SOFTWARE RELEASE NOTICE

1. SRN Number: CSPE - SRN - 275

2. Project Title: CLST	Project No. 20.01402.571
3. SRN Title: OLI Stream Analyzer Software Version 1.1	
4. Originator/Requestor: Vijay Jain	Date: 8/30/02

5. Summary of Actions

■ Release of new software ☐ Change of access software

☐ Release of modified software: ☐ Software Retirement

☐ Enhancements made

☐ Corrections made

6. Validation Status

☐ Validated

☐ Limited Validation

■ Not Validated Explain: Validation process underway

7. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
V. Jain	RO	A
N. Sridhar	RO	A
L. Yang	RO	A
R. Pabalan	RO	A

8. Element Manager Approval: Date: 8/30/02

9. Remarks: Installation test performed 8/30/02 by V. Jain and recorded in notebook 484 pg 37. Results confirmed with tests performed using ESP module of the software (Scientific note books 135 (pg 10,11) and 430 (pg. 30-35).
The results of this test and past verifications using ESP 6.0 and 6.2 versions are attached.
Test results are acceptable.

CNWRA Form TOP-6 (09/01)

SOFTWARE SUMMARY FORM

01. Summary Date: 8/30/02	02. Summary prepared by (Name and phone) Vijay Jain, 5439	03. Summary Action: Acceptance testing for Stream Analyzer Ver 1.1
04. Software Date: 11/16/02	05. Short Title: Thermodynamic Speciation Software	
06. Software Title: Stream Analyzer Version 1.1 (OLI software)		07. Internal Software ID:

08. Software Type: ☐ Automated Data System ■ Computer Program ☐ Subroutine/Module	09. Processing Mode: ■ Interactive ☐ Batch ☐ Combination	10. Application Area a. General: ■ Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific:
11. Submitting Organization and Address: CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: Vijay Jain (210) 522 5439
13. Software Application: Speciation of aqueous solutions		

14. Computer Platform PC	15. Computer Operating System: NT	16. Programming Language(s): NA	17. Number of Source Program Statements: NA
18. Computer Memory Requirements: 100MB	19. Tape Drives: NA	20. Disk Units: NA	21. Graphics: NA
22. Other Operational Requirements NA			

23. Software Availability: ☐ Available ■ Limited ☐ In-House ONLY	24. Documentation Availability: ■ Available ☐ Preliminary ☐ In-House ONLY
25. USER - Vijay Jain Software Developer: _____	Date: 8/30/02

CNWRA Form TOP-4-1 (05/98)

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Title/Name: OLI Stream Analyzer

Version: 1.1

Demonstration workstation: LOKI

Operating System: MS-NT

User: Vijay Jain

NOTE: Acquired software may or may not meet all requirements and will be evaluated on a case-by-case basis.

Installation Testing [TOP-018, Section 5.6]

Has *installation testing* been conducted for each intended computer platform and operating system?

Yes: ☑ No: ☐ N/A: ☐

Computer Platforms: PC Operating Systems: NT

Location of ~~Acceptance~~ Test Results: See SRN & Notebook #484 pg. 37

Comments:. [signature] 7/3/02

Software Output [TOP-018, Section 5.5.4]

Is software designed so that individual runs are uniquely identified by date, time, name of software and version?

Yes: ☐ No: ☑ N/A: ☐

Date and Time Displayed: 8/30/02, 8:25:29 Am

Name/Version Displayed: Stream Analyzer

Comments: (No version)

See acceptance test results.

NOTE: Output identification content and format is typically taken as is.

Medium Documentation [TOP-018, Section 5.5.6]

The physical labeling of software medium (tapes, disks, etc.) contains: Program Name, Module/Name/Title, Module Revision, File type (ASCII, OBJ, EXE), Recording Date, and Operating System(s)?

Yes: ☑ No: ☐ N/A: ☐

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ACQUIRED SOFTWARE NOT TO BE MODIFIED←

User Documentation [TOP-018, Section 5.5.7]

Is there a Users' Manual for the software and is it up-to-date?

Yes: ☑ No: ☐ N/A: ☐

User's Manual Version and Date: OLI Analyzers Manual.pdf (10/04/01)

Comments: See enclosed CD.

Are there basic instructions for the *installation* and *use* of the software?

Yes: ☑ No: ☐ N/A: ☐

Location of Instructions: OLI Analyzer Installation.pdf (07/27/01)

Comments: See enclosed CD.

Configuration Control [TOP-018, Section 5.7, 5.9.3]

Is the Software Summary Form (Form TOP-4-1) completed and signed?

Yes: ☑ No: ☐ N/A: ☐

Date of Approval: August 30, 2002

Is the list of files attached to the Software Summary Form complete and accurate?

Yes: ☑ No: ☐ N/A: ☐

Comments: List attached to SSF.

Is the source code available or, is the executable code available in the case of (acquired/commercial codes)?

Yes: ☑ No: ☐ N/A: ☐

Location of Source Code: Enclosed CD.

Comments:

Have all the script/make files and executable files been submitted to the Software Custodian?

Only the executable files are being submitted.

Yes: ☑ No: ☐ N/A: ☐

Location of executable files: Enclosed CD.

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ACQUIRED SOFTWARE NOT TO BE MODIFIED←

Software Release [TOP-018, Section 5.9]

Upon acceptance of the software as verified above, has a Software Release Notice (SRN), Form TOP-6 been issued and does the version number of the software match the documentation?

Yes: ☑ No: ☐ N/A: ☐

SRN Number: CSPE-SRN-275
Comments:

Software Validation [TOP-018, Section 5.10]

Has a Software Validation Test Plan (SVTP) been prepared for the ***range of application*** of the software?

Yes: ☐ No: ☑ N/A: ☐

Version and Date of SVTP: ___

Date Reviewed and Approved via QAP-002: ___

Comments: Validation process underway

Has a Software Validation Test Report (SVTR) been prepared that documents the results of the validation cases, interpretation of the results, and determination if the software has been validated?

Yes: ☐ No: ☑ N/A: ☐

Version and Date of SVTR: ____

Date Reviewed and Approved via QAP-002: _____

Comments.: Validation Process underway

Additional Comments:

9/24/02 — Software Evaluator/User/Date

Sept 24, 2002 — Software Custodian/Date

NOTE: Product serial number and hardware Key is required to run program. This information is Maintained by CNWRA MIS Dept..

STREAM ANALYZER, VERSION 1.1

```
 Volume in drive E is OLIAnalyzer
 Volume Serial Number is E993-098E


 Directory of E:\

08/23/00  04:00p        <DIR>          .
08/23/00  04:00p        <DIR>          ..
03/26/01  12:36p        <DIR>          acrobat
10/29/01  02:42p             2,808,147 data1.cab
10/29/01  02:42p               279,522 data1.hdr
10/29/01  02:42p            58,802,971 data2.cab
10/05/00  05:11p               339,565 ikernel.ex_
10/29/01  02:42p                   435 layout.bin
12/19/00  03:12p        <DIR>          Manuals
07/19/01  11:44a               491,286 setup.bmp
10/05/00  04:00p                54,272 Setup.exe
10/29/01  02:41p                    83 Setup.ini
08/28/01  02:39p               161,895 setup.inx
              13 File(s)     62,938,176 bytes

 Directory of E:\acrobat

03/26/01  12:36p        <DIR>          .
08/23/00  04:00p        <DIR>          ..
03/19/99  02:25p             5,455,526 ACRD4ENU.EXE
               3 File(s)      5,455,526 bytes

 Directory of E:\Manuals

12/19/00  03:12p        <DIR>          .
08/23/00  04:00p        <DIR>          ..
02/13/01  11:31a             4,161,283 CorrosionAnalyzerManual.PDF
09/28/01  02:08p             1,347,372 Corrosion of Iron in Aqueous.PDF
07/27/01  08:40a               282,901 OLIAnalyzerInstallation.pdf
10/04/01  08:16a             6,075,620 OLIAnalyzers Manual.PDF
10/01/01  01:34p             2,016,549 Removal of Nickel.pdf
               7 File(s)     13,883,725 bytes

     Total Files Listed:
              23 File(s)     82,277,427 bytes
                                      0 bytes free
```

INSTALLATION TEST FOR
~~EVOLUTION OF SOLUTION CHEMISTRY~~
STREAM ANALYZER VER. 1.1. VJ 8/30

Project No. 01402.571
Book No. 484.

37

Page No.

OBJECTIVE: TO CONDUCT INSTALLATION TEST ON STREAM ANALYZER VER. 1.1. (a COMPONENT OF OLI SOFTWARE).

METHOD: USE THE SAME TEST SAMPLE THAT WAS USED BY SRIDHAR (NOTEBOOK 135, PP. ~~36-37~~ 10, 11) 1998 VJ 8/30

AND REPEATED BY L. YANG ON 11/29/2000 IN (NOTE BOOK 430, PP. 30-35).

TEST WAS PERFORMED IN ACCORDANCE WITH TOP-018. S-6.3.

RESULTS:

SOLUTION USED

HCl - 0.5 M.
$CrCl_3$ - variable
25°C at 1 atm. pressure

Filename: Stream Analyzer Acceptance Test. STA.
(This file will be included as a part of Data CD, attached to this Notebook)

Results acceptance test for Stream Anlyzer ver 1.1

Conc. CrCl3 moles	VJ NB 484	NS NB 135	LY NB 430
pH			
4	-0.43	-0.43	-0.43
6	-0.80	-0.81	-0.80
8	-1.08	-1.09	-1.09
CrCl2 (+1)			
4	0.19	0.19	0.19
6	0.34	0.34	0.34
8	0.52	0.53	0.53
CrCl(2+)			
4	3.6	3.6	3.6
6	5.6	5.6	5.6
8	7.5	7.5	7.5

Acceptance test results are acceptable

To Page No. N/A

Invented by [signature] Date 8/30/02
Recorded by

From Notebook #430

Installation Test of OLI Software ESP V6.2e/CSP V2.0e

Date: November 29, 2000
Prepared by: Lietai Yang

In accordance with TOP-018, 5.6.3, the OLI Software ESP V6.2e/CSP V2.0e was tested by N. Sridhar on 11/29/00. Page A-1 to A-3 present the results obtained from ESP V6.2e/V2.0e and Page B-1 to B-2 present the results from Scientific Notebook #135 (page 10 and 11). The results in Page B-1 to B-2 were obtained from ESP V6.0. The two sets of results compares well.

This documentation is recorded in Scientific Notebook #430 (pages 30 through 35).

L. Yang 11/29/00

```
==========================================================================

      O   O   O          L                    I I I I
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  O               O      L                       I
 O                 O     L                       I
 O                 O     L                       I
 O                 O     L                       I
  O               O      L                       I
    O           O        L                       I
      O   O   O          L L L L L L L L      I I I I

E N V I R O N M E N T A L   S I M U L A T I O N   P R O G R A M

V - 6.2   July 1, 1999

SURVEY: FECL2

CHEMISTRY MODEL: FECL2

THIS FILE NAME: FECL2.LIS

DATE: 11/29/2000

==========================================================================
```

TABLE OF CONTENTS

STREAM SECTION

SURVEY VARIABLES SECTION
CRIIICL3IN..... 2
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CRIIICLION..... 2
CRIIIION..... 2
CRIIICL2ION..... 2
CROH3AQ..... 2

J. Young
3/14/02

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CRIIICL3IN moles	PH	CRIIICLION moles	CRIIIION moles	CRIIICL2ION moles	CROH3AQ moles
0.0000	0.4163	0.0000	0.0000	0.0000	0.0000
0.2500	0.4104	0.7557E-01	0.1728	0.1660E-02	0.2121E-19
0.5000	0.3542	0.1832	0.3118	0.4979E-02	0.1556E-19
0.7500	0.2899	0.3276	0.4120	0.1041E-01	0.1051E-19
1.000	0.2254	0.5074	0.4745	0.1811E-01	0.7111E-20
1.250	0.1629	0.7168	0.5053	0.2792E-01	0.4872E-20
1.500	0.1027	0.9488	0.5117	0.3947E-01	0.3377E-20
1.750	0.4449E-01	1.197	0.5002	0.5236E-01	0.2360E-20
2.000	-0.1211E-01	1.457	0.4764	0.6622E-01	0.1658E-20
2.250	-0.6741E-01	1.725	0.4444	0.8075E-01	0.1168E-20
2.500	-0.1217	1.997	0.4075	0.9575E-01	0.8224E-21
2.750	-0.1752	2.271	0.3682	0.1111	0.5786E-21
3.000	-0.2280	2.545	0.3284	0.1267	0.4062E-21
3.250	-0.2802	2.818	0.2896	0.1425	0.2844E-21
3.500	-0.3318	3.089	0.2528	0.1586	0.1985E-21
3.750	-0.3829	3.356	0.2188	0.1750	0.1382E-21
4.000	-0.4334	3.620	0.1880	0.1917	0.9605E-22
4.250	-0.4831	3.881	0.1606	0.2088	0.6667E-22
4.500	-0.5321	4.137	0.1367	0.2263	0.4627E-22
4.750	-0.5803	4.390	0.1160	0.2442	0.3215E-22
5.000	-0.6274	4.639	0.9834E-01	0.2627	0.2240E-22
5.250	-0.6735	4.885	0.8344E-01	0.2817	0.1567E-22
5.500	-0.7184	5.128	0.7097E-01	0.3013	0.1102E-22
5.750	-0.7621	5.368	0.6060E-01	0.3214	0.7795E-23
6.000	-0.8043	5.606	0.5203E-01	0.3421	0.5557E-23
6.250	-0.8452	5.842	0.4496E-01	0.3633	0.3996E-23
6.500	-0.8845	6.076	0.3917E-01	0.3851	0.2900E-23
6.750	-0.9222	6.308	0.3445E-01	0.4074	0.2126E-23
7.000	-0.9582	6.539	0.3060E-01	0.4303	0.1575E-23
7.250	-0.9926	6.769	0.2750E-01	0.4536	0.1181E-23
7.500	-1.025	6.998	0.2502E-01	0.4775	0.8959E-24
7.750	-1.056	7.225	0.2307E-01	0.5018	0.6881E-24
8.000	-1.085	7.452	0.2158E-01	0.5266	0.5354E-24

From Notebook #135

9/17/98 ~~9/18/98~~

Speciation modeling of simulated pit solutions

Objective : The objective is to understand the speciation in concentrated chloride solutions in pits of stainless steels and Ni-base alloys. Such an understanding will aid in an understanding of repassivation mechanisms in pits and in understanding the analyses performed

Approach : Used ESP version 6.0 from OLI Systems, Inc. to determine speciation in $CrCl_3$, $FeCl_2$ and $NiCl_2$ and mixtures.

chemistry Model : $FeCl_2$

Specified Inflows :

H_2O	$FeBr_2$	H_2SO_4
HCl	$FeCl_2$	$NaCl$
$NaOH$	$FeSO_4$	$CrCl_3$
$NiCl_2$	$FeCO_3$	

Temp : 25°C

$Fe\,II\,Cl_2$ = 0
$Ni\,II\,Cl_2$ = 0
$Cr\,III\,Cl_3$ = variable.
HCl = 0.5M

Output of survey : $FeCl_2$.lis saved as excel file $CrCl_3$sur.txt.

No precipitation was noted for $CrCl_3$ upto 8 ~~mm~~ Hence the conc. was increased to 15 m. No ~~0.5~~ 9/18 HCl No precipitation was seen even in this case. Output saved as $CrCl_3$surr.txt

N. Sridhar
9/17/98

From Notebook # 13

-37-

9/17/98 D
~~9/18/98~~

$CrCl_3$ + 0.5M HCl survey

SURVEY: CrCl3
CHEMISTRY MODEL: FECL2
THIS FILE NAME: FECL2.LIS
DATE: 9/17/98

ESP V-6.0 SURVEY-VA 9/17/98 PAGE 2

CRIIICL3IN lmoles	PH lmoles	CRIIICLION lmoles	CRIIIION lmoles	CRIIICL2ION lmoles	CROH3AQ
0	0.4163	0	0	0	0
0.25	0.4103	7.56E-02	0.1728	1.66E-03	2.12E-20
0.5	0.354	0.1832	0.3118	4.98E-03	1.55E-20
0.75	0.2896	0.3277	0.4119	1.04E-02	1.05E-20
1	0.2251	0.5076	0.4742	1.81E-02	7.09E-21
1.25	0.1626	0.7172	0.5049	2.80E-02	4.86E-21
1.5	0.1023	0.9494	0.5111	3.95E-02	3.37E-21
1.75	4.40E-02	1.198	0.4996	5.24E-02	2.35E-21
2	-1.26E-02	1.458	0.4757	6.63E-02	1.65E-21
2.25	-6.80E-02	1.726	0.4436	8.08E-02	1.16E-21
2.5	-0.1223	1.998	0.4066	9.58E-02	8.18E-22
2.75	-0.1759	2.272	0.3673	0.1112	5.76E-22
3	-0.2287	2.546	0.3276	0.1268	4.04E-22
3.25	-0.281	2.819	0.2888	0.1426	2.83E-22
3.5	-0.3327	3.089	0.252	0.1587	1.97E-22
3.75	-0.3838	3.357	0.2181	0.1751	1.37E-22
4	-0.4343	3.621	0.1873	0.1918	9.53E-23
4.25	-0.4841	3.881	0.16	0.2089	6.61E-23
4.5	-0.5331	4.138	0.1361	0.2264	4.59E-23
4.75	-0.5813	4.39	0.1155	0.2444	3.19E-23
5	-0.6285	4.639	9.79E-02	0.2629	2.22E-23
5.25	-0.6746	4.885	8.31E-02	0.282	1.55E-23
5.5	-0.7195	5.128	7.06E-02	0.3015	1.09E-23
5.75	-0.7632	5.368	6.03E-02	0.3217	7.72E-24
6	-0.8055	5.606	5.18E-02	0.3424	5.50E-24
6.25	-0.8463	5.842	4.48E-02	0.3636	3.96E-24
6.5	-0.8856	6.076	3.90E-02	0.3854	2.87E-24
6.75	-0.9233	6.308	3.43E-02	0.4077	2.10E-24
7	-0.9594	6.539	3.05E-02	0.4306	1.56E-24
7.25	-0.9937	6.769	2.74E-02	0.454	1.17E-24
7.5	-1.026	6.997	2.49E-02	0.4778	8.87E-25
7.75	-1.057	7.225	2.30E-02	0.5022	6.81E-25
8	-1.086	7.451	2.15E-02	0.527	5.30E-25

J. Jones 8/19/02

M Sridhar 9/18/98 17 D

Page B = 2

Calculation Summary

Survey1 Calculation for Survey1 - Workstream

Acceptance Test Results for Stream analyzer Ver 1.1.

AUTHOR – V.JAIN 8/30/02

Automatic Chemistry Model
- Public Databank
- Geochem Databank
- Corrosion Databank
- Lab Databank
- Oxidation / Reduction selected.

Composition survey

Chromium(III) chloride

Range	0.0 to 8.0000 mol
Step size	1.0000 mol
No. steps	8
No. points	9

No secondary survey selected

Survey Stream Parameters

CrCl3	Stream Amt	Temp	Pres	pH	ORP	OsPres
mol	mol	°C	atm	pH	V	atm
0.0	56.008	25.000	1.0000	0.41588	0.78995	24.060
1.0000	57.008	25.000	1.0000	0.22699	0.82969	75.067
2.0000	58.008	25.000	1.0000	-8.9819e-3	0.84861	95.768
3.0000	59.008	25.000	1.0000	-0.22340	0.86475	93.324
4.0000	60.008	25.000	1.0000	-0.42740	0.87822	84.466
5.0000	61.008	25.000	1.0000	-0.62042	0.88797	77.864
6.0000	62.008	25.000	1.0000	-0.79678	0.89484	75.376
7.0000	63.008	25.000	1.0000	-0.95075	0.90009	75.392
8.0000	64.008	25.000	1.0000	-1.0780	0.90417	76.157

CrCl3	onic Strengt	H2O	ECond, sp	ECond, mol	Visc, abs	Visc, rel
mol	mol/kg H2O	Activity	1/ohm	cm2/ohm-mol	cP	cP/cP H2O
0.0	0.50001	0.98254	0.17820	360.79	0.91934	1.0321
1.0000	4.8945	0.94788	0.20366	142.04	0.91502	1.0273
2.0000	7.8144	0.93468	0.27290	118.54	0.92140	1.0345
3.0000	10.252	0.93675	0.36035	115.89	0.92932	1.0433
4.0000	12.698	0.94299	0.44462	115.10	0.92461	1.0381
5.0000	15.282	0.94768	0.51977	113.85	0.91977	1.0326
6.0000	17.980	0.94964	0.58706	112.43	0.91522	1.0275
7.0000	20.738	0.94988	0.64874	111.29	0.91063	1.0224
8.0000	23.517	0.94958	0.70739	110.66	0.90591	1.0171

CrCl3	DensityAq	DensityVap	DensitySolid	ensity2nd Li	Enthalpy	EnthAq
mol	g/ml	g/ml	g/ml	g/ml	cal	cal
0.0	1.0058	0.0	0.0	0.0	-3.8118e6	-3.8118e6
1.0000	1.1247	0.0	0.0	0.0	-3.9801e6	-3.9801e6
2.0000	1.2293	0.0	0.0	0.0	-4.1470e6	-4.1470e6
3.0000	1.3266	0.0	0.0	0.0	-4.3131e6	-4.3131e6
4.0000	1.4179	0.0	0.0	0.0	-4.4791e6	-4.4791e6
5.0000	1.5025	0.0	0.0	0.0	-4.6453e6	-4.6453e6
6.0000	1.5812	0.0	0.0	0.0	-4.8117e6	-4.8117e6
7.0000	1.6530	0.0	0.0	0.0	-4.9782e6	-4.9782e6
8.0000	1.7185	0.0	0.0	0.0	-5.1449e6	-5.1449e6

CrCl3	EnthVap	EnthSolid	EnthOrg
mol	cal	cal	cal
0.0	0.0	0.0	0.0
1.0000	0.0	0.0	0.0
2.0000	0.0	0.0	0.0
3.0000	0.0	0.0	0.0
4.0000	0.0	0.0	0.0
5.0000	0.0	0.0	0.0
6.0000	0.0	0.0	0.0
7.0000	0.0	0.0	0.0
8.0000	0.0	0.0	0.0

Stream Inflows

CrCl3	H2O	HCl
mol	mol	mol
0.0	55.508	0.50000
1.0000	55.508	0.50000
2.0000	55.508	0.50000
3.0000	55.508	0.50000
4.0000	55.508	0.50000
5.0000	55.508	0.50000
6.0000	55.508	0.50000
7.0000	55.508	0.50000
8.0000	55.508	0.50000

Species Output (True Species)

CrCl3	H2O	H2O - Vap	HCl - Aq	HCl - Vap	CrCl3	Cr(OH)3 - Aq
mol	mol	mol	mol	mol	mol	mol
0.0	55.508	0.0	8.6358e-8	0.0	0.0	0.0
1.0000	55.508	0.0	5.8249e-7	0.0	0.0	7.2367e-21
2.0000	55.508	0.0	1.2470e-6	0.0	0.0	1.7045e-21
3.0000	55.508	0.0	2.0534e-6	0.0	0.0	4.2250e-22
4.0000	55.508	0.0	3.1265e-6	0.0	0.0	1.0117e-22
5.0000	55.508	0.0	4.5899e-6	0.0	0.0	2.3854e-23
6.0000	55.508	0.0	6.4516e-6	0.0	0.0	5.9578e-24
7.0000	55.508	0.0	8.5425e-6	0.0	0.0	1.6920e-24
8.0000	55.508	0.0	1.0531e-5	0.0	0.0	5.7324e-25

CrCl3	Cr(OH)3	H+1	Cr(OH)4-1	Cr(OH)2+1	Cr+3	CrCl2+1
mol	mol	mol	mol	mol	mol	mol
0.0	0.0	0.50000	0.0	0.0	0.0	0.0
1.0000	0.0	0.50001	1.7612e-31	2.5426e-15	0.47681	0.017985
2.0000	0.0	0.50000	3.3236e-32	1.0585e-15	0.48200	0.065864
3.0000	0.0	0.50000	7.7349e-33	4.3057e-16	0.33483	0.12625
4.0000	0.0	0.50000	1.7153e-33	1.6563e-16	0.19331	0.19114
5.0000	0.0	0.50000	3.5694e-34	6.1991e-17	0.10177	0.26193
6.0000	0.0	0.50000	7.7106e-35	2.4022e-17	0.053974	0.34095
7.0000	0.0	0.50000	1.9285e-35	1.0193e-17	0.031645	0.42868
8.0000	0.0	0.49999	6.0160e-36	4.9067e-18	0.022100	0.52460

CrCl3	CrCl+2	CrOH+2	OH-1	Cl-1	Cr2O3	CrO2
mol	mol	mol	mol	mol	mol	mol
0.0	0.0	0.0	4.2287e-14	0.50000	0.0	0.0
1.0000	0.50521	3.5357e-6	1.7862e-14	2.9589	0.0	0.0
2.0000	1.4521	2.3202e-6	1.1750e-14	4.9162	0.0	0.0
3.0000	2.5389	1.3271e-6	9.2184e-15	6.7086	0.0	0.0
4.0000	3.6156	6.9235e-7	7.1348e-15	8.5022	0.0	0.0
5.0000	4.6363	3.4337e-7	5.2392e-15	10.340	0.0	0.0
6.0000	5.6051	1.7096e-7	3.7575e-15	12.213	0.0	0.0
7.0000	6.5397	8.9322e-8	2.7397e-15	14.103	0.0	0.0
8.0000	7.4534	5.0233e-8	2.0879e-15	15.998	0.0	0.0

CrCl3	CrO3	O2 - Aq	O2 - Vap	Cr	CrCl2	H2 - Aq
mol	mol	mol	mol	mol	mol	mol
0.0	0.0	1.1264e-31	0.0	0.0	0.0	2.2527e-31
1.0000	0.0	7.0262e-30	0.0	0.0	0.0	1.9118e-32
2.0000	0.0	1.2191e-29	0.0	0.0	0.0	1.0710e-32
3.0000	0.0	1.7575e-29	0.0	0.0	0.0	6.8552e-33
4.0000	0.0	1.8550e-29	0.0	0.0	0.0	5.1501e-33
5.0000	0.0	1.2049e-29	0.0	0.0	0.0	4.8918e-33
6.0000	0.0	5.7731e-30	0.0	0.0	0.0	5.3658e-33
7.0000	0.0	2.6284e-30	0.0	0.0	0.0	6.0123e-33
8.0000	0.0	1.2733e-30	0.0	0.0	0.0	6.5226e-33

CrCl3	H2 - Vap	Cr2O7-2	Cr+2	HCrO4-1	CrO4-2
mol	mol	mol	mol	mol	mol
0.0	0.0	0.0	0.0	0.0	0.0
1.0000	0.0	5.5998e-52	6.3811e-27	2.1177e-27	1.1303e-32
2.0000	0.0	6.2864e-53	2.0195e-27	6.5691e-28	2.4510e-33
3.0000	0.0	5.2896e-54	6.2210e-28	1.8394e-28	4.6167e-34
4.0000	0.0	2.6145e-55	1.9398e-28	3.9929e-29	6.7323e-35
5.0000	0.0	6.3742e-57	6.6513e-29	6.1095e-30	7.0067e-36
6.0000	0.0	1.1997e-58	2.5550e-29	8.2269e-31	6.6060e-37
7.0000	0.0	2.9954e-60	1.0885e-29	1.2781e-31	7.5076e-38
8.0000	0.0	1.3140e-61	5.1591e-30	2.6360e-32	1.1973e-38