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Performance Assessment
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subject: Recommended μ^0/RT Values for Modeling the Solubility of Oxalate Solids in WIPP Brines

For consistency with the parameter values recommended for modeling organic ligands in WIPP brines (Giambalvo, 2002), it is necessary to recalculate the normalized chemical potentials (μ^0/RT, where R is the ideal gas constant and T is temperature in Kelvin) assigned to the oxalate (Ox) solid phases ($H_2Ox \cdot 2H_2O_{(s)}$, $NaHOx \cdot H_2O_{(s)}$, $Na_2Ox_{(s)}$) in the version of the Fracture Matrix Transport (FMT) database used in compliance baseline performance assessment calculations (baseline database)[1]. Novak (1996) calculated the values used in the current baseline database. I used the nonlinear parameter estimation program NONLIN[2] (SNL, 1996) to recalculate μ^0/RT values from the same solubility data sets that Novak (1996) used. The difference between the two sets of calculations is in the input parameters describing the deprotonation of oxalic acid and the interaction of aqueous oxalate species with Na^+. The current calculation uses input parameters recommended by Giambalvo (2002).

Table 1 compares input parameters used by Novak (1996) to those used in the current calculation. Table 2 compares the μ^0/RT values in the baseline database to those calculated here. Figures 1-3 compare measured solubilities to the solubilities predicted using the new μ^0/RT values. Input and output files necessary to reconstruct the current calculations are attached as an appendix. The new μ^0/RT values should be used in conjunction with organic ligand parameters recommended by Giambalvo (2002).

References

Choppin, G.R., A.H. Bond, M. Borkowski, M. Bronikowski, J.-F. Chen, S. Lis, J. Mizera, O.S. Pokrovsky, N.A. Wall, Y.X. Xia and R.C. Moore, 2001. "Waste Isolation Pilot Plant actinide source term test program: Solubility studies and development of modeling parameters," April 2001, Sandia National Laboratories, Albuquerque, SAND99-0943.

[1] The baseline database is identical to the database used for the Performance Assessment Verification Test (PAVT), and is the most recent documented version of the database (Novak, 1997). It is stored in the CHEMDAT file FMT_970407.CHEMDAT in Sandia National Laboratories' Configuration Management System on the WIPP Alpha Cluster in the library WP$NONPA_CMSROOT:[FMT].

[2] The NONLIN executable is stored in Sandia National Laboratories' Configuration Management System in the library WP$NONPA_CMSROOT:[NL] and class PA96 as NL_NONLIN_PA96.EXE. It runs under the VMS operating system on Sandia's WIPP DEC/COMPAQ Alpha cluster.

WIPP:1.3.5.1.2.1:PA:QA:FMT Database for the CRA

Giambalvo, E.R., 2002. "Recommended Parameter Values for Modeling Organic Ligands in WIPP Brines," Memo to L. H. Brush, 25 July 2002, Carlsbad, NM: Sandia National Laboratories. ERMS 522981.

Mizera, J., A.H. Bond, G.R. Choppin and R.C. Moore, 1999. Dissociation constants of carboxylic acids at high ionic strengths in *Actinide Speciation in High Ionic Strength Media*, eds. Reed et al., Kluwer Academic/Plenum Publishers, New York, pp. 113-124.

Novak, C.F., 1996. "Thermodynamic parameters for the solubility of $H_2Ox \cdot 2H_2O(s)$, $NaHOx \cdot H_2O(s)$, and $Na_2Ox(s)$," memo to R. C. Moore, 16 April 1996, Albuquerque: Sandia National Laboratories. WPO 37048.

Novak, C.F., 1997. "Calculation of actinide solubilities in WIPP SPC and ERDA-6 brines under MgO backfill scenarios containing either nesquehonite or hydromagnesite as the $Mg\text{-}CO_3$ solubility-limiting phase," Memo to R. V. Bynum, April 21, 1997, Albuquerque, NM: Sandia National Laboratories. WPO 46124.

SNL, 1996. "User's Manual for NONLIN, Version 2.0," 31 January 1996, Sandia National Laboratories, Albuquerque, NM, 75 pp. WPO 30740.

ERG:6821:erg/(2002-1010, Rev. A)

Copy to:

MS-1395,	M.K. Knowles	[Dept. 6821]
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MS-1395,	E.R. Giambalvo	[Dept. 6821]
MS-1395,	Day File	[Dept. 6821]

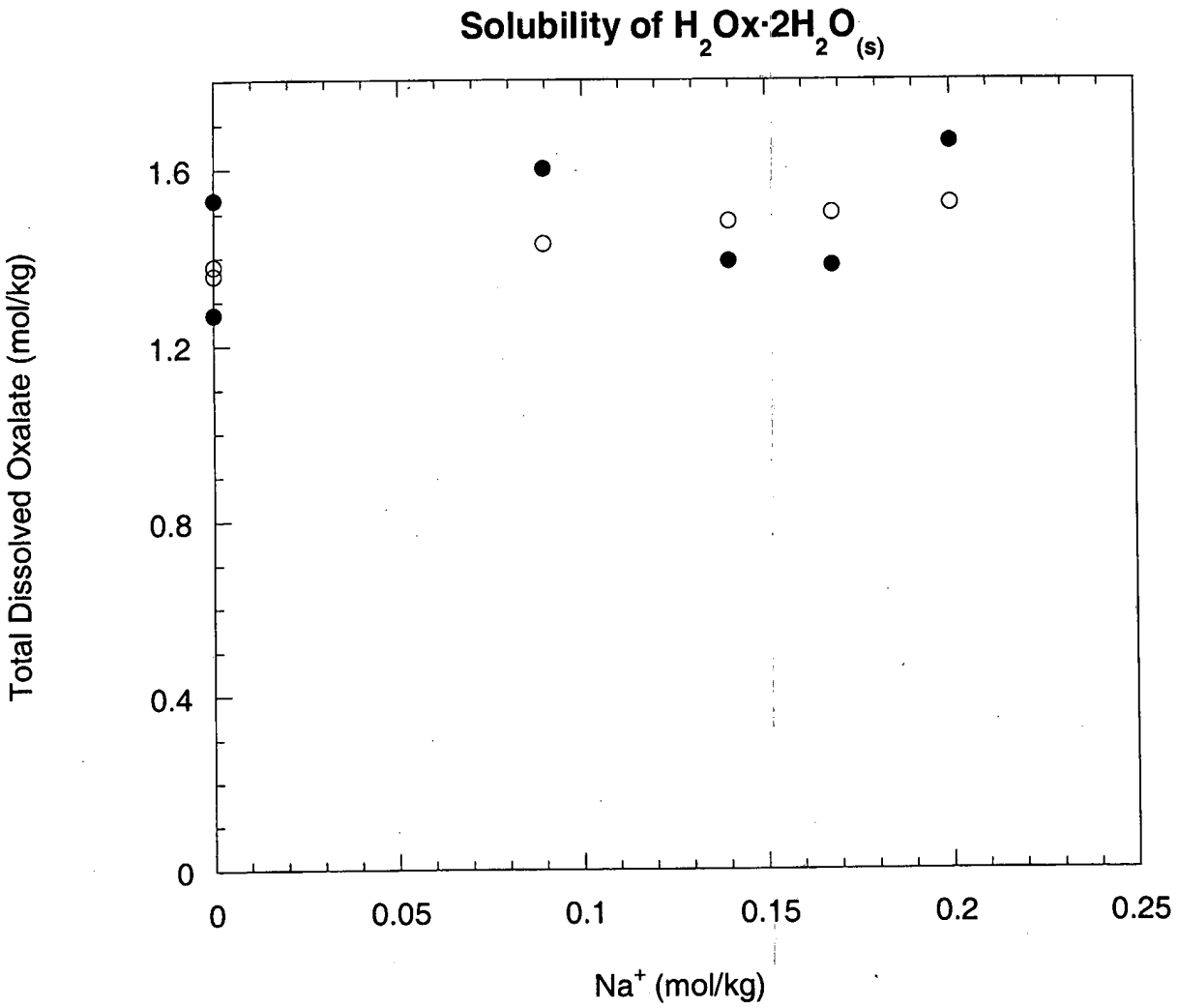

Figure 1. Solubility of $H_2Ox \cdot 2H_2O_{(s)}$ in the H_2Ox-NaOH system. Filled circles: measured solubility (Novak, 1996); open circles: model predictions.

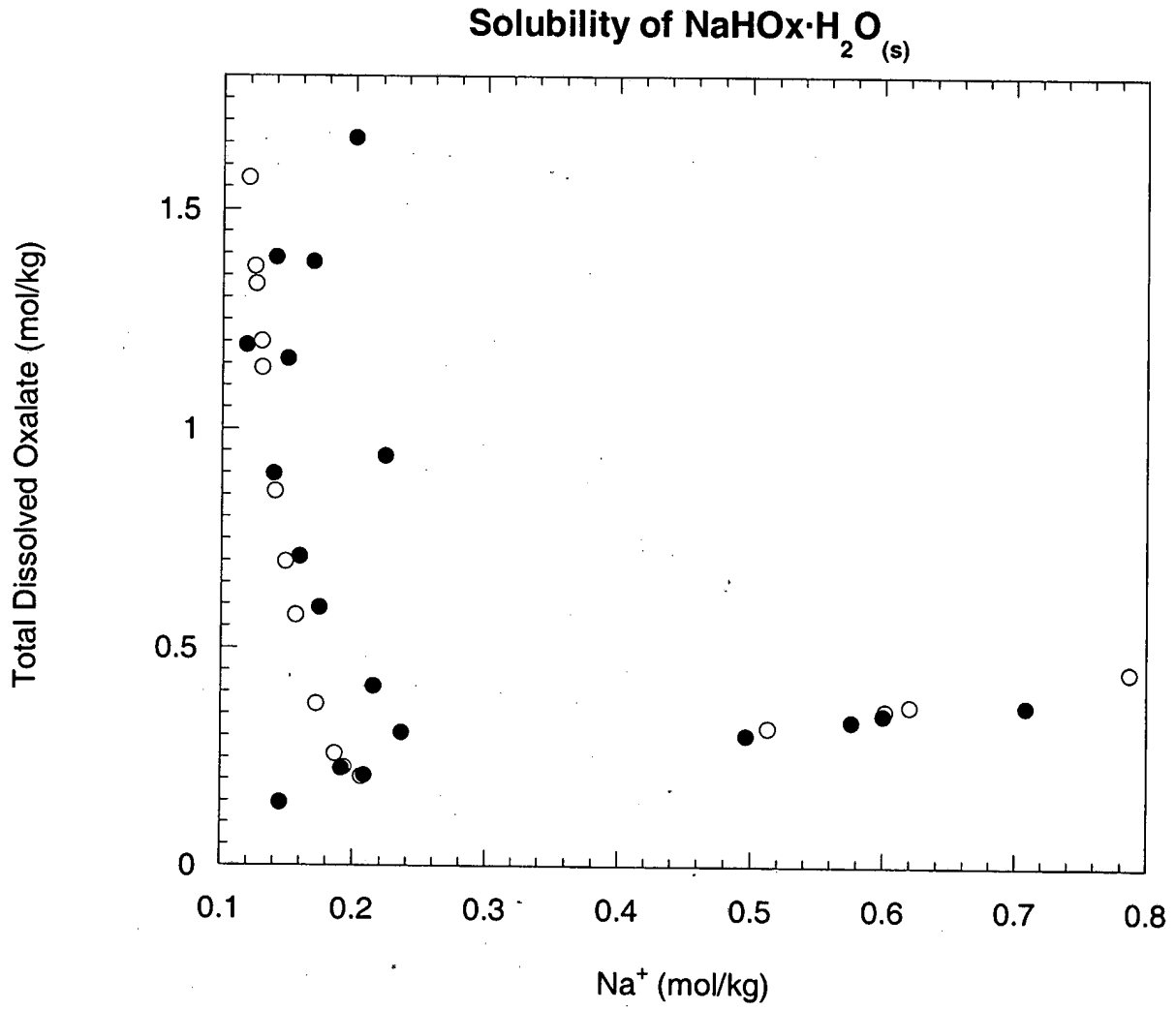

Figure 2. Solubility of $NaHOx \cdot H_2O_{(s)}$ in the H_2Ox-NaOH system. Filled circles: measured solubility (Novak, 1996); open circles: model predictions.

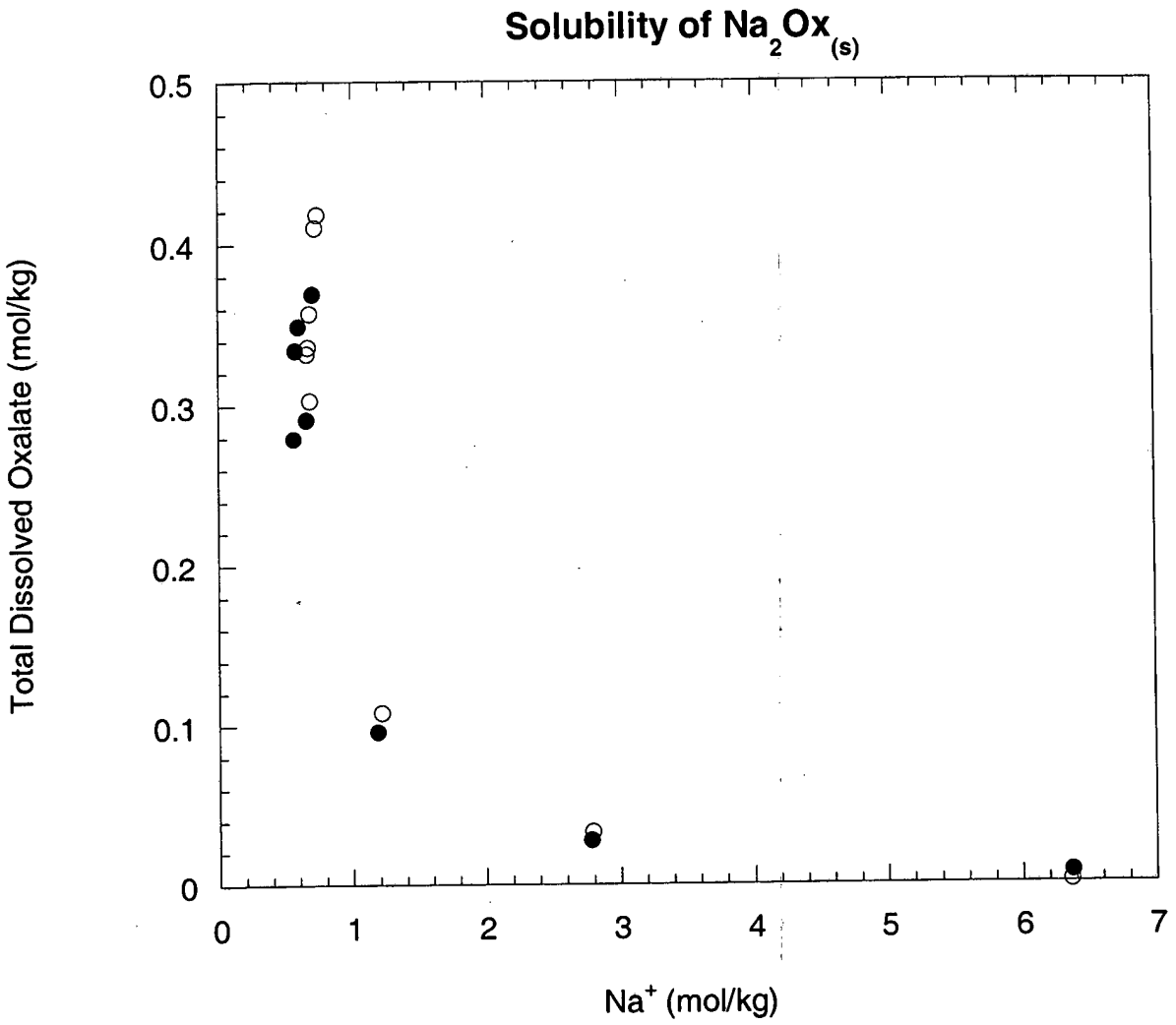

Figure 3. Solubility of $Na_2Ox_{(s)}$ in the H_2Ox-NaOH system. Filled circles: measured solubility (Novak, 1996); open circles: model predictions.

Table 1. Input Parameters that Differ Between Novak (1996) Calculations and This Work

	Novak (1996)	This work[a]
μ^0/RT ($H_2Ox_{(aq)}$)	0.00 [b]	0.000
μ^0/RT (HOx^-)	3.05 [b,c]	3.209
μ^0/RT (Ox^{2-})	12.79 [b]	13.017
$\beta^{(0)}$ (Na^+ - HOx^-)	-0.0307	-0.2448
$\beta^{(1)}$ (Na^+ - HOx^-)	0	0.29
C^ϕ (Na^+ - HOx^-)	0	0.068
$\beta^{(0)}$ (Na^+ - Ox^{2-})	0.0028	-0.2176
$\beta^{(1)}$ (Na^+ - Ox^{2-})	1.661	1.74
C^ϕ (Na^+ - Ox^{2-})	0.027	0.122

[a]Values recommended by Giambalvo, 2002 (original sources are Choppin et al. (2002) and Mizera et al. (1999)).

[b]Normalized to μ^0/RT ($H_2Ox_{(aq)}$) = 0.

[c]Novak (1996) reported μ^0/RT values to two decimal places. This value is listed as 3.052 in the baseline (PAVT) database.

Table 2. Oxalate Solid μ^0/RT Values

	Current baseline[a]	Recommended[b]
$H_2Ox \cdot 2H_2O_{(s)}$	-191.370	-191.346
$NaHOx \cdot H_2O_{(s)}$	-202.245 [c]	-202.253
$Na_2Ox_{(s)}$	-203.651	-203.823

[a]Novak (1996), normalized to μ^0/RT ($H_2Ox_{(aq)}$) = 0.

[b]This work.

[c]The source of this value is unknown. On the basis of Novak (1996) calculations this value should be -202.291.

```
001080H2O            0       -95.6635  1 2.0 8 1.0
001000H+             1        000.000  1 1.0
000080OH-           -1        -63.435  1 1.0 8 1.0
011000Na+            1       -105.651 11 1.0
012000Mg++           2       -183.468 12 1.0
012001Mg++F          2       -183.468 12 1.072 1.0
000170Cl-           -1       -52.9550 17 1.0

090000Th++++         4       -284.227 90 1.0
090001Th++++F        4       -284.227 90 1.072 1.0
095000Am+++          3       -241.694 95 1.0
095001Am+++F         3       -241.694 95 1.072 1.0

095890AmAc++         2       -395.356 95 1.089 1.0
095891AmAc++F        2        999.999 95 1.089 1.073 1.0
095892AmAc++moore    2       -395.239 95 1.089 1.0

090870ThEDTA         0       -285.419 90 1.087 1.0
090871ThEDTAF        0        999.999 90 1.087 1.073 1.0

000890Ac-           -1       -147.347 89 1.0
000891Ac-F          -1       -147.347 89 1.071 1.0

000990Ox=           -2         13.017 99 1.0
000991Ox=F          -2         13.017 99 1.071 1.0
001990HOx-          -1          3.209 99 1.0 1 1.0
001991H2Ox(aq)       0          0.000 99 1.0 1 2.0

000870EDTA==        -4          53.05 87 1.0
000871EDTA==F       -4          53.05 87 1.071 1.0

000860Cit=-         -3         33.410 86 1.0
000861Cit=-F        -3         33.410 86 1.071 1.0

012890MgAc+          1       -333.378 89 1.012 1.0
012891MgAc+F         1        999.999 89 1.012 1.073 1.0

012990MgOx           0       -179.185 99 1.012 1.0
012991MgOxF          0        999.99  99 1.012 1.073 1.0

012870MgEDTA=       -2       -153.734 87 1.012 1.0
012871MgEDTA=F      -2        999.999 87 1.012 1.073 1.0

012860MgCit-        -1       -162.261 86 1.012 1.0
012861MgCit-F       -1        999.999 86 1.012 1.073 1.0

195890AmAc/Am/Ac(s)  0          0.000 73 1.071-1.072-1.0
190870ThEDTA/Th/EDT  0          0.000 73 1.071-1.072-1.0
112890MgAc/Mg/Ac(s)  0          0.000 73 1.071-1.072-1.0
112990MgOx/Mg/Ox(s)  0          0.000 73 1.071-1.072-1.0
112870MgEDTA/Mg/EDT  0          0.000 73 1.071-1.072-1.0
112860MgCit/Mg/Cit   0          0.000 73 1.071-1.072-1.0

111990Na2Ox(s)       0        999.999 11 2.099 1.0
111991NaHOx.H2O(s)   0        999.999 11 1.099 1.001 3.008 1.0
101990H2Ox.2H2O(s)   0        999.999 01 6.099 1.008 2.0

    -1


Reference keys in order are:
H2O HMW84
H+ HMW84
OH- HMW84
```

Na+ HMW84
Mg++ HMW84
Cl- HMW84
Th++++ FRM91
Am+++ FRF90
AmAc++moore SAND99/Moore et al. 99
Ac- NBC96
Ox= SAND99/Mizera
EDTA== SAND99/Mizera
Cit=- SAND99/Mizera

References:
HMW84 = Harvie, Moller, and Weare, 1984. Geochimica et Cosmochimica Acta 48:723-
SAND99 = Choppin et al., 2001. SAND99-0943.
Moore et al 99 = Moore et al., 1999. J. Soln. Chem. 28:521-531.
Mizera = Mizera et al., 1999. in Actinide Speciation in High Ionic Strength Medi
Reed et al., p. 113-124.
FRF90 = Felmy, Rai, and Fulton, 1990. Radiochimica Acta 50:193-204.
NBC96 = Novak, Borkowski, and Choppin, 1996. Radiochimica Acta 74:111-116.
FRM91 = Felmy, Rai, and Mason, 1991. Radiochimica Acta 55:177-185.

011000	000170	.0765	.2664	.000	.00127	Na+ - Cl-	HMW84
011000	000080	.0864	.253	.000	.0044	Na+ - OH-	HMW84
001000	000170	.1775	.2945	.000	.0008	H+ - Cl-	HMW84
095000	000170	.6117	5.403	.000	-.0284	Am+++ - Cl-	FRF90
095001	000170	.6117	5.403	.000	-.0284	Am+++F - Cl-	
090000	000170	1.092	13.7	-160.	-.112	Th++++ - Cl-	Roy92
090001	000170	1.092	13.7	-160.	-.112	Th++++F - Cl-	
012000	000170	.35235	1.6815	.0	.00519	Mg++ - Cl-	HMW84
012001	000170	.35235	1.6815	.0	.00519	Mg++F - Cl-	
011000	000990	-.2176	1.74	.000	.122	Na+ - Ox=	SAND99/Mizera
011000	000991	-.2176	1.74	.000	.122	Na+ - Ox=F	
011000	001990	-.2448	.29	.000	.068	Na+ - HOx-	SAND99/Mizera
011000	000890	.1426	.22	.000	-.00629	Na+ - Ac-	NBC96
011000	000891	.1426	.22	.000	-.00629	Na+ - Ac-F	
011000	000860	0.0887	5.22	.0	.047	Na+ - Cit=-	SAND99/Mizera
011000	000861	0.0887	5.22	.0	.047	Na+ - Cit=-F	
011000	000870	1.016	11.6	.0	.001	Na+ - EDTA==	SAND99/Mizera
011000	000871	1.016	11.6	.0	.001	Na+ - EDTA==F	
011000	012861	.000	0.29	.0	.000	Na+ - MgCit-F	Fix Beta(1) followin
011000	012860	.1742	0.29	.0	-.06923	Na+ - MgCit-	
011000	012870	.2134	1.74	.0	.00869	Na+ - MgEDTA=	
011000	012871	.000	1.74	.0	.000	Na+ - MgEDTA=F	Fix Beta(1) followin
095890	000170	0.3088	1.74	.000	-.132	AmAc++ - Cl-	
095891	000170	0.000	1.74	.000	-.000	AmAc++F - Cl-	Fix Beta(1) followin
095892	000170	1.014	1.74	.000	-.265	AmAc++moore - Cl-	SAND99/Moore et
012890	000170	-.0833	0.29	.000	.0987	MgAc+ - Cl-	
012891	000170	0.0	0.29	.000	.000	MgAc+F - Cl-	Fix Beta(1) followin

000000

cation anion beta0 beta1 beta2 cphi

References:

HMW84 = Harvie, Moller, and Weare, 1984. Geochimica et Cosmochimica Acta 48:723-
SAND99 = Choppin et al., 2001. SAND99-0943.
Moore et al 99 = Moore et al., 1999. J. Soln. Chem. 28:521-531.
Mizera = Mizera et al., 1999. in Actinide Speciation in High Ionic Strength Medi
Reed et al., p. 113-124.
FRF90 = Felmy, Rai, and Fulton, 1990. Radiochimica Acta 50:193-204.
Roy92 = Roy et al., 1992. J. Phys. Chem. 96:11065-11072.
NBC96 = Novak, Borkowski, and Choppin, 1996. Radiochimica Acta 74:111-116.

```
012990 000170 0.0189
012991 000170  0.000
090870 000170 0.1111
090871 000170 0.0000
000000

MgOx Cl lambda
MgOxF Cl lambda
ThEDTA Cl lambda
ThEDTAF Cl lambda

Neutral/ion interaction parameters
```

```
011000 001000   .036 000170   -.004
011000 012000   .07  000170   -.012
011000 012001   .07  000170   -.012
012000 001000   .10  000170   -.011
012001 001000   .10  000170   -.011
000170 000080   -.05 011000   -.006  012000  0.0
000170 000890  -.090 011000  .01029
000170 000891  -.090 011000  .01029
090000 001000   .600 000170  .37
090001 001000   .600 000170  .37
090000 011000   .420 000170  .21
090001 011000   .420 000170  .21
000000
```

Na+	H+	theta	Cl-	psi	HMW84
Na+	Mg++	theta	Cl-	psi	HMW84
Na+	Mg++F	theta	Cl-	psi	
Mg++	H+	theta	Cl-	psi	HMW84
Mg++F	H+	theta	Cl-	psi	
Cl-	OH-	theta	Na+	psi	HMW84
Cl-	Ac-	theta	Na+	psi	NBC96
Cl-	Ac-F	theta	Na+	psi	
Th++++	H+	theta	Cl-	psi	Roy92
Th++++F	H+	theta	Cl-	psi	
Th++++	Na+	theta	Cl-	psi	RFSMMN
Th++++F	Na+	theta	Cl-	psi	

References:
RFSMMN = Rai et al., 1997. Radiochimica Acta 79:239-247.
HMW84 = Harvie, Moller, and Weare, 1984. Geochimica et Cosmochimica Acta 48:723-
Roy92 = Roy et al., 1992. J. Phys. Chem. 96:11065-11072.
NBC96 = Novak, Borkowski, and Choppin, 1996. Radiochimica Acta 74:111-116.

```
$ set def u1:[ergiamb.nonlin.oxsolid]
$!
$ define GMIN u1:[ergiamb.nonlin.oxsolid]h2ox.gmin
$ define INPUT u1:[ergiamb.nonlin.oxsolid]h2ox.in
$ define COMP u1:[ergiamb.nonlin.oxsolid]comp.dat
$ define BINARYP u1:[ergiamb.nonlin.oxsolid]binaryp.dat
$ define LAMBDA u1:[ergiamb.nonlin.oxsolid]lambda.dat
$ define TERNARYP u1:[ergiamb.nonlin.oxsolid]ternaryp.dat
$ define OUTPUT u1:[ergiamb.nonlin.oxsolid]h2ox.out
$!
run u1:[ergiamb.nonlin.cms_files]nl_nonlin_pa96.exe
$!
$ deassign GMIN
$ deassign INPUT
$ deassign COMP
$ deassign BINARYP
$ deassign LAMBDA
$ deassign TERNARYP
$ deassign OUTPUT
end
```

```
     0    0    0    0
0
001080      0.00000000        H2O
001000      0.00000000        H+
011000      0.00000000        Na+
001990      0.00000000        HOx-
000990      0.00000000        Ox=
001991      0.00000000        H2Ox(aq)
000000
101990      .000000000        H2Ox.2H2O(s)
-1
-1
```

```
000007    -476.0          u0(H2Ox.2H2O(s))
-1
  07   -1
0         0        1.14E-00     1.000E-12  1.140E-00  1.00E-10  1.262e-01
0         0        1.07E-00     1.683e-01  1.240E-00  1.00E-10  1.374e-01
0         0        1.14E-00     1.000e-12  1.140E-00  1.00E-10  1.262E-01
0         0        1.11E-00     1.397e-01  1.250E-00  1.00E-10  1.385E-01
0         0        1.38E-00     1.000e-12  1.380E-00  1.00E-10  1.532E-01
0         0        1.35E-00     8.942e-02  1.440E-00  1.00E-10  1.598E-01
0         0        1.29E-00     2.004e-01  1.490E-00  1.00E-10  1.655E-01
-1
-1

 0    0             H             Na         HOx         Ox         H2Ox
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.OXSOLID]H2OX.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.OXSOLID]H2OX.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.OXSOLID]H2OX.OUT;5

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
1000	H+	0.000000000000	1.	0.000
11000	Na+	0.000000000000	1.	-105.651
1990	HOx-	0.000000000000	-1.	3.209
990	Ox=	0.000000000000	-2.	13.017
1991	H2Ox(aq)	0.000000000000	0.	0.000

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
101990	H2Ox.2H2O(s)	0.000000000000	0.	999.999

CONSTRAINT EQUATIONS

	0	1	8	11	99
H2O	0.0	2.0	1.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0
HOx-	-1.0	1.0	0.0	0.0	1.0
Ox=	-2.0	0.0	0.0	0.0	1.0
H2Ox(aq)	0.0	2.0	0.0	0.0	1.0
H2Ox.2H2O(s)	0.0	6.0	2.0	0.0	1.0

Closed input files GMIN and COMP

COMP file name is U1:[ERGIAMB.NONLIN.OXSOLID]COMP.DAT;1
BINARYP file name is U1:[ERGIAMB.NONLIN.OXSOLID]BINARYP.DAT;1
TERNARYP file name is U1:[ERGIAMB.NONLIN.OXSOLID]TERNARYP.DAT;1
LAMBDA file name is U1:[ERGIAMB.NONLIN.OXSOLID]LAMBDA.DAT;1

non-ideal electrolyte parameters

single electrolyte parameters

H+	HOx-	0.00000	0.00000	0.00000	0.00000
H+	Ox=	0.00000	0.00000	0.00000	0.00000
Na+	HOx-	-0.24480	0.29000	0.00000	0.06800
Na+	Ox=	-0.21760	1.74000	0.00000	0.12200

ternary electrolyte parameters

			HOx-	Ox=
H+	Na+	0.03600	0.00000	0.00000

			H+	Na+
HOx-	Ox=	0.00000	0.00000	0.00000

neutral ion parameters

	H2Ox(aq)
H+	0.0000
Na+	0.0000
HOx-	0.0000
Ox=	0.0000
H2Ox(aq)	0.0000

higher order lambdas

		HOx-	Ox=
H2Ox(aq)	H+	0.00000	0.00000
H2Ox(aq)	Na+	0.00000	0.00000

TOTAL NUMBER OF SPECIES = 7
NUMBER OF COMPONENTS = 5
INDEPENDENT CONSTRAINTS = 4

SOLUBILITY DATA

input molalities

H+	Na+	HOx-	Ox=	H2Ox(aq)
1.140E+00	1.000E-12	1.140E+00	1.000E-10	1.262E-01
1.070E+00	1.683E-01	1.240E+00	1.000E-10	1.374E-01
1.140E+00	1.000E-12	1.140E+00	1.000E-10	1.262E-01
1.110E+00	1.397E-01	1.250E+00	1.000E-10	1.385E-01
1.380E+00	1.000E-12	1.380E+00	1.000E-10	1.532E-01
1.350E+00	8.942E-02	1.440E+00	1.000E-10	1.598E-01
1.290E+00	2.004E-01	1.490E+00	1.000E-10	1.655E-01

-4.7600E+02
L2 NORM OF THE RESIDUALS 7.5312432E+02

-1.9135E+02
L2 NORM OF THE RESIDUALS 2.5412871E-01

-1.9135E+02
L2 NORM OF THE RESIDUALS 2.5412871E-01

ADJUSTED PARAMETERS
u0rt(H2Ox.2H2O(s)) -1.9134578E+02

DATA SET(1)

input	calc	diff
0.000000000000000E+000	8.322425715954193E-002	
0.000000000000000E+000	9.664381498101701E-002	
0.000000000000000E+000	8.322425715954193E-002	
0.000000000000000E+000	6.771054644123263E-002	
0.000000000000000E+000	-0.117502997553888	
0.000000000000000E+000	-0.117801815967318	
0.000000000000000E+000	-9.549806222026247E-002	

AVERAGE DEVIATION = 9.4515E-02

STANDARD DEVIATION = 9.6052E-02

FINAL MOLALITIES

H+	Na+	HOx-	Ox=	H2Ox(aq)
3.135E-01	1.000E-12	3.127E-01	4.154E-04	9.531E-01
2.620E-01	1.683E-01	4.306E-01	7.176E-04	9.461E-01
3.135E-01	1.000E-12	3.127E-01	4.154E-04	9.531E-01
2.751E-01	1.397E-01	4.138E-01	6.573E-04	9.741E-01
3.563E-01	1.000E-12	3.554E-01	1.590E-04	1.177E+00

3.285E-01	8.942E-02	4.173E-01	5.953E-04	1.182E+00
2.967E-01	2.004E-01	4.951E-01	8.002E-04	1.160E+00

FINAL LOG ACTIVITIES

H+	Na+	HOx-	Ox=	H2Ox(aq)
-7.066E-01	-1.222E+01	-7.079E-01	-4.261E+00	-2.087E-02
-8.065E-01	-1.034E+00	-6.112E-01	-4.064E+00	-2.405E-02
-7.066E-01	-1.222E+01	-7.079E-01	-4.261E+00	-2.087E-02
-7.828E-01	-1.109E+00	-6.223E-01	-4.099E+00	-1.140E-02
-6.608E-01	-1.223E+01	-6.620E-01	-4.261E+00	7.092E-02
-7.071E-01	-1.301E+00	-6.140E-01	-4.166E+00	7.258E-02
-7.633E-01	-9.767E-01	-5.661E-01	-4.062E+00	6.430E-02

Calculated Log Activity Coefficients

H+	Na+	HOx-	Ox=	H2Ox(aq)
-0.2029	-0.2178	-0.2030	-0.8792	0.0000
-0.2248	-0.2601	-0.2452	-0.9202	0.0000
-0.2029	-0.2178	-0.2030	-0.8792	0.0000
-0.2222	-0.2542	-0.2390	-0.9168	0.0000
-0.2125	-0.2309	-0.2126	-0.9225	0.0000
-0.2236	-0.2528	-0.2345	-0.9412	0.0000
-0.2356	-0.2786	-0.2608	-0.9656	0.0000

SOLID PHASE NOW IN EQUILIBRIUM

DATA SET(1)

input	calc	diff
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

H+	Na+	HOx-	Ox=	H2Ox(aq)
3.318E-01	1.000E-12	3.309E-01	4.344E-04	1.044E+00
2.834E-01	1.683E-01	4.519E-01	7.290E-04	1.052E+00
3.318E-01	1.000E-12	3.309E-01	4.344E-04	1.044E+00
2.902E-01	1.397E-01	4.289E-01	6.674E-04	1.049E+00
3.285E-01	1.000E-12	3.276E-01	4.300E-04	1.034E+00
3.002E-01	8.942E-02	3.891E-01	5.708E-04	1.037E+00
2.740E-01	2.004E-01	4.724E-01	7.896E-04	1.043E+00

FINAL LOG ACTIVITIES

H+	Na+	HOx-	Ox=	H2Ox(aq)
-6.877E-01	-1.222E+01	-6.889E-01	-4.261E+00	1.708E-02
-7.779E-01	-1.041E+00	-5.958E-01	-4.077E+00	1.999E-02
-6.877E-01	-1.222E+01	-6.889E-01	-4.261E+00	1.708E-02
-7.634E-01	-1.114E+00	-6.108E-01	-4.107E+00	1.947E-02
-6.877E-01	-1.222E+01	-6.889E-01	-4.261E+00	1.707E-02
-7.385E-01	-1.291E+00	-6.366E-01	-4.158E+00	1.860E-02
-7.923E-01	-9.694E-01	-5.808E-01	-4.048E+00	2.059E-02

Calculated Log Activity Coefficients

H+	Na+	HOx-	Ox=	H2Ox(aq)
-0.2086	-0.2248	-0.2087	-0.8986	-0.0017
-0.2302	-0.2672	-0.2508	-0.9402	-0.0020
-0.2086	-0.2248	-0.2087	-0.8986	-0.0017
-0.2262	-0.2594	-0.2431	-0.9313	-0.0014
-0.2042	-0.2204	-0.2043	-0.8942	0.0027
-0.2159	-0.2429	-0.2266	-0.9142	0.0027
-0.2300	-0.2713	-0.2551	-0.9455	0.0022

FINAL L2 NORM OF THE RESIDUALS 2.5412871E-01

EXIT PARAMETER 3

FINAL APPROXIMATE SOLUTION

0 0 7 -1.9134578E+02

```
$ set def u1:[ergiamb.nonlin.oxsolid]
$!
$ define GMIN u1:[ergiamb.nonlin.oxsolid]nahox.gmin
$ define INPUT u1:[ergiamb.nonlin.oxsolid]nahox.in
$ define COMP u1:[ergiamb.nonlin.oxsolid]comp.dat
$ define BINARYP u1:[ergiamb.nonlin.oxsolid]binaryp.dat
$ define LAMBDA u1:[ergiamb.nonlin.oxsolid]lambda.dat
$ define TERNARYP u1:[ergiamb.nonlin.oxsolid]ternaryp.dat
$ define OUTPUT u1:[ergiamb.nonlin.oxsolid]nahox.out
$!
run u1:[ergiamb.nonlin.cms_files]nl_nonlin_pa96.exe
$!
$ deassign GMIN
$ deassign INPUT
$ deassign COMP
$ deassign BINARYP
$ deassign LAMBDA
$ deassign TERNARYP
$ deassign OUTPUT
end
```

```
     0    0    0    0
0
001080      0.00000000        H2O
001000      0.00000000        H+
011000      0.00000000        Na+
000080      0.00000000        OH-
001990      0.00000000        HOx-
000990      0.00000000        Ox=
001991      0.00000000        H2Ox(aq)
000000
111991      .000000000        NaHOx.2H2O(s)
-1
-1
```

```
000008    -10.0          u0(NaHOx.2H2O(s))
-1
   18   -1
0        0        1.07E-00  1.683E-01  1.000E-13  1.240E-00  1.000e-12  1.374e-01
0        0        1.00E-07  1.488e-01  1.000e-07  1.488e-01  1.000e-12  1.008e+00
0        0        1.00E-07  1.593e-01  1.000e-07  1.593e-01  1.000e-12  5.486e-01
0        0        1.00E-07  1.736e-01  1.000e-07  1.736e-01  1.000e-12  4.181e-01
0        0        1.00E-07  5.759e-01  1.000e-07  1.000e-12  2.879e-01  4.630e-02
0        0        1.11E-00  1.397e-01  1.000e-13  1.250e-00  1.000e-12  1.385e-01
0        0        1.00E-07  1.176e-01  1.000e-07  1.176e-01  1.000e-12  1.069e-00
0        0        1.00E-07  1.391e-01  1.000e-07  1.391e-01  1.000e-12  7.587e-01
0        0        1.00E-07  1.911e-01  1.000e-07  1.911e-01  1.000e-12  3.415e-02
0        0        1.00E-07  4.958e-01  4.960e-01  1.000e-12  1.000e-12  3.020e-01
0        0        1.00E-07  6.003e-01  6.000e-01  1.000e-12  1.000e-12  3.490e-01
0        0        1.29e-00  2.004e-01  1.000e-13  1.490e-00  1.000e-12  1.655e-01
0        0        1.00e-07  2.226e-01  1.000e-07  2.226e-01  1.000e-12  7.167e-01
0        0        1.00e-07  2.147e-01  1.000e-07  2.147e-01  1.000e-12  1.995e-01
0        0        1.00e-07  2.357e-01  1.000e-07  2.357e-01  1.000e-12  7.137e-02
0        0        1.00e-07  7.076e-01  1.000e-07  1.000e-12  3.538e-01  1.509e-02
0        0        1.00e-07  1.452e-01  1.000e-07  1.452e-01  1.000e-12  1.000e-12
0        0        1.00e-07  2.083e-01  1.000e-07  2.083e-01  1.000e-12  1.000e-12
-1
-1

 0   0            H          Na         OH          HOx         Ox         H2Ox
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.OXSOLID]NAHOX.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.OXSOLID]NAHOX.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.OXSOLID]NAHOX.OUT;6

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
1000	H+	0.000000000000	1.	0.000
11000	Na+	0.000000000000	1.	-105.651
80	OH-	0.000000000000	-1.	-63.435
1990	HOx-	0.000000000000	-1.	3.209
990	Ox=	0.000000000000	-2.	13.017
1991	H2Ox(aq)	0.000000000000	0.	0.000

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
111991	NaHOx.H2O(s)	0.000000000000	0.	999.999

CONSTRAINT EQUATIONS

	0	1	8	11	99
H2O	0.0	2.0	1.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0
OH-	-1.0	1.0	1.0	0.0	0.0
HOx-	-1.0	1.0	0.0	0.0	1.0
Ox=	-2.0	0.0	0.0	0.0	1.0
H2Ox(aq)	0.0	2.0	0.0	0.0	1.0
NaHOx.H2O(s)	0.0	3.0	1.0	1.0	1.0

Closed input files GMIN and COMP

COMP file name is U1:[ERGIAMB.NONLIN.OXSOLID]COMP.DAT;1
BINARYP file name is U1:[ERGIAMB.NONLIN.OXSOLID]BINARYP.DAT;1
TERNARYP file name is U1:[ERGIAMB.NONLIN.OXSOLID]TERNARYP.DAT;1
LAMBDA file name is U1:[ERGIAMB.NONLIN.OXSOLID]LAMBDA.DAT;1

non-ideal electrolyte parameters

single electrolyte parameters

H+	OH-	0.00000	0.00000	0.00000	0.00000
H+	HOx-	0.00000	0.00000	0.00000	0.00000
H+	Ox=	0.00000	0.00000	0.00000	0.00000
Na+	OH-	0.08640	0.25300	0.00000	0.00440
Na+	HOx-	-0.24480	0.29000	0.00000	0.06800
Na+	Ox=	-0.21760	1.74000	0.00000	0.12200

ternary electrolyte parameters

			OH-	HOx-	Ox=
H+	Na+	0.03600	0.00000	0.00000	0.00000
			H+	Na+	
OH-	HOx-	0.00000	0.00000	0.00000	
OH-	Ox=	0.00000	0.00000	0.00000	
HOx-	Ox=	0.00000	0.00000	0.00000	

neutral ion parameters

	H2Ox(aq)
H+	0.0000

Na+	0.0000
OH-	0.0000
HOx-	0.0000
Ox=	0.0000
H2Ox(aq)	0.0000

higher order lambdas

		OH-	HOx-	Ox=
H2Ox(aq)	H+	0.00000	0.00000	0.00000
H2Ox(aq)	Na+	0.00000	0.00000	0.00000

TOTAL NUMBER OF SPECIES = 8
NUMBER OF COMPONENTS = 5
INDEPENDENT CONSTRAINTS = 4

SOLUBILITY DATA

input molalities

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
1.070E+00	1.683E-01	1.000E-13	1.240E+00	1.000E-12	1.374E-01
1.000E-07	1.488E-01	1.000E-07	1.488E-01	1.000E-12	1.008E+00
1.000E-07	1.593E-01	1.000E-07	1.593E-01	1.000E-12	5.486E-01
1.000E-07	1.736E-01	1.000E-07	1.736E-01	1.000E-12	4.181E-01
1.000E-07	5.759E-01	1.000E-07	1.000E-12	2.879E-01	4.630E-02
1.110E+00	1.397E-01	1.000E-13	1.250E+00	1.000E-12	1.385E-01
1.000E-07	1.176E-01	1.000E-07	1.176E-01	1.000E-12	1.069E+00
1.000E-07	1.391E-01	1.000E-07	1.391E-01	1.000E-12	7.587E-01
1.000E-07	1.911E-01	1.000E-07	1.911E-01	1.000E-12	3.415E-02
1.000E-07	4.958E-01	4.960E-01	1.000E-12	1.000E-12	3.020E-01
1.000E-07	6.003E-01	6.000E-01	1.000E-12	1.000E-12	3.490E-01
1.290E+00	2.004E-01	1.000E-13	1.490E+00	1.000E-12	1.655E-01
1.000E-07	2.226E-01	1.000E-07	2.226E-01	1.000E-12	7.167E-01
1.000E-07	2.147E-01	1.000E-07	2.147E-01	1.000E-12	1.995E-01
1.000E-07	2.357E-01	1.000E-07	2.357E-01	1.000E-12	7.137E-02
1.000E-07	7.076E-01	1.000E-07	1.000E-12	3.538E-01	1.509E-02
1.000E-07	1.452E-01	1.000E-07	1.452E-01	1.000E-12	1.000E-12
1.000E-07	2.083E-01	1.000E-07	2.083E-01	1.000E-12	1.000E-12

-1.0000E+01
L2 NORM OF THE RESIDUALS 8.1566463E+02

-2.0225E+02
L2 NORM OF THE RESIDUALS 1.7762456E+00

-2.0225E+02
L2 NORM OF THE RESIDUALS 1.7762456E+00

ADJUSTED PARAMETERS
u0rt(NaHOx.H2O(s)) -2.0225354E+02

DATA SET(1)

input calc diff
0.000000000000000E+000 -0.329817979335654
0.000000000000000E+000 -0.148013499040960

```
 0.000000000000000E+000 -8.488694901513925E-002
 0.000000000000000E+000 -0.134411878358377
 0.000000000000000E+000  0.249055907123721
 0.000000000000000E+000 -0.131391267215302
 0.000000000000000E+000  9.785649492400517E-002
 0.000000000000000E+000 -1.534964415988256E-003
 0.000000000000000E+000  1.248886583409871E-002
 0.000000000000000E+000  0.159465291073130
 0.000000000000000E+000  0.193574980792176
 0.000000000000000E+000 -0.559890915572380
 0.000000000000000E+000 -0.539098442678339
 0.000000000000000E+000 -0.299675139430694
 0.000000000000000E+000 -0.343732983230486
 0.000000000000000E+000   1.30881623325661
 0.000000000000000E+000  0.567307885688962
 0.000000000000000E+000 -1.613688700162922E-002

 AVERAGE DEVIATION  =  2.8762E-01

 STANDARD DEVIATION =  4.1867E-01
```

FINAL MOLALITIES

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
2.620E-01	1.683E-01	9.954E-14	4.306E-01	7.176E-04	9.461E-01
2.321E-01	1.488E-01	1.086E-13	3.796E-01	6.549E-04	7.766E-01
1.420E-01	1.593E-01	1.640E-13	2.999E-01	6.825E-04	4.073E-01
1.115E-01	1.736E-01	2.042E-13	2.836E-01	7.692E-04	3.074E-01
1.729E-04	5.759E-01	1.959E-10	9.226E-02	2.419E-01	8.216E-05
2.751E-01	1.397E-01	9.451E-14	4.138E-01	6.573E-04	9.741E-01
2.494E-01	1.176E-01	1.010E-13	3.658E-01	5.923E-04	8.202E-01
1.880E-01	1.391E-01	1.281E-13	3.258E-01	6.168E-04	5.714E-01
1.215E-02	1.911E-01	1.686E-12	1.960E-01	3.645E-03	2.565E-02
2.267E-04	4.958E-01	1.420E-10	1.075E-01	1.944E-01	1.401E-04
1.812E-04	6.003E-01	1.926E-10	9.764E-02	2.513E-01	8.843E-05
2.967E-01	2.004E-01	9.113E-14	4.951E-01	8.002E-04	1.160E+00
1.656E-01	2.226E-01	1.494E-13	3.865E-01	8.644E-04	5.520E-01
5.537E-02	2.147E-01	3.983E-13	2.674E-01	1.317E-03	1.454E-01
2.131E-02	2.357E-01	1.014E-12	2.510E-01	2.994E-03	5.306E-02
4.724E-05	7.076E-01	7.956E-10	3.012E-02	3.388E-01	6.115E-06
3.185E-03	1.452E-01	6.061E-12	1.321E-01	8.140E-03	4.955E-03
3.825E-03	2.083E-01	5.476E-12	1.894E-01	1.138E-02	7.551E-03

FINAL LOG ACTIVITIES

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
-8.065E-01	-1.034E+00	-1.320E+01	-6.112E-01	-4.064E+00	-2.405E-02
-8.498E-01	-1.072E+00	-1.316E+01	-6.537E-01	-4.063E+00	-1.098E-01
-1.045E+00	-1.019E+00	-1.296E+01	-7.383E-01	-3.952E+00	-3.901E-01
-1.146E+00	-9.771E-01	-1.286E+01	-7.597E-01	-3.873E+00	-5.123E-01
-4.045E+00	-4.707E-01	-9.957E+00	-1.434E+00	-1.648E+00	-4.085E+00
-7.828E-01	-1.109E+00	-1.323E+01	-6.223E-01	-4.099E+00	-1.140E-02
-8.162E-01	-1.169E+00	-1.319E+01	-6.635E-01	-4.107E+00	-8.607E-02
-9.300E-01	-1.085E+00	-1.308E+01	-7.068E-01	-4.036E+00	-2.431E-01
-2.086E+00	-9.057E-01	-1.191E+01	-8.982E-01	-3.071E+00	-1.591E+00
-3.915E+00	-5.301E-01	-1.009E+01	-1.336E+00	-1.681E+00	-3.857E+00
-4.032E+00	-4.604E-01	-9.970E+00	-1.420E+00	-1.648E+00	-4.058E+00
-7.633E-01	-9.767E-01	-1.325E+01	-5.661E-01	-4.062E+00	6.430E-02
-9.967E-01	-9.030E-01	-1.301E+01	-6.550E-01	-3.918E+00	-2.581E-01
-1.446E+00	-8.816E-01	-1.256E+01	-7.850E-01	-3.599E+00	-8.373E-01
-1.857E+00	-8.368E-01	-1.214E+01	-8.116E-01	-3.214E+00	-1.275E+00
-4.632E+00	-3.890E-01	-9.370E+00	-1.975E+00	-1.603E+00	-5.214E+00
-2.651E+00	-9.978E-01	-1.115E+01	-1.048E+00	-2.657E+00	-2.305E+00
-2.593E+00	-8.693E-01	-1.141E+01	-9.223E-01	-2.589E+00	-2.122E+00

Calculated Log Activity Coefficients

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
-0.2248	-0.2601	-0.2012	-0.2452	-0.9202	0.0000
-0.2154	-0.2450	-0.1939	-0.2329	-0.8796	0.0000
-0.1977	-0.2213	-0.1733	-0.2153	-0.7865	0.0000
-0.1935	-0.2167	-0.1666	-0.2124	-0.7591	0.0000
-0.2828	-0.2310	-0.2485	-0.3989	-1.0319	0.0000
-0.2222	-0.2542	-0.2024	-0.2390	-0.9168	0.0000
-0.2130	-0.2395	-0.1959	-0.2268	-0.8794	0.0000
-0.2040	-0.2285	-0.1831	-0.2198	-0.8266	0.0000
-0.1709	-0.1870	-0.1399	-0.1904	-0.6331	0.0000
-0.2704	-0.2254	-0.2385	-0.3675	-0.9693	-0.0039
-0.2900	-0.2388	-0.2546	-0.4096	-1.0478	-0.0047
-0.2356	-0.2786	-0.2085	-0.2608	-0.9656	0.0000
-0.2157	-0.2505	-0.1837	-0.2421	-0.8545	0.0000
-0.1892	-0.2134	-0.1556	-0.2123	-0.7182	0.0000
-0.1859	-0.2092	-0.1491	-0.2113	-0.6901	0.0000
-0.3064	-0.2388	-0.2709	-0.4540	-1.1325	0.0000
-0.1537	-0.1598	-0.1305	-0.1689	-0.5676	0.0000
-0.1759	-0.1880	-0.1446	-0.1996	-0.6445	0.0000

SOLID PHASE NOW IN EQUILIBRIUM

DATA SET(1)

input	calc	diff
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
2.710E-01	1.245E-01	9.488E-14	3.959E-01	6.250E-04	9.371E-01
2.359E-01	1.303E-01	1.061E-13	3.649E-01	6.131E-04	7.728E-01
1.438E-01	1.484E-01	1.609E-13	2.910E-01	6.471E-04	4.054E-01
1.141E-01	1.558E-01	1.972E-13	2.686E-01	6.981E-04	3.047E-01
2.228E-04	6.007E-01	1.524E-10	1.169E-01	2.420E-01	1.319E-04
2.785E-01	1.238E-01	9.288E-14	4.013E-01	6.253E-04	9.707E-01
2.470E-01	1.286E-01	1.023E-13	3.743E-01	6.154E-04	8.226E-01
1.880E-01	1.389E-01	1.281E-13	3.257E-01	6.164E-04	5.713E-01
1.212E-02	1.927E-01	1.692E-12	1.971E-01	3.692E-03	2.572E-02
2.663E-04	5.130E-01	1.213E-10	1.246E-01	1.945E-01	1.882E-04

2.208E-04	6.202E-01	1.584E-10	1.174E-01	2.513E-01	1.279E-04
3.132E-01	1.192E-01	8.446E-14	4.307E-01	6.389E-04	1.143E+00
1.794E-01	1.404E-01	1.329E-13	3.186E-01	6.186E-04	5.379E-01
5.910E-02	1.723E-01	3.606E-13	2.294E-01	9.940E-04	1.414E-01
2.295E-02	1.862E-01	8.971E-13	2.051E-01	2.074E-03	5.049E-02
1.785E-04	7.871E-01	2.108E-10	1.093E-01	3.390E-01	8.018E-05
3.809E-03	2.064E-01	5.498E-12	1.877E-01	1.128E-02	7.471E-03
3.805E-03	2.062E-01	5.491E-12	1.874E-01	1.127E-02	7.463E-03

FINAL LOG ACTIVITIES

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
-7.857E-01	-1.153E+00	-1.322E+01	-6.359E-01	-4.110E+00	-2.788E-02
-8.399E-01	-1.125E+00	-1.317E+01	-6.656E-01	-4.085E+00	-1.118E-01
-1.038E+00	-1.046E+00	-1.297E+01	-7.480E-01	-3.970E+00	-3.920E-01
-1.132E+00	-1.018E+00	-1.287E+01	-7.774E-01	-3.905E+00	-5.160E-01
-3.937E+00	-4.597E-01	-1.006E+01	-1.336E+00	-1.659E+00	-3.880E+00
-7.752E-01	-1.157E+00	-1.323E+01	-6.313E-01	-4.116E+00	-1.281E-02
-8.220E-01	-1.134E+00	-1.319E+01	-6.566E-01	-4.094E+00	-8.489E-02
-9.298E-01	-1.086E+00	-1.308E+01	-7.069E-01	-4.037E+00	-2.431E-01
-2.088E+00	-9.028E-01	-1.191E+01	-8.957E-01	-3.068E+00	-1.590E+00
-3.847E+00	-5.205E-01	-1.015E+01	-1.276E+00	-1.689E+00	-3.729E+00
-3.948E+00	-4.520E-01	-1.005E+01	-1.344E+00	-1.656E+00	-3.898E+00
-7.294E-01	-1.181E+00	-1.328E+01	-6.056E-01	-4.136E+00	5.866E-02
-9.479E-01	-1.079E+00	-1.306E+01	-7.144E-01	-4.026E+00	-2.687E-01
-1.407E+00	-9.614E-01	-1.259E+01	-8.358E-01	-3.688E+00	-8.492E-01
-1.811E+00	-9.193E-01	-1.219E+01	-8.789E-01	-3.327E+00	-1.296E+00
-4.059E+00	-3.643E-01	-9.944E+00	-1.431E+00	-1.631E+00	-4.097E+00
-2.595E+00	-8.729E-01	-1.140E+01	-9.258E-01	-2.590E+00	-2.127E+00
-2.595E+00	-8.729E-01	-1.140E+01	-9.258E-01	-2.590E+00	-2.127E+00

Calculated Log Activity Coefficients

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
-0.2186	-0.2482	-0.2007	-0.2334	-0.9056	0.0003
-0.2125	-0.2398	-0.1935	-0.2277	-0.8728	0.0001
-0.1955	-0.2178	-0.1727	-0.2118	-0.7808	0.0001
-0.1897	-0.2107	-0.1653	-0.2064	-0.7486	0.0001
-0.2849	-0.2384	-0.2479	-0.4044	-1.0427	-0.0002
-0.2199	-0.2499	-0.2023	-0.2348	-0.9117	0.0001
-0.2147	-0.2426	-0.1960	-0.2298	-0.8833	-0.0001
-0.2040	-0.2285	-0.1831	-0.2197	-0.8265	0.0000
-0.1714	-0.1877	-0.1402	-0.1911	-0.6348	0.0000
-0.2723	-0.2307	-0.2384	-0.3717	-0.9777	-0.0040
-0.2916	-0.2446	-0.2541	-0.4139	-1.0562	-0.0048
-0.2252	-0.2575	-0.2085	-0.2398	-0.9412	0.0006
-0.2018	-0.2258	-0.1806	-0.2176	-0.8175	0.0006
-0.1787	-0.1976	-0.1508	-0.1963	-0.6857	0.0003
-0.1720	-0.1894	-0.1415	-0.1908	-0.6441	0.0004
-0.3110	-0.2603	-0.2674	-0.4695	-1.1610	-0.0006
-0.1758	-0.1876	-0.1447	-0.1992	-0.6427	-0.0005
-0.1753	-0.1871	-0.1442	-0.1987	-0.6422	0.0000

FINAL L2 NORM OF THE RESIDUALS 1.7762456E+00

EXIT PARAMETER 3

FINAL APPROXIMATE SOLUTION

0 0 8 -2.0225354E+02

```
$ set def u1:[ergiamb.nonlin.oxsolid]
$!
$ define GMIN u1:[ergiamb.nonlin.oxsolid]na2ox.gmin
$ define INPUT u1:[ergiamb.nonlin.oxsolid]na2ox.in
$ define COMP u1:[ergiamb.nonlin.oxsolid]comp.dat
$ define BINARYP u1:[ergiamb.nonlin.oxsolid]binaryp.dat
$ define LAMBDA u1:[ergiamb.nonlin.oxsolid]lambda.dat
$ define TERNARYP u1:[ergiamb.nonlin.oxsolid]ternaryp.dat
$ define OUTPUT u1:[ergiamb.nonlin.oxsolid]na2ox.out
$!
run u1:[ergiamb.nonlin.cms_files]nl_nonlin_pa96.exe
$!
$ deassign GMIN
$ deassign INPUT
$ deassign COMP
$ deassign BINARYP
$ deassign LAMBDA
$ deassign TERNARYP
$ deassign OUTPUT
end
```

```
     0    0    0    0
0
001080      0.00000000        H2O
001000      0.00000000        H+
011000      0.00000000        Na+
000080      0.00000000        OH-
001990      0.00000000        HOx-
000990      0.00000000        Ox=
001991      0.00000000        H2Ox(aq)
000000
111990      .000000000        Na2Ox(s)
-1
-1
```

```
000008    -488.0          u0(Na2Ox(s))
-1
   09   -1
0        0        1.00E-07   0.5759  1.000E-07  1.00E-12  0.2879      0.0463
0        0        1.00E-07   0.5574  1.000E-07  1.00E-12  0.2787      1.00E-12

0        0        1.00E-07   0.6003  6.000E-01  1.00E-12  1.000E-12   3.49E-01
0        0        1.00E-07   0.5574  5.570E-01  1.00E-12  1.000E-12   2.79E-01

0        0        1.00E-07   0.7076  1.000E-07  1.00E-12  3.538E-01   1.509E-02
0        0        1.00E-07   0.6576  7.471E-02  1.00E-12  2.914E-01   1.000E-12
0        0        1.00E-07   1.183   9.914E-01  1.00E-12  9.598E-02   1.000E-12
0        0        1.00E-07   2.777   2.721E+00  1.00E-12  2.770E-02   1.000E-12
0        0        1.00E-07   6.371   6.358E+00  1.00E-12  6.856E-03   1.000E-12
-1
-1

 0   0   H      Na       OH     HOx     Ox      H2Ox
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.OXSOLID]NA2OX.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.OXSOLID]NA2OX.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.OXSOLID]NA2OX.OUT;7

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
1000	H+	0.000000000000	1.	0.000
11000	Na+	0.000000000000	1.	-105.651
80	OH-	0.000000000000	-1.	-63.435
1990	HOx-	0.000000000000	-1.	3.209
990	Ox=	0.000000000000	-2.	13.017
1991	H2Ox(aq)	0.000000000000	0.	0.000

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
111990	Na2Ox(s)	0.000000000000	0.	999.999

CONSTRAINT EQUATIONS

	0	1	8	11	99
H2O	0.0	2.0	1.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0
OH-	-1.0	1.0	1.0	0.0	0.0
HOx-	-1.0	1.0	0.0	0.0	1.0
Ox=	-2.0	0.0	0.0	0.0	1.0
H2Ox(aq)	0.0	2.0	0.0	0.0	1.0
Na2Ox(s)	0.0	0.0	0.0	2.0	1.0

Closed input files GMIN and COMP

COMP file name is U1:[ERGIAMB.NONLIN.OXSOLID]COMP.DAT;1
BINARYP file name is U1:[ERGIAMB.NONLIN.OXSOLID]BINARYP.DAT;1
TERNARYP file name is U1:[ERGIAMB.NONLIN.OXSOLID]TERNARYP.DAT;1
LAMBDA file name is U1:[ERGIAMB.NONLIN.OXSOLID]LAMBDA.DAT;1

non-ideal electrolyte parameters

single electrolyte parameters

H+	OH-	0.00000	0.00000	0.00000	0.00000
H+	HOx-	0.00000	0.00000	0.00000	0.00000
H+	Ox=	0.00000	0.00000	0.00000	0.00000
Na+	OH-	0.08640	0.25300	0.00000	0.00440
Na+	HOx-	-0.24480	0.29000	0.00000	0.06800
Na+	Ox=	-0.21760	1.74000	0.00000	0.12200

ternary electrolyte parameters

			OH-	HOx-	Ox=
H+	Na+	0.03600	0.00000	0.00000	0.00000

			H+	Na+
OH-	HOx-	0.00000	0.00000	0.00000
OH-	Ox=	0.00000	0.00000	0.00000
HOx-	Ox=	0.00000	0.00000	0.00000

neutral ion parameters

	H2Ox(aq)
H+	0.0000

Na+	0.0000
OH-	0.0000
HOx-	0.0000
Ox=	0.0000
H2Ox(aq)	0.0000

higher order lambdas

		OH-	HOx-	Ox=
H2Ox(aq)	H+	0.00000	0.00000	0.00000
H2Ox(aq)	Na+	0.00000	0.00000	0.00000

TOTAL NUMBER OF SPECIES = 8
NUMBER OF COMPONENTS = 5
INDEPENDENT CONSTRAINTS = 4

SOLUBILITY DATA

input molalities

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
1.000E-07	5.759E-01	1.000E-07	1.000E-12	2.879E-01	4.630E-02
1.000E-07	5.574E-01	1.000E-07	1.000E-12	2.787E-01	1.000E-12
1.000E-07	6.003E-01	6.000E-01	1.000E-12	1.000E-12	3.490E-01
1.000E-07	5.574E-01	5.570E-01	1.000E-12	1.000E-12	2.790E-01
1.000E-07	7.076E-01	1.000E-07	1.000E-12	3.538E-01	1.509E-02
1.000E-07	6.576E-01	7.471E-02	1.000E-12	2.914E-01	1.000E-12
1.000E-07	1.183E+00	9.914E-01	1.000E-12	9.598E-02	1.000E-12
1.000E-07	2.777E+00	2.721E+00	1.000E-12	2.770E-02	1.000E-12
1.000E-07	6.371E+00	6.358E+00	1.000E-12	6.856E-03	1.000E-12

-4.8800E+02
L2 NORM OF THE RESIDUALS 8.5253406E+02

-2.0382E+02
L2 NORM OF THE RESIDUALS 1.8762571E+00

-2.0382E+02
L2 NORM OF THE RESIDUALS 1.8762571E+00

ADJUSTED PARAMETERS
u0rt(Na2Ox(s)) -2.0382267E+02

DATA SET(1)

input	calc	diff
0.000000000000000E+000	0.425445627910774	
0.000000000000000E+000	0.297868648171734	
0.000000000000000E+000	0.376622742615447	
0.000000000000000E+000	0.317265532299033	
0.000000000000000E+000	-5.589186591127794E-002	
0.000000000000000E+000	6.175843325691539E-002	
0.000000000000000E+000	0.124120261648272	
0.000000000000000E+000	0.172150402315071	
0.000000000000000E+000	-1.719339788534594	

AVERAGE DEVIATION = 3.9450E-01

STANDARD DEVIATION = 6.2542E-01

FINAL MOLALITIES

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
1.729E-04	5.759E-01	1.959E-10	9.226E-02	2.419E-01	8.216E-05
7.635E-09	5.574E-01	4.609E-06	4.602E-06	2.787E-01	1.761E-13
1.812E-04	6.003E-01	1.926E-10	9.764E-02	2.513E-01	8.843E-05
1.665E-06	5.574E-01	2.146E-08	9.984E-04	2.780E-01	8.315E-09
4.724E-05	7.076E-01	7.956E-10	3.012E-02	3.388E-01	6.115E-06
4.808E-13	6.576E-01	7.471E-02	2.810E-10	2.914E-01	7.000E-15
3.142E-14	1.183E+00	9.914E-01	5.142E-12	9.598E-02	7.000E-15
9.817E-15	2.777E+00	2.721E+00	2.983E-13	2.770E-02	7.000E-15
7.000E-15	6.371E+00	6.358E+00	1.383E-14	6.856E-03	7.000E-15

FINAL LOG ACTIVITIES

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
-4.045E+00	-4.707E-01	-9.957E+00	-1.434E+00	-1.648E+00	-4.085E+00
-8.404E+00	-4.680E-01	-5.597E+00	-5.743E+00	-1.598E+00	-1.275E+01
-4.032E+00	-4.604E-01	-9.970E+00	-1.420E+00	-1.648E+00	-4.058E+00
-6.069E+00	-4.716E-01	-7.932E+00	-3.409E+00	-1.599E+00	-8.084E+00
-4.632E+00	-3.890E-01	-9.370E+00	-1.975E+00	-1.603E+00	-5.214E+00
-1.262E+01	-4.023E-01	-1.387E+00	-9.983E+00	-1.627E+00	-1.415E+01
-1.381E+01	-1.162E-01	-2.014E-01	-1.178E+01	-2.227E+00	-1.415E+01
-1.436E+01	3.216E-01	3.130E-01	-1.322E+01	-3.123E+00	-1.415E+01
-1.447E+01	9.541E-01	9.531E-01	-1.441E+01	-3.567E+00	-1.415E+01

Calculated Log Activity Coefficients

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
-0.2828	-0.2310	-0.2485	-0.3989	-1.0319	0.0000
-0.2873	-0.2141	-0.2603	-0.4063	-1.0435	0.0000
-0.2900	-0.2388	-0.2546	-0.4096	-1.0478	-0.0047
-0.2906	-0.2178	-0.2638	-0.4083	-1.0435	-0.0043
-0.3064	-0.2388	-0.2709	-0.4540	-1.1325	0.0000
-0.2970	-0.2202	-0.2607	-0.4314	-1.0917	0.0000
-0.3086	-0.1891	-0.1977	-0.4895	-1.2087	0.0000
-0.3481	-0.1220	-0.1217	-0.6941	-1.5654	0.0000
-0.3118	0.1499	0.1498	-0.5463	-1.4026	0.0000

SOLID PHASE NOW IN EQUILIBRIUM

DATA SET(1)

input	calc	diff
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	
0.000000000000000E+000	0.000000000000000E+000	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)

1.535E-04	7.277E-01	2.399E-10	9.232E-02	3.177E-01	6.143E-05
7.613E-09	6.642E-01	4.905E-06	4.897E-06	3.321E-01	1.654E-13
1.630E-04	7.388E-01	2.307E-10	9.770E-02	3.205E-01	6.819E-05
1.554E-06	6.716E-01	2.451E-08	9.986E-04	3.351E-01	6.813E-09
4.788E-05	6.843E-01	7.762E-10	3.012E-02	3.271E-01	6.352E-06
4.868E-13	6.812E-01	7.471E-02	2.893E-10	3.032E-01	7.000E-15
3.175E-14	1.208E+00	9.914E-01	5.759E-12	1.083E-01	7.000E-15
9.820E-15	2.787E+00	2.721E+00	3.530E-13	3.284E-02	7.000E-15
7.000E-15	6.360E+00	6.358E+00	7.000E-15	1.248E-03	7.000E-15

FINAL LOG ACTIVITIES

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
-4.118E+00	-3.884E-01	-9.884E+00	-1.487E+00	-1.628E+00	-4.212E+00
-8.421E+00	-4.065E-01	-5.581E+00	-5.754E+00	-1.592E+00	-1.278E+01
-4.097E+00	-3.876E-01	-9.906E+00	-1.467E+00	-1.630E+00	-4.171E+00
-6.116E+00	-4.063E-01	-7.886E+00	-3.449E+00	-1.592E+00	-8.171E+00
-4.623E+00	-4.006E-01	-9.379E+00	-1.967E+00	-1.604E+00	-5.197E+00
-1.261E+01	-3.900E-01	-1.390E+00	-9.978E+00	-1.625E+00	-1.415E+01
-1.381E+01	-1.090E-01	-2.037E-01	-1.174E+01	-2.187E+00	-1.415E+01
-1.436E+01	3.231E-01	3.130E-01	-1.315E+01	-3.051E+00	-1.415E+01
-1.447E+01	9.522E-01	9.520E-01	-1.470E+01	-4.309E+00	-1.415E+01

Calculated Log Activity Coefficients

H+	Na+	OH-	HOx-	Ox=	H2Ox(aq)
-0.3045	-0.2504	-0.2643	-0.4522	-1.1301	0.0000
-0.3029	-0.2288	-0.2712	-0.4437	-1.1133	0.0000
-0.3093	-0.2561	-0.2686	-0.4573	-1.1356	-0.0047
-0.3072	-0.2334	-0.2754	-0.4481	-1.1176	-0.0043
-0.3034	-0.2359	-0.2689	-0.4463	-1.1185	0.0000
-0.3003	-0.2233	-0.2630	-0.4396	-1.1067	0.0000
-0.3110	-0.1909	-0.1999	-0.4972	-1.2217	0.0000
-0.3482	-0.1221	-0.1217	-0.6955	-1.5676	0.0000
-0.3125	0.1488	0.1487	-0.5481	-1.4056	0.0000

FINAL L2 NORM OF THE RESIDUALS 1.8762571E+00

EXIT PARAMETER 2

FINAL APPROXIMATE SOLUTION

0 0 8 -2.0382267E+02