                                      B 690
    IF (I.EQ.IEQU(J)) ISIG=SIGN(2)                                      B 700
 20 CONTINUE                                                            B 710
    WRITE (6,650) I,NREACT(I),DH(I),LOGKTO(I),ISIG,I,NSPEC(I),Z(I),     B 720
   1DHA(I),GFW(I)                                                       B 730
 30 CONTINUE                                                            B 740
    DD=D+1                                                              B 750
    DO 50 I=DD,E                                                        B 760
    ISIG=SIGN(1)                                                        B 770
    DO 40 J=1,NEQU                                                      B 780
    IF (I.EQ.IEQU(J)) ISIG=SIGN(2)                                      B 790
 40 CONTINUE                                                            B 800
    WRITE (6,660) I,NREACT(I),DH(I),LOGKTO(I),ISIG                      B 810
 50 CONTINUE                                                            B 820
    WRITE (6,570)                                                       B 830
    DO 60 I=1,NEQU                                                      B 840
    WRITE (6,580)IEQU(I),NREACT(IEQU(I)),COEF(1,IEQU(I)),COEF(2,IEQU(I  B 850
   1)),COEF(3,IEQU(I)),COEF(4,IEQU(I)),COEF(5,IEQU(I)),COEF(6,IEQU(I))  B 860
 60 CONTINUE                                                            B 870
 70 CONTINUE                                                            B 880
    IPRT=1                                                              B 890
    WRITE (6,670) TITL                                                  B 900
    READ (5,680) (CUNITS(INPT(I)),I=1,6)                                B 910
    READ (5,680) (CUNITS(INPT(I)),I=7,12)                               B 920
    IF (ISPEC.GT.0) READ (5,590) (KSPEC(I),I=1,ISPEC)                   B 930
    IF (IMIN.GT.0) READ (5,590) (KMIN(I),I=1,IMIN)                      B 940
 80 CALL READ (WORD,INT,VAL)                                            B 950
    IF (WORD.NE.CARD(1)) GO TO 100                                      B 960
    DO 90 I=1,5                                                         B 970
    IF (INT(I).EQ.0) GO TO 90                                           B 980
    CUNITS(INT(I))=VAL(I)                                               B 990
 90 CONTINUE                                                            B1000
    GO TO 80                                                            B1010
100 CONTINUE                                                            B1020
    IF (WORD.NE.CARD(2)) GO TO 110                                      B1030
    EROR1=VAL(1)                                                        B1040
    EROR2=VAL(2)                                                        B1050
    EROR3=VAL(3)                                                        B1060
    EROR4=VAL(4)                                                        B1070
    EROR5=VAL(5)                                                        B1080
    CALL READ (WORD,INT,VAL)                                            B1090
    GO TO 100                                                           B1100
110 IF (WORD.NE.CARD(3)) GO TO 130                                      B1110
    DO 120 I=1,5                                                        B1120
    IF (INT(I).EQ.0) GO TO 120                                          B1130
    DH(INT(I))=VAL(I)                                                   B1140
    JJ=JJ+1                                                             B1150
    IDH(JJ)=INT(I)                                                      B1160
    WRITE (6,700) INT(I),NREACT(INT(I)),VAL(I)                          B1170
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  120 CONTINUE                                                          B1180
      CALL READ (WORD,INT,VAL)                                          B1190
      GO TO 110                                                         B1200
  130 IF (WORD.NE.CARD(4)) GO TO 150                                    B1210
      DO 140 I=1,5                                                      B1220
      IF (INT(I).EQ.0) GO TO 140                                        B1230
      LOGKTO(INT(I))=VAL(I)                                             B1240
      JK=JK+1                                                           B1250
      IKTT(JK)=INT(I)                                                   B1260
      WRITE (6,710) INT(I),NREACT(INT(I)),VAL(I)                        B1270
  140 CONTINUE                                                          B1280
      CALL READ (WORD,INT,VAL)                                          B1290
      GO TO 130                                                         B1300
  150 CONTINUE                                                          B1310
C                                                                       B1320
C                                                                       B1330
C     VANT HOFF EQUATION FOR EFFECT OF T ON K                           B1340
C                                                                       B1350
      T=TEMP+273.15                                                     B1360
      C1=(298.15-T)/(298.15*T*C*R)                                      B1370
      DO 170 I=1,E                                                      B1380
      LOGKT(I)=LOGKTO(I)-DH(I)*C1                                       B1390
      LCHEK(I)=0                                                        B1400
      IF (LOGKT(I).LT.-38.0.OR.LOGKT(I).GT.38.0) LCHEK(I)=1             B1410
      IF (LCHEK(I).EQ.1) GO TO 160                                      B1420
      KT(I)=10.**LOGKT(I)                                               B1430
  160 CONTINUE                                                          B1440
  170 CONTINUE                                                          B1450
      KW=KT(153)                                                        B1460
C                                                                       B1470
C                                                                       B1480
C     ANALYTICAL EXPRESSIONS FOR EFFECT OF T ON K                       B1490
  180 IF (WORD.NE.CARD(5)) GO TO 220                                    B1500
      IF (INT(1).EQ.0) GO TO 210                                        B1510
      DO 190 I=1,6                                                      B1520
      COEF(I,INT(1))=VAL(I)                                             B1530
  190 CONTINUE                                                          B1540
      IEQ=0                                                             B1550
      DO 200 I=1,NEQU                                                   B1560
      IF (IEQU(I).EQ.INT(1)) IEQ=1                                      B1570
  200 CONTINUE                                                          B1580
      IF (IEQ.EQ.0) NEQU=NEQU+1                                         B1590
      IF (IEQ.EQ.0) IEQU(NEQU)=INT(1)                                   B1600
      WRITE (6,720) INT(1),NREACT(INT(1)),COEF(1,INT(1)),COEF(2,INT(1)) B1610
     1,COEF(3,INT(1)),COEF(4,INT(1)),COEF(5,INT(1)),COEF(6,INT(1))      B1620
  210 CONTINUE                                                          B1630
      CALL READ (WORD,INT,VAL)                                          B1640
      GO TO 180                                                         B1650
  220 CONTINUE                                                          B1660
      IF (WORD.EQ.CARD(6)) GO TO 230                                    B1670
      WRITE (6,600)                                                     B1680
      CALL READ (WORD,INT,VAL)                                          B1690
      GO TO 220                                                         B1700
  230 CONTINUE                                                          B1710
      DO 280 I=1,NEQU                                                   B1720
      IF (JJ.EQ.0) GO TO 250                                            B1730
      DO 240 I1=1,JJ                                                    B1740
      IF (IEQU(I).EQ.IDH(I1)) GO TO 280                                 B1750
  240 CONTINUE                                                          B1760
  250 IF (JK.EQ.0) GO TO 270                                            B1770
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      DO 260 I1=1,JK                                                    B1780
      IF (IEQU(I).EQ.IKTT(I1)) GO TO 280                                B1790
  260 CONTINUE                                                          B1800
  270 CONTINUE                                                          B1810
      LOGKT(IEQU(I))=COEF(1,IEQU(I))+COEF(2,IEQU(I))*T+COEF(3,IEQU(I))/T B1820
     1+COEF(4,IEQU(I))*T*T+COEF(5,IEQU(I))/(T*T)+COEF(6,IEQU(I))        B1830
     2*DLOG10(T)                                                        B1840
      IF (IEQU(I).EQ.26) LOGKT(26)=LOGKT(26)+DLOG10(KW)                 B1850
      KT(IEQU(I))=1E1**(LOGKT(IEQU(I)))                                 B1860
  280 CONTINUE                                                          B1870
      KW=KT(153)                                                        B1880
C                                                                       B1890
C                                                                       B1900
C     CALCULATION OF ANALYZED MOLALITY                                  B1910
      IF (FLAG.NE.0) GO TO 300                                          B1920
      DO 290 I=1,22                                                     B1930
      CUNITS(INPT(I))=CUNITS(INPT(I))*GFW(INPT(I))                      B1940
  290 CONTINUE                                                          B1950
      FLAG=2                                                            B1960
      GO TO 320                                                         B1970
  300 CONTINUE                                                          B1980
      IF (FLAG.NE.1) GO TO 320                                          B1990
      DO 310 I=1,22                                                     B2000
      CUNITS(INPT(I))=CUNITS(INPT(I))*GFW(INPT(I))/V(INPT(I))           B2010
  310 CONTINUE                                                          B2020
      FLAG=2                                                            B2030
  320 CONTINUE                                                          B2040
      IF (FLAG.NE.2) GO TO 340                                          B2050
      DO 330 I=1,22                                                     B2060
      CUNITS(INPT(I))=CUNITS(INPT(I))/DENS                              B2070
  330 CONTINUE                                                          B2080
      FLAG=3                                                            B2090
  340 CONTINUE                                                          B2100
      IF (FLAG.NE.3) GO TO 370                                          B2110
      C1=0.0                                                            B2120
      DO 350 I=1,22                                                     B2130
      C1=C1+CUNITS(INPT(I))                                             B2140
  350 CONTINUE                                                          B2150
      C1SAVE=C1                                                         B2160
      C1=1.0/(1.0-1.0E-06*C1SAVE)                                       B2170
      DO 360 I=1,22                                                     B2180
      MI(INPT(I))=(CUNITS(INPT(I))/(1.0E+03*GFW(INPT(I))))*C1           B2190
      IF (MI(INPT(I)).GT.0.0) XLMI(INPT(I))=DLOG10(MI(INPT(I)))         B2200
      GRAMS(INPT(I))=CUNITS(INPT(I))*DENS                               B2210
  360 CONTINUE                                                          B2220
      C1=1.0/C1                                                         B2230
      GO TO 410                                                         B2240
  370 CONTINUE                                                          B2250
      C1=0.0                                                            B2260
      IF (FLAG.NE.4) GO TO 530                                          B2270
      DO 390 J=1,3                                                      B2280
      C2=0.0                                                            B2290
      C1=1.0-C1*1.0E-06                                                 B2300
      DO 380 I=1,22                                                     B2310
      MI(INPT(I))=CUNITS(INPT(I))                                       B2320
      C2=C2+MI(INPT(I))*GFW(INPT(I))*1000.*C1                           B2330
  380 CONTINUE                                                          B2340
      C1=C2                                                             B2350
  390 CONTINUE                                                          B2360
      C1SAVE=C1                                                         B2370
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      C1=(1.0-C1SAVE*1.0E-06)                                              B2380
      DO 400 I=1,22                                                        B2390
      GRAMS(INPT(I))=MI(INPT(I))*1000.*GFW(INPT(I))*C1                     B2400
      IF (MI(INPT(I)).GT.0.0) XLMI(INPT(I))=DLOG10(MI(INPT(I)))            B2410
  400 CONTINUE                                                             B2420
  410 CONTINUE                                                             B2430
      TDS=0.0                                                              B2440
      DO 420 I=1,22                                                        B2450
      ANALMI(INPT(I))=MI(INPT(I))                                          B2460
      TDS=TDS+GRAMS(INPT(I))                                               B2470
  420 CONTINUE                                                             B2480
      EPMCAT=0.0                                                           B2490
      EPMAN=0.0                                                            B2500
C                                                                          B2510
C                                                                          B2520
C     CALCULATION OF CATION-ANION BALANCE                                  B2530
      DO 430 I=1,22                                                        B2540
      IF (Z(INPT(I)).GT.0) GO TO 425                                       B2550
      EPMAN=EPMAN-Z(INPT(I))*MI(INPT(I))*C1                                B2560
      GO TO 430                                                            B2570
  425 EPMCAT=EPMCAT+Z(INPT(I))*MI(INPT(I))*C1                              B2580
  430 CONTINUE                                                             B2590
      EPMCAT=EPMCAT*1000.                                                  B2600
      EPMAN=EPMAN*1000.                                                    B2610
C                                                                          B2620
C                                                                          B2630
C     CALCULATION OF EH FROM FIELD DATA                                    B2640
      IF (EHM.LT.9.0) GO TO 470                                            B2650
      IF (EMFZ.GT.9.0) GO TO 440                                           B2660
      C1=0.429+2.4E-03*(25.0-TEMP)-EMFZ                                    B2670
      GO TO 450                                                            B2680
  440 C1=0.244+8.6E-04*(25.0-TEMP)                                         B2690
  450 CONTINUE                                                             B2700
      IF (EHMC.LT.9.0) GO TO 460                                           B2710
      GO TO 470                                                            B2720
  460 EHM=EHMC+C1                                                          B2730
  470 CONTINUE                                                             B2740
      PEEH=EHM/(C*R*T/F)                                                   B2750
      IF (PECALC.NE.0) GO TO 475                                           B2760
      PE=100.                                                              B2770
      MI(8)=0.0                                                            B2780
      MI(101)=0.0                                                          B2790
      WRITE (6,560)                                                        B2800
  475 IF (EHM.GE.9.0) PEEH=100.                                            B2810
      WRITE (6,620)                                                        B2820
      WRITE (6,730)                                                        B2830
      WRITE (6,740) TEMP,PH,EPMCAT,EPMAN                                   B2840
      WRITE (6,750) DOX,EHMC,EMFZ,IFLAG,CORALK,PECALC,IDAVES,EHM,PEEH      B2850
      IF (PECALC.EQ.1) PE=PEEH                                             B2860
      WRITE (6,620)                                                        B2870
      WRITE (6,760)                                                        B2880
      DO 480 I=1,22                                                        B2890
      IF (MI(INPT(I)).LE.0.0) GO TO 480                                    B2900
      WRITE (6,790) NSPEC(INPT(I)),Z(INPT(I)),MI(INPT(I)),XLMI(INPT(I))    B2910
     1,GRAMS(INPT(I))                                                      B2920
  480 CONTINUE                                                             B2930
      WRITE (6,620)                                                        B2940
      WRITE (6,620)                                                        B2950
      IF (PRT(2).NE.0) GO TO 490                                           B2960
      WRITE (6,620)                                                        B2970
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      C1=(1.0-C1SAVE*1.0E-06)                                          B2380
      DO 400 I=1,22                                                    B2390
      GRAMS(INPT(I))=MI(INPT(I))*1000.*GFW(INPT(I))*C1                 B2400
      IF (MI(INPT(I)).GT.0.0) XLMI(INPT(I))=DLOG10(MI(INPT(I)))        B2410
  400 CONTINUE                                                         B2420
  410 CONTINUE                                                         B2430
      TDS=0.0                                                          B2440
      DO 420 I=1,22                                                    B2450
      ANALMI(INPT(I))=MI(INPT(I))                                      B2460
      TDS=TDS+GRAMS(INPT(I))                                           B2470
  420 CONTINUE                                                         B2480
      EPMCAT=0.0                                                       B2490
      EPMAN=0.0                                                        B2500
C                                                                      B2510
C                                                                      B2520
C     CALCULATION OF CATION-ANION BALANCE                              B2530
      DO 430 I=1,22                                                    B2540
      IF (Z(INPT(I)).GT.0) GO TO 425                                   B2550
      EPMAN=EPMAN-Z(INPT(I))*MI(INPT(I))*C1                            B2560
      GO TO 430                                                        B2570
  425 EPMCAT=EPMCAT+Z(INPT(I))*MI(INPT(I))*C1                          B2580
  430 CONTINUE                                                         B2590
      EPMCAT=EPMCAT*1000.                                              B2600
      EPMAN=EPMAN*1000.                                                B2610
C                                                                      B2620
C                                                                      B2630
C     CALCULATION OF EH FROM FIELD DATA                                B2640
      IF (EHM.LT.9.0) GO TO 470                                        B2650
      IF (EMFZ.GT.9.0) GO TO 440                                       B2660
      C1=0.429+2.4E-03*(25.0-TEMP)-EMFZ                                B2670
      GO TO 450                                                        B2680
  440 C1=0.244+8.6E-04*(25.0-TEMP)                                     B2690
  450 CONTINUE                                                         B2700
      IF (EHMC.LT.9.0) GO TO 460                                       B2710
      GO TO 470                                                        B2720
  460 EHM=EHMC+C1                                                      B2730
  470 CONTINUE                                                         B2740
      PEEH=EHM/(C*R*T/F)                                               B2750
      IF (PECALC.NE.0) GO TO 475                                       B2760
      PE=100.                                                          B2770
      MI(8)=0.0                                                        B2780
      MI(101)=0.0                                                      B2790
      WRITE (6,560)                                                    B2800
  475 IF (EHM.GE.9.0) PEEH=100.                                        B2810
      WRITE (6,620)                                                    B2820
      WRITE (6,730)                                                    B2830
      WRITE (6,740) TEMP,PH,EPMCAT,EPMAN                               B2840
      WRITE (6,750) DOX,EHMC,EMFZ,IFLAG,CORALK,PECALC,IDAVES,EHM,PEEH  B2850
      IF (PECALC.EQ.1) PE=PEEH                                         B2860
      WRITE (6,620)                                                    B2870
      WRITE (6,760)                                                    B2880
      DO 480 I=1,22                                                    B2890
      IF (MI(INPT(I)).LE.0.0) GO TO 480                                B2900
      WRITE (6,790) NSPEC(INPT(I)),Z(INPT(I)),MI(INPT(I)),XLMI(INPT(I))B2910
     1,GRAMS(INPT(I))                                                  B2920
  480 CONTINUE                                                         B2930
      WRITE (6,620)                                                    B2940
      WRITE (6,620)                                                    B2950
      IF (PRT(2).NE.0) GO TO 490                                       B2960
      WRITE (6,620)                                                    B2970
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      WRITE (6,770)                                                     B2980
  490 CONTINUE                                                          B2990
      IF (IGO.EQ.1) GO TO 500                                           B3000
      IF (PH.LT.3.0.OR.PH.GT.11.0) GO TO 540                            B3010
      DUM=((EPMCAT-EPMAN)/(1.+EPMCAT+EPMAN))*100.                       B3020
      IF (ABS(DUM).GT.30.) GO TO 540                                    B3030
  500 CONTINUE                                                          B3040
C                                                                       B3050
C                                                                       B3060
C     TEMPERATURE EFFECTS ON DEBYE-HUCKEL SOLVENT CONSTANTS             B3070
      S1=374.11-TEMP                                                    B3080
      S2=S1**0.333333                                                   B3090
      S3=SQRT((1.0+0.1342489*S2-3.946263E-03*S1)/(3.1975E0-.3151548E0*S2 B3100
     1-1.203374E-3*S1+7.48908E-13*S1**4))                               B3110
      IF (T.LT.373.15) GO TO 510                                        B3120
      C1=5321E0/T+233.76E0-T*(T*(8.292E-7*T-1.417E-3)+.9297E0)          B3130
      GO TO 520                                                         B3140
  510 C1=87.74E0-TEMP*(TEMP*(1.41E-6*TEMP-9.398E-4)+.4008E0)            B3150
  520 CONTINUE                                                          B3160
      C1=SQRT(C1*T)                                                     B3170
      A=18246.0E02*S3/C1**3                                             B3180
      B=50.29*S3/C1                                                     B3190
      GO TO 550                                                         B3200
  530 WRITE (6,780)                                                     B3210
      ICK=1                                                             B3220
      GO TO 550                                                         B3230
  540 WRITE (6,610)                                                     B3240
      ICK=1                                                             B3250
  550 CONTINUE                                                          B3260
      RETURN                                                            B3270
C                                                                       B3280
C                                                                       B3290
C                                                                       B3300
  560 FORMAT (5X,'IRON AND/OR MANGANESE HAVE BEEN SPECIFIED WITHOUT REDO B3310
     1X',/5X,'INFORMATION, IRON AND MANGANESE TOTALS HAVE BEEN CHANGED', B3320
     2' TO ZERO.',/)                                                    B3330
  570 FORMAT (//,1X,'*** DENOTES THAT AN ANALYTICAL EXPRESSION FOR RT HA B3340
     1S BEEN USED',////,1X,'SUMMARY OF ANALYTICAL EXPRESSIONS OF THE FOR B3350
     2M',/1X,'  LOG K = A+B*T+C/T+D*T**2+E/T**2+F*LOG T'///,2X,'I   NREA B3360
     3CT',9X,'A              B              C              D              E B3370
     4       F'/)                                                       B3380
  580 FORMAT (1X,I3,2X,A8,1X,F11.4,1X,F14.9,1X,F11.4,1X,1PE11.4,1X,     B3390
     11PE13.6,1X,1PE14.7)                                               B3400
  590 FORMAT (16I5)                                                     B3410
  600 FORMAT (/,2X,'WARNING--- INPUT ERROR, SEARCHING FOR BLANK CARD')  B3420
  610 FORMAT (/,2X,'WARNING---CHECK INPUT PH AND/OR CATION-ANION BALANCE B3430
     1',/12X,'...CALCULATION TERMINATED')                               B3440
  620 FORMAT (//)                                                       B3450
  630 FORMAT (5(F6.0,1X),2F5.0,1X,9I1,2I3)                              B3460
  640 FORMAT (//,37X,'----',/,37X,'DATA',/,37X,'----',//,3X,'I',1X,'NREA B3470
     1CT',8X,'DH',7X,'LOGKTO',10X,'I',1X,'NSPEC',6X,'Z',2X,'DHA',5X,'GFW B3480
     2',/)                                                              B3490
  650 FORMAT(1X,I3,1X,A8,2(1X,F10.4),A1,6X,I3,1X,A8,2X,I2,2X,F3.1       B3500
     1,1X,F10.4)                                                        B3510
  660 FORMAT (1H ,I3,1X,A8,2(1X,F10.4),A1)                              B3520
  670 FORMAT (1H1,(A80),//)                                             B3530
  680 FORMAT (6(E12.5),8X)                                              B3540
  690 FORMAT (A4,1X,5(I3,E12.5))                                        B3550
  700 FORMAT (1X,'NEW DATA *** DELTA H FOR REACTION ',I3,1X,A8,' HAS BEE B3560
     1N CHANGED TO ',F9.4)                                              B3570
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  710 FORMAT (1X,'NEW DATA *** LOGKTO  FOR REACTION ',I3,1X,A8,' HAS BEE  B3580
     1N CHANGED TO ',F9.4)                                                B3590
  720 FORMAT(1X,'NEW DATA *** LOGKT   FOR REACTION ',I3,1X,A8,' = ',/1X,  B3600
     11PE15.8,'+',E15.8,'*T+',E15.8,'/T+',E15.8,'*T**2+',E15.8,'*T**2+',  B3610
     2E15.8,'*LOG T')                                                     B3620
  730 FORMAT (30X,'----------',/,30X,'INITIAL SOLUTION',/,30X,'--        B3630
     1----------',///)                                                    B3640
  740 FORMAT (10X,'TEMPERATURE = ',F6.2,' DEGREES C    PH = ',F6.3,/,10X  B3650
     1,'ANALYTICAL EPMCAT = ',F8.3,'    ANALYTICAL EPMAN = ',F8.3,//)     B3660
  750 FORMAT (5X,'***** OXIDATION - REDUCTION *****',///,1X,'DISSOLVED O  B3670
     1XYGEN = ',F6.3,' MG/L',/,1X,'EH MEASURED WITH CALOMEL = ',F7.4,' V  B3680
     2OLTS',9X,'FLAG CORALK PECALC IDAVES',/,1X,'MEASURED EH OF ZOBE',    B3690
     3'LL SOLUTION = ',F7.4,' VOLTS',5X,I1,4X,I1,6X,I1,6X,I1,/,1X         B3700
     4,'CORRECTED EH = ',F7.4,' VOLTS',/,1X,'PE COMPUTED FROM CORRECTED   B3710
     5EH = ',F7.3,/)                                                      B3720
  760 FORMAT (15X,'*** TOTAL CONCENTRATIONS OF INPUT SPECIES ***',//,25X  B3730
     1,'TOTAL',13X,'LOG TOTAL',12X,'TOTAL',/,8X,'SPECIES',8X,'MOLALITY'   B3740
     2,12X,'MOLALITY',11X,'MG/LITRE',/,8X,'----------',8X,'----------',12X,'-  B3750
     3----------',11X,'----------',/)                                     B3760
  770 FORMAT (22X,'*** CONVERGENCE ITERATIONS ***',//,1X,'ITERATION',2X   B3770
     1,'S1-ANALCO3',3X,'S2-SO4TOT',4X,'S3-FTOT',5X,'S4-PTOT',4X,'S5-CLTO  B3780
     2T',/)                                                               B3790
  780 FORMAT (1X,'INPUT ERROR--UNITS OF CONCENTRATION ARE NOT KNOWN',/    B3800
     1//)                                                                 B3810
  790 FORMAT (1H ,7X,A8,I3,3X,1PE12.5,9X,0PF9.4,8X,1PE12.5)               B3820
      END                                                                 B3830
      SUBROUTINE SET                                                      C  10
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                                 C  20
      INTEGER D,E,DD,RBIT,CORALK,Z(120),PRT(4),PECALC,PECK                C  30
      DOUBLE PRECISION MI(120),KT(200),LOGKT(200),LOGKTO(200),MWTOT,LH2O  C  40
     1,MJ,NATOT,KTOT,MGTOT,LITOT,NH4TOT,KW                                C  50
      CHARACTER *8 NSPEC(120),NREACT(200)                                 C  60
      CHARACTER *80 TITL                                                  C  70
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDO,P  C  80
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA  C  90
     2LFA(120),Z,CUNITS(120),ANALMI(120),GFW(120),DHA(120),NSPEC,NREACT,  C 100
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EH4,DENS,DOX,XLMI(  C 110
     4120),ITER,RBIT,C1SAVE,COPALK,MJ,LCHEX(200),CO2TIT,ANALCO,SITOT,CAT  C 120
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT  C 130
     6,SRTOT,BATOT,CLTOT,MWTOT,ICK,PRT,TITL,EPMCAT,EPMAN,NEQU,ISPEC,      C 140
     7KSPEC(120),IMIN,KMIN(200),TDS,IDAVES,IPRT,JJ,JK                     C 150
C                                                                         C 160
C                                                                         C 170
C     INITIALIZE STARTING VALUES FOR ITERATIVE LOOP                       C 180
      AH2O=1.0                                                            C 190
      DO 10 I=1,D                                                         C 200
      GAMMA(I)=1.0                                                        C 210
   10 CONTINUE                                                            C 220
      CO2TIT=MI(7)+2.0*MI(18)                                             C 230
      ANALCO=CO2TIT                                                       C 240
      IF (CORALK.EQ.2) CO2TIT=MI(7)+MI(18)+MI(86)                         C 250
      SITOT=MI(35)                                                        C 260
      CATOT=MI(1)                                                         C 270
      MGTOT=MI(2)                                                         C 280
      NATOT=MI(3)                                                         C 290
      KTOT=MI(4)                                                          C 300
      SO4TOT=MI(6)                                                        C 310
      FETOT=MI(8)                                                         C 320
      PTOT=MI(45)                                                         C 330
      PION10=PTOT                                                         C 340
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      ALTOT=MI(51)                                                      C 350
      FTOT=MI(62)                                                       C 360
      BTOT=MI(87)                                                       C 370
      LITOT=MI(81)                                                      C 380
      NH4TOT=MI(39)                                                     C 390
      SRTOT=MI(88)                                                      C 400
      BATOT=MI(90)                                                      C 410
      CLTOT=MI(5)                                                       C 420
      MNTOT=MI(101)                                                     C 430
      MI(35)=0.0                                                        C 440
      MI(87)=0.0                                                        C 450
      TENPH=10.**PH                                                     C 460
      ALFA(64)=10.**(-PH)                                               C 470
C                                                                       C 480
CC                                                                      C 490
C     CALCULATION OF ANION ACTIVITIES EXCEPT CO2 AND PO4 SPECIES        C 500
      ALFA(5)=MI(5)*GAMMA(5)                                            C 510
      ALFA(6)=MI(6)*GAMMA(6)                                            C 520
      ALFA(62)=MI(62)*GAMMA(62)                                         C 530
      ALFA(85)=MI(85)*GAMMA(85)                                         C 540
      ALFA(98)=MI(98)*GAMMA(98)                                         C 550
      ALFA(27)=AH2O*KW*TENPH                                            C 560
      MI(27)=ALFA(27)/GAMMA(27)                                         C 570
      MI(64)=1E0/(TENPH*GAMMA(64))                                      C 580
      ALFA(63)=ALFA(6)*KT(90)/TENPH                                     C 590
      MI(63)=ALFA(63)/GAMMA(63)                                         C 600
C                                                                       C 610
CC                                                                      C 620
C     CO2 SPECIES                                                       C 630
      IF (CORALK.EQ.2) GO TO 20                                         C 640
      C1=2.0*TENPH/(GAMMA(18)*KT(69))                                   C 650
      MI(7)=CO2TIT/(1.+GAMMA(7)*C1)                                     C 660
      C2=KT(36)/(TENPH*GAMMA(86))                                       C 670
      ALFA(7)=MI(7)*GAMMA(7)                                            C 680
      MI(18)=C1*ALFA(7)/2.                                              C 690
      MI(86)=C2*ALFA(7)                                                 C 700
      ALFA(18)=MI(18)*GAMMA(18)                                         C 710
      ALFA(86)=MI(86)*GAMMA(86)                                         C 720
      GO TO 30                                                          C 730
   20 CONTINUE                                                          C 740
      MI(7)=CO2TIT/(1.0+GAMMA(7)*((KT(36)/(TENPH*GAMMA(86)))+TENPH/(KT(6 C 750
     19)*GAMMA(18))))                                                   C 760
      MI(18)=MI(7)*GAMMA(7)*TENPH/(GAMMA(18)*KT(69))                    C 770
      MI(86)=MI(7)*GAMMA(7)*KT(36)/(TENPH*GAMMA(86))                    C 780
      ALFA(7)=MI(7)*GAMMA(7)                                            C 790
      ALFA(18)=MI(18)*GAMMA(18)                                         C 800
      ALFA(86)=MI(86)*GAMMA(86)                                         C 810
   30 CONTINUE                                                          C 820
C                                                                       C 830
CC                                                                      C 840
C     PHOSPHATE SPECIES                                                 C 850
      MI(45)=PTOT/(1.+(KT(17)*GAMMA(45)/(GAMMA(48)*TENPH**2))+(KT(16)*GA C 860
     1MMA(45)/(TENPH*GAMMA(47))))                                       C 870
      ALFA(45)=MI(45)*GAMMA(45)                                         C 880
      ALFA(47)=KT(16)*ALFA(45)/TENPH                                    C 890
      MI(47)=ALFA(47)/GAMMA(47)                                         C 900
      ALFA(48)=KT(17)*ALFA(45)/(TENPH**2)                               C 910
      MI(48)=ALFA(48)/GAMMA(48)                                         C 920
      ITER=0                                                            C 930
      RETURN                                                            C 940
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      END                                                                C 950
      SUBROUTINE READ (WORD,INT,VAL)                                     D  10
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                                D  20
      CHARACTER *8 WORD                                                  D  30
      DIMENSION INT(6),VAL(6)                                            D  40
      CHARACTER *80 LINE                                                 D  50
      READ(5,10)LINE                                                     D  60
   10 FORMAT (A80)                                                       D  70
      READ (LINE,20)WORD,(INT(I),VAL(I),I=1,5)                           D  80
      IF (WORD.NE.'LOGK') RETURN                                         D  90
      READ (LINE,20)WORD,(INT(I),VAL(I),I=1,6)                           D 100
   20 FORMAT (A4,1X,6(I3,E12.5))                                         D 110
      RETURN                                                             D 120
      END                                                                D 130
      SUBROUTINE MODEL                                                   E  10
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                                E  20
      INTEGER D,E,DD,RBIT,CORALK,Z(120),LIST(8),LIST1(5),LIST2(18),LIST3 E  30
     1(9),PRT(4),PECALC,PECK                                             E  40
      DOUBLE PRECISION MI(120),KT(200),LOGKT(200),LOGKTO(200),MNTOT,H2O  E  50
     1,MU,NATOT,KTOT,MGTOT,LITOT,NH4TOT,KW,MUHALF,L1ALK(11)              E  60
      CHARACTER *8 NSPEC(120),NREACT(200)                                E  70
      CHARACTER *80 TITL                                                 E  80
      DIMENSION NPAIR(5),L1M(11),L1K(11),L1C(11),L1A(11), L2M(14), L2K(1 E  90
     14), L2C(14), L3M(7), L3K(7), L3C(7), L4M(14), L4K(14), L4C(14), L4 E 100
     2A(14), L5M(9), L5K(9), L5C(9)                                      E 110
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDO,P E 120
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA E 130
     2LFA(120),Z,CUNITS(120),ANALMI(120),GFW(120),DHA(120),NSPEC,NREACT, E 140
     3DH(200),AH2O,BH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XLMI( E 150
     4120),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT E 160
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT E 170
     6,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL,EPMCAT,EPMAN,NEQU,LSPEC,     E 180
     7KSPEC(120),IMIN,FMIN(200),TDS,IDAVES,IPRT,JJ,JK                    E 190
      DATA LIST/17,35,66,70,71,72,84,87/                                 E 200
      DATA LIST1/42,43,44,50,94/                                         E 210
      DATA LIST2/8,9,10,11,12,13,15,16,28,33,34,65,77,78,79,80,100,99/   E 220
      DATA LIST3/82,83,88,89,69,97,90,91,114/                            E 230
      DATA L1M/7,21,22,30,31,42,43,86,111,69,97/,L1K/69,74,75,78,79,70,  E 240
     171,36,167,149,170/,L1C/64,2,2,1,1,3,3,64,101,88,88/,L1A/18,18,7,7, E 250
     &18,18,7,7,7,7,18/,L1ALK/1.0,2.0,1.0,1.0,2.0,2.0,1.0,0.0,1.0,1.0    E 260
     2,2.0/,L2M/15,23,32,34,44,46,59,60,63,83,92,96,109,114/,L2K/5,76,24 E 270
     3,9,72,73,88,89,90,127,132,136,165,182/,L2C/8,2,1,8,3,4,51,51,64,81 E 280
     4,39,64,101,88/,L3M/20,55,56,57,58,108,49/,L3K/23                   E 290
     5,84,85,86,87,164,80/,L3C/2,51,51,51,51,101,1/,L4M/13,40,41,47,48,5 E 300
     60,61,65,73,74,75,76,99,100/,L4K/140,124,125,16,17,31,33,121,34,35, E 310
     7122,123,157,139/,L4C/8,2,2,64,64,3,4,8,2,1,1,1,8,8/,L4A/47,45,48,4 E 320
     85,45,47,47,48,47,47,45,48,48,47/,L5M/16,28,33,93,94,95,103,104,105 E 330
     9/,L5K/6,7,8,133,134,135,159,160,161/,L5C/8,8,8,64,3,4,101,101,101/ E 340
     $,NPAIR/11,14,7,14,9/                                               E 350
      ITER=ITER+1                                                        E 360
C                                                                        E 370
C                                                                        E 380
C     CALCULATION OF TOTAL MOLALITY AND AH2O                             E 390
      J=1                                                                E 400
      C1=0.0                                                             E 410
      DO 20 I=1,D                                                        E 420
      IF (J.GT.8) GO TO 5                                                E 430
      IF (I.EQ.LIST(J)) GO TO 10                                         E 440
    5 C1=C1+MI(I)                                                        E 450
      GO TO 20                                                           E 460
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   10 J=J+1                                                              E 470
   20 CONTINUE                                                           E 480
      AH2O=1.0-0.017*C1                                                  E 490
      LH2O=DLOG10(AH2O)                                                  E 500
      IF (DOX.GT.0.0) PEDO=-(DLOG10(KT(152))+PH+0.5*LH2O-0.25*DLOG10(DOX E 510
     1/32E3))                                                            E 520
      IF (DOX.GT.0.0) PESATO=-(DLOG10(KT(137))+PH+0.5*LH2O-0.25*DLOG10(D E 530
     1OX/32E3))                                                          E 540
      IF (PECALC.EQ.2) PE=PEDO                                           E 550
      IF (PECALC.EQ.3) PE=PESATO                                         E 560
C                                                                        E 570
C                                                                        E 580
C     CALCULATION OF ACTIVITY COEFFICIENTS                               E 590
      MU=0.0                                                             E 600
      J=1                                                                E 610
      DO 40 I=1,D                                                        E 620
      IF (I.EQ.LIST(J)) GO TO 30                                         E 630
      MU=MU+0.5*M(I)*Z(I)*Z(I)                                           E 640
      GO TO 40                                                           E 650
   30 J=J+1                                                              E 660
   40 CONTINUE                                                           E 670
      MUHALF=SQRT(MU)                                                    E 680
      C1=-A*4E0*MUHALF                                                   E 690
      GAMMA(1)=1E1**(C1/(1E0+B*5E0*MUHALF)+0.165*MU)                     E 700
      GAMMA(2)=1E1**(C1/(1E0+B*5.5*MUHALF)+0.2*MU)                       E 710
      GAMMA(3)=1E1**(-A*MUHALF/(1E0+B*4E0*MUHALF)+0.075*MU)              E 720
      GAMMA(4)=1E1**(-A*MUHALF/(1E0+B*3.5*MUHALF)+0.015*MU)              E 730
      GAMMA(5)=GAMMA(4)                                                  E 740
      GAMMA(6)=1E1**(C1/(1E0+B*5E0*MUHALF)-0.04*MU)                      E 750
      DO 60 I=8,D                                                        E 760
      IF (Z(I).EQ.0) GO TO 50                                            E 770
      IF(IDAVES.EQ.1) GAMMA(I)=1E1**(-A*Z(I)**2*((MUHALF/(1.0+MUHALF)    E 780
     1-0.3*MU)))                                                         E 790
      IF (IDAVES.EQ.1) GO TO 60                                          E 800
      GAMMA(I)=1E1**(-A*MUHALF*Z(I)**2/(1E0+DHA(I)*B*MUHALF))            E 810
      GO TO 60                                                           E 820
   50 GAMMA(I)=10.**(0.1*MU)                                             E 830
   60 CONTINUE                                                           E 840
      GAMMA(7)=1E1**(-A*MUHALF*Z(7)**2/(1E0+DHA(7)*B*MUHALF))            E 850
      GAMMA(18)=1E1**(-A*MUHALF*Z(18)**2/(1E0+DHA(18)*B*MUHALF))         E 860
      GAMMA(86)=1E1**(MU*(170.01/T-.8798+.0013935*T)+MU*MU*(28.81/T-.210 E 870
     18+.0003641*T))                                                     E 880
      GAMMA(30)=GAMMA(7)                                                 E 890
      GAMMA(31)=1E1**(-0.5*MU)                                           E 900
C                                                                        E 910
C                                                                        E 920
C     SULFUR SPECIES AND PE CALCULATION FROM S                           E 930
      C1=KT(92)*TENPH/GAMMA(67)                                          E 940
      C2=KT(92)*KT(93)*TENPH**2/GAMMA(68)                                E 950
      MI(14)=MI(17)/(1E0+GAMMA(14)*(C1+C2))                              E 960
      ALFA(14)=MI(14)*GAMMA(14)                                          E 970
      ALFA(17)=MI(17)*GAMMA(17)                                          E 980
      MI(67)=ALFA(14)*C1                                                 E 990
      MI(68)=ALFA(14)*C2                                                E1000
      ALFA(67)=MI(67)*GAMMA(67)                                         E1010
      ALFA(68)=MI(68)*GAMMA(68)                                         E1020
      C1=ALFA(6)*ALFA(14)                                               E1030
      IF (C1.GT.0.0) GO TO 70                                           E1040
      GO TO 80                                                          E1050
   70 PES=0.125*LOGKT(91)+0.125*DLOG10(ALFA(6))-1.25*PH-0.125*DLOG10    E1060
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     1(ALFA(14))-0.5*LH2O                                                    £1070
      IF (PECALC.EQ.4) PE=PES                                                £1080
   80 CONTINUE                                                               £1090
      IF (PECALC.EQ.0.0.OR.PE.GE.100.) GO TO 90                              £1100
      TENMPE=10.**(-PE)                                                      £1110
      GO TO 100                                                              £1120
   90 TENMPE=1.0                                                             £1130
  100 CONTINUE                                                               £1140
C                                                                            £1150
C                                                                            £1160
C     SILICA SPECIES                                                         £1170
      C1=KT(14)*TENPH/GAMMA(25)                                              £1180
      C2=KT(15)*TENPH**2/GAMMA(26)                                           £1190
      MI(24)=SITOT/(1.0+GAMMA(24)*(C1+C2))                                   £1200
      ALFA(24)=MI(24)*GAMMA(24)                                              £1210
      MI(25)=ALFA(24)*C1                                                     £1220
      MI(26)=ALFA(24)*C2                                                     £1230
      ALFA(25)=MI(25)*GAMMA(25)                                              £1240
      ALFA(26)=MI(26)*GAMMA(26)                                              £1250
C                                                                            £1260
C                                                                            £1270
C     BORON SPECIES                                                          £1280
      C1=GAMMA(36)*KT(26)*TENPH/GAMMA(37)                                    £1290
      MI(36)=BTOT/(1.0+C1)                                                   £1300
      MI(37)=C1*MI(36)                                                       £1310
      ALFA(36)=MI(36)*GAMMA(36)                                              £1320
      ALFA(37)=MI(37)*GAMMA(37)                                              £1330
C                                                                            £1340
C                                                                            £1350
C     NITROGEN SPECIES                                                       £1360
      C1=TENPH*KT(27)/GAMMA(38)                                              £1370
      C2=ALFA(6)*KT(132)/GAMMA(92)                                           £1380
      MI(39)=NH4TOT/(1E0+GAMMA(39)*(C1+C2))                                  £1390
      ALFA(39)=MI(39)*GAMMA(39)                                              £1400
      MI(38)=ALFA(39)*C1                                                     £1410
      ALFA(38)=MI(38)*GAMMA(38)                                              £1420
      MI(92)=ALFA(39)*C2                                                     £1430
      ALFA(92)=MI(92)*GAMMA(92)                                              £1440
C                                                                            £1450
C                                                                            £1460
C     MAGNESIUM SPECIES                                                      £1470
      MI(19)=ALFA(27)*KT(25)/GAMMA(19)                                       £1480
      MI(20)=ALFA(62)*KT(23)/GAMMA(20)                                       £1490
      MI(21)=ALFA(18)*KT(74)/GAMMA(21)                                       £1500
      MI(22)=ALFA(7)*KT(75)/GAMMA(22)                                        £1510
      MI(23)=ALFA(6)*KT(76)/GAMMA(23)                                        £1520
      MI(40)=ALFA(45)*KT(124)/GAMMA(40)                                      £1530
      MI(41)=ALFA(48)*KT(125)/GAMMA(41)                                      £1540
      MI(73)=ALFA(47)*KT(34)/GAMMA(73)                                       £1550
      MI(2)=MGTOT/(1.0+GAMMA(2)*(MI(19)+MI(20)+MI(21)+MI(22)+MI(23)+MI(4     £1560
     10)+MI(41)+MI(73)))                                                     £1570
      ALFA(2)=MI(2)*GAMMA(2)                                                 £1580
      C1=ALFA(2)                                                             £1590
      DO 110 I=19,23                                                         £1600
      MI(I)=C1*MI(I)                                                         £1610
      ALFA(I)=MI(I)*GAMMA(I)                                                 £1620
  110 CONTINUE                                                               £1630
      MI(40)=C1*MI(40)                                                       £1640
      ALFA(40)=MI(40)*GAMMA(40)                                              £1650
      MI(41)=C1*MI(41)                                                       £1660
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      ALFA(41)=MI(41)*GAMMA(41)                                          01670
      MI(73)=C1*MI(73)                                                   01680
      ALFA(73)=MI(73)*GAMMA(73)                                          01690
C                                                                        01700
C                                                                        01710
C     CALCIUM SPECIES                                                    01720
      MI(29)=ALFA(27)*KT(77)/GAMMA(29)                                   01730
      MI(30)=ALFA(7)*KT(78)/GAMMA(30)                                    01740
      MI(31)=ALFA(18)*KT(79)/GAMMA(31)                                   01750
      MI(32)=ALFA(6)*KT(24)/GAMMA(32)                                    01760
      MI(74)=ALFA(47)*KT(35)/GAMMA(74)                                   01770
      MI(76)=ALFA(48)*KT(123)/GAMMA(76)                                  01780
      MI(75)=ALFA(45)*KT(122)/GAMMA(75)                                  01790
      MI(49)=ALFA(62)*KT(80)/GAMMA(49)                                   01800
      MI(1)=CATOT/(1.0+GAMMA(1)*(MI(29)+MI(30)+MI(31)+MI(32)+MI(74)+MI(7 01810
     15)+MI(76)+MI(49)))                                                 01820
      C1=MI(1)*GAMMA(1)                                                  01830
      ALFA(1)=C1                                                         01840
      DO 120 I=29,32                                                     01850
      MI(I)=C1*MI(I)                                                     01860
      ALFA(I)=MI(I)*GAMMA(I)                                             01870
  120 CONTINUE                                                           01880
      MI(74)=C1*MI(74)                                                   01890
      ALFA(74)=MI(74)*GAMMA(74)                                          01900
      MI(75)=C1*MI(75)                                                   01910
      ALFA(75)=MI(75)*GAMMA(75)                                          01920
      MI(76)=C1*MI(76)                                                   01930
      ALFA(76)=MI(76)*GAMMA(76)                                          01940
      MI(49)=C1*MI(49)                                                   01950
      ALFA(49)=MI(49)*GAMMA(49)                                          01960
C                                                                        01970
C                                                                        01980
C     SODIUM SPECIES                                                     01990
      MI(42)=ALFA(18)*KT(70)/GAMMA(42)                                   02000
      MI(43)=ALFA(7)*KT(71)/GAMMA(43)                                    02010
      MI(44)=ALFA(6)*KT(72)/GAMMA(44)                                    02020
      MI(50)=ALFA(47)*KT(31)/GAMMA(50)                                   02030
      MI(94)=ALFA(5)*KT(134)/GAMMA(94)                                   02040
      MI(3)=NATOT/(1.0+GAMMA(3)*(MI(42)+MI(43)+MI(44)+MI(50)+MI(94)))    02050
      ALFA(3)=MI(3)*GAMMA(3)                                             02060
      C1=ALFA(3)                                                         02070
      DO 130 I=1,5                                                       02080
      MI(LIST1(I))=C1*MI(LIST1(I))                                       02090
      ALFA(LIST1(I))=MI(LIST1(I))*GAMMA(LIST1(I))                        02100
  130 CONTINUE                                                           02110
C                                                                        02120
C                                                                        02130
C     POTASSIUM SPECIES                                                  02140
      MI(46)=ALFA(6)*KT(73)/GAMMA(46)                                    02150
      MI(61)=ALFA(47)*KT(33)/GAMMA(61)                                   02160
      MI(95)=ALFA(5)*KT(135)/GAMMA(95)                                   02170
      MI(4)=KTOT/(1.0+GAMMA(4)*(MI(46)+MI(61)+MI(95)))                   02180
      ALFA(4)=MI(4)*GAMMA(4)                                             02190
      C1=ALFA(4)                                                         02200
      MI(46)=C1*MI(46)                                                   02210
      ALFA(46)=MI(46)*GAMMA(46)                                          02220
      MI(61)=C1*MI(61)                                                   02230
      ALFA(61)=MI(61)*GAMMA(61)                                          02240
      MI(95)=C1*MI(95)                                                   02250
      ALFA(95)=MI(95)*GAMMA(95)                                          02260
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C                                                                       E2270
C                                                                       E2280
C     ALUMINIUM SPECIES                                                 E2290
      MI(52)=ALFA(27)*KT(81)/GAMMA(52)                                  E2300
      MI(53)=ALFA(27)**2*KT(82)/GAMMA(53)                               E2310
      MI(54)=ALFA(27)**4*KT(83)/GAMMA(54)                               E2320
      MI(55)=ALFA(62)*KT(84)/GAMMA(55)                                  E2330
      MI(56)=ALFA(62)**2*KT(85)/GAMMA(56)                               E2340
      MI(57)=ALFA(62)**3*KT(86)/GAMMA(57)                               E2350
      MI(58)=ALFA(62)**4*KT(87)/GAMMA(58)                               E2360
      MI(59)=ALFA(6)*KT(88)/GAMMA(59)                                   E2370
      MI(60)=ALFA(6)**2*KT(89)/GAMMA(60)                                E2380
      MI(51)=ALTOT/(1.0+GAMMA(51)*(MI(52)+MI(53)+MI(54)+MI(55)+MI(56)+MI E2390
     1(57)+MI(58)+MI(59)+MI(60)))                                       E2400
      ALFA(51)=MI(51)*GAMMA(51)                                         E2410
      C1=ALFA(51)                                                       E2420
      DO 140 I=52,60                                                    E2430
      MI(I)=C1*MI(I)                                                    E2440
      ALFA(I)=MI(I)*GAMMA(I)                                            E2450
  140 CONTINUE                                                          E2460
C                                                                       E2470
C                                                                       E2480
C     IRON SPECIES                                                      E2490
      IF (ABS(PE).LT.20.0.AND.FETOT.GT.0.0) GO TO 150                   E2500
      GO TO 170                                                         E2510
  150 MI(9)=KT(1)/(TENMPE*GAMMA(9))                                     E2520
      MI(10)=KT(2)*AH2O*TENPH/(TENMPE*GAMMA(10))                        E2530
      MI(11)=KT(3)*AH2O*TENPH/GAMMA(11)                                 E2540
      MI(12)=KT(4)*AH2O**3*TENPH**3/GAMMA(12)                           E2550
      MI(13)=KT(140)*ALFA(47)/(GAMMA(13)*TENMPE)                        E2560
      MI(15)=KT(5)*ALFA(6)/(TENMPE*GAMMA(15))                           E2570
      MI(16)=KT(6)*ALFA(5)/(TENMPE*GAMMA(16))                           E2580
      MI(28)=KT(7)*ALFA(5)**2/(TENMPE*GAMMA(28))                        E2590
      MI(33)=KT(8)*ALFA(5)**3/(TENMPE*GAMMA(33))                        E2600
      MI(34)=KT(9)*ALFA(6)/GAMMA(34)                                    E2610
      MI(65)=KT(121)*ALFA(48)/GAMMA(65)                                 E2620
      MI(77)=KT(103)*(AH2O*TENPH)**2/(TENMPE*GAMMA(77))                 E2630
      MI(78)=KT(104)*(AH2O*TENPH)**3/(TENMPE*GAMMA(78))                 E2640
      MI(79)=KT(105)*(AH2O*TENPH)**4/(TENMPE*GAMMA(79))                 E2650
      MI(80)=KT(106)*(AH2O*TENPH)**2/GAMMA(80)                          E2660
      MI(99)=KT(157)*ALFA(48)/(TENMPE*GAMMA(99))                        E2670
      MI(100)=KT(139)*ALFA(47)/GAMMA(100)                               E2680
      MI(8)=FETOT/(1.0+GAMMA(8)*(MI(9)+MI(10)+MI(11)+MI(12)+MI(13)+MI(15 E2690
     1)+MI(16)+MI(28)+MI(33)+MI(34)+MI(65)+MI(77)+MI(78)+MI(79)+MI(80)+M E2700
     2I(100)+MI(99)))                                                   E2710
      ALFA(8)=MI(8)*GAMMA(8)                                            E2720
      C1=ALFA(8)                                                        E2730
      DO 160 I=2,18                                                     E2740
      MI(LIST2(I))=C1*MI(LIST2(I))                                      E2750
      ALFA(LIST2(I))=MI(LIST2(I))*GAMMA(LIST2(I))                       E2760
  160 CONTINUE                                                          E2770
      GO TO 190                                                         E2780
  170 CONTINUE                                                          E2790
      DO 180 I=2,18                                                     E2800
      MI(LIST2(I))=0.0                                                  E2810
  180 CONTINUE                                                          E2820
      ALFA(8)=MI(8)*GAMMA(8)                                            E2830
  190 CONTINUE                                                          E2840
C                                                                       E2850
C     MANGANESE SPECIES                                                 E2860
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C                                                                       2870
      IF (ABS(PE).LT.20.0.AND.MNTOT.GT.0.0) GO TO 200                   2880
      GO TO 240                                                         2890
  200 MI(102)=KT(158)/(GAMMA(102)*TEMPE)                                2900
      MI(103)=KT(159)*MI(5)*GAMMA(5)/GAMMA(103)                         2910
      MI(104)=KT(160)*MI(5)**2*GAMMA(5)**2/GAMMA(104)                   2920
      MI(105)=KT(161)*MI(5)**3*GAMMA(5)**3/GAMMA(105)                   2930
      MI(106)=KT(162)*MI(27)*GAMMA(27)/GAMMA(106)                       2940
      MI(107)=KT(163)*MI(27)**3*GAMMA(27)**3/GAMMA(107)                 2950
      MI(108)=KT(164)*MI(62)*GAMMA(62)/GAMMA(108)                       2960
      MI(109)=KT(165)*MI(6)*GAMMA(6)/GAMMA(109)                         2970
      MI(110)=KT(166)*MI(85)**2*GAMMA(85)**2/GAMMA(110)                 2980
      MI(111)=KT(167)*MI(7)*GAMMA(7)/GAMMA(111)                         2990
      XMI112=LOGKT(168)+4*LH2O-(DLOG10(GAMMA(112))-8*PH-5*PE)           3000
      IF (XMI112.LT.-38.) MI(112)=0.0                                   3010
      IF (XMI112.LT.-38.) GO TO 210                                     3020
      MI(112)=10.**XMI112                                               3030
  210 CONTINUE                                                          3040
      XMI113=LOGKT(169)+4*LH2O-(DLOG10(GAMMA(113))-8*PH-4*PE)           3050
      IF (XMI113.LT.-38.) MI(113)=0.0                                   3060
      IF (XMI113.LT.-38.) GO TO 220                                     3070
      MI(113)=10.**XMI113                                               3080
  220 CONTINUE                                                          3090
      MI(115)=KT(171)*AH2O**2/(GAMMA(115)*ALFA(64)**3)                  3100
      MI(101)=MNTOT/(1.0+GAMMA(101)*(MI(102)+MI(103)+MI(104)+MI(105)+MI(  3110
     1106)+MI(107)+MI(108)+MI(109)+MI(110)+MI(111)+MI(112)+MI(113)+MI(11  3120
     25)))                                                              3130
      ALFA(101)=MI(101)*GAMMA(101)                                      3140
      C1=ALFA(101)                                                      3150
      DO 230 I=102,113                                                  3160
      MI(I)=C1*MI(I)                                                    3170
      ALFA(I)=MI(I)*GAMMA(I)                                            3180
  230 CONTINUE                                                          3190
      MI(115)=C1*MI(115)                                                3200
      ALFA(115)=MI(115)*GAMMA(115)                                      3210
      GO TO 260                                                         3220
  240 DO 250 I=101,113                                                  3230
      MI(I)=0.0                                                         3240
  250 CONTINUE                                                          3250
      MI(115)=0.0                                                       3260
  260 CONTINUE                                                          3270
C                                                                       3280
C                                                                       3290
C     CALCULATION OF PCO2 AND PCH4                                      3300
      IF (ABS(PE).LT.19.0) GO TO 270                                    3310
      GO TO 280                                                         3320
  270 C1=DLOG10(KT(94))+PH+PE+0.5*LH2O                                  3330
      ALFA(70)=10.**(4.0*C1)                                            3340
  280 CONTINUE                                                          3350
      IF (ABS(PE).LT.19.0.AND.ALFA(7).GT.0.0) GO TO 290                 3360
      GO TO 300                                                         3370
  290 XLALFA(71)=(DLOG10(KT(95))-8.0*PH-9.0*PH-3.0*LH2O+DLOG10(ALFA(7)))  3380
      IF (XLALFA(71).LT.-38.) GO TO 300                                 3390
      ALFA(71)=10.**XLALFA(71)                                          3400
  300 CONTINUE                                                          3410
C                                                                       3420
C                                                                       3430
C     LITHIUM, STRONTIUM, BARIUM SPECIES                                3440
      C1=KT(126)*ALFA(27)/GAMMA(82)                                     3450
      C2=KT(127)*ALFA(6)/GAMMA(83)                                      3460
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      MI(81)=LITOT/(1.0+GAMMA(81)*(C1+C2))                              E3470
      ALFA(81)=MI(81)*GAMMA(81)                                         E3480
      MI(82)=C1*ALFA(81)                                                E3490
      MI(83)=C2*ALFA(81)                                                E3500
      C1=KT(130)*ALFA(27)/GAMMA(89)                                     E3510
      C2=KT(149)*ALFA(7)/GAMMA(69)                                      E3520
      C3=KT(170)*ALFA(18)/GAMMA(97)                                     E3530
      C5=KT(182)*ALFA(6)/GAMMA(114)                                     E3540
      MI(88)=SRTOT/(1.0+GAMMA(88)*(C1+C2+C3+C5))                        E3550
      C4=GAMMA(88)*MI(88)                                               E3560
      MI(89)=C1*C4                                                      E3570
      MI(69)=C2*C4                                                      E3580
      MI(97)=C3*C4                                                      E3590
      MI(114)=C5*C4                                                     E3600
      C1=KT(131)*ALFA(27)/GAMMA(91)                                     E3610
      MI(90)=BATOT/(1.0+GAMMA(90)*C1)                                   E3620
      MI(91)=GAMMA(90)*MI(90)*C1                                        E3630
      DO 310 I=1,9                                                      E3640
      ALFA(LIST3(I))=MI(LIST3(I))*GAMMA(LIST3(I))                       E3650
  310 CONTINUE                                                          E3660
C     SUMMATION OF ANION SPECIES                                        E3670
      N=NPAIR(1)                                                        E3680
      IF (CORALK.NE.2) GO TO 330                                        E3690
      S1=MI(18)                                                         E3700
      DO 320 I=1,N                                                      E3710
      S1=S1+MI(L1M(I))                                                  E3720
  320 CONTINUE                                                          E3730
      GO TO 350                                                         E3740
  330 CONTINUE                                                          E3750
      S1=2.0*MI(18)                                                     E3760
      DO 340 I=1,N                                                      E3770
      S1=S1+L1ALK(I)*MI(L1M(I))                                         E3780
  340 CONTINUE                                                          E3790
  350 CONTINUE                                                          E3800
      N=NPAIR(2)                                                        E3810
      S2=MI(6)+MI(60)                                                   E3820
      DO 360 I=1,N                                                      E3830
      S2=S2+MI(L2M(I))                                                  E3840
  360 CONTINUE                                                          E3850
      N=NPAIR(3)                                                        E3860
      S3=MI(62)+MI(56)+2.0*MI(57)+3.0*MI(58)                            E3870
      DO 370 I=1,N                                                      E3880
      S3=S3+MI(L3M(I))                                                  E3890
  370 CONTINUE                                                          E3900
      N=NPAIR(4)                                                        E3910
      S4=MI(45)                                                         E3920
      DO 380 I=1,N                                                      E3930
      S4=S4+MI(L4M(I))                                                  E3940
  380 CONTINUE                                                          E3950
      N=NPAIR(5)                                                        E3960
      S5=MI(5)+MI(28)+MI(104)+2.0*(MI(33)+MI(105))                      E3970
      DO 390 I=1,N                                                      E3980
      S5=S5+MI(L5M(I))                                                  E3990
  390 CONTINUE                                                          E4000
      ANALCO=CO2TIT                                                     E4010
C     MASS BALANCE ON CARBON                                            E4020
      IF (CO2TIT.LE.0.0) GO TO 460                                      E4030
      ACT=KT(69)*ALFA(64)                                               E4040
      SUM=0.0                                                           E4050
      SUM1=0.0                                                          E4060
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      N=NPAIR(1)                                                        E4070
      DO 400 I=1,N                                                      E4080
      MI(L1M(I))=KT(L1K(I))*ALFA(L1C(I))/GAMMA(L1M(I))                  E4090
      IF (L1A(I).EQ.7) MI(L1M(I))=MI(L1M(I))*ACT                        E4100
      SUM=SUM+MI(L1M(I))                                                E4110
      SUM1=SUM1+L1ALK(I)*MI(L1M(I))                                     E4120
  400 CONTINUE                                                          E4130
      IF (CORALK.NE.2) GO TO 420                                        E4140
      MI(18)=ANALCO/(1.0+GAMMA(18)*SUM)                                 E4150
      ALFA(18)=MI(18)*GAMMA(18)                                         E4160
      DO 410 I=1,N                                                      E4170
      MI(L1M(I))=MI(L1M(I))*ALFA(18)                                    E4180
      ALFA(L1M(I))=MI(L1M(I))*GAMMA(L1M(I))                             E4190
  410 CONTINUE                                                          E4200
      GO TO 460                                                         E4210
  420 CONTINUE                                                          E4220
      IF (CORALK.EQ.1) GO TO 440                                        E4230
      IF (CORALK.EQ.3) GO TO 430                                        E4240
      ANALCO=CO2TIT-MI(25)-2.0*MI(26)-MI(27)-MI(37)-2.0*MI(45)-MI(47)-MI E4250
     1(54)-MI(67)-2.0*MI(68)-MI(82)                                     E4260
      GO TO 440                                                         E4270
  430 CONTINUE                                                          E4280
      SUMALK=MI(29)+MI(76)+MI(19)+MI(41)+MI(11)+MI(10)+MI(99)+MI(52)+MI( E4290
     1106)+MI(25)+MI(37)+MI(82)+MI(89)+MI(91)+MI(38)+MI(67)+MI(48)+MI(27 E4300
     2)+2.0*(MI(74)+MI(73)+MI(50)+MI(61)+MI(80)+MI(100)+MI(13)+MI(77)+MI E4310
     3(53)+MI(26)+MI(68)+MI(47))+3.0*(MI(75)+MI(40)+MI(12)+MI(78)+MI(107 E4320
     4)+MI(115)+MI(45))+4.0*(MI(79)+MI(54))-MI(64)-MI(63)-MI(93)-2.0*MI( E4330
     596)+MI(69)+2.0*MI(97)                                             E4340
      ANALCO=CO2TIT-SUMALK                                              E4350
  440 CONTINUE                                                          E4360
      IF (ANALCO.LT.0.0) ANALCO=0.0                                     E4370
      MI(18)=ANALCO/(2.0+GAMMA(18)*SUM1)                                E4380
      ALFA(18)=MI(18)*GAMMA(18)                                         E4390
      DO 450 I=1,N                                                      E4400
      MI(L1M(I))=MI(L1M(I))*ALFA(18)                                    E4410
      ALFA(L1M(I))=MI(L1M(I))*GAMMA(L1M(I))                             E4420
  450 CONTINUE                                                          E4430
  460 CONTINUE                                                          E4440
C     MASS BALANCE ON SULFATE                                           E4450
      IF (SO4TOT.LE.0.0) GO TO 500                                      E4460
      N=NPAIR(2)                                                        E4470
      DO 470 I=1,N                                                      E4480
      MI(L2M(I))=KT(L2K(I))*ALFA(L2C(I))/GAMMA(L2M(I))                  E4490
  470 CONTINUE                                                          E4500
      MI(15)=MI(15)/TEMPK                                               E4510
      MI(60)=MI(60)*ALFA(6)                                             E4520
      MI(96)=MI(96)*ALFA(64)                                            E4530
      SUM=MI(60)                                                        E4540
      DO 480 I=1,N                                                      E4550
      SUM=SUM+MI(L2M(I))                                                E4560
  480 CONTINUE                                                          E4570
      MI(6)=SO4TOT/(1.0+GAMMA(6)*SUM)                                   E4580
      ALFA(6)=MI(6)*GAMMA(6)                                            E4590
      DO 490 I=1,N                                                      E4600
      MI(L2M(I))=MI(L2M(I))*ALFA(6)                                     E4610
      ALFA(L2M(I))=MI(L2M(I))*GAMMA(L2M(I))                             E4620
  490 CONTINUE                                                          E4630
  500 CONTINUE                                                          E4640
C     MASS BALANCE ON FLUORIDE                                          E4650
      IF (FTOT.LE.0.0) GO TO 540                                        E4660
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      N=NPAIR(3)                                                        E4670
      DO 510 I=1,N                                                      E4680
      MI(L3M(I))=KT(L3K(I))*ALFA(L3C(I))/GAMMA(L3M(I))                  E4690
  510 CONTINUE                                                          E4700
      MI(56)=MI(56)*ALFA(62)                                            E4710
      MI(57)=MI(57)*ALFA(62)*ALFA(62)                                   E4720
      MI(58)=MI(58)*ALFA(62)*ALFA(62)*ALFA(62)                          E4730
      SUM=MI(56)+2.0*MI(57)+3.0*MI(58)                                  E4740
      DO 520 I=1,N                                                      E4750
      SUM=SUM+MI(L3M(I))                                                E4760
  520 CONTINUE                                                          E4770
      MI(62)=PTOT/(1.0+GAMMA(62)*SUM)                                   E4780
      ALFA(62)=MI(62)*GAMMA(62)                                         E4790
      DO 530 I=1,N                                                      E4800
      MI(L3M(I))=MI(L3M(I))*ALFA(62)                                    E4810
      ALFA(L3M(I))=MI(L3M(I))*GAMMA(L3M(I))                             E4820
  530 CONTINUE                                                          E4830
  540 CONTINUE                                                          E4840
C     MASS BALANCE ON PHOSPHATE                                         E4850
      IF (PTOT.LE.0.0) GO TO 580                                        E4860
      N=NPAIR(4)                                                        E4870
      C1=KT(16)*ALFA(64)                                                E4880
      C2=KT(17)*ALFA(64)*ALFA(64)                                       E4890
      DO 550 I=1,N                                                      E4900
      MI(L4M(I))=KT(L4K(I))*ALFA(L4C(I))/GAMMA(L4M(I))                  E4910
      IF (L4A(I).EQ.47) MI(L4M(I))=MI(L4M(I))*C1                        E4920
      IF (L4A(I).EQ.48) MI(L4M(I))=MI(L4M(I))*C2                        E4930
  550 CONTINUE                                                          E4940
      MI(13)=MI(13)/TENMPE                                              E4950
      MI(48)=MI(48)*ALFA(64)                                            E4960
      MI(99)=MI(99)/TENMPE                                              E4970
      SUM=0.0                                                           E4980
      DO 560 I=1,N                                                      E4990
      SUM=SUM+MI(L4M(I))                                                E5000
  560 CONTINUE                                                          E5010
      MI(45)=PTOT/(1.0+GAMMA(45)*SUM)                                   E5020
      ALFA(45)=MI(45)*GAMMA(45)                                         E5030
      DO 570 I=1,N                                                      E5040
      MI(L4M(I))=MI(L4M(I))*ALFA(45)                                    E5050
      ALFA(L4M(I))=MI(L4M(I))*GAMMA(L4M(I))                             E5060
  570 CONTINUE                                                          E5070
  580 CONTINUE                                                          E5080
C     MASS BALANCE ON CHLORIDE                                          E5090
      IF (CLTOT.LE.0.0) GO TO 620                                       E5100
      N=NPAIR(5)                                                        E5110
      DO 590 I=1,N                                                      E5120
      MI(L5M(I))=KT(L5K(I))*ALFA(L5C(I))/GAMMA(L5M(I))                  E5130
  590 CONTINUE                                                          E5140
      MI(16)=MI(16)/TENMPE                                              E5150
      MI(28)=MI(28)*ALFA(5)/TENMPE                                      E5160
      MI(33)=MI(33)*ALFA(5)*ALFA(5)/TENMPE                              E5170
      MI(104)=MI(104)*ALFA(5)                                           E5180
      MI(105)=MI(105)*ALFA(5)*ALFA(5)                                   E5190
      SUM=MI(28)+2.0*MI(33)+MI(104)+2.0*MI(105)                         E5200
      DO 600 I=1,N                                                      E5210
      SUM=SUM+MI(L5M(I))                                                E5220
  600 CONTINUE                                                          E5230
      MI(5)=CLTOT/(1.0+GAMMA(5)*SUM)                                    E5240
      ALFA(5)=MI(5)*GAMMA(5)                                            E5250
      DO 610 I=1,N                                                      E5260
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      MI(LSM(I))=MI(LSM(I))*ALFA(5)                                     E5270
      ALFA(LSM(I))=MI(LSM(I))*GAMMA(LSM(I))                             E5280
  610 CONTINUE                                                          E5290
  620 CONTINUE                                                          E5300
      ALFA(85)=MI(85)*GAMMA(85)                                         E5310
      ALFA(98)=MI(98)*GAMMA(98)                                         E5320
      ALFA(27)=AH2O*KW*TENPH                                            E5330
      MI(27)=ALFA(27)/GAMMA(27)                                         E5340
      MI(64)=1.ED/(TENPH*GAMMA(64))                                     E5350
      TEST1=S1-ANALCO                                                   E5360
      TEST2=S2-SO4TOT                                                   E5370
      TEST3=S3-FTOT                                                     E5380
      TEST4=S4-PTOT                                                     E5390
      TEST5=S5-CLTOT                                                    E5400
      RBIT=0                                                            E5410
      IF (S1.EQ.0.0.OR.ANALCO.LE.0.0) GO TO 630                         E5420
      IF (ABS(TEST1).GT.EROR1*ANALCO) RBIT=1                            E5430
      GO TO 640                                                         E5440
  630 ANALCO=0.0                                                        E5450
  640 CONTINUE                                                          E5460
      IF (S2.EQ.0.0) GO TO 650                                          E5470
      IF (ABS(TEST2).GT.EROR2*SO4TOT) RBIT=1                            E5480
  650 CONTINUE                                                          E5490
      IF (S3.EQ.0.0) GO TO 660                                          E5500
      IF (ABS(TEST3).GT.EROR3*FTOT) RBIT=1                              E5510
  660 CONTINUE                                                          E5520
      IF (S4.EQ.0.0) GO TO 670                                          E5530
      IF (ABS(TEST4).GT.EROR4*PTOT) RBIT=1                              E5540
  670 CONTINUE                                                          E5550
      IF (S5.EQ.0.0) GO TO 680                                          E5560
      IF (ABS(TEST5).GT.EROR5*CLTOT) RBIT=1                             E5570
  680 CONTINUE                                                          E5580
      IF (PRT(2).NE.0) GO TO 690                                        E5590
      WRITE (6,700) ITER,TEST1,TEST2,TEST3,TEST4,TEST5                  E5600
  690 CONTINUE                                                          E5610
      RETURN                                                            E5620
C                                                                       E5630
C                                                                       E5640
C                                                                       E5650
  700 FORMAT (1H ,3X,I3,5X,5(1PE10.3,2X))                               E5660
      END                                                               E5670
      SUBROUTINE PRINT                                                  P  10
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                               P  20
      INTEGER D,E,DD,RBIT,CORALK,Z(120),LIST4(106),LIST5(8),PRT(4)      P  30
      INTEGER PECALC,PECK                                               P  40
      DOUBLE PRECISION MI(120),KT(200),LOGKT(200),LOGKTO(200),MNTOT,LH2O P  50
     1,MU,NATOT,KTOT,MGTOT,LITOT,NH4TOT,KW,RATIO1(10),RATIO2(10),RATIO3 P  60
     2(8),XLGAM(120)                                                    P  70
      CHARACTER *8 NSPEC(120),NREACT(200)                               P  80
      CHARACTER *80 TITL                                                P  90
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDO,P P 100
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA P 110
     2LFA(120),Z,CUNITS(120),ANALMI(120),GFW(120),DHA(120),NSPEC,NREACT, P 120
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EBM,DENS,DOX,XLMI( P 130
     4120),ITER,RBIT,CLSAVE,CORALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT P 140
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT P 150
     6,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL,EPMCAT,EPMAN,NEQU,ISPEC,    P 160
     7KSPEC(120),IMIN,KMIN(200),IDS,IDAVES,IPRT,JJ,JK                   P 170
      DATA LIST4/1,2,3,4,64,5,6,7,18,86,27,62,98,19,23,22,21,20,29,32,30 P 180
     1,31,49,44,43,42,94,46,95,63,96,93,24,25,26,14,67,68,8,9,10,11,12,7 P 190
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     27,78,79,80,13,100,65,99,15,16,28,33,34,101,102,106,107,111,109,110   F 200
     3,103,104,105,108,112,113,115,51,52,53,54,55,56,57,58,59,60,45,47,4   F 210
     48,40,73,41,75,74,76,61,50,36,37,85,38,39,92,81,82,83,88,69,97,89,    F 220
     590,91/                                                               F 230
      DATA LIST5/1,2,3,4,51,8,6,7/                                         F 240
      CEPMAN=0.0                                                           F 250
      CEPMCT=0.0                                                           F 260
      ELECT=0.0                                                            F 270
      DO 20 I=1,D                                                          F 280
      ELECT=ELECT+Z(I)*MI(I)                                               F 290
      IF (Z(I).GT.0) GO TO 10                                              F 300
      CEPMAN=CEPMAN-Z(I)*MI(I)                                             F 310
      GO TO 20                                                             F 320
   10 CEPMCT=CEPMCT+Z(I)*MI(I)                                             F 330
   20 CONTINUE                                                             F 340
      ELECT=ELECT*1000.                                                    F 350
      CEPMAN=CEPMAN*1000.*(1.0-C1SAVE*1.0E-06)                             F 360
      CEPMCT=CEPMCT*1000.*(1.0-C1SAVE*1.0E-06)                             F 370
      S1=MI(7)+MI(18)+MI(21)+MI(22)+MI(30)+MI(31)+MI(42)+MI(43)+MI(86)+M   F 380
     1I(111)+MI(69)+2.0*MI(97)                                             F 390
      PCO2=0.0                                                             F 400
      XLPCO2=-99.9                                                         F 410
      IF (S1.GT.0.0) GO TO 30                                              F 420
      GO TO 40                                                             F 430
   30 PCO2=ALFA(86)/10.0**(108.3865+0.01985076*T-6919.53/T-40.45154        F 440
     1*DLOG10(T)+669365.0/T**2.0)                                          F 450
      XLPCO2=DLOG10(PCO2)                                                  F 460
   40 CONTINUE                                                             F 470
      EHPE=PE*C*R*T/F                                                      F 480
      SUMALK=MI(30)+MI(29)+MI(76)+MI(19)+MI(22)+MI(41)+MI(43)+MI(11)+MI(   F 490
     110)+MI(99)+MI(52)+MI(106)+MI(111)+MI(25)+MI(37)+MI(82)+MI(89)+MI(9   F 500
     21)+MI(38)+MI(67)+MI(7)+MI(48)+MI(27)+2.0*(MI(74)+MI(31)+MI(21)+MI(   F 510
     373)+MI(42)+MI(50)+MI(61)+MI(80)+MI(100)+MI(13)+MI(77)+MI(53)+MI(26   F 520
     4)+MI(68)+MI(18)+MI(47))+3.0*(MI(75)+MI(40)+MI(12)+MI(78)+MI(107)+M   F 530
     5I(115)+MI(45))+4.0*(MI(79)+MI(54))-MI(64)-MI(63)-MI(93)-2.0*MI(96)   F 540
     6+MI(69)+2*MI(97)                                                     F 550
      SUMALK=SUMALK*1000.                                                  F 560
      CARBAL=MI(7)+MI(30)+MI(22)+MI(43)+MI(111)+2.0*(MI(31)+MI(21)+MI(42   F 570
     1)+MI(18))+MI(69)+2.0*MI(97)                                          F 580
      CARBAL=CARBAL*1000.                                                  F 590
      WRITE (6,110) TITL                                                   F 600
      WRITE (6,120)                                                        F 610
      WRITE (6,120)                                                        F 620
      WRITE (6,130) AH2O,EPMCAT,CEPMCT,PH,PCO2,EPMAN,CEPMAN,XLPCO2         F 630
     1,ALFA(70),EHM,PE,TEMP,ALFA(71),PES,S1,PEDO,DENS,PESATO,MU,TDS        F 640
     2,SUMALK,CARBAL,ELECT                                                 F 650
      IF (PECALC.NE.0) WRITE (6,140) PE,EHPE                               F 660
      WRITE (6,150)                                                        F 670
      DUM=10.**(-38)                                                       F 680
      DO 50 I=1,D                                                          F 690
      CUNITS(I)=0.0                                                        F 700
      IF (MI(I).LT.DUM) GO TO 50                                           F 710
      CUNITS(I)=MI(I)*1000.*GFW(I)*(1.0-1.0E-06*C1SAVE)                    F 720
      XLMI(I)=DLOG10(MI(I))                                                F 730
      XLALFA(I)=DLOG10(ALFA(I))                                            F 740
      XLGAM(I)=DLOG10(GAMMA(I))                                            F 750
   50 CONTINUE                                                             F 760
      DO 80 I=1,104                                                        F 770
      IF (MI(LIST4(I)).LT.DUM) GO TO 80                                    F 780
      IF (ISPEC.EQ.0) GO TO 70                                             F 790
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      DO 60 J=1,ISPEC                                                    F 800
      IF (LIST(I).EQ.KSPEC(J)) GO TO 70                                  F 810
   60 CONTINUE                                                           F 820
      GO TO 80                                                           F 830
   70 CONTINUE                                                           F 840
      WRITE (6,160) LIST4(I),NSPEC(LIST4(I)),Z(LIST4(I)),CUNITS(LIST4(I)) F 850
     1),MI(LIST4(I)),ALFA(LIST4(I)),XLALFA(LIST4(I)),GAMMA(LIST4(I))     F 860
   80 CONTINUE                                                           F 870
      IF (PRT(3).NE.0) GO TO 100                                         F 880
C                                                                        F 890
C                                                                        F 900
C     CALCULATION OF MOLAR RATIOS AND LOG ACTIVITY RATIOS.               F 910
      DO 90 I=1,8                                                        F 920
      IF (ANALMI(LIST5(I)).LT.1E-30) ANALMI(LIST5(I))=1E-30              F 930
      IF (MI(LIST5(I)).LT.1E-30) MI(LIST5(I))=1E-30                      F 940
      IF (MI(LIST5(I)).LT.1E-30) XLALFA(LIST5(I))=-30.                   F 950
      RATIO1(I)=ANALMI(5)/ANALMI(LIST5(I))                               F 960
      RATIO2(I)=MI(5)/MI(LIST5(I))                                       F 970
   90 CONTINUE                                                           F 980
      RATIO1(9)=ANALMI(1)/ANALMI(2)                                      F 990
      RATIO1(10)=ANALMI(3)/ANALMI(4)                                     F1000
      RATIO2(9)=MI(1)/MI(2)                                              F1010
      RATIO2(10)=MI(3)/MI(4)                                             F1020
      RATIO3(1)=XLALFA(1)+PH*2.                                          F1030
      RATIO3(2)=XLALFA(2)+PH*2.                                          F1040
      RATIO3(3)=XLALFA(3)+PH                                             F1050
      RATIO3(4)=XLALFA(4)+PH                                             F1060
      RATIO3(5)=XLALFA(51)+PH*3.                                         F1070
      RATIO3(6)=XLALFA(8)+PH*2.                                          F1080
      RATIO3(7)=XLALFA(1)-XLALFA(2)                                      F1090
      RATIO3(8)=XLALFA(3)-XLALFA(4)                                      F1100
      WRITE (6,120)                                                      F1110
      WRITE (6,170) (RATIO1(I),RATIO2(I),RATIO3(I),I=1,8),(RATIO1(I)     F1120
     1,RATIO2(I),I=9,10)                                                 F1130
  100 CONTINUE                                                           F1140
      WRITE (6,110) TITL                                                 F1150
      RETURN                                                             F1160
C                                                                        F1170
C                                                                        F1180
C                                                                        F1190
  110 FORMAT (/1X,A80)                                                   F1200
  120 FORMAT (//)                                                        F1210
  130 FORMAT (//,22X,'****DESCRIPTION OF SOLUTION ****',//,10X,'ANAL.'   F1220
     1,5X,'COMP.',9X,'PH',11X,'ACTIVITY H2O = ',F7.4,/,1X,'EPMCAT ',     F1230
     2F8.2,2X,F8.2,6X,F6.3,9X,'PCO2= ',1PE13.6,/,1X,'EPMAN  ',0PF8.2     F1240
     3,2X,F8.2,21X,'LOG PCO2 = ',F8.4,/,30X,'TEMPERATURE',6X,'PO2 = ',   F1250
     41PE13.6,/,1X,'EH = ',0PF6.4,2X,'PE = ',F7.3,4X,F6.2,' DEG C',5X,   F1260
     5'PCH4 = ',1PE13.6,/,1X,'PE CALC S = ',0PF8.3,26X,'CO2 TOT = ',1PE1 F1270
     63.6,/,1X,'PE CALC DOX=',0PF7.3,9X,'IONIC STRENGTH',4X,'DENSITY = ' F1280
     7,F8.4,/,1X,'PE SATO DOX=',F7.3,9X,1PE13.6,5X,'TDS = '0PF9.1,       F1290
     8'MG/L',/,1X,'TOT ALK = ',1PE10.3,' MEQ',22X,'CARB ALK',           F1300
     9' = ',E10.3,' MEQ',/,1X,'ELECT  = ',E10.3,' MEQ',/)               F1310
  140 FORMAT (1X,'IN COMPUTING THE DISTRIBUTION OF SPECIES,'/,1X,'PE = ' F1320
     1,F7.3,5X,'EQUIVALENT EH =',F7.3,'VOLTS',//)                       F1330
  150 FORMAT (///,25X,'-------------------------',/,25X,'DISTRIBUTION OF S F1340
     1PECIES',/,25X,'-------------------------',//,2X,'I',2X,'SPECIES',9X F1350
     2,'PPM',7X,'MOLALITY',3X,'ACTIVITY',4X,'LOG ACT',4X,'GAMMA',/)      F1360
  160 FORMAT(1H ,I3,1X,A8,I3,1X,1PE11.4,1X,E11.4,1X,1PE11.4              F1370
     1,1X,0PF7.3,1X,1PE11.4)                                             F1380
  170 FORMAT (//,3X,'MOLE RATIOS FROM',9X,'MOLE RATIOS FROM',/,2X,       F1390
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     1'ANALYTICAL MOLALITY',7X,'COMPUTED MOLALITY',7X,'LOG ACTIVITY',      F1400
     2' RATIOS',/,1X,3(21('-'),4X),/,1X,'CL/CA   = ',1PE11.4,4X,'CL/CA'    F1410
     3,'   = ',E11.4,4X,'LOG CA/H2 = ',0PF9.4,/1X,'CL/MG   = ',1PE11.4,    F1420
     44X,'CL/MG   = ',E11.4,4X,'LOG MG/H2 = ',0PF9.4,/1X,'CL/NA   = ',     F1430
     51PE11.4,4X,                                                          F1440
     6'CL/NA   = ',E11.4,4X,'LOG NA/H1 = ',0PF9.4,/,1X,'CL/K    = ',       F1450
     71PE11.4,4X,'CL/K    = ',E11.4,4X,'LOG K/H1  = ',0PF9.4,/,1X,'CL/AL   F1460
     8   = ',1PE11.4,4X,'CL/AL   = ',E11.4,4X,'LOG AL/H3 = ',0PF9.4,/,     F1470
     91X,'CL/FE   = ',1PE11.4,4X,'CL/FE   = ',E11.4,4X,'LOG FE/H2 = ',     F1480
     $0PF9.4,/,1X,'CL/SO4  = ',1PE11.4,4X,'CL/SO4  = ',E11.4,4X,'LOG CA/   F1490
     $MG = ',0PF9.4,/,1X,'CL/HCO3 = ',1PE11.4,4X,'CL/HCO3 = ',E11.4,       F1500
     $4X,'LOG NA/K  = ',0PF9.4,/,1X,'CA/MG   = ',1PE11.4,4X,'CA/MG   = '   F1510
     $,E11.4,/,1X,'NA/K    = ',E11.4,4X,'NA/K    = ',E11.4)               F1520
      END                                                                  F1530
      SUBROUTINE SAT                                                       G  10
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                                  G  20
      INTEGER D,E,DD,RBIT,CORALK,Z(120),LIST6(24),PRT(4)                   G  30
      INTEGER PECALC,PECK                                                  G  40
      DIMENSION LIST7(101), LIST8(15),LIST9(25),LIST0(101)                 G  50
      DOUBLE PRECISION MI(120),KT(200),LOGKT(200),LOGKTO(200),MWTOT,LH2O   G  60
     1,MU,NATOT,KTOT,MGTOT,LITOT,NH4TOT,KW                                 G  70
      CHARACTER *8 NSPEC(120),NREACT(200)                                  G  80
      CHARACTER *80 TITL                                                   G  90
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDO,P   G 100
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA   G 110
     2LFA(120),Z,CUNITS(120),ANALMI(120),GFW(120),DHA(120),NSPEC,NREACT,   G 120
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOK,XLMI(   G 130
     4120),ITER,RBIT,CISAVE,CORALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT   G 140
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT   G 150
     6,SRTOT,BATOT,CLTOT,MWTOT,ICK,PRT,TITL,EPMCAT,EPMAN,NEQU,ISPEC,       G 160
     7KSPEC(120),IMIN,KMIN(200),TDS,IDAVES,IPRT,JJ,JK                      G 170
      DATA LIST6/1,2,3,4,5,6,7,8,9,11,18,24,27,40,45,47,51,54,62,67,88,9   G 180
     10,101,102/                                                           G 190
      DATA LIST7/40,41,141,51,43,18,114,42,22,151,145,49,53,20,13,144,98   G 200
     1,50,21,30,57,100,29,12,56,113,120,97,63,28,52,111,112,119,19,65,48   G 210
     2,109,118,39,96,46,47,44,129,148,68,99,110,11,108,64,116,117,58,67,   G 220
     359,61,150,55,45,142,115,54,102,37,10,101,147,143,38,66,62,32,60,10   G 230
     47,146,154,155,156,172,173,174,175,176,177,178,179,180,181,183,184,   G 240
     5185,186,187,188,189,190,191,192,193/                                 G 250
      DATA LIST8/107,108,109,110,111,112,113,114,115,119,120,173,174,175   G 260
     1,177/                                                                G 270
      DATA LIST9/13,12,10,181,19,144,145,96,107,63,113,111,109,52,174      G 280
     1,180,100,101,98,102,47,154,37,120,68/                                G 290
C                                                                          G 300
C                                                                          G 310
C     CALCULATION OF ION ACTIVITY PRODUCTS                                 G 320
      DO 20 I=1,24                                                         G 330
      IF (ALFA(LIST6(I)).LT.1.E-38) GO TO 10                               G 340
      ALFA(LIST6(I))=DLOG10(ALFA(LIST6(I)))                                G 350
      GO TO 20                                                             G 360
   10 ALFA(LIST6(I))=-2E4                                                  G 370
   20 CONTINUE                                                             G 380
      AP(10)=ALFA(8)+ALFA(18)                                              G 390
      AP(11)=ALFA(2)+ALFA(18)                                              G 400
      AP(12)=ALFA(1)+AP(11)+ALFA(18)                                       G 410
      AP(13)=ALFA(1)+ALFA(18)                                              G 420
      AP(18)=ALFA(1)+ALFA(6)                                               G 430
      AP(19)=AP(18)+2E0*LH2O                                               G 440
      AP(20)=ALFA(2)+2E0*ALFA(27)                                          G 450
      AP(21)=3E0*ALFA(2)+2E0*ALFA(24)+6E0*ALFA(27)-5E0*LH2O                G 460
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      AP(22)=AP(13)                                                     G 470
      AP(28)=2E0*ALFA(2)+ALFA(24)+4E0*(ALFA(27)-LH2O)                   G 480
      AP(29)=ALFA(1)+ALFA(2)+2E0*ALFA(24)+4E0*ALFA(27)-6E0*LH2O         G 490
      AP(30)=ALFA(2)+ALFA(24)+2E0*ALFA(27)-3E0*LH2O                     G 500
      AP(32)=2E0*ALFA(1)+5E0*ALFA(2)+8E0*ALFA(24)+14E0*ALFA(27)-22E0*LH2 G 510
     10                                                                 G 520
      AP(37)=2E0*ALFA(2)+3E0*ALFA(24)+4E0*ALFA(27)-4.5E0*LH2O           G 530
      AP(38)=3E0*ALFA(2)+4E0*ALFA(24)+6E0*ALFA(27)-1E1*LH2O             G 540
      AP(39)=5E0*ALFA(2)+4E0*ALFA(18)+2E0*ALFA(27)+4E0*LH2O             G 550
      AP(40)=ALFA(4)+ALFA(54)+3E0*ALFA(24)-8E0*LH2O                     G 560
      AP(41)=AP(40)-ALFA(4)+ALFA(3)                                     G 570
      AP(42)=ALFA(1)+2E0*(ALFA(54)+ALFA(24))-8E0*LH2O                   G 580
      AP(43)=ALFA(3)+ALFA(54)+2E0*ALFA(24)-5E0*LH2O                     G 590
      AP(44)=ALFA(4)+3E0*(ALFA(54)+ALFA(24))-2E0*PH-12E0*LH2O           G 600
      AP(45)=ALFA(4)+ALFA(54)+3E0*(ALFA(2)+ALFA(24))+6E0*ALFA(27)-1E1*LH G 610
     12O                                                                G 620
      AP(46)=.6E0*ALFA(4)+.25E0*ALFA(2)+2.3E0*ALFA(54)+3.5E0*ALFA(24)-1. G 630
     12E0*PH-11.2E0*LH2O                                                G 640
      AP(47)=2E0*(ALFA(54)+ALFA(24)-PH)-7E0*LH2O                        G 650
      AP(48)=AP(47)                                                     G 660
      C1=(SQRT(MI(1)*GAMMA(1)+MI(2)*GAMMA(2)+MI(3)*GAMMA(3)))           G 670
      IF (C1.GT.0.0) C1=DLOG10(C1)                                      G 680
      IF (C1.LE.0.0) C1=-2E4                                            G 690
      AP(49)=.33E0*C1+2.33E0*ALFA(54)+3.67E0*ALFA(24)-2E0*PH-12E0*LH2O  G 700
      AP(50)=5E0*ALFA(2)+2E0*ALFA(54)+3E0*ALFA(24)+8E0*ALFA(27)-1E1*LH2O G 710
      AP(51)=ALFA(4)+3E0*ALFA(51)+6E0*ALFA(27)+2E0*ALFA(6)              G 720
      AP(52)=ALFA(51)+3E0*ALFA(27)                                      G 730
      AP(53)=AP(52)-LH2O                                                G 740
      AP(54)=2E0*ALFA(54)+4E0*ALFA(24)-2E0*PH-12.0*LH2O                 G 750
      AP(55)=.5E0*(ALFA(3)+ALFA(4))+ALFA(54)+3E0*ALFA(24)-7E0*LH2O      G 760
      AP(56)=ALFA(3)+ALFA(54)+3.5E0*ALFA(24)-6E0*LH2O                   G 770
      C2=(MI(3)*GAMMA(3)+MI(4)*GAMMA(4))                                G 780
      IF (C2.GT.0.0) C2=DLOG10(C2)                                      G 790
      IF (C2.LE.0.0) C1=-2E4                                            G 800
      AP(57)=.5E0*C2+ALFA(54)+5E0*ALFA(24)-8.5E0*LH2O                   G 810
      AP(58)=.5E0*C2+ALFA(54)+4.5E0*ALFA(24)-8E0*LH2O                   G 820
      AP(59)=ALFA(3)+ALFA(7)                                            G 830
      AP(60)=3E0*ALFA(3)+ALFA(7)+ALFA(18)+2E0*LH2O                      G 840
      AP(62)=2E0*ALFA(3)+ALFA(18)+LH2O                                  G 850
      AP(61)=AP(62)+9E0*LH2O                                            G 860
      AP(63)=ALFA(1)+2E0*ALFA(62)                                       G 870
      AP(64)=.167E0*ALFA(1)+2.33E0*ALFA(54)+3.67E0*ALFA(24)-2E0*PH-12E0* G 880
     1LH2O                                                              G 890
      AP(65)=ALFA(3)+ALFA(5)                                            G 900
      AP(66)=2E0*ALFA(3)+ALFA(6)                                        G 910
      AP(67)=AP(66)+1E1*LH2O                                            G 920
      AP(68)=ALFA(8)+ALFA(67)+PH                                        G 930
      AP(96)=5E0*ALFA(1)+3E0*(ALFA(47)-LH2O)+4E0*ALFA(27)               G 940
      AP(97)=5E0*ALFA(1)+3E0*(ALFA(47)-LH2O)+3E0*ALFA(27)+ALFA(62)      G 950
      AP(98)=ALFA(24)-2E0*LH2O                                          G 960
      AP(99)=ALFA(4)+7E0*ALFA(24)+PH-9E0*LH2O                           G 970
      AP(100)=AP(98)                                                    G 980
      AP(101)=AP(98)                                                    G 990
      AP(102)=AP(98)                                                   G1000
      IF (ABS(PE).LT.20.0) GO TO 30                                    G1010
      GO TO 40                                                         G1020
   30 CONTINUE                                                         G1030
      AP(107)=3E0*ALFA(8)+2E0*ALFA(45)+8E0*LH2O                        G1040
      AP(108)=3E0*ALFA(9)-PE+4E0*LH2O+8E0*PH                           G1050
      AP(109)=2E0*ALFA(9)+3E0*LH2O+6E0*PH                              G1060
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      AP(110)=AP(109)                                                   G1070
      AP(111)=ALFA(9)+3E0*ALFA(27)-LH2O                                 G1080
      AP(112)=3E0*ALFA(8)+2E0*ALFA(24)+6E0*ALFA(27)-5E0*LH2O            G1090
      AP(113)=ALFA(9)+3E0*(LH2O+PH)                                     G1100
      AP(114)=AP(45)+3E0*(ALFA(8)-ALFA(2))                              G1110
      AP(115)=ALFA(8)+2E0*(ALFA(67)+PE+PH)                              G1120
      AP(119)=3E0*ALFA(8)+4E0*ALFA(67)+2E0*PE+4E0*PH                    G1130
      AP(120)=AP(68)                                                    G1140
      AP(173)=ALFA(102)+2*LH2O+4*PH+PE                                  G1150
      AP(174)=AP(173)                                                   G1160
      AP(175)=AP(173)                                                   G1170
      AP(177)=3*ALFA(101)+4*LH2O+8*PH+2*PE                              G1180
      GO TO 60                                                          G1190
   40 CONTINUE                                                          G1200
      DO 50 I=1,15                                                      G1210
      J1=LIST8(I)                                                       G1220
      AP(J1)=-6000.                                                     G1230
   50 CONTINUE                                                          G1240
      PECK=1                                                            G1250
   60 CONTINUE                                                          G1260
      AP(116)=.29*ALFA(2)+.23*ALFA(9)+1.58*ALFA(54)+3.93*ALFA(24)-10.*LH G1270
     120                                                                G1280
      AP(117)=.45*ALFA(2)+.34*ALFA(9)+1.47*ALFA(54)+3.82*ALFA(24)-9.2*LH G1290
     120+.76*PH                                                         G1300
      AP(118)=3E0*ALFA(2)+ALFA(1)+4E0*ALFA(18)                          G1310
      AP(129)=ALFA(1)+2E0*ALFA(54)+4E0*ALFA(24)-8E0*LH2O                G1320
      AP(141)=AP(52)                                                    G1330
      AP(142)=2E0*(ALFA(1)+ALFA(54)+PH)+3E0*ALFA(24)-8E0*LH2O           G1340
      AP(143)=ALFA(88)+ALFA(18)                                         G1350
      AP(144)=ALFA(88)+ALFA(6)                                          G1360
      AP(145)=ALFA(90)+ALFA(6)                                          G1370
      AP(146)=ALFA(90)+ALFA(18)                                         G1380
      AP(147)=ALFA(9)+ALFA(45)+2E0*LH2O                                 G1390
      AP(148)=2E0*ALFA(1)+4E0*ALFA(54)+8E0*ALFA(24)-17E0*LH2O           G1400
      AP(150)=ALFA(2)+ALFA(18)+3E0*LH2O                                 G1410
      AP(151)=2E0*ALFA(1)+ALFA(18)+2E0*ALFA(27)+3E0*LH2O                G1420
      AP(172)=ALFA(101)+LH2O+2*PH                                       G1430
      AP(176)=2*ALFA(102)+3*LH2O+6*PH                                   G1440
      AP(178)=ALFA(101)+2*ALFA(27)                                      G1450
      AP(179)=ALFA(102)+3*ALFA(27)                                      G1460
      AP(180)=ALFA(102)+2*LH2O+3*PH                                     G1470
      AP(181)=ALFA(101)+ALFA(18)                                        G1480
      AP(183)=ALFA(101)+2*ALFA(5)                                       G1490
      AP(184)=AP(183)+LH2O                                              G1500
      AP(185)=AP(183)+2*LH2O                                            G1510
      AP(186)=AP(183)+4*LH2O                                            G1520
      AP(187)=2*ALFA(101)+ALFA(24)+4*PH                                 G1530
      AP(188)=2*ALFA(101)+ALFA(24)+2*PH-LH2O                            G1540
      AP(189)=ALFA(101)+ALFA(67)+PH                                     G1550
      AP(190)=ALFA(101)+ALFA(6)                                         G1560
      AP(191)=2*ALFA(102)+3*ALFA(6)                                     G1570
      AP(192)=3*ALFA(101)+2*ALFA(45)                                    G1580
      AP(193)=ALFA(101)+ALFA(47)                                        G1590
      AP(154)=AP(37)                                                    G1600
      AP(155)=AP(52)-LH2O                                               G1610
      AP(156)=AP(129)-2*LH2O                                            G1620
      WRITE (6,140)                                                     G1630
      WRITE (6,150)                                                     G1640
      IF (PRT(4).NE.9)  GO TO  67                                       G1650
      INPRINT=25                                                        G1660
```

```
      DO 66 I=1,INPRINT                                                 G1670
      LIST0(I)=LIST9(I)                                                 G1680
   66 CONTINUE                                                          G1690
      GO TO 65                                                          G1700
   67 INPRINT=101                                                       G1710
      DO 68 I=1,INPRINT                                                 G1720
      LIST0(I)=LIST7(I)                                                 G1730
   68 CONTINUE                                                          G1740
   65 DO 100 I=1,INPRINT                                                G1750
      IF (IMIN.EQ.0) GO TO 80                                           G1760
      K=0                                                               G1770
      DO 70 J=1,IMIN                                                    G1780
      IF (LIST0(I).EQ.KMIN(J)) K=1                                      G1790
   70 CONTINUE                                                          G1800
      IF (K.EQ.1) GO TO 80                                              G1810
      GO TO 100                                                         G1820
   80 CONTINUE                                                          G1830
      IF (AP(LIST0(I)).LT.-38.0.OR.AP(LIST0(I)).GT.38.0) GO TO 90       G1840
      IF (LCHEK(LIST0(I)).EQ.1) GO TO 90                                G1850
      DUM=AP(LIST0(I))-DLOG10(KT(LIST0(I)))                             G1860
      IF (DUM.GT.75.) GO TO 90                                          G1870
      XIAP=10.**AP(LIST0(I))                                            G1880
      RAT=XIAP/KT(LIST0(I))                                             G1890
      XLRAT=DLOG10(RAT)                                                 G1900
      DELGR=C*R*T*XLRAT                                                 G1910
      WRITE (6,160) LIST0(I),NREACT(LIST0(I)),XIAP,KT(LIST0(I)),AP(LIST0 G1920
     1(I)),LOGKT(LIST0(I)),RAT,XLRAT                                    G1930
      GO TO 100                                                         G1940
   90 IF (AP(LIST0(I)).LT.-5000.0.OR.AP(LIST0(I)).GT.5000.0) GO TO 100  G1950
      XLRAT=AP(LIST0(I))-LOGKT(LIST0(I))                                G1960
      DELGR=C*R*T*XLRAT                                                 G1970
      WRITE (6,170) LIST0(I),NREACT(LIST0(I)),AP(LIST0(I)),LOGKT(LIST0( G1980
     1I)),XLRAT                                                         G1990
  100 CONTINUE                                                          G2000
      IF (PECK.EQ.1.AND.PECALC.NE.0) GO TO 110                          G2010
      GO TO 130                                                         G2020
  110 WRITE (6,180)                                                     G2030
      DO 120 I=1,15                                                     G2040
      WRITE (6,190) NREACT(LIST8(I))                                    G2050
  120 CONTINUE                                                          G2060
  130 CONTINUE                                                          G2070
      RETURN                                                            G2080
C                                                                       G2090
C                                                                       G2100
  140 FORMAT (//)                                                       G2110
  150 FORMAT (//,6X,'PHASE',6X,'IAP',7X,'KT',6X,'LOG IAP',2X,'LOG KT',  G2120
     14X,'IAP/KT',2X,'LOG IAP/KT',/)                                    G2130
  160 FORMAT(1H ,I3,1X,A8,2(1PE10.3),2(1X,0PF8.3),1X,1PE10.3,           G2140
     11X,0PF8.3)                                                        G2150
  170 FORMAT (1H ,I3,1X,A8,21X,2(F8.3,1X),9X,F10.3)                     G2160
  180 FORMAT (///,1X,'PE IS GREATER THAN 20 OR LESS THAN -20',/,1X,'AN', G2170
     1'D THE FOLLOWING MINERAL REACTIONS HAVE BEEN DISREGARDED',/)      G2180
  190 FORMAT (1H ,20X,A8)                                               G2190
      END                                                               G2200
```

DATA TABLE

'CA	2	40.0800	6.0
'MG	2	24.3120	6.5
'NA	1	22.9898	4.0
'K	1	39.1020	3.0
'CL	-1	35.4530	3.0
'SO4	-2	96.0616	4.0
'HCO3	-1	61.0173	5.4
'FE	2	55.8470	6.0
'FE	3	55.8470	9.0
'FEOH	2	72.8544	5.0
'FEOH	1	72.8549	5.0
'FE(OH)3	-1	106.8690	5.0
'FEHPO4	1	151.8200	5.4
'H2S AQ	0	34.0799	0.0
'FESO4	1	151.9086	5.0
'FECL	2	91.3000	5.0
'ANAL H2S	0	34.0799	0.0
'CO3	-2	60.0094	5.4
'MGOH	1	41.3194	6.5
'MGF	1	43.3104	4.5
'MGCO3 AQ	0	84.3214	0.0
'MGHCO3	1	85.3293	4.0
'MGSO4 AQ	0	120.3736	0.0
'H4SIO4AQ	0	96.1155	0.0
'H3SIO4	-1	95.1075	4.0
'H2SIO4	-2	94.0995	5.4
'OH	-1	17.0074	3.5
'FECL2	1	126.7530	5.0
'CAOH	1	57.0874	6.0
'CAHCO3	1	101.0973	6.0
'CACO3 AQ	0	100.0890	0.0
'CASO4 AQ	0	136.1416	0.0
'FECL3	0	162.2060	0.0
'FESO4	0	151.9086	0.0
'SIO2 TOT	0	60.0848	0.0
'H3BO3 AQ	0	61.8331	0.0
'H2BO3	-1	60.8251	2.5
'NH3 AQ	0	17.0306	0.0
'NH4	1	18.0386	2.5
'MGPO4	-1	119.2834	5.4
'MGH2PO4	1	121.2993	5.4
'NACO3	-1	82.9992	5.4
'NAHCO3	0	83.9909	0.0
'NASO4	-1	119.0514	5.4
'PO4	-3	94.9714	5.0
'KSO4	-1	135.1636	5.4
'HPO4	-2	95.9794	5.0
'H2PO4	-1	96.9873	5.4
'CAF+	1	59.0784	5.0
'NAHPO4	-1	118.9692	5.4
'AL	3	26.9815	9.0
'AL(OH)	2	43.9889	5.4
'AL(OH)2	1	60.9962	5.4
'AL(OH)4	-1	95.0110	4.5
'ALF	2	45.9799	5.4
'ALF2	1	64.9783	5.4
'ALF3	0	83.9767	0.0
'ALF4	-1	102.9751	4.5
'ALSO4	1	123.0431	4.5
'AL(SO4)2	-1	219.1047	4.5

'KHPO4	'	-1	135.0814	5.4
'F	'	-1	18.9984	3.5
'HSO4	'	-1	97.0696	4.5
'H	'	1	1.0080	9.0
'FEH2PO4	'	1	152.8340	5.4
'H2S CALC	'	0	34.0799	0.0
'HS	'	-1	33.0720	3.5
'S	'	-2	32.0640	5.0
'SRHCO3	'	1	148.6373	5.4
'PO2	'	0	31.9988	0.0
'PCH4	'	0	16.0430	0.0
'AH2O	'	0	18.0153	0.0
'MGHPO4	'	0	120.2914	0.0
'CAHPO4	'	0	136.0594	0.0
'CAPO4	'	-1	135.0514	5.4
'CAH2PO4	'	1	137.0673	5.4
'FE(OH)2	'	1	89.8616	5.4
'FE(OH)3	'	0	106.8689	0.0
'FE(OH)4	'	-1	123.8762	5.4
'FE(OH)2	'	0	89.8616	0.0
'LI	'	1	6.9390	6.0
'LIOH	'	0	23.9464	0.0
'LISO4	'	-1	103.0006	5.0
'NH4CALC	'	1	18.0386	2.5
'NO3	'	-1	62.0049	3.0
'H2CO3	'	0	62.0253	0.0
'B TOT	'	0	10.8100	0.0
'SR	'	2	87.6200	5.0
'SROH	'	1	104.6274	5.0
'BA	'	2	137.3400	5.0
'BAOH	'	1	154.3474	5.0
'NH4SO4	'	-1	114.1002	5.0
'HCL	'	0	36.4610	0.0
'NACL	'	0	58.4428	0.0
'KCL	'	0	74.5550	0.0
'H2SO4	'	0	98.0775	0.0
'SRCO3	'	0	147.6294	0.0
'BR	'	-1	79.9090	4.0
'FEH2PO4	'	2	152.8340	5.4
'FEHPO4	'	0	151.8200	0.0
'MN	'	2	54.9400	6.0
'MN	'	3	54.9400	9.0
'MNCL	'	1	90.3970	5.0
'MNCL2	'	0	125.8540	0.0
'MNCL3	'	-1	161.3110	5.0
'MNOH	'	1	71.8480	5.0
'MN(OH)3	'	-1	105.9640	5.0
'MNP	'	1	73.9400	5.0
'MNSO4	'	0	151.0060	0.0
'MN(NO3)2	'	0	178.9560	0.0
'MNHCO3	'	1	115.9590	5.0
'MNO4	'	-1	118.9400	3.0
'MNO4	'	-2	118.9400	5.0
'SRSO4	'	0	183.6800	0.0
'HMNO2	'	-1	87.9480	5.0
'KFE +3	'	9.7000	-13.038	
'KFEH+2	'	20.1150	-15.228	
'KFEOH+	'	13.2180	-9.500	
'KFEOH3	'	30.3	-31.000	
'KFESO4	'	13.61	-9.118	

'KFECL	'	18.1520 -11.6000
'KFECL2	'	0.0 -10.9190
'KFECL3	'	0.0 -11.9250
'KFESO	'	3.23 2.25
'SIDERITE	'	-6.14 -10.57
'MAGNESIT	'	-6.1690 -8.2400
'DOLOMITE	'	-9.4360 -17.09
'CALCITE	'	-2.2970 -8.4800
'KH3SIO4	'	8.9350 -9.9290
'KH2SIO4	'	29.7170 -21.6170
'KHPO4	'	-3.5300 12.3460
'KH2PO4	'	-4.5200 19.5530
'ANHYDRIT	'	-4.3 -4.384
'GYPSUM	'	-0.028 -4.602
'BRUCITE	'	0.8500 -11.4100
'CHRYSOTL	'	27.5850 -51.8000
'ARAGONIT	'	-2.5890 -8.3360
'KMGF	'	4.6740 1.8200
'KCASO4	'	1.5000 2.3090
'KMGOH	'	2.0900 2.2100
'KH3BO3	'	3.2190 -9.2350
'KNH3	'	12.4770 -9.2440
'FORSTRIT	'	4.8700 -28.1100
'DIOPSIDE	'	21.1000 -36.2200
'CLENSTIT	'	6.6750 -16.8700
'KNAHPO	'	0.0 ^.2900
'TREMOLIT	'	90.2150 -140.3000
'KKHPO4	'	0.0 0.2900
'KMGHPO4	'	3.3000 2.8700
'KCAHPO4	'	3.3000 2.7390
'KH2CO3	'	-2.1770 6.3520
'SEPIOLIT	'	26.5320 -40.1000
'TALC	'	45.0650 -62.2900
'HYDMAG	'	-25.5200 -37.8200
'ADULAR	'	30.8200 -20.570[illegible]
'ALBITE	'	25.8950 -18.0000
'ANORTH	'	17.5300 -19.3300
'ANALCM	'	18.2060 -12.7000
'KMICA	'	67.8600 -49.0900
'PHLOG	'	0.0 -63.5300
'ILLITE	'	54.6840 -40.3100
'KAOLIN	'	49.1500 -36.9100
'HALLOY	'	44.6800 -32.8200
'BEIDEL	'	60.3550 -45.2600
'CHLOR	'	54.7600 -90.6100
'ALUNIT	'	29.8200 -85.3200
'GIBCRS	'	14.4700 -32.7700
'BOEHM	'	11.9050 -33.4100
'PYROPH	'	0.0 -42.4300
'PHILIP	'	0.0 -19.8600
'ERION	'	0.0 0.0
'CLINOP	'	0.0 0.0
'MORDEN	'	0.0 0.0
'NAHCOL	'	3.7200 -0.5480
'TRONA	'	-18.0000 -0.7950
'NATRON	'	15.7450 -1.3110
'THRNAT	'	-2.8020 0.1250
'FLUOR	'	4.71 -10.96
'MONTCA	'	58.3730 -45.0000
'HALITE	'	0.9180 1.5820

'THENAR '	-0.5720	-0.1790
'MIRABI '	18.9870	-1.1130
'MACKIT '	0.0	-4.6310
'KHCO3 '	-3.5610	10.329
'KNACO3 '	8.9110	1.2680
'KNAHCO3 '	0.0	-0.2500
'KNASO4 '	1.12	0.7200
'KKSO4 '	2.25	0.8470
'KMGCO3 '	2.7100	2.9800
'KMGHCO3 '	1.0770	1.0660
'KMGSO4 '	4.6	2.2380
'KCAOH '	1.1900	1.4000
'KCAHCO3 '	4.1100	1.0950
'KCACO3 '	3.5560	3.2240
'KCAF+ '	4.1200	0.9400
'KALOH '	1.43	9.030
'KALOH2 '	0.0	18.700
'KALOH4 '	-11.16	33.00
'KALF '	0.0	7.0100
'KALF2 '	20.0000	12.7500
'KALF3 '	2.5000	17.0200
'KALF4 '	0.0	19.7200
'KALSO4 '	2.15	3.02
'KASO42 '	2.84	4.92
'KHSO4 '	4.91	1.987
'KH2SC '	-65.4400	40.6440
'KH2S '	5.2990	-6.9420
'KHS '	12.1000	-12.9180
'KCXY '	34.1570	-20.7800
'KCH4 '	-57.4350	30.7410
'HYXAPT '	17.2250	-59.3500
'FLUAPT '	19.6950	-66.7900
'CHALC '	4.6150	-3.5230
'MAGADI '	0.0	-14.3000
'SILGEL '	5.5000	-2.70
'SILGLAS '	4.4400	-3.0170
'QUARTZ '	6.2200	-4.0050
'KFEOH2 '	0.0	-18.708
'KFEOH3 '	0.0	-26.638
'KFEOH4 '	0.0	-34.638
'KFEOH2 '	28.5650	-20.5700
'VIVIAN '	0.0	-36.0000
'BIOTNET '	-40.6600	-9.5650
'HEMATI '	-30.8450	-4.0070
'MAGHEM '	0.0	6.3700
'GOETH '	25.5550	-44.197
'GREENA '	0.0	-63.1900
'FEOH3A '	0.0	4.8850
'ANNITE '	62.4800	-84.2400
'PYRITE '	11.3000	-18.4800
'MONTBP '	0.0	-34.9700
'MONTAB '	0.0	-29.7800
'HUNTITE '	-25.7600	-30.5100
'GREGITE '	0.0	-17.9700
'FESPPT '	0.0	-3.9150
'KFEH2P '	0.0	2.7000
'KCAPO4 '	3.1000	6.4590
'KCAH2P '	3.4000	1.4080
'KMGPO4 '	3.1000	6.5890
'KMGH2P '	3.4000	1.5130

'KLICH	4.8320	0.2000
'KLISO4	0.0	0.6400
'KNH4R	-187.0550	119.0770
'LAUMON	39.6100	-30.9600
'KSRCH	1.1500	0.8200
'KBACH	1.7500	0.6400
'KNH4SO	0.0	1.1100
'KHCL	0.0	-30.0
'KNACL	0.0	-30.0
'KKCL	0.0	-30.0
'KH2SO4	0.0	-30.0
'KCO2 SATO	0.0	-11.3850
'KCO2	-4.776	-1.468
'KFEHPO	0.0	3.6000
'KFEHP+	0.0	-7.6130
'ALOH3A	12.9900	-31.6100
'PREHNT	10.3900	-11.5200
'STRONT	-0.400	-9.271
'CELEST	0.228	-6.578
'BARITE	6.1410	-9.978
'WITHERIT	6.9500	-8.585
'STRENGIT	-2.0300	-26.4000
'LEON	90.0700	-69.5700
'KSRHCO3	6.05	1.18
'NESQUE	-5.789	-5.2110
'ARTIN	-1.842	-18.4000
'K CO2AQ	33.4570	-21.4950
'KW	13.3410	-13.9920
'SEP FT	0.0	-37.2120
'DIASP	-15.4050	-35.0600
'WAIRKT	26.1400	-26.6200
'KFEHP2	0.0	-7.5830
'KMN 3+	25.7600	-25.5070
'KMNCL+	0.0	0.6070
'KMNCL2	0.0	0.0410
'KMNCL3-	0.0	-0.3050
'KMNOH+	0.0	3.4490
'KMN(OH)3	0.0	7.7820
'KMNF+	0.0	0.8500
'KMNSO4	3.7000	1.7080
'KMNNO3,2	-0.3960	0.0590
'KMNHCO3+	0.0	1.7160
'KMNO4-	176.6200	-127.8240
'KMNO4—	150.0200	-118.4400
'KSRCO3	5.22	2.81
'KHMNO2—	0.0	-34.4400
'MANGANO	-24.0250	17.9380
'PYROLUST	-29.1800	15.8610
'BIRNSITE	0.0	18.0910
'NUSTITE	0.0	17.5040
'BIXBYITE	-15.2450	-0.6110
'HAUSMITE	-80.1400	61.5400
'MNOH2	4.1000	-12.9120
'MNOH3	20.0900	-35.6440
'MANGANIT	0.0	-0.2380
'RHODOCHR	-2.0790	-10.5390
'KSRSO4	1.6	2.55
'MNCL2	-17.6220	8.7600
'MNCL2,1W	-7.1750	5.5220
'MNCL2,2W	1.7100	3.9740

'MNCL2,4W '	17.3800	2.7100
'TEPHRITE '	-40.0600	23.1220
'RHODONIT '	-21.8850	9.5220
'MNS GRN '	-5.7900	3.8000
'MNSO4 '	-15.4800	2.6690
'MN2SO4,3 '	-39.0600	-5.7110
'MN3PO4,2 '	2.1200	-23.8270
'MNHPO4 '	0.0	-12.9470

NUMBER	MINERAL NAMES	MINERAL OR SPECIES ABR.	REACTION
1	-----	KFE +3	$Fe^{+2} = Fe^{+3} + e^-$
2	-----	KFEH+2	$Fe^{+2} + H_2O = FeOH^{+2} + e^- + H^+$
3	-----	KFEOH+	$Fe^{+2} + H_2O = FeOH^+ + H^+$
4	-----	KFEOOH	$Fe^{+2} + 2H_2O = FeOOH^- + 3H^+$
5	-----	KFESO4	$Fe^{+2} + SO_4^{-2} = FeSO_4^+ + e^-$
6	-----	KFECL	$Fe^{+2} + Cl^- = FeCl^{+2} + e^-$
7	-----	KFECL2	$Fe^{+2} + 2Cl^- = FeCl_2^+ + e^-$
8	-----	KFECL3	$Fe^{+2} + 3Cl^- = FeCl_3^\circ + e^-$
9	-----	KFESO	$Fe^{+2} + SO_4^{-2} = FeSO_4^\circ$
10	siderite	SIDERITE	$FeCO_3 = Fe^{+2} + CO_3^{-2}$
11	magnesite	MAGNESIT	$MgCO_3 = Mg^{+2} + CO_3^{-2}$
12	dolomite	DOLOMITE	$CaMg(CO_3)_2 = Ca^{+2} + Mg^{+2} + 2CO_3^{-2}$
13	calcite	CALCITE	$CaCO_3 = Ca^{+2} + CO_3^{-2}$
14	-----	KH3SIO	$H_4SiO_4 = H_3SiO_4^- + H^+$
15	-----	KH2SIO	$H_4SiO_4 = H_2SiO_4^{-2} + 2H^+$
16	-----	KHPO4	$H^+ + PO_4^{-3} = HPO_4^{-2}$
17	-----	KH2PO4	$2H^+ + PO_4^{-3} = H_2PO_4^-$
18	anhydrite	ANHYDRIT	$CaSO_4 = Ca^{+2} + SO_4^{-2}$

19	gypsum	GYPSUM	$CaSO_4 \cdot 2H_2O = Ca^{+2} + SO_4^{-2} + 2H_2O$
20	brucite	BRUCITE	$Mg(OH)_2 = Mg^{+2} + 2OH^-$
21	chrysotile	CHRYSOTL	$Mg_3Si_2O_5(OH)_4 + 5H_2O = 3Mg^{+2} + 2H_4SiO_4 + 6OH^-$
22	aragonite	ARAGONIT	$CaCO_3 = Ca^{+2} + CO_3^{-2}$
23	-----	KMGF	$Mg^{+2} + F^- = MgF^+$
24	-----	KCASO4	$Ca^{+2} + SO_4^{-2} = CaSO_4^\circ$
25	-----	KMGOH	$Mg^{+2} + OH^- = MgOH^+$
26	-----	KH3BO3	$H_3BO_3 = H^+ + H_2BO_3^-$
27	-----	KNH3	$NH_4^+ = NH_3 + H^+$
28	forsterite	FORSTRIT	$Mg_2SiO_4 + 4H_2O = 2Mg^{+2} + 2H_4SiO_4 + 4OH^-$
29	diopside	DIOPSIDE	$CaMgSi_2O_6 + 6H_2O = Ca^{+2} + Mg^{+2} + 2H_4SiO_4 + 4OH^-$
30	clinoenstatite	CLENSTIT	$MgSiO_3 + 3H_2O = Mg^{2+} + H_4SiO_4 + 2OH^-$
31	-----	KNAHPO	$Na^+ + HPO_4^{-2} = NaHPO_4^-$
32	tremolite	TREMOLIT	$Ca_2Mg_5Si_8O_{22}(OH)_2 + 22H_2O = 2Ca^{+2} + 5Mg^{+2} + 8H_4SiO_4 + 14OH^-$
33	-----	KKHPO	$K^+ + HPO_4^{-2} = KHPO_4^-$
34	-----	KMGHPO	$Mg^{+2} + HPO_4^{-2} = MgHPO_4^\circ$
35	-----	KCAHPO	$Ca^{+2} + HPO_4^{-2} = CaHPO_4^\circ$
36	-----	KH2CO3	$HCO_3^- + H^+ = CO_2(aq) + H_2O$
37	sepiolite	SEPIALIT	$Mg_2Si_3O_{7.5}(OH) \cdot 3H_2O + 4.5H_2O = 2Mg^{+2} + 3H_4SiO_4 + 4(OH)^-$

38	talc	TALC	$Mg_3Si_4O_{10}(OH)_2 + 10H_2O = 3Mg^{+2} + 4H_4SiO_4 + 6OH^-$
39	hydromagnesite	HYDMAG	$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O = 5Mg^{+2} + 4CO_3^{-2} + 2OH^- + 4H_2O$
40	adularia	ADULAR	$KAlSi_3O_8 + 8H_2O = K^+ + Al(OH)_4^- + 3H_4SiO_4$
41	albite	ALBITE	$NaAlSi_3O_8 + 8H_2O = Na^+ + Al(OH)_4^- + 3H_4SiO_4$
42	anorthite	ANORTH	$CaAl_2Si_2O_8 + 8H_2O = Ca^{+2} + 2Al(OH)_4^- + 2H_4SiO_4$
43	analcime	ANALCM	$NaAlSi_2O_6 \cdot H_2O + 5H_2O = Na^+ + Al(OH)_4^- + 2H_4SiO_4$
44	muscovite	KMICA	$KAl_3Si_3O_{10}(OH)_2 + 12H_2O = K^+ + 3Al(OH)_4^- + 3H_4SiO_4 + 2H^+$
45	phlogopite	PHLOG	$KMg_3AlSi_3O_{10}(OH)_2 + 10H_2O = K^+ + 3Mg^{+2} + Al(OH)_4^- + 3H_4SiO_4 + 6OH^-$
46	illite	ILLITE	$K_{.6}Mg_{.25}Al_{2.3}Si_{3.5}O_{10}(OH)_2 + 11.2H_2O = .6K^+ + .25Mg^{+2} + 2.3Al(OH)_4^- + 3.5H_4SiO_4 + 1.2H^+$
47	kaolinite	KAOLIN	$Al_2Si_2O_5(OH)_4 + 7H_2O = 2Al(OH)_4^- + 2H_4SiO_4 + 2H^+$
48	halloysite	HALLOY	$Al_2Si_2O_5(OH)_4 + 7H_2O = 2Al(OH)_4^- + 2H_4SiO_4 + 2H^+$
49	beidellite	BEIDEL	$(Na,K,\frac{1}{2}Mg)_{.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 12H_2O = .33(Na,K,\frac{1}{2}Mg)^+ + 2.33Al(OH)_4^- + 3.67H_4SiO_4 + 2H^+$
50	chlorite	CHLOR	$Mg_5Al_2Si_3O_{10}(OH)_8 + 10H_2O = 5Mg^{+2} + 2Al(OH)_4^- + 3H_4SiO_4 + 8OH^-$
51	alunite	ALUNIT	$KAl_3(SO_4)_2(OH)_6 = K^+ + 3Al^{+3} + 2SO_4^{-2} + 6OH^-$
52	gibbsite	GIBCRS	$Al(OH)_3 = Al^{+3} + 3OH^-$
53	boehmite	BOEHM	$AlO(OH) + H_2O = Al^{+3} + 3OH^-$
54	pyrophyllite	PYROPH	$Al_2Si_4O_{10}(OH)_2 + 12H_2O = 2Al(OH)_4^- + 4H_4SiO_4 + 2H^+$
55	phillipsite	PHILIP	$Na_{.5}K_{.5}AlSi_3O_8 \cdot H_2O + 7H_2O = 0.5Na^+ + 0.5K^+ + Al(OH)_4^- + 3H_4SiO_4$
56	erionite	ERION	$NaAlSi_{3.5}O_9 \cdot 3H_2O + 6H_2O = Na^+ + Al(OH)_4^- + 3.5H_4SiO_4$

57	clinoptilolite	CLINOP	$(K,Na)AlSi_5O_{12}\cdot 3.5H_2O + 8.5H_2O = (K,Na)^+ + Al(OH)_4^- + 5H_4SiO_4$
58	mordenite	MORDEN	$(Na,K)AlSi_{4.5}O_{11}\cdot 3H_2O + 8H_2O = (Na,K)^+ + Al(OH)_4^- + 4.5H_4SiO_4$
59	nahcolite	NAHCOL	$NaHCO_3 = Na^+ + HCO_3^-$
60	trona	TRONA	$NaHCO_3\cdot Na_2CO_3\cdot 2H_2O = 3Na^+ + HCO_3^- + CO_3^{-2} + 2H_2O$
61	natron	NATRON	$Na_2CO_3\cdot 10H_2O = 2Na^+ + CO_3^{-2} + 10H_2O$
62	thermonatrite	THRNAT	$Na_2CO_3\cdot H_2O = 2Na^+ + CO_3^{-2} + H_2O$
63	fluorite	FLUOR	$CaF_2 = Ca^{+2} + 2F^-$
64	Ca-montmorillonite	MONTCA	$Ca_{.17}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 12H_2O = .17Ca^{+2} + 2.33Al(OH)_4^- + 3.67H_4SiO_4 + 2H^+$
65	halite	HALITE	$NaCl = Na^+ + Cl^-$
66	thenardite	THENAR	$Na_2SO_4 = 2Na^+ + SO_4^{-2}$
67	mirabilite	MIRABI	$Na_2SO_4\cdot 10H_2O = 2Na^+ + SO_4^{-2} + 10H_2O$
68	mackinawite	MACKIT	$FeS + H^+ = Fe^{+2} + HS^-$
69	-----	KHCO3	$CO_3^{-2} + H^+ = HCO_3^-$
70	-----	KNACO3	$Na^+ + CO_3^{-2} = NaCO_3^-$
71	-----	KNAHCO3	$Na^+ + HCO_3^- = NaHCO_3^\circ$
72	-----	KNASO4	$Na^+ + SO_4^{-2} = NaSO_4^-$
73	-----	KKSO4	$K^+ + SO_4^{-2} = KSO_4^-$
74	-----	KMGCO3	$Mg^{+2} + CO_3^{-2} = MgCO_3^\circ$
75	-----	KMGHCO3	$Mg^{+2} + HCO_3^- = MgHCO_3^+$

76	-----	KMGSO4	$Mg^{+2} + SO_4^{-2} = MgSO_4^{\circ}$
77	-----	KCAOH	$Ca^{+2} + OH^{-} = CaOH^{+}$
78	-----	KCAHCO3	$Ca^{+2} + HCO_3^{-} = CaHCO_3^{+}$
79	-----	KCACO3	$Ca^{+2} + CO_3^{-2} = CaCO_3^{\circ}$
80	-----	KCAF+	$Ca^{+2} + F^{-} = CaF^{+}$
81	-----	KALOH	$Al^{+3} + OH^{-} = AlOH^{+2}$
82	-----	KALOH2	$Al^{+3} + 2OH^{-} = Al(OH)_2^{+}$
83	-----	KALOH4	$Al^{+3} + 4OH^{-} = Al(OH)_4^{-}$
84	-----	KALF	$Al^{+3} + F^{-} = AlF^{+2}$
85	-----	KALF2	$Al^{+3} + 2F^{-} = AlF_2^{+}$
86	-----	KALF3	$Al^{+3} + 3F^{-} = AlF_3^{\circ}$
87	-----	KALF4	$Al^{+3} + 4F^{-} = AlF_4^{-}$
88	-----	KALSO4	$Al^{+3} + SO_4^{-2} = AlSO_4^{+}$
89	-----	KASO42	$Al^{+3} + 2SO_4^{-2} = Al(SO_4)_2^{-}$
90	-----	KHSO4	$H^{+} + SO_4^{-2} = HSO_4^{-}$
91	-----	KH2SC	$SO_4^{-2} + 10H^{+} + 8e^{-} = H_2S + 4H_2O$
92	-----	KH2S	$H_2S = H^{+} + HS^{-}$
93	-----	KHS	$HS^{-} = H^{+} + S^{-2}$
94	-----	KOXY	$.5H_2O = .25O_2 + H^{+} + e^{-}$

95	-----	KCH4	$HCO_3^- + 8e^- + 9H^+ = CH_4 + 3H_2O$
96	hydroxyapatite	HYXAPT	$Ca_5(PO_4)_3(OH) + 3H_2O = 5Ca^{+2} + 3HPO_4^{-2} + 4OH^-$
97	fluorapatite	FLUAPT	$Ca_5(PO_4)_3F + 3H_2O = 5Ca^{+2} + 3HPO_4^{-2} + 3OH^- + F^-$
98	chalcedony	CHALC	$SiO_2 + 2H_2O = H_4SiO_4$
99	magadiite	MAGADI	$NaSi_7O_{13}(OH)_3 \cdot 3H_2O + H^+ + 9H_2O = Na^+ + 7H_4SiO_4$
100	cristobalite	CRISTO	$SiO_2 + 2H_2O = H_4SiO_4$
101	silica gel	SILGEL	$SiO_2 + 2H_2O = H_4SiO_4$
102	quartz	QUARTZ	$SiO_2 + 2H_2O = H_4SiO_4$
103	-----	KFEOH2	$Fe^{+2} + 2H_2O = Fe(OH)_2^+ + 2H^+ + e^-$
104	-----	KFEOH3	$Fe^{+2} + 3H_2O = Fe(OH)_3^o + 3H^+ + e^-$
105	-----	KFEOH4	$Fe^{+2} + 4H_2O = Fe(OH)_4^- + 4H^+ + e^-$
106	-----	KFEOH2	$Fe^{+2} + 2H_2O = Fe(OH)_2^o + 2H^+$
107	vivianite	VIVIAN	$Fe_3(PO_4)_2 \cdot 8H_2O = 3Fe^{+2} + 2PO_4^{-3} + 8H_2O$
108	magnetite	MAGNET	$Fe_3O_4 + 8H^+ = 3Fe^{+3} + 4H_2O + e^-$
109	hematite	HEMATI	$Fe_2O_3 + 6H^+ = 2Fe^{+3} + 3H_2O$
110	maghemite	MAGHEM	$Fe_2O_3 + 6H^+ = 2Fe^{+3} + 3H_2O$
111	goethite	GOETH	$FeO(OH) + H_2O = Fe^{+3} + 3OH^-$
112	greenalite	GREENA	$Fe_3Si_2O_5(OH)_4 + 5H_2O = 3Fe^{+2} + 2H_2SiO_4 + 6OH^-$
113	rphous $Fe(OH)_3$	FEOH3A	$Fe(OH)_3 + 3H^+ = Fe^{+3} + 3H_2O$

114	annite	ANNITE	$KFE_3AlSi_3O_{10}(OH)_2 + 10H_2O = K^+ + 3Fe^{+2} + Al(OH)_4^- + 3H_4SiO_4 + 6OH^-$
115	pyrite	PYRITE	$FeS_2 + 2H^+ + 2e^- = Fe^{+2} + 2HS^-$
116	montmorillonite	MONTBF	$(H,Na,K)_{0.28}Mg_{0.29}Fe^{3+}_{0.23}Al_{1.58}Si_{3.93}O_{10}(OH)_2 + 10.04H_2O =$ $0.28(H,Na,K)^+ + 0.29Mg^{+2} + 0.23Fe^{+3} + 1.58\ Al(OH)_4^-$ $+3.93\ H_4SiO_4$
117	montmorillonite	MONTAB	$(H,Na,K)_{0.42}Mg_{0.45}Fe^{+3}_{0.34}Al_{1.47}Si_{3.82}O_{10}(OH)_2 + 9.16H_2O + 0.84H^+$ $=0.42(H,Na,K)^+ + 0.45Mg^{+2} + 0.34Fe^{+3} + 1.47Al(OH)_4^- + 3.82\ H_4SiO_4$
118	huntite	HUNTITE	$CaMg_3(CO_3)_4 = 3Mg^{+2} + Ca^{+2} + 4CO_3^{-2}$
119	greigite	GREGITE	$Fe_3S_4 + 4H^+ + 2e^- = 3Fe^{+2} + 4HS^-$
120	amorphous FeS	FESPPT	$FeS + H^+ = Fe^{+2} + HS^-$
121	--------	KFEH2P	$Fe^{+2} + H_2PO_4^- = FeH_2PO_4^+$
122	--------	KCAPO4	$Ca^{+2} + PO_4^{-3} = CaPO_4^-$
123	--------	KCAH2P	$Ca^{+2} + H_2PO_4^- = CaH_2PO_4^+$
124	--------	KMGPO4	$Mg^{+2} + PO_4^{-3} = MgPO_4^-$
125	---------	KMGH2P	$Mg^{+2} + H_2PO_4^- = MgH_2PO_4^+$
126	---------	KLIOH	$Li^+ + OH^- = LiOH^o$
127	---------	KLISO4	$Li^+ + SO_4^{-2} = LiSO_4^-$
128	---------	KNH4R	$NO_3^- + 10H^+ + 8e^- = NH_4^+ + 3H_2O$
129	Laumontite	LAUMON	$CaAl_2Si_4O_{12}\cdot 4H_2O + 8H_2O = Ca^{+2} + 2Al(OH)_4^- + 4H_4SiO_4$
130	---------	KSROH	$Sr^{+2} + OH^- = SrOH^+$
131	---------	KBAOH	$Ba^{+2} + OH^- = BaOH^+$
132	---------	KNH4SO	$NH_4^+ + SO_4^{-2} = NH_4SO_4^-$

133	-----	KHCL	$H^+ + Cl^- = HCl^\circ$
134	-----	KNACL	$Na^+ + Cl^- = NaCl^\circ$
135	-----	KKCL	$K^+ + Cl^- = KCl^\circ$
136	-----	KH2SO4	$2H^+ + SO_4^{-2} = H_2SO_4^o$
137	-----	KO2SATO	$0.5H_2O = 0.25O_{2(aq)} + H^+ + e^-$
138	-----	KCO2	$CO_{2(g)} + H_2O = H_2CO_3^*$
139	-----	KFEHPO	$Fe^{+2} + HPO_4^{-2} = FeHPO_4^\circ$
140	-----	KFEHP+	$Fe^{+2} + HPO_4^{-2} = FeHPO_4^+ + e^-$
141	amorphous $Al(OH)_3$	ALOH3A	$Al(OH)_3 = Al^{+3} + 3OH^-$
142	prehnite	PREHNT	$Ca_2Al_2Si_3O_{10}(OH)_2 + 8H_2O + 2H^+ = 2Ca^{+2} + 2Al(OH)_4^- + 3H_4SiO_4$
143	strontianite	STRONT	$SrCO_3 = Sr^{+2} + CO_3^{-2}$
144	celestite	CELEST	$SrSO_4 = Sr^{+2} + SO_4^{-2}$
145	barite	BARITE	$BaSO_4 = Ba^{+2} + SO_4^{-2}$
146	witherite	WITHERIT	$BaCO_3 = Ba^{+2} + CO_3^{-2}$
147	strengite	STRENGIT	$FePO_4 \cdot 2H_2O = Fe^{+3} + PO_4^{-3} + 2H_2O$
148	leonhardite	LEON	$Ca_2Al_4Si_8O_{24} \cdot 7H_2O + 17H_2O = 2Ca^{+2} + 4Al(OH)_4^- + 8H_4SiO_4$
149	-----	KSRHCO3	$Sr^{2+} + HCO_3^- = SrHCO_3^+$
150	nesquehonite	NESQUE	$MgCO_3 \cdot 3H_2O = Mg^{+2} + CO_3^{-2} + 3H_2O$
151	-tinite	ARTIN	$Mg_2(OH)_2CO_3 \cdot 3H_2O = 2Mg^{+2} + CO_3^{-2} + 2OH^- + 3H_2O$

152	-----	KO2AQ	$0.5H_2O = 0.25O_2(aq) + H^+ + e^-$
153	-----	KW	$H_2O = H^+ + OH^-$
154	sepiolite	SEP PT	$Mg_2Si_3O_{7.5}(OH).3H_2O + 4.5H_2O = 2Mg^{+2} + 3H_4SiO_4 + 4OH^-$
155	diaspore	DIASP	$AlOOH + H_2O = Al^{+3} + 3OH^-$
156	wairakite	WAIRKT	$CaAl_2Si_4O_{12}.2H_2O + 10H_2O = Ca^{+2} + 2Al(OH)_4^- + 4H_4SiO_4$
157	-----	KFEHP2	$Fe^{+2} + H_2PO_4^- = FeH_2PO_4^{+2} + e^-$
158	-----	KMN3+	$Mn^{+2} = Mn^{+3} + e^-$
159	-----	KMNCL+	$Mn^{+2} + Cl^- = MnCl^+$
160	-----	KMNCL2	$Mn^{+2} + 2Cl^- = MnCl_2^o$
161	-----	KMNCL3-	$Mn^{+2} + 3Cl^- = MnCl_3^-$
162	-----	KMNOH+	$Mn^{+2} + OH^- = MnOH^+$
163	-----	KMN(OH)3	$Mn^{+2} + 3OH^- = Mn(OH)_3^-$
164	-----	KMNF+	$Mn^{+2} + F^- + MnF^+$
165	-----	KMNSO4	$Mn^{+2} + SO_4^= = MnSO_4^o$
166	-----	KMNNO3,2	$Mn^{+2} + 2NO_3^- = Mn(NO_3)_2^o$
167	-----	KMNHCO3+	$Mn^{+2} + HCO_3^- = MnHCO_3^+$

168	-----	KMNO4-	$Mn^{+2} + 4H_2O = MnO_4^- + 8H^+ + 5e^-$
169	-----	KMNO4--	$Mn^{+2} + 4H_2O = MnO_4^{--} + 8H^+ + 4e^-$
170	-----	KSRCO3	$Sr^{2+} + CO_3^{2-} = SrCO_3^o$
171	-----	KHMNO2--	$Mn^{+2} + 2H_2O = HMnO_2^- + 3H^+$
172	manganosite	MANGANO	$MnO + 2H^+ = Mn^{+2} + H_2O$
173	pyrolusite	PYROLUST	$MnO_2 + 4H^+ + e^- = Mn^{+3} + 2H_2O$
174	δ, birnessite	BIRNSITE	$MnO_2 + 4H^+ + e^- = Mn^{+3} + 2H_2O$
175	nsutite	NUSTITE	$MnO_2 + 4H^+ + e^- = Mn^{+3} + 2H_2O$
176	bixbyite	BIXBYITE	$Mn_2O_3 + 6H^+ = 2Mn^{+3} + 3H_2O$
177	hausmanite	HAUSMITE	$Mn_3O_4 + 8H^+ + 2e^- = 3Mn^{+2} + 4H_2O$
178	pyrochrosite	MNOH2	$Mn(OH)_2 = Mn^{+2} + 2OH^-$
179	$Mn(OH)_3$	MNOH3	$Mn(OH)_3 = Mn^{+3} + 3OH^-$
180	manganite	MANGANIT	$MnOOH + 3H^+ = Mn^{+3} + 2H_2O$
181	rhodochrosite	RHODOCHR	$MnCO_3 = Mn^{+2} + CO_3^=$
182	--------	$KSRSO_4$	$Sr^{2+} + SO_4^{2-} = SrSO_4^o$

183	$MnCl_2$	MNCL2	$MnCl_2 = Mn^{+2} + 2Cl^-$
184	$MnCl_2.H_2O$	MNCL2,1W	$MnCl_2.H_2O = Mn^{+2} + 2Cl^- + H_2O$
185	$MnCl_2.2H_2O$	MNCL2,2W	$MnCl_2.2H_2O = Mn^{+2} + 2Cl^- + 2H_2O$
186	$MnCl_2.4H_2O$	MNCL2,4W	$MnCl_2 \cdot 4H_2O = Mn^{+2} + 2Cl^- + 4H_2O$
187	tephroite	TEPHRITE	$Mn_2SiO_4 + 4H^+ = 2Mn^{+2} + H_4SiO_4$
188	rhodonite	RHODONIT	$MnSiO_3 + 2H^+ + H_2O = Mn^{+2} + H_4SiO_4$
189	MnS(green)	MNS GRN	$MnS + H^+ = Mn^{+2} + HS^-$
190	$MnSO_4$	$MNSO_4$	$MnSO_4 = Mn^{+2} + SO_4^{-2}$
191	$Mn_2(SO_4)3$	MN2SO4,3	$Mn_2(SO_4)_3 = 2Mn^{+3} + 3SO_4^{-2}$
192	$Mn_3(PO_4)_2$	MN3PO4,2	$Mn_3(PO_4)_2 = 3Mn^{+2} + 2PO_4^{-3}$
193	$MnHPO_4$	MNHPO4	$MnHPO_4 = Mn^{+2} + HPO_4^{-2}$