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subject: Recommended Parameter Values for Modeling Organic Ligands in WIPP Brines

1. INTRODUCTION

Tables 1-5 list values for parameters (normalized chemical potential and Pitzer parameters) pertaining to protonation of organic ligands and complexation of organic ligands with actinides and with Mg that are recommended for use in the next release of the FMT (Fracture-Matrix Transport) geochemical database. Also listed are the parameter values contained in the version of the database used for the Performance Assessment Verification Test (PAVT) (Novak, 1997)[1]. All recommended values were calculated using the nonlinear parameter estimation code NONLIN and a consistent set of input parameters describing interaction of organic species and of actinide ions (or Mg^{2+}) with Na^+, Cl^-, and H^+ (Novak et al., 1996; Pokrovsky et al., 1998; Mizera et al., 1999; Moore et al., 1999; Borkowski et al., 2001; Choppin et al., 2001; this work).

2. NEW PARAMETER VALUES FROM THE LITERATURE

Most recommended parameter values were taken from Choppin et al. (2001) and other documents derived from the same experimental data and published concurrently (Pokrovsky et al., 1998; Mizera et al., 1999; Moore et al., 1999; Borkowski et al., 2001). The data analysis contained in these recent documents is based on essentially the same data set used by Moore (1996) to derive most of the parameter values contained in the PAVT version of the database. Differences between the PAVT values and the new recommended values are due primarily to refinements to the parameter fitting process.

The choice of parameters from the literature for two species ($AmLac^{2+}$ and $ThAc^{3+}$) requires further explanation.

[1] The PAVT database is the most recent documented version of the FMT 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].

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

Recommended parameters pertaining to $AmLac^{2+}$ (normalized chemical potential (μ^0/RT, where R is the ideal gas constant and T is temperature in Kelvin) and the binary Pitzer parameters describing interaction with Cl^-) are from Choppin et al. (2001). Moore et al. (1999) had access to the same data set, and deemed it insufficient to calculate parameters for this species. Collection of more data might improve the reliability of this parameter set, but such improvement is not currently necessary because performance assessment calculations of actinide solubility in the Waste Isolation Pilot Plant (WIPP) do not include lactate interactions with metals.

Choppin et al. (2001) and Moore et al. (1999) list two different sets of values for parameters pertaining to $ThAc^{3+}$ (μ^0/RT and the binary Pitzer parameters describing interaction with Cl^-). The differences occur because the two parameter calculations used two different apparent stability constants (β_{101}) for $ThAc^{3+}$ at 0.3 m NaCl. Choppin et al. (2001) report log (β_{101}) = 4.41±0.02, while Moore et al. (1999) report log (β_{101}) = 3.73±0.02. Choppin et al. (2001) refer to the original laboratory notebook documenting the calculation of the apparent stability constant. Comparison of the two reported β_{101} values to those recorded in the notebook (Xia, 1995) allowed determination of the individual experimental runs from which each value was derived. The value reported by Choppin et al. (2001) was apparently derived from a run at low total acetate concentrations (Xia, 1995, pg. 96), and is therefore based on eight data points, all of which were collected in the acetate concentration range in which the 101 complex dominates Th-Ac speciation. The value reported by Moore et al. (1999) was apparently derived from a run at high total acetate concentrations (Xia, 1995, pp. 80-81). β_{101} and β_{102} (the appparent stability constant for $ThAc_2^{2+}$) were fit simultaneously using a data set of seven points, only two of which were collected in the acetate concentration range in which the 101 complex is predominant. Therefore, the recommended values for parameters pertaining to $ThAc^{3+}$ are those listed in Choppin et al. (2001).

3. NEWLY CALCULATED PARAMETER VALUES

Satisfactory references were not available for parameters pertaining to $AmAc^{2+}$, $ThEDTA_{(aq)}$, $MgAc^{2+}$, $MgOx_{(aq)}$, $MgCit^-$, and $MgEDTA^{2-}$. Parameter sets (μ^0/RT and appropriate Pitzer parameters) for each of these species were calculated using NONLIN version 2.0[2] and the apparent stability constant (β_{101}) versus ionic strength data given in Choppin et al. (2001). Calculation and verification of each set of parameters involves two NONLIN calculations (SNL, 1996). In the first calculation, best-fit parameters are determined from log β_{101} versus NaCl molality data. In the second (or verification) calculation the newly determined parameter values are used to predict log β_{101} as a function of NaCl molality. The verification calculation provides the information necessary to visualize the accuracy of the fit.

3.1. $AmAc^{2+}$

A verification calculation run using the the $AmAc^{2+}$ parameter values listed in Choppin et al. (2001; their Tables 43 and 44) and Moore et al. (1999; their Tables II and III(A)) resulted in an inaccurate prediction of the log β_{101} values listed by these authors (Choppin et al., 2001, Tables 26-31; Moore et al., 1999, Table I). I used the β_{101} values listed in Tables 26-31 of Choppin et al. (2001) to

[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.

calculate new values for μ^0/RT and the binary Pitzer parameters describing interaction of $AmAc^{2+}$ with Cl^-. The resulting parameters (Tables 1 and 2) provide a much improved fit to the data (Figure 1).

3.2. $ThEDTA_{(aq)}$

Choppin et al. (2001), concerned that Th hydrolysis species and Na-EDTA complexes were affecting their measurements of $ThEDTA_{(aq)}$ complexation, expressed the opinion that more data should be collected before calculation of μ^0/RT and Pitzer parameters for $ThEDTA_{(aq)}$. They recommended, however, that their β_{101} values for $ThEDTA_{(aq)}$ be used for performance assessment, because their values implicitly account for these additional species, which can be expected to occur in the WIPP. I used their β_{101} values (Choppin et al., 2001, Tables Th55-Th63) to calculate μ^0/RT and the neutral-ion interaction parameter (λ) describing interaction of $ThEDTA_{(aq)}$ with Cl^- (Figure 2; Tables 1 and 3).

3.3. Mg-organic complexes

Choppin et al. (2001) did not calculate parameter sets for the species $MgAc^{2+}$, $MgOx_{(aq)}$, $MgCit^-$, and $MgEDTA^{2-}$, although they did provide values for log β_{101} versus NaCl molality. I used the β_{101} values listed in Tables 32-37 of Choppin et al. (2001) to calculate μ^0/RT and the appropriate Pitzer parameters for each of these species. Figures 3a-d show the data and the model predictions resulting from the recommended parameter values listed in Tables 1-3. No parameter values for $MgLac^+$ were calculated, because no $MgLac^+$ complexation data is available.

All input, output, and database files related to the calculations described in the preceding three paragraphs are attached as an appendix.

4. Parameters for Species that Could be Added to the Database if Desired

Four actinide-organic complexes could be added to the FMT database if desired. These are $NpO_2H_2EDTA^-$, NpO_2HEDTA^{2-}, $ThAc_2^{2+}$, and $ThLac_2^{2+}$. Recommended values for parameters pertaining to these species are listed in Tables 1-2. Values come from the literature (Pokrovsky et al., 1998; Moore et al., 1999; Choppin et al., 2001).

Choppin et al. (2001) listed the same value for $C^\phi(ThAc_2^{2+}\text{-}Cl^-)$ that Moore et al. (1999) listed for $C^\phi(ThLac_2^{2+}\text{-}Cl^-)$, and vice versa. The switch is likely due to a typographical error in one of the two documents. Bob Moore performed the NONLIN modeling for both of these documents. Values obtained from his NONLIN database files (Moore, 2002) match those in Moore et al. (1999). Therefore the Moore et al. (1999) values of $C^\phi(ThAc_2^{2+}\text{-}Cl^-)$ and $C^\phi(ThLac_2^{2+}\text{-}Cl^-)$ are the recommended values (Table 2).

5. Other

The PAVT database also contains values for Pitzer parameters describing interaction of aqueous organic species with ClO_4^-. These parameters are not required for modeling the behavior of organic ligands in WIPP brines. Therefore, they are not considered here.

6. REFERENCES

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Figure 1. Log β_{101} versus NaCl molality for $AmAc^{2+}$. Filled circles: values from Choppin et al. (2001); open squares: model prediction calculated using parameters listed in Choppin et al. (2001) and Moore et al. (1999); open circles: model prediction calculated using parameters listed in Tables 1 and 3.

Figure 2. Log β_{101} versus NaCl molality for $ThEDTA_{(aq)}$. Filled circles: values from Choppin et al. (2001), points at 0.3 and 1 m NaCl are average values calculated from values plotted with X; open circles: model prediction calculated using parameters listed in Tables 1 and 3. Parameter fit used average values at 0.3 and 1 m NaCl.

Figure 3a. Log β_{101} versus NaCl molality for $MgAc^{+}$. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

Figure 3b. Log β_{101} versus NaCl molality for $MgOx_{(aq)}$. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

Figure 3c. Log β_{101} versus NaCl molality for $MgCit^{-}$. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

Figure 3d. Log β_{101} versus NaCl molality for $MgEDTA^{2-}$. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

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1. Appendix notes

2. NONLIN database files (COMP.DAT, BINARYP.DAT, TERNARYP.DAT, and LAMBDA.DAT) containing all of the input parameter values required to calculate the parameter values presented here, as well as all of the calculated parameter values. The calculations presented here can be reproduced from these database files without alteration.

3. Input and output files (IN, GMIN, and OUT files) for all parameter calculations and verification calculations discussed in this memo. These files include:

- amac.in, amac.gmin, amac.out
- rev_amac.in, rev_amac.gmin, rev_amac.out
- rev_amac_moore.in, rev_amac_moore.gmin, rev_amac_moore.out
- thedta.in, thedta.gmin, thedta.out
- rev_thedta.in, rev_thedta.gmin, rev_thedta.out
- mgac.in, mgac.gmin, mgac.out
- rev_mgac.in, rev_mgac.gmin, rev_mgac.out
- mgox.in, mgox.gmin, mgox.out
- rev_mgox.in, rev_mgox.gmin, rev_mgox.out
- mgcit.in, mgcit.gmin, mgcit.out
- rev_mgcit.in, rev_mgcit.gmin, rev_mgcit.out
- mgedta.in, mgedta.gmin, mgedta.out
- rev_mgedta.in, rev_mgedta.gmin, rev_mgedta.out

Files beginning with "rev_" were used or produced in a verification calculation. Other files were used or produced in a parameter calculation. File names are descriptive.

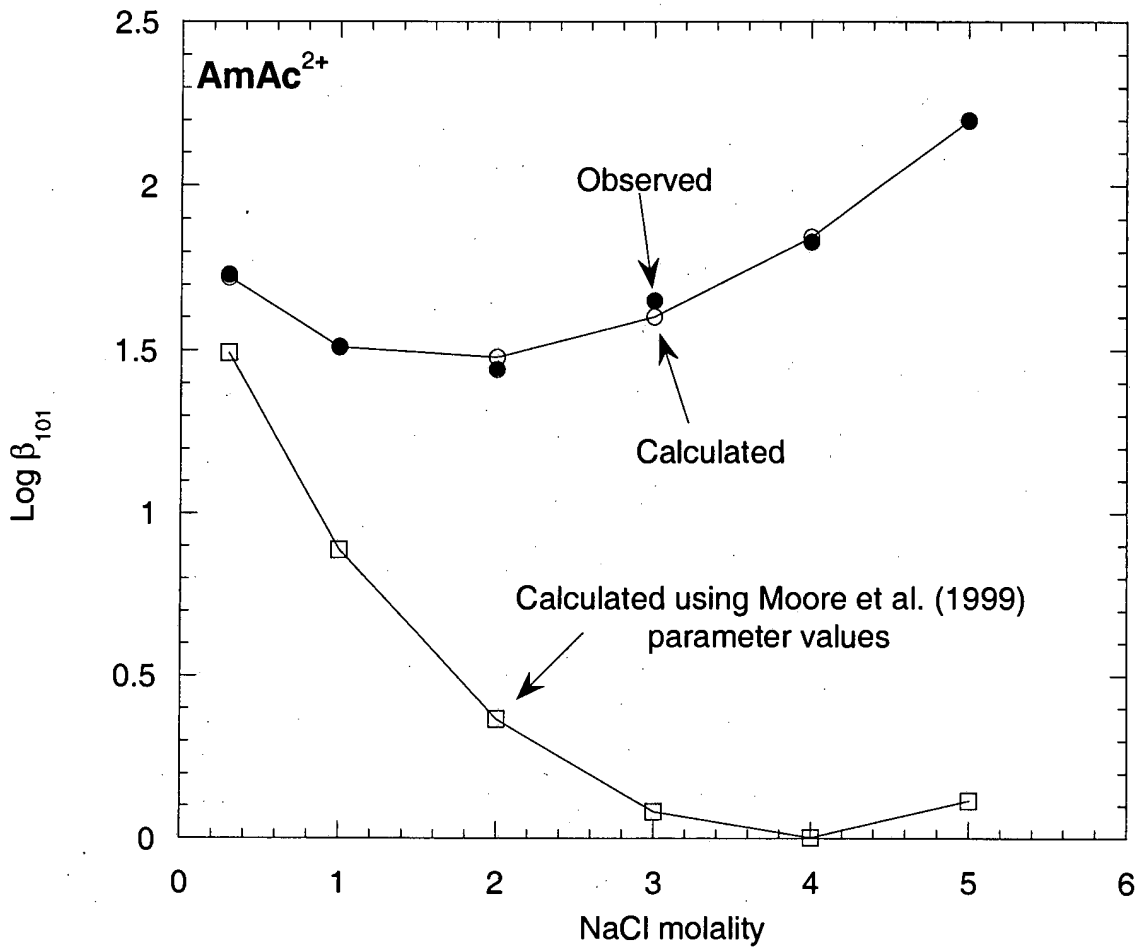

Figure 1. Log β_{101} versus NaCl molality for $AmAc^{2+}$. Filled circles: values from Choppin et al. (2001); open squares: model prediction calculated using parameters listed in Choppin et al. (2001) and Moore et al. (1999); open circles: model prediction calculated using parameters listed in Tables 1 and 3.

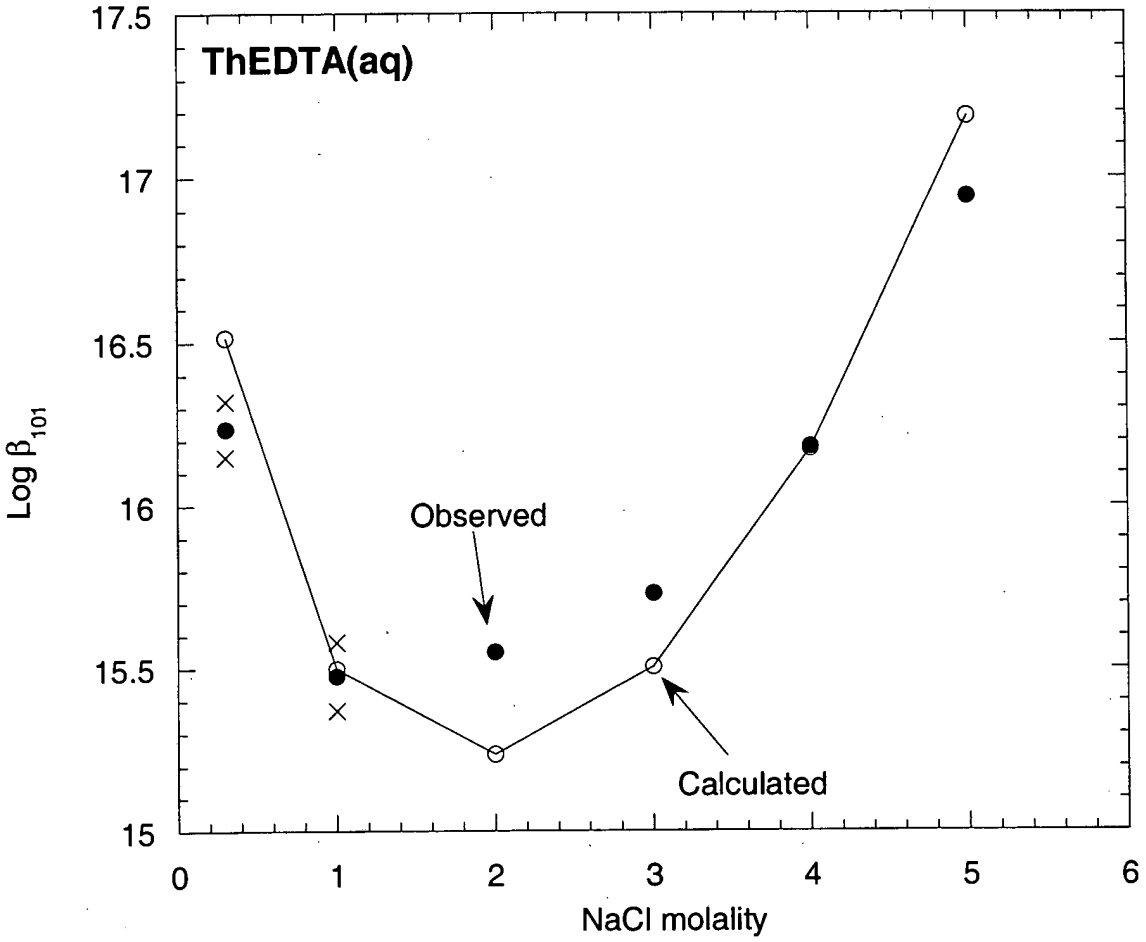

Figure 2. Log β_{101} versus NaCl molality for $ThEDTA_{(aq)}$. Filled circles: values from Choppin et al. (2001), points at 0.3 and 1 m NaCl are average values calculated from values plotted with X; open circles: model prediction calculated using parameters listed in Tables 1 and 3. Parameter fit used average values at 0.3 and 1 m NaCl.

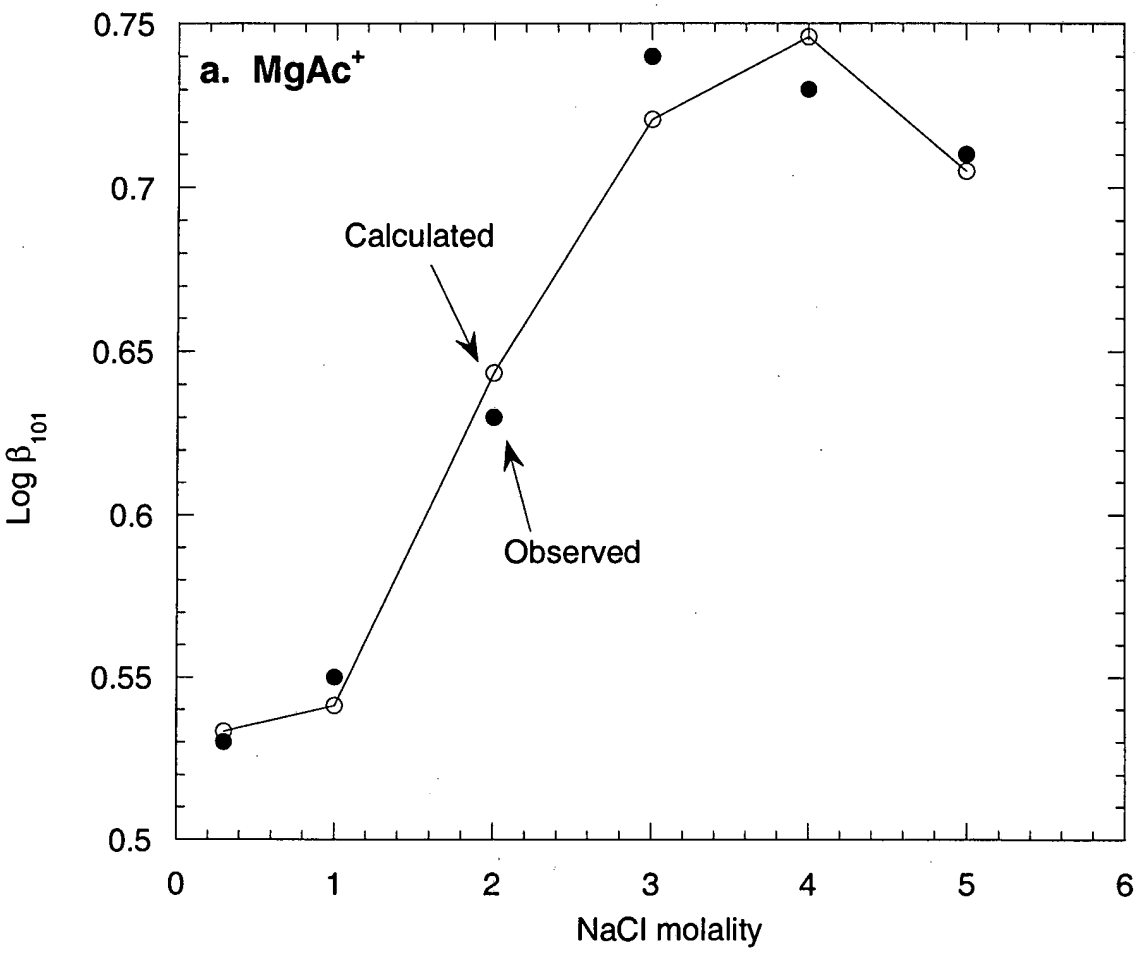

Figure 3a. Log β_{101} versus NaCl molality for $MgAc^+$. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

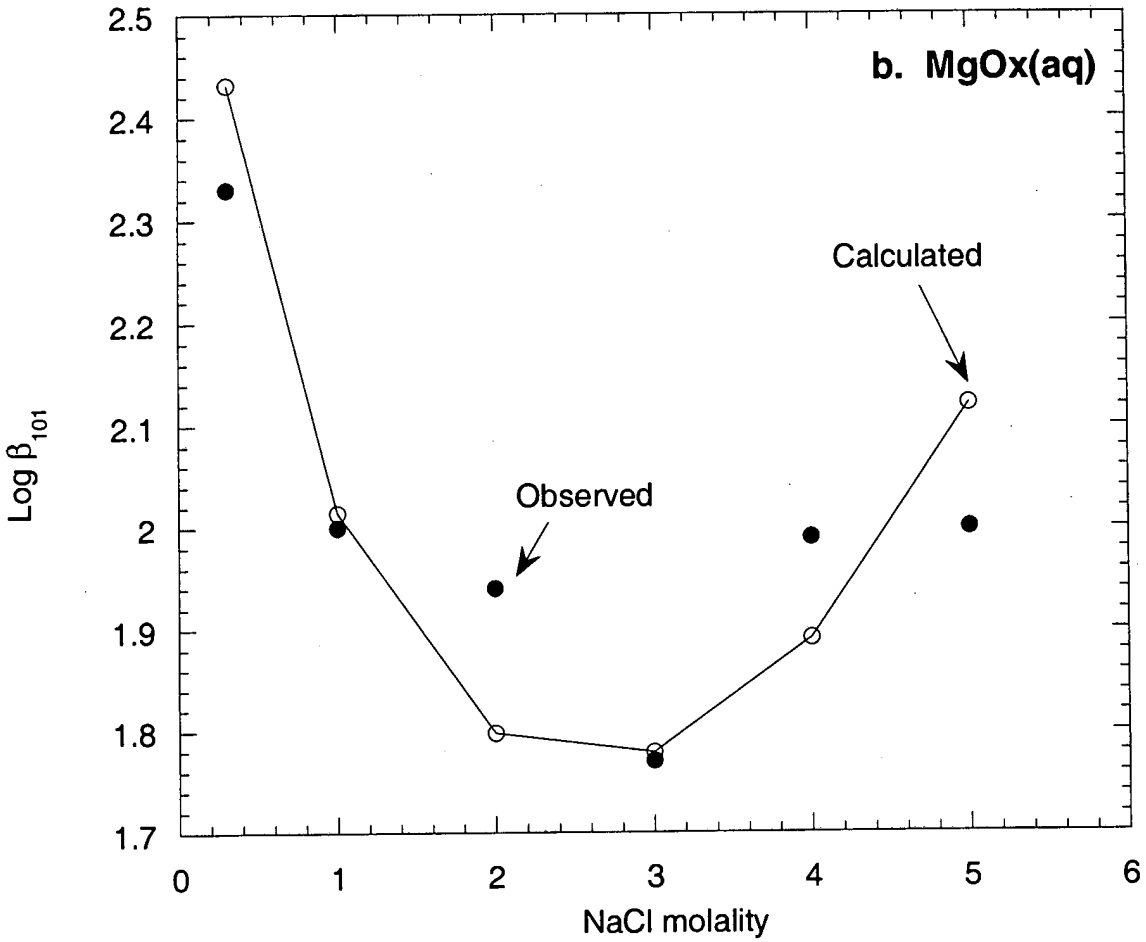

Figure 3b. Log β_{101} versus NaCl molality for $MgOx_{(aq)}$. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

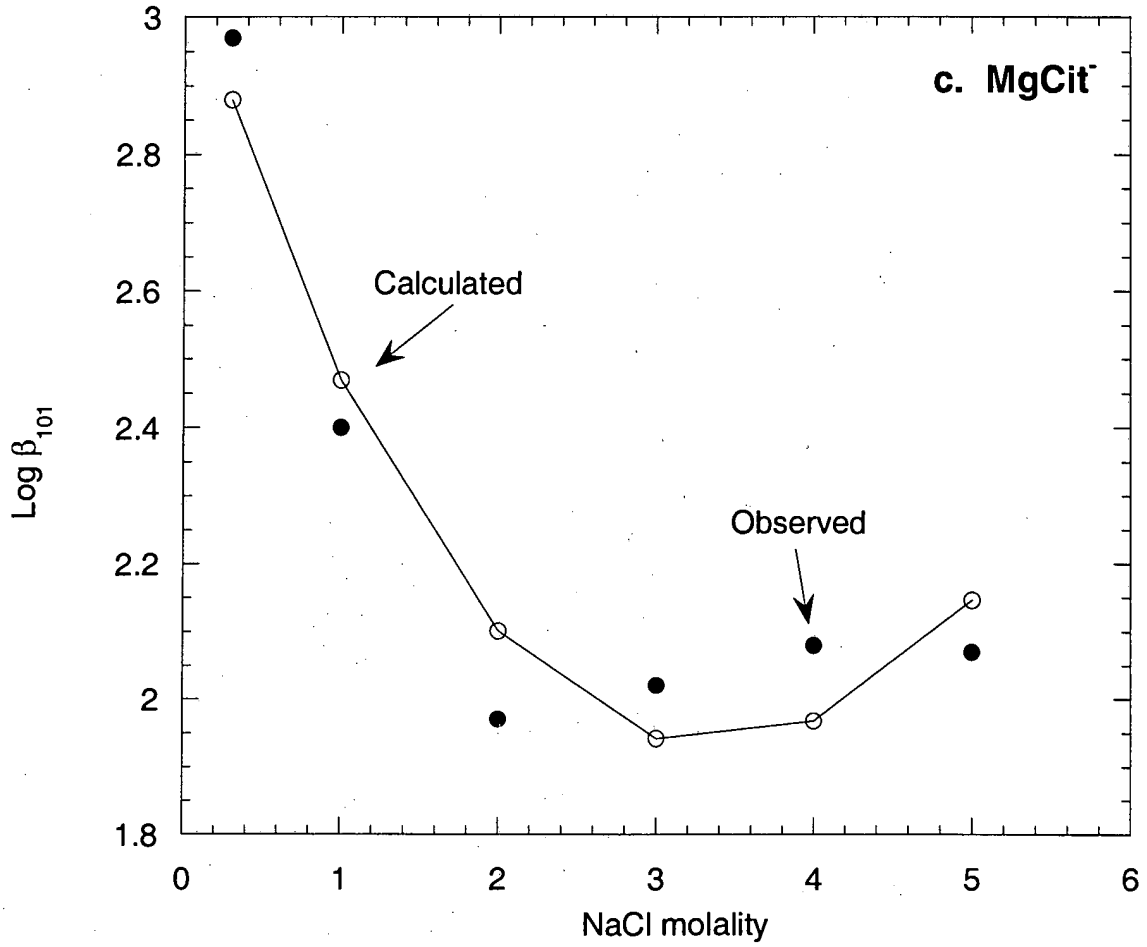

Figure 3c. Log β_{101} versus NaCl molality for $MgCit^-$. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

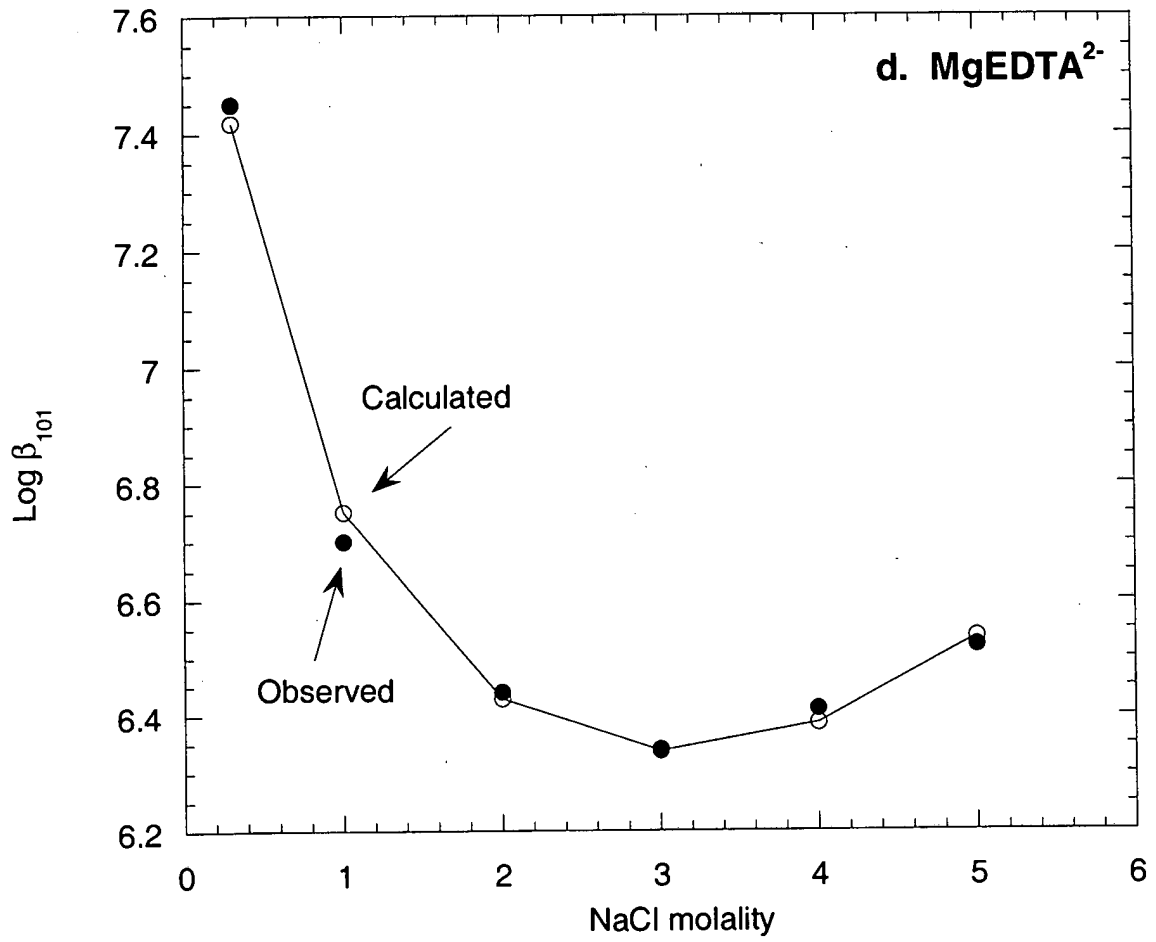

Figure 3d. Log β_{101} versus NaCl molality for $MgEDTA^{2-}$. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

Table 1. Normalized Chemical Potential (μ^0/RT)

Species[a]	PAVT	Recommended	Source of recommended value
$HAc_{(aq)}$	-158.300	-158.300	Choppin et al. (2001); Novak et al. (1996)
Ac^-	-147.347	-147.347	Choppin et al. (2001); Novak et al. (1996)
$H_3Cit_{(aq)}$	0.000	0.000	Choppin et al. (2001); Mizera et al. (1999)
H_2Cit^-	7.245	7.476	Choppin et al. (2001); Mizera et al. (1999)
$HCit^{2-}$	18.300	18.620	Choppin et al. (2001); Mizera et al. (1999)
Cit^{3-}	33.068	33.410	Choppin et al. (2001); Mizera et al. (1999)
$H_4EDTA_{(aq)}$	0.000	0.000	Choppin et al. (2001); Mizera et al. (1999)
H_3EDTA^-	5.360	5.761	Choppin et al. (2001); Mizera et al. (1999)
H_2EDTA^{2-}	11.659	12.870	Choppin et al. (2001); Mizera et al. (1999)
$HEDTA^{3-}$	26.700	28.710	Choppin et al. (2001); Mizera et al. (1999)
$EDTA^{4-}$	52.109	53.050	Choppin et al. (2001); Mizera et al. (1999)
$H_2Ox_{(aq)}$	0.000	0.000	Choppin et al. (2001); Mizera et al. (1999)
HOx^-	3.052	3.209	Choppin et al. (2001); Mizera et al. (1999)
Ox^{2-}	12.790	13.017	Choppin et al. (2001); Mizera et al. (1999)
$HLac_{(aq)}$	0.000	0.000	Choppin et al. (2001)
Lac^-	9.002	8.798	Choppin et al. (2001)
$AmAc^{2+}$	-395.358	-395.356	This work
$AmCit_{(aq)}$	-228.687	-228.543	Choppin et al. (2001)
$AmEDTA^-$	-232.977	-232.324	Choppin et al. (2001)
$AmOx^+$	-243.483	-242.853	Choppin et al. (2001); Borkowski et al. (2001)
$AmLac^{2+}$	-242.339	-241.436	Choppin et al. (2001)

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Table 1. Normalized Chemical Potential (μ^0/RT) (continued)

Species[a]	PAVT	Recommended	Source of recommended value
$ThAc^{3+}$	-448.639	-448.525	Choppin et al. (2001)
$ThCit^{+}$	-285.706	-285.898	Choppin et al. (2001)
$ThEDTA_{(aq)}$	-285.817	-285.419	This work
$ThOx^{2+}$	-297.076	-297.428	Choppin et al. (2001); Borkowski et al. (2001)
$ThLac^{3+}$	-291.182	-291.152	Choppin et al. (2001); Moore et al. (1999)
$NpO_2Ac_{(aq)}$	-519.809	-526.061	Choppin et al. (2001)
NpO_2Cit^{2-}	-343.066	-343.747	Choppin et al. (2001)
NpO_2EDTA^{3-}	-337.030	-335.708	Choppin et al. (2001); Pokrovsky et al. (1998)
NpO_2Ox^{-}	-366.452	-365.851	Choppin et al. (2001); Borkowski et al. (2001)
$NpO_2Lac_{(aq)}$	-364.266	-364.837	Choppin et al. (2001); Moore et al. (1999)
$MgAc^{+}$	-333.346	-333.378	This work
$MgCit^{-}$	-161.979	-162.261	This work
$MgEDTA^{2-}$	-160.325	-153.734	This work
$MgOx_{(aq)}$	-178.880	-179.185	This work
$MgLac^{+}$	999.999	999.999	No $MgLac^{+}$ data[b]
		Species not in the PAVT database	
NpO_2HEDTA^{2-}	xx	-351.852	Choppin et al. (2001); Pokrovsky et al. (1998)
$NpO_2H_2EDTA^{-}$	xx	-364.098	Choppin et al. (2001); Pokrovsky et al. (1998)
$ThAc_2^{2+}$	xx	-604.800	Moore et al. (1999)[c]
$ThLac_2^{2+}$	xx	-292.400	Moore et al. (1999)[c]

[a]Ac = Acetate; Cit = Citrate; Ox = Oxalate; Lac = Lactate

[b]This species is in the FMT database, but its formation is prevented by setting μ^0/RT to a large positive value.

[c]Choppin et al. (2001) did not list values of μ^0/RT for these species, although they did list binary Pitzer parameters (Table 2).

Table 2. Binary Pitzer Parameters ($\beta^{(0)}$, $\beta^{(1)}$, $\beta^{(2)}$, C^{ϕ})

		PAVT				Recommended				Source of Recommended Value
Cation	Anion	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^{ϕ}	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^{ϕ}	
Na^+	Ac^-	0.1426	0.22	0	-0.00629	0.1426	0.22	0	-0.00629	Choppin et al. (2001); Novak et al. (1996)
Na^+	H_2Cit^-	-0.0613	0.5548	0	0	-0.1296	0.29	0	0.013	Choppin et al. (2001); Mizera et al. (1999)
Na^+	$HCit^{2-}$	-0.0014	2.339	0	0	-0.0989	1.74	0	0.027	Choppin et al. (2001); Mizera et al. (1999)
Na^+	Cit^{3-}	0.2823	5.411	0	0	0.0887	5.22	0	0.047	Choppin et al. (2001); Mizera et al. (1999)
Na^+	H_3EDTA^-	-0.0908	0.0825	0	0	-0.2345	0.29	0	0.059	Choppin et al. (2001); Mizera et al. (1999)
Na^+	H_2EDTA^{2-}	-0.1272	2.863	0	0	-0.1262	1.74	0	0.054	Choppin et al. (2001); Mizera et al. (1999)
Na^+	$HEDTA^{3-}$	0.2619	8.325	0	0	0.5458	5.22	0	-0.048	Choppin et al. (2001); Mizera et al. (1999)
Na^+	$EDTA^{4-}$	1.034	11.34	0	0	1.016	11.6	0	0.001	Choppin et al. (2001); Mizera et al. (1999)
Na^+	HOx^-	-0.0307	0	0	0	-0.2448	0.29	0	0.068	Choppin et al. (2001); Mizera et al. (1999)
Na^+	Ox^{2-}	0.0028	1.661	0	0.027	-0.2176	1.74	0	0.122	Choppin et al. (2001); Mizera et al. (1999)
Na^+	Lac^-	0.1349	-0.7242	0	0	-0.0563	0.29	0	0.047	Choppin et al. (2001); Moore et al. (1999)
Na^+	$AmEDTA^-$	-0.2307	0	0	0	-0.2239	0.29	0	0.002	Choppin et al. (2001)
Na^+	NpO_2Cit^{2-}	-0.4092	1.221	0	0.213	-0.4226	1.75	0	0.142	Choppin et al. (2001)
Na^+	NpO_2EDTA^{3-}	0.5067	7.738	0	0	0.683	5.911	0	0	Choppin et al. (2001); Pokrovsky et al. (1998)
Na^+	NpO_2Ox^-	-0.1893	0	0	0	-0.5418	0.29	0	0.095	Choppin et al. (2001); Borkowski et al. (2001)
Na^+	$MgCit^-$	0.2317	0	0	0	0.1742	0.29	0	-0.06923	This work
Na^+	$MgEDTA^{2-}$	0.9289	0	0	0	0.2134	1.74	0	0.00869	This work
K^+	Ac^-	0.1587	0.3251	0	-0.0066	0.1587	0.3251	0	-0.0066	Pitzer (1991)
H^+	Ac^-	0	0	0	0	0	0	0	0	Novak et al. (1996)

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Table 2. Binary Pitzer Parameters ($\beta^{(0)}$, $\beta^{(1)}$, $\beta^{(2)}$, C^{ϕ}) (continued)

		PAVT				Recommended				Source of Recommended Value
Cation	Anion	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^{ϕ}	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^{ϕ}	
$AmAc^{2+}$	Cl^-	0.227	2.154	0	-0.102	0.309	1.74	0	-0.132	This work
$AmOx^{+}$	Cl^-	-0.3219	0	0	0	-0.9374	0.29	0	0.248	Choppin et al. (2001); Borkowski et al. (2001)
$AmLac^{2+}$	Cl^-	-0.0572	6.331	0	0	0.8397	1.74	0	-0.332	Choppin et al. (2001); Moore et al. (1999)
$ThAc^{3+}$	Cl^-	1.239	4.934	0	0	1.061	5.22	0	0.109	Choppin et al. (2001)
$ThCit^{+}$	Cl^-	-0.604	-1.607	0	0	-0.7467	0.29	0	0.319	Choppin et al. (2001)
$ThOx^{2+}$	Cl^-	-0.2061	-0.525	0	0	-0.343	1.74	0	0.5	Choppin et al. (2001); Borkowski et al. (2001)
$ThLac^{3+}$	Cl^-	0.2138	5.371	0	0	0.6677	5.22	0	0.341	Choppin et al. (2001); Moore et al. (1999)
$MgAc^{+}$	Cl^-	0.1696	0	0	0	-0.0833	0.29	0	0.0987	This work
					Species not in the PAVT database					
Na^{+}	NpO_2HEDTA^{2-}	xx	xx	xx	xx	0.4733	-1.504	0	0	Pokrovsky et al. (1998)[a]
Na^{+}	$NpO_2H_2EDTA^{-}$	xx	xx	xx	xx	-0.8285	0.2575	0	0.256	Pokrovsky et al. (1998)[a]
$ThAc_2^{2+}$	Cl^-	xx	xx	xx	xx	0.4671	1.74	0	0.143	Moore et al. (1999)[b]
$ThLac_2^{2+}$	Cl^-	xx	xx	xx	xx	0.5058	1.74	0	0.225	Moore et al. (1999)[b]

[a]Choppin et al. (2001) did not list values for binary Pitzer parameters for these species, although they did list μ^0/RT (Table 1).

[b]Choppin et al. (2001) list the same values except that they switched the C^{ϕ} values. The Moore et al. (1999) values are preferred (see text).

Table 3. Neutral-Ion Interaction Parameter (λ)

Neutral	Ion	PAVT λ	Recommended λ	Source of Recommended Value[a]
$HAc_{(aq)}$	Cl^-	0	0	Choppin et al. (2001); Novak et al. (1996)
$H_3Cit_{(aq)}$	Cl^-	0	0	Choppin et al. (2001); Mizera et al. (1999)
$H_4EDTA_{(aq)}$	Cl^-	0	0	Choppin et al. (2001); Mizera et al. (1999)
$H_2Ox_{(aq)}$	Cl^-	0.035	0	Choppin et al. (2001); Mizera et al. (1999)
$H_2Ox_{(aq)}$	HSO_4^-	0.126	0	[b]
$HLac_{(aq)}$	Cl^-	0	0	Choppin et al. (2001)
$AmCit_{(aq)}$	Cl^-	-0.2731	-0.406	Choppin et al. (2001)
$ThEDTA_{(aq)}$	Cl^-	-0.832	0.1111	This work.
$NpO_2Ac_{(aq)}$	Cl^-	0	0	Choppin et al. (2001); Novak et al. (1996)
$NpO_2Lac_{(aq)}$	Cl^-	-0.1853	0.015	Choppin et al. (2001); Moore et al. (1999)
$MgOx_{(aq)}$	Cl^-	-0.00514	0.0189	This work.

[a]Novak et al. (1996) explicitly stated that all λ values were set to zero. I assumed that Choppin et al. (2001), Mizera et al. (1999), and Moore et al. (1999) set λ values to zero if they did not explicitly list them.

[b]Source of this value in the PAVT database is unknown. Therefore, I recommend setting it to zero.

Table 4. Neutral-Cation-Anion Interaction Parameter (ζ)

Neutral	Cation	Anion	PAVT ζ	Recommended ζ	Source of Recommended Value[a]
$NpO_2Lac_{(aq)}$	Na^+	Cl^-	0.059	0	Choppin et al. (2001); Moore et al. (1999)

[a]I assumed that Choppin et al. (2001) and Moore et al. (1999) set ζ values to zero because neither explicitly listed them.

Table 5. Ternary Pitzer Parameters (θ, ψ)

Anion *i*	Anion *j*	Cation *k*	PAVT		Recommended		Source for Recommended Value
			$\theta_{i,j}$	$\psi_{i,j,k}$	$\theta_{i,j}$	$\psi_{i,j,k}$	
Ac^-	Cl^-	Na^+	-0.09	0.01029	-0.09	0.01029	Novak et al. (1996); Moore et al. (1999)[a]

[a]Choppin et al. (2001) did not explicitly list these values, but it is reasonable to assume that they used them. Choppin et al. (2001) referenced Novak et al. (1996) for other values; and Choppin et al. (2001) and Moore et al. (1999) presented almost identical calculated parameters.

10. APPENDIX

10.1. Appendix Notes

NONLIN does not return the binary Pitzer parameter C^{ϕ}. Instead it returns the parameter C_{MX}, from which C^{ϕ} can be calculated according to:

$$C^{\phi} = C_{MX} \times 2 \times \sqrt{|z_a z_c|}, \quad \text{(A1)}$$

where z_a is the charge of the anion, and z_c is the charge of the cation. OUT files resulting from calculations of binary Pitzer parameters give C_{MX} values. C^{ϕ} values in Table 2 were calculated from these values according the Equation A1.

Each set of calculated log β_{101} values plotted in Figures 1-4 was calculated from the first listing of "FINAL MOLALITIES" in a rev_*.out file. In order to use NONLIN to calculate μ^0/RT for aqueous complexes, it is necessary to trick NONLIN into believing that it is calculating the solubility of a solid phase. The fictional solid phase is removed for verification calculations, although NONLIN expects it to be there. In the verification calculation, NONLIN first equilibrates the aqueous phase (resulting in the first listing of "FINAL MOLALITIES"), then attempts to equilibrate the aqueous phase with a nonexistant solid (resulting in garbage). See the NONLIN User's Manual (SNL, 1996) for more information.

```
001080H2O            0       -95.6635  1 2.0 8 1.0
001000H+             1        000.000  1 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

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

    -1


Reference keys in order are:
H+ 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
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 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.

```
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 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-	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.

```
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
```

```
000005 -300.0          u0 AmAc++F
010401  0.1            b0 AmAc++F Cl-
040401  0.1            cMX AmAc++F Cl-
-1
   .6   -1
0  0  0.3000  1.543E-05  1.0000E-08  3.276E-08  0.30000  0.061
0  0  1.0000  1.563E-05  1.0000E-08  1.974E-08  1.00000  0.061
0  0  2.0000  1.535E-05  1.0000E-08  1.680E-08  2.00000  0.061
0  0  3.0000  1.169E-05  1.0000E-08  2.725E-08  3.00000  0.061
0  0  4.0000  1.040E-05  1.0000E-08  4.124E-08  4.00000  0.061
0  0  5.0000  8.974E-06  1.0000E-08  1.585E-07  5.00000  0.100
-1

0  0  Na+      H+         Am3+        AmAc++   Cl-      Ac-
```

```
     0    0    0    0
0
001080      0.00000000       1   0 H2O
011000      0.00000000       2   1 Na+
001000      0.00000000       3   2 H+
095001      0.00000000       4   3 Am+++F
095891      0.00000000       5   4 AmAc++F
000170      0.00000000       6   1 Cl-
000891      0.00000000       7   2 Ac-F
000000
195890      0.00000000       8    AmAc/Am/Ac(s)
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

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

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
95001	Am+++F	0.000000000000	3.	-241.694
95891	AmAc++F	0.000000000000	2.	999.999
170	Cl-	0.000000000000	-1.	-52.955
891	Ac-F	0.000000000000	-1.	-147.347

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
195890	AmAc/Am/Ac(s	0.000000000000	0.	0.000

CONSTRAINT EQUATIONS

	0	1	8	11	95	72	89	73	17
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Am+++F	3.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
AmAc++F	2.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
Ac-F	-1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
AmAc/Am/Ac(s	0.0	0.0	0.0	0.0	0.0	-1.0	0.0	1.0	0.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	Ac-F	0.14260	0.22000	0.00000	-0.00629
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	Ac-F	0.00000	0.00000	0.00000	0.00000
Am+++F	Cl-	0.61170	5.40300	0.00000	-0.02840
Am+++F	Ac-F	0.00000	0.00000	0.00000	0.00000
AmAc++F	Cl-	0.00000	1.74000	0.00000	0.00000
AmAc++F	Ac-F	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	Ac-F
Na+	H+	0.03600	-0.00400	0.00000
Na+	Am+++F	0.00000	0.00000	0.00000
Na+	AmAc++F	0.00000	0.00000	0.00000
H+	Am+++F	0.00000	0.00000	0.00000
H+	AmAc++F	0.00000	0.00000	0.00000
Am+++F	AmAc++F	0.00000	0.00000	0.00000

		Na+	H+	Am+++F	AmAc

Cl- Ac-F -0.09000 0.01029 0.00000 0.00000 0.00

TOTAL NUMBER OF SPECIES = 8
NUMBER OF COMPONENTS = 10
INDEPENDENT CONSTRAINTS = 7

SOLUBILITY DATA

input molalities

Na+	H+	Am+++F	AmAc++F	Cl-	Ac-F
3.000E-01	1.543E-05	1.000E-08	3.276E-08	3.000E-01	6.100E-02
1.000E+00	1.563E-05	1.000E-08	1.974E-08	1.000E+00	6.100E-02
2.000E+00	1.535E-05	1.000E-08	1.680E-08	2.000E+00	6.100E-02
3.000E+00	1.169E-05	1.000E-08	2.725E-08	3.000E+00	6.100E-02
4.000E+00	1.040E-05	1.000E-08	4.124E-08	4.000E+00	6.100E-02
5.000E+00	8.974E-06	1.000E-08	1.585E-07	5.000E+00	1.000E-01

-3.0000E+02 1.0000E-01 1.0000E-01
L2 NORM OF THE RESIDUALS 2.3768669E+02

-3.9536E+02 3.0876E-01 -4.6823E-02
L2 NORM OF THE RESIDUALS 1.4869226E-01

-3.9536E+02 3.0876E-01 -4.6823E-02
L2 NORM OF THE RESIDUALS 1.4869226E-01

ADJUSTED PARAMETERS

u0rt(		AmAc++F	)	-3.9535597E+02
b0(	AmAc++F	Cl-	)	3.0876051E-01
cmx(	AmAc++F	Cl-	)	-4.6822821E-02

DATA SET(1)

input	calc	diff
0.000000000000000E+000		-1.660113707291089E-002
0.000000000000000E+000		-1.717283835233729E-003
0.000000000000000E+000		8.852777900085584E-002
0.000000000000000E+000		-0.110911777906608
0.000000000000000E+000		4.113469835297678E-002
0.000000000000000E+000		-4.322785390229456E-004

AVERAGE DEVIATION = 4.3221E-02

STANDARD DEVIATION = 6.0703E-02

FINAL MOLALITIES

Na+	H+	Am+++F	AmAc++F	Cl-	Ac-F
3.000E-01	1.543E-05	1.000E-08	3.276E-08	3.000E-01	6.100E-02
1.000E+00	1.563E-05	1.000E-08	1.974E-08	1.000E+00	6.100E-02
2.000E+00	1.535E-05	1.000E-08	1.680E-08	2.000E+00	6.100E-02
3.000E+00	1.169E-05	1.000E-08	2.725E-08	3.000E+00	6.100E-02
4.000E+00	1.040E-05	1.000E-08	4.124E-08	4.000E+00	6.100E-02
5.000E+00	8.974E-06	1.000E-08	1.585E-07	5.000E+00	1.000E-01

FINAL LOG ACTIVITIES

Na+	H+	Am+++F	AmAc++F	Cl-	Ac-F
-6.691E-01	-4.932E+00	-9.468E+00	-8.104E+00	-6.869E-01	-1.386E+00
-1.771E-01	-4.870E+00	-9.761E+00	-8.452E+00	-1.926E-01	-1.434E+00
1.321E-01	-4.753E+00	-9.873E+00	-8.615E+00	1.179E-01	-1.446E+00
3.371E-01	-4.732E+00	-9.876E+00	-8.519E+00	3.236E-01	-1.433E+00
5.022E-01	-4.636E+00	-9.819E+00	-8.501E+00	4.892E-01	-1.406E+00
6.518E-01	-4.551E+00	-9.730E+00	-8.143E+00	6.312E-01	-1.156E+00

Calculated Log Activity Coefficients

Na+	H+	Am+++F	AmAc++F	Cl-	Ac-F
-0.1462	-0.1203	-1.4679	-0.6195	-0.1641	-0.1714
-0.1771	-0.0639	-1.7606	-0.7469	-0.1926	-0.2196
-0.1690	0.0606	-1.8732	-0.8404	-0.1832	-0.2313
-0.1400	0.2003	-1.8765	-0.9545	-0.1535	-0.2187
-0.0999	0.3468	-1.8188	-1.1159	-0.1128	-0.1918
-0.0472	0.4956	-1.7303	-1.3434	-0.0678	-0.1559

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Am+++F	AmAc++F	Cl-	Ac-F
3.000E-01	1.543E-05	1.000E-08	3.276E-08	3.000E-01	6.100E-02
1.000E+00	1.563E-05	1.000E-08	1.974E-08	1.000E+00	6.100E-02
2.000E+00	1.535E-05	1.000E-08	1.680E-08	2.000E+00	6.100E-02
3.000E+00	1.169E-05	1.000E-08	2.725E-08	3.000E+00	6.100E-02
4.000E+00	1.040E-05	1.000E-08	4.124E-08	4.000E+00	6.100E-02
5.000E+00	8.974E-06	1.000E-08	1.585E-07	5.000E+00	1.000E-01

FINAL LOG ACTIVITIES

Na+	H+	Am+++F	AmAc++F	Cl-	Ac-F
-6.691E-01	-4.932E+00	-9.468E+00	-8.104E+00	-6.869E-01	-1.386E+00
-1.771E-01	-4.870E+00	-9.761E+00	-8.452E+00	-1.926E-01	-1.434E+00
1.321E-01	-4.753E+00	-9.873E+00	-8.615E+00	1.179E-01	-1.446E+00
3.371E-01	-4.732E+00	-9.876E+00	-8.519E+00	3.236E-01	-1.433E+00
5.022E-01	-4.636E+00	-9.819E+00	-8.501E+00	4.892E-01	-1.406E+00
6.518E-01	-4.551E+00	-9.730E+00	-8.143E+00	6.312E-01	-1.156E+00

Calculated Log Activity Coefficients

Na+	H+	Am+++F	AmAc++F	Cl-	Ac-F
-0.1462	-0.1203	-1.4679	-0.6195	-0.1641	-0.1714
-0.1771	-0.0639	-1.7606	-0.7469	-0.1926	-0.2196
-0.1690	0.0606	-1.8732	-0.8404	-0.1832	-0.2313
-0.1400	0.2003	-1.8765	-0.9545	-0.1535	-0.2187
-0.0999	0.3468	-1.8188	-1.1159	-0.1128	-0.1918
-0.0472	0.4956	-1.7303	-1.3434	-0.0678	-0.1559

FINAL L2 NORM OF THE RESIDUALS 1.4869226E-01

EXIT PARAMETER 3

FINAL APPROXIMATE SOLUTION

```
0 0 5  -3.9535597E+02
1 4 1   3.0876051E-01
4 4 1  -4.6822821E-02
```

```
-1
     6   -1
0   0   0.3000   1.543E-05   1.0000E-08   3.276E-08   0.30000   0.061
0   0   1.0000   1.563E-05   1.0000E-08   1.974E-08   1.00000   0.061
0   0   2.0000   1.535E-05   1.0000E-08   1.680E-08   2.00000   0.061
0   0   3.0000   1.169E-05   1.0000E-08   2.725E-08   3.00000   0.061
0   0   4.0000   1.040E-05   1.0000E-08   4.124E-08   4.00000   0.061
0   0   5.0000   8.974E-06   1.0000E-08   1.585E-07   5.00000   0.100
-1

0   0   Na+      H+          Am3+         AmAc++   Cl-      Ac-
```

```
     0    0    0    0
0
001080      0.00000000       1  0 H2O
011000      0.00000000       2  1 Na+
001000      0.00000000       3  2 H+
095000      0.00000000       4  3 Am+++
095890      0.00000000       5  4 AmAc++
000170      0.00000000       6  1 Cl-
000890      0.00000000       7  2 Ac-
000000
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_AMAC.IN;2
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_AMAC.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_AMAC.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
95000	Am+++	0.000000000000	3.	-241.694
95890	AmAc++	0.000000000000	2.	-395.356
170	Cl-	0.000000000000	-1.	-52.955
890	Ac-	0.000000000000	-1.	-147.347

SOLID PHASES

ID	NAME	MOLES	Z	u0rt

CONSTRAINT EQUATIONS

	0	1	8	11	95	89	17
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Am+++	3.0	0.0	0.0	0.0	1.0	0.0	0.0
AmAc++	2.0	0.0	0.0	0.0	1.0	1.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	1.0
Ac-	-1.0	0.0	0.0	0.0	0.0	1.0	0.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	Ac-	0.14260	0.22000	0.00000	-0.00629
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	Ac-	0.00000	0.00000	0.00000	0.00000
Am+++	Cl-	0.61170	5.40300	0.00000	-0.02840
Am+++	Ac-	0.00000	0.00000	0.00000	0.00000
AmAc++	Cl-	0.30880	1.74000	0.00000	-0.13200
AmAc++	Ac-	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	Ac-
Na+	H+	0.03600	-0.00400	0.00000
Na+	Am+++	0.00000	0.00000	0.00000
Na+	AmAc++	0.00000	0.00000	0.00000
H+	Am+++	0.00000	0.00000	0.00000
H+	AmAc++	0.00000	0.00000	0.00000
Am+++	AmAc++	0.00000	0.00000	0.00000

			Na+	H+	Am+++	AmAc
Cl-	Ac-	-0.09000	0.01029	0.00000	0.00000	0.00

TOTAL NUMBER OF SPECIES = 7
NUMBER OF COMPONENTS = 7
INDEPENDENT CONSTRAINTS = 6

SOLUBILITY DATA

input molalities

Na+	H+	Am+++	AmAc++	Cl-	Ac-
3.000E-01	1.543E-05	1.000E-08	3.276E-08	3.000E-01	6.100E-02
1.000E+00	1.563E-05	1.000E-08	1.974E-08	1.000E+00	6.100E-02
2.000E+00	1.535E-05	1.000E-08	1.680E-08	2.000E+00	6.100E-02
3.000E+00	1.169E-05	1.000E-08	2.725E-08	3.000E+00	6.100E-02
4.000E+00	1.040E-05	1.000E-08	4.124E-08	4.000E+00	6.100E-02
5.000E+00	8.974E-06	1.000E-08	1.585E-07	5.000E+00	1.000E-01

ADJUSTED PARAMETERS

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Am+++	AmAc++	Cl-	Ac-
3.000E-01	1.543E-05	1.013E-08	3.263E-08	3.000E-01	6.100E-02
1.000E+00	1.563E-05	1.001E-08	1.973E-08	1.000E+00	6.100E-02
2.000E+00	1.535E-05	9.460E-09	1.734E-08	2.000E+00	6.100E-02
3.000E+00	1.169E-05	1.085E-08	2.640E-08	3.000E+00	6.100E-02
4.000E+00	1.040E-05	9.714E-09	4.153E-08	4.000E+00	6.100E-02
5.000E+00	8.974E-06	1.008E-08	1.584E-07	5.000E+00	1.000E-01

FINAL LOG ACTIVITIES

Na+	H+	Am+++	AmAc++	Cl-	Ac-
-6.691E-01	-4.932E+00	-9.462E+00	-8.106E+00	-6.869E-01	-1.386E+00
-1.771E-01	-4.870E+00	-9.760E+00	-8.452E+00	-1.926E-01	-1.434E+00
1.321E-01	-4.753E+00	-9.897E+00	-8.601E+00	1.179E-01	-1.446E+00
3.371E-01	-4.732E+00	-9.841E+00	-8.532E+00	3.236E-01	-1.433E+00
5.022E-01	-4.636E+00	-9.831E+00	-8.495E+00	4.892E-01	-1.406E+00
6.518E-01	-4.551E+00	-9.727E+00	-8.140E+00	6.312E-01	-1.156E+00

Calculated Log Activity Coefficients

Na+	H+	Am+++	AmAc++	Cl-	Ac-
-0.1462	-0.1203	-1.4679	-0.6195	-0.1641	-0.1714
-0.1771	-0.0639	-1.7606	-0.7467	-0.1926	-0.2196
-0.1690	0.0606	-1.8732	-0.8398	-0.1832	-0.2313
-0.1400	0.2003	-1.8765	-0.9532	-0.1535	-0.2187
-0.0999	0.3468	-1.8188	-1.1136	-0.1128	-0.1918
-0.0472	0.4956	-1.7303	-1.3399	-0.0678	-0.1559

SOLID PHASE NOW IN EQUILIBRIUM

```
 DATA SET( 1)

   input    calc      diff
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
 0.000000000000000E+000  0.000000000000000E+000
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
 0.000000000000000E+000  0.000000000000000E+000
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
 0.000000000000000E+000  0.000000000000000E+000
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
 0.000000000000000E+000  0.000000000000000E+000
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
 0.000000000000000E+000  0.000000000000000E+000
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
 0.000000000000000E+000  0.000000000000000E+000
```

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Am+++	AmAc++	Cl-	Ac-
7.000E-15	2.100E+18	2.677E+34	2.350E+18	8.032E+34	7.000E-15
7.000E-15	2.299E+19	2.931E+35	2.573E+19	8.793E+35	7.000E-15
7.000E-15	9.004E+19	1.148E+36	1.008E+20	3.444E+36	7.000E-15
7.000E-15	1.984E+20	2.530E+36	2.220E+20	7.589E+36	7.000E-15
7.000E-15	3.455E+20	4.405E+36	3.867E+20	1.322E+37	7.000E-15
7.000E-15	5.289E+20	6.744E+36	5.919E+20	2.023E+37	7.000E-15

FINAL LOG ACTIVITIES

Na+	H+	Am+++	AmAc++	Cl-	Ac-
-3.463E+28	-4.576E+28	-5.823E+29	-2.339E+30	-1.941E+29	-6.470E+28
-3.806E+29	-5.028E+29	-6.399E+30	-2.571E+31	-2.133E+30	-7.110E+29
-1.498E+30	-1.980E+30	-2.519E+31	-1.012E+32	-8.398E+30	-2.799E+30
-3.319E+30	-4.385E+30	-5.581E+31	-2.242E+32	-1.860E+31	-6.201E+30
-5.809E+30	-7.676E+30	-9.768E+31	-3.924E+32	-3.256E+31	-1.085E+31
-8.938E+30	-1.181E+31	-1.503E+32	-6.037E+32	-5.010E+31	-1.670E+31

Calculated Log Activity Coefficients

Na+	H+	Am+++	AmAc++	Cl-	Ac-
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********

FINAL L2 NORM OF THE RESIDUALS 0.0000000E+00

EXIT PARAMETER 0

FINAL APPROXIMATE SOLUTION

```
-1
     6    -1
0   0   0.3000   1.543E-05   1.0000E-08   3.276E-08   0.30000   0.061
0   0   1.0000   1.563E-05   1.0000E-08   1.974E-08   1.00000   0.061
0   0   2.0000   1.535E-05   1.0000E-08   1.680E-08   2.00000   0.061
0   0   3.0000   1.169E-05   1.0000E-08   2.725E-08   3.00000   0.061
0   0   4.0000   1.040E-05   1.0000E-08   4.124E-08   4.00000   0.061
0   0   5.0000   8.974E-06   1.0000E-08   1.585E-07   5.00000   0.100
-1

0   0   Na+      H+          Am3+         AmAc++    Cl-       Ac-
```

```
     0    0    0    0
0
001080      0.00000000      1  0 H2O
011000      0.00000000      2  1 Na+
001000      0.00000000      3  2 H+
095000      0.00000000      4  3 Am+++
095892      0.00000000      5  4 AmAc++moore
000170      0.00000000      6  1 Cl-
000890      0.00000000      7  2 Ac-
000000
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_AMAC_MOORE.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_AMAC_MOORE.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_AMAC_MOORE.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
95000	Am+++	0.000000000000	3.	-241.694
95892	AmAc++moore	0.000000000000	2.	-395.239
170	Cl-	0.000000000000	-1.	-52.955
890	Ac-	0.000000000000	-1.	-147.347

SOLID PHASES

ID	NAME	MOLES	Z	u0rt

CONSTRAINT EQUATIONS

	0	1	8	11	95	89	17
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Am+++	3.0	0.0	0.0	0.0	1.0	0.0	0.0
AmAc++moore	2.0	0.0	0.0	0.0	1.0	1.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	1.0
Ac-	-1.0	0.0	0.0	0.0	0.0	1.0	0.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	Ac-	0.14260	0.22000	0.00000	-0.00629
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	Ac-	0.00000	0.00000	0.00000	0.00000
Am+++	Cl-	0.61170	5.40300	0.00000	-0.02840
Am+++	Ac-	0.00000	0.00000	0.00000	0.00000
AmAc++moore	Cl-	1.01400	1.74000	0.00000	-0.26500
AmAc++moore	Ac-	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	Ac-
Na+	H+	0.03600	-0.00400	0.00000
Na+	Am+++	0.00000	0.00000	0.00000
Na+	AmAc++moore	0.00000	0.00000	0.00000
H+	Am+++	0.00000	0.00000	0.00000
H+	AmAc++moore	0.00000	0.00000	0.00000
Am+++	AmAc++moore	0.00000	0.00000	0.00000

			Na+	H+	Am+++	AmAc
Cl-	Ac-	-0.09000	0.01029	0.00000	0.00000	0.00

TOTAL NUMBER OF SPECIES = 7
NUMBER OF COMPONENTS = 7
INDEPENDENT CONSTRAINTS = 6

SOLUBILITY DATA

input molalities

Na+	H+	Am+++	AmAc++moore	Cl-	Ac-
3.000E-01	1.543E-05	1.000E-08	3.276E-08	3.000E-01	6.100E-02
1.000E+00	1.563E-05	1.000E-08	1.974E-08	1.000E+00	6.100E-02
2.000E+00	1.535E-05	1.000E-08	1.680E-08	2.000E+00	6.100E-02
3.000E+00	1.169E-05	1.000E-08	2.725E-08	3.000E+00	6.100E-02
4.000E+00	1.040E-05	1.000E-08	4.124E-08	4.000E+00	6.100E-02
5.000E+00	8.974E-06	1.000E-08	1.585E-07	5.000E+00	1.000E-01

ADJUSTED PARAMETERS

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Am+++	AmAc++moore	Cl-	Ac-
3.000E-01	1.543E-05	1.477E-08	2.799E-08	3.000E-01	6.100E-02
1.000E+00	1.563E-05	2.022E-08	9.525E-09	1.000E+00	6.100E-02
2.000E+00	1.535E-05	2.346E-08	3.338E-09	2.000E+00	6.100E-02
3.000E+00	1.169E-05	3.469E-08	2.564E-09	3.000E+00	6.100E-02
4.000E+00	1.040E-05	4.827E-08	2.966E-09	4.000E+00	6.100E-02
5.000E+00	8.974E-06	1.491E-07	1.939E-08	5.000E+00	1.000E-01

FINAL LOG ACTIVITIES

Na+	H+	Am+++	AmAc++moore	Cl-	Ac-
-6.691E-01	-4.932E+00	-9.298E+00	-7.993E+00	-6.869E-01	-1.386E+00
-1.771E-01	-4.870E+00	-9.455E+00	-8.197E+00	-1.926E-01	-1.434E+00
1.321E-01	-4.753E+00	-9.503E+00	-8.257E+00	1.179E-01	-1.446E+00
3.371E-01	-4.732E+00	-9.336E+00	-8.078E+00	3.236E-01	-1.433E+00
5.022E-01	-4.636E+00	-9.135E+00	-7.850E+00	4.892E-01	-1.406E+00
6.518E-01	-4.551E+00	-8.557E+00	-7.021E+00	6.312E-01	-1.156E+00

Calculated Log Activity Coefficients

Na+	H+	Am+++	AmAc++moore	Cl-	Ac-
-0.1462	-0.1203	-1.4679	-0.4398	-0.1641	-0.1714
-0.1771	-0.0639	-1.7606	-0.1763	-0.1926	-0.2196
-0.1690	0.0606	-1.8732	0.2194	-0.1832	-0.2313
-0.1400	0.2003	-1.8765	0.5131	-0.1535	-0.2187
-0.0999	0.3468	-1.8188	0.6781	-0.1128	-0.1918
-0.0472	0.4956	-1.7303	0.6915	-0.0678	-0.1559

SOLID PHASE NOW IN EQUILIBRIUM

```
 DATA SET( 1)

   input    calc      diff
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
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 projected hessian indefinite
  0.000000000000000E+000  0.000000000000000E+000
 projected hessian indefinite
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  0.000000000000000E+000  0.000000000000000E+000
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  0.000000000000000E+000  0.000000000000000E+000
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  0.000000000000000E+000  0.000000000000000E+000
 projected hessian indefinite
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 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
  0.000000000000000E+000  0.000000000000000E+000
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
 projected hessian indefinite
```

projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
0.000000000000000E+000 0.000000000000000E+000

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Am+++	AmAc++moore	Cl-	Ac-
7.000E-15	2.100E+18	2.677E+34	2.350E+18	8.032E+34	7.000E-15
7.000E-15	2.299E+19	2.931E+35	2.573E+19	8.793E+35	7.000E-15
7.000E-15	9.004E+19	1.148E+36	1.008E+20	3.444E+36	7.000E-15
7.000E-15	1.984E+20	2.530E+36	2.220E+20	7.589E+36	7.000E-15
7.000E-15	3.455E+20	4.405E+36	3.867E+20	1.322E+37	7.000E-15
7.000E-15	5.289E+20	6.744E+36	5.919E+20	2.023E+37	7.000E-15

FINAL LOG ACTIVITIES

Na+	H+	Am+++	AmAc++moore	Cl-	Ac-
-3.463E+28	-4.576E+28	-5.823E+29	-4.566E+30	-1.941E+29	-6.470E+28
-3.806E+29	-5.028E+29	-6.399E+30	-5.017E+31	-2.133E+30	-7.110E+29
-1.498E+30	-1.980E+30	-2.519E+31	-1.975E+32	-8.398E+30	-2.799E+30
-3.319E+30	-4.385E+30	-5.581E+31	-4.376E+32	-1.860E+31	-6.201E+30
-5.809E+30	-7.676E+30	-9.768E+31	-7.659E+32	-3.256E+31	-1.085E+31
-8.938E+30	-1.181E+31	-1.503E+32	-1.178E+33	-5.010E+31	-1.670E+31

Calculated Log Activity Coefficients

Na+	H+	Am+++	AmAc++moore	Cl-	Ac-
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********
**********	**********	**********	**********	**********	**********

FINAL L2 NORM OF THE RESIDUALS 0.0000000E+00

EXIT PARAMETER 0

FINAL APPROXIMATE SOLUTION

```
000005 -300.0          u0 ThEDTA(aq)
100101  0.1            lambda MgOxF Cl-
-1
    6   -1
0  0  0.3000  1.000E-03  1.0000E-10  1.718E-04  0.30000  1.0E-10
0  0  1.0000  1.000E-03  1.0000E-10  2.985E-05  1.00000  1.0E-10
0  0  2.0000  1.000E-03  1.0000E-10  3.548E-05  2.00000  1.0E-10
0  0  3.0000  1.000E-03  1.0000E-10  5.370E-05  3.00000  1.0E-10
0  0  4.0000  1.000E-03  1.0000E-10  1.514E-04  4.00000  1.0E-10
0  0  5.0000  1.000E-03  1.0000E-10  8.710E-04  5.00000  1.0E-10
-1

0  0  Na+      H+         Th++++       ThEDTA    Cl-      EDTA==
```

```
     0    0    0    0
0
001080      0.00000000       1  0 H2O
011000      0.00000000       2  1 Na+
001000      0.00000000       3  2 H+
090001      0.00000000       4  3 Th++++F
090871      0.00000000       5  1 ThEDTAF
000170      0.00000000       6  1 Cl-
000871      0.00000000       7  2 EDTA==F
000000
190870      0.00000000       8   ThEDTA/Th/EDTA
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]THEDTA.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]THEDTA.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]THEDTA.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
90001	Th++++F	0.000000000000	4.	-284.227
90871	ThEDTAF	0.000000000000	0.	999.999
170	Cl-	0.000000000000	-1.	-52.955
871	EDTA==F	0.000000000000	-4.	53.050

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
190870	ThEDTA/Th/ED	0.000000000000	0.	0.000

CONSTRAINT EQUATIONS

	0	1	8	11	90	72	87	73	17
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Th++++F	4.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
ThEDTAF	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
EDTA==F	-4.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
ThEDTA/Th/ED	0.0	0.0	0.0	0.0	0.0	-1.0	0.0	1.0	0.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	EDTA==F	1.01600	11.60000	0.00000	0.00100
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	EDTA==F	0.00000	0.00000	0.00000	0.00000
Th++++F	Cl-	1.09200	13.70000	-160.00000	-0.11200
Th++++F	EDTA==F	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	EDTA==F
Na+	H+	0.03600	-0.00400	0.00000
Na+	Th++++F	0.42000	0.21000	0.00000
H+	Th++++F	0.60000	0.37000	0.00000

			Na+	H+	Th++++F
Cl-	EDTA==F	0.00000	0.00000	0.00000	0.00000

neutral ion parameters

	ThEDTAF
Na+	0.0000

```
H+              0.0000
Th++++F         0.0000
Cl-             0.0000
EDTA==F         0.0000
ThEDTAF         0.0000

        higher order lambdas

                      Cl-          EDTA==F
ThEDTAF     Na+           0.00000      0.00000
ThEDTAF     H+            0.00000      0.00000
ThEDTAF     Th++++F       0.00000      0.00000

 TOTAL NUMBER OF SPECIES =  8
 NUMBER OF COMPONENTS    = 10
 INDEPENDENT CONSTRAINTS =  7

          SOLUBILITY DATA

          input molalities

   Na+          H+           Th++++F      ThEDTAF      Cl-          EDTA==F
   3.000E-01    1.000E-03    1.000E-10    1.718E-04    3.000E-01    1.000E-10
   1.000E+00    1.000E-03    1.000E-10    2.985E-05    1.000E+00    1.000E-10
   2.000E+00    1.000E-03    1.000E-10    3.548E-05    2.000E+00    1.000E-10
   3.000E+00    1.000E-03    1.000E-10    5.370E-05    3.000E+00    1.000E-10
   4.000E+00    1.000E-03    1.000E-10    1.514E-04    4.000E+00    1.000E-10
   5.000E+00    1.000E-03    1.000E-10    8.710E-04    5.000E+00    1.000E-10

 -3.0000E+02  1.0000E-01
          L2 NORM OF THE RESIDUALS  3.5877168E+01


 -2.8542E+02  1.1112E-01
          L2 NORM OF THE RESIDUALS  1.2356648E+00


 -2.8542E+02  1.1112E-01
          L2 NORM OF THE RESIDUALS  1.2356648E+00


        ADJUSTED PARAMETERS
  u0rt(                        ThEDTAF      )  -2.8541866E+02
lambda(           ThEDTAF      Cl-          )   1.1112193E-01

 DATA SET( 1)

  input    calc       diff
 0.000000000000000E+000  0.642008119066638
 0.000000000000000E+000  5.188313108466856E-002
 0.000000000000000E+000 -0.723811722606282
 0.000000000000000E+000 -0.519777812527454
 0.000000000000000E+000 -1.398043412079985E-002
 0.000000000000000E+000  0.563678498212074

 AVERAGE DEVIATION   =  4.1919E-01

 STANDARD DEVIATION =  5.0446E-01

 FINAL MOLALITIES
```

Na+	H+	Th++++F	ThEDTAF	Cl-	EDTA==F
3.000E-01	1.000E-03	1.000E-10	1.718E-04	3.000E-01	1.000E-10
1.000E+00	1.000E-03	1.000E-10	2.985E-05	1.000E+00	1.000E-10
2.000E+00	1.000E-03	1.000E-10	3.548E-05	2.000E+00	1.000E-10
3.000E+00	1.000E-03	1.000E-10	5.370E-05	3.000E+00	1.000E-10
4.000E+00	1.000E-03	1.000E-10	1.514E-04	4.000E+00	1.000E-10
5.000E+00	1.000E-03	1.000E-10	8.710E-04	5.000E+00	1.000E-10

FINAL LOG ACTIVITIES

Na+	H+	Th++++F	ThEDTAF	Cl-	EDTA==F
-6.737E-01	-3.112E+00	-1.426E+01	-3.736E+00	-6.734E-01	-1.276E+01
-1.839E-01	-3.060E+00	-1.443E+01	-4.429E+00	-1.836E-01	-1.354E+01
1.249E-01	-2.937E+00	-1.411E+01	-4.257E+00	1.250E-01	-1.402E+01
3.297E-01	-2.797E+00	-1.351E+01	-3.980E+00	3.299E-01	-1.425E+01
4.947E-01	-2.651E+00	-1.265E+01	-3.434E+00	4.949E-01	-1.434E+01
6.394E-01	-2.502E+00	-1.157E+01	-2.577E+00	6.397E-01	-1.432E+01

Calculated Log Activity Coefficients

Na+	H+	Th++++F	ThEDTAF	Cl-	EDTA==F
-0.1508	-0.1116	-4.2581	0.0290	-0.1505	-2.7559
-0.1839	-0.0596	-4.4272	0.0965	-0.1836	-3.5356
-0.1762	0.0635	-4.1124	0.1930	-0.1760	-4.0157
-0.1474	0.2026	-3.5082	0.2896	-0.1473	-4.2548
-0.1073	0.3487	-2.6542	0.3861	-0.1072	-4.3425
-0.0595	0.4983	-1.5718	0.4826	-0.0593	-4.3176

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Th++++F	ThEDTAF	Cl-	EDTA==F
3.000E-01	1.000E-03	1.000E-10	1.718E-04	3.000E-01	1.000E-10
1.000E+00	1.000E-03	1.000E-10	2.985E-05	1.000E+00	1.000E-10
2.000E+00	1.000E-03	1.000E-10	3.548E-05	2.000E+00	1.000E-10
3.000E+00	1.000E-03	1.000E-10	5.370E-05	3.000E+00	1.000E-10
4.000E+00	1.000E-03	1.000E-10	1.514E-04	4.000E+00	1.000E-10
5.000E+00	1.000E-03	1.000E-10	8.710E-04	5.000E+00	1.000E-10

FINAL LOG ACTIVITIES

Na+	H+	Th++++F	ThEDTAF	Cl-	EDTA==F
-6.737E-01	-3.112E+00	-1.426E+01	-3.736E+00	-6.734E-01	-1.276E+01
-1.839E-01	-3.060E+00	-1.443E+01	-4.429E+00	-1.836E-01	-1.354E+01
1.249E-01	-2.937E+00	-1.411E+01	-4.257E+00	1.250E-01	-1.402E+01
3.297E-01	-2.797E+00	-1.351E+01	-3.980E+00	3.299E-01	-1.425E+01
4.947E-01	-2.651E+00	-1.265E+01	-3.434E+00	4.949E-01	-1.434E+01
6.394E-01	-2.502E+00	-1.157E+01	-2.577E+00	6.397E-01	-1.432E+01

Calculated Log Activity Coefficients

Na+	H+	Th++++F	ThEDTAF	Cl-	EDTA==F
-0.1508	-0.1116	-4.2581	0.0290	-0.1505	-2.7559
-0.1839	-0.0596	-4.4272	0.0965	-0.1836	-3.5356
-0.1762	0.0635	-4.1124	0.1930	-0.1760	-4.0157
-0.1474	0.2026	-3.5082	0.2896	-0.1473	-4.2548
-0.1073	0.3487	-2.6542	0.3861	-0.1072	-4.3425
-0.0595	0.4983	-1.5718	0.4826	-0.0593	-4.3176

FINAL L2 NORM OF THE RESIDUALS 1.2356648E+00

EXIT PARAMETER 3

FINAL APPROXIMATE SOLUTION

0 0 5 -2.8541866E+02
10 1 1 1.1112193E-01

```
-1
     6   -1
0   0   0.3000   1.000E-03   1.0000E-10   1.718E-04   0.30000   1.0E-10
0   0   1.0000   1.000E-03   1.0000E-10   2.985E-05   1.00000   1.0E-10
0   0   2.0000   1.000E-03   1.0000E-10   3.548E-05   2.00000   1.0E-10
0   0   3.0000   1.000E-03   1.0000E-10   5.370E-05   3.00000   1.0E-10
0   0   4.0000   1.000E-03   1.0000E-10   1.514E-04   4.00000   1.0E-10
0   0   5.0000   1.000E-03   1.0000E-10   8.710E-04   5.00000   1.0E-10
-1

0   0   Na+      H+          Th++++        ThEDTA     Cl-       EDTA==
```

```
     0    0    0    0
0
001080      0.00000000       1  0 H2O
011000      0.00000000       2  1 Na+
001000      0.00000000       3  2 H+
090000      0.00000000       4  3 Th++++
090870      0.00000000       5  1 ThEDTA
000170      0.00000000       6  1 Cl-
000870      0.00000000       7  2 EDTA==
000000
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_THEDTA.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_THEDTA.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_THEDTA.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
90000	Th++++	0.000000000000	4.	-284.227
90870	ThEDTA	0.000000000000	0.	-285.419
170	Cl-	0.000000000000	-1.	-52.955
870	EDTA==	0.000000000000	-4.	53.050

SOLID PHASES

ID	NAME	MOLES	Z	u0rt

CONSTRAINT EQUATIONS

	0	1	8	11	90	87	17
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Th++++	4.0	0.0	0.0	0.0	1.0	0.0	0.0
ThEDTA	0.0	0.0	0.0	0.0	1.0	1.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	1.0
EDTA==	-4.0	0.0	0.0	0.0	0.0	1.0	0.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	EDTA==	1.01600	11.60000	0.00000	0.00100
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	EDTA==	0.00000	0.00000	0.00000	0.00000
Th++++	Cl-	1.09200	13.70000	-160.00000	-0.11200
Th++++	EDTA==	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	EDTA==
Na+	H+	0.03600	-0.00400	0.00000
Na+	Th++++	0.42000	0.21000	0.00000
H+	Th++++	0.60000	0.37000	0.00000

			Na+	H+	Th++++
Cl-	EDTA==	0.00000	0.00000	0.00000	0.00000

neutral ion parameters

	ThEDTA
Na+	0.0000
H+	0.0000
Th++++	0.0000

```
Cl-              0.1111
EDTA==           0.0000
ThEDTA           0.0000
```

higher order lambdas

		Cl-	EDTA==
ThEDTA	Na+	0.00000	0.00000
ThEDTA	H+	0.00000	0.00000
ThEDTA	Th++++	0.00000	0.00000

TOTAL NUMBER OF SPECIES = 7
NUMBER OF COMPONENTS = 7
INDEPENDENT CONSTRAINTS = 6

SOLUBILITY DATA

input molalities

Na+	H+	Th++++	ThEDTA	Cl-	EDTA==
3.000E-01	1.000E-03	1.000E-10	1.718E-04	3.000E-01	1.000E-10
1.000E+00	1.000E-03	1.000E-10	2.985E-05	1.000E+00	1.000E-10
2.000E+00	1.000E-03	1.000E-10	3.548E-05	2.000E+00	1.000E-10
3.000E+00	1.000E-03	1.000E-10	5.370E-05	3.000E+00	1.000E-10
4.000E+00	1.000E-03	1.000E-10	1.514E-04	4.000E+00	1.000E-10
5.000E+00	1.000E-03	1.000E-10	8.710E-04	5.000E+00	1.000E-10

ADJUSTED PARAMETERS

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Th++++	ThEDTA	Cl-	EDTA==
3.000E-01	1.000E-03	7.253E-11	1.718E-04	3.000E-01	7.253E-11
1.000E+00	1.000E-03	9.742E-11	2.985E-05	1.000E+00	9.742E-11
2.000E+00	1.000E-03	1.436E-10	3.548E-05	2.000E+00	1.436E-10
3.000E+00	1.000E-03	1.296E-10	5.370E-05	3.000E+00	1.296E-10
4.000E+00	1.000E-03	1.007E-10	1.514E-04	4.000E+00	1.007E-10
5.000E+00	1.000E-03	7.542E-11	8.710E-04	5.000E+00	7.542E-11

FINAL LOG ACTIVITIES

Na+	H+	Th++++	ThEDTA	Cl-	EDTA==
-6.737E-01	-3.112E+00	-1.440E+01	-3.736E+00	-6.734E-01	-1.290E+01
-1.839E-01	-3.060E+00	-1.444E+01	-4.429E+00	-1.836E-01	-1.355E+01
1.249E-01	-2.937E+00	-1.396E+01	-4.257E+00	1.250E-01	-1.386E+01
3.297E-01	-2.797E+00	-1.340E+01	-3.981E+00	3.299E-01	-1.414E+01
4.947E-01	-2.651E+00	-1.285E+01	-3.434E+00	4.949E-01	-1.434E+01
6.394E-01	-2.502E+00	-1.169E+01	-2.577E+00	6.397E-01	-1.444E+01

Calculated Log Activity Coefficients

Na+	H+	Th++++	ThEDTA	Cl-	EDTA==
-0.1508	-0.1116	-4.2581	0.0290	-0.1505	-2.7559
-0.1839	-0.0596	-4.4272	0.0965	-0.1836	-3.5356
-0.1762	0.0635	-4.1124	0.1930	-0.1760	-4.0157
-0.1474	0.2026	-3.5082	0.2895	-0.1473	-4.2548
-0.1073	0.3487	-2.6542	0.3860	-0.1072	-4.3425
-0.0595	0.4983	-1.5718	0.4825	-0.0593	-4.3176

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Th++++	ThEDTA	Cl-	EDTA==
3.000E-01	1.000E-03	1.718E-04	7.000E-15	3.007E-01	7.000E-15
1.000E+00	1.000E-03	2.985E-05	7.000E-15	1.000E+00	7.000E-15
2.000E+00	1.000E-03	3.548E-05	7.000E-15	2.000E+00	7.000E-15
3.000E+00	1.000E-03	5.370E-05	7.000E-15	3.000E+00	7.000E-15
4.000E+00	1.000E-03	1.514E-04	7.000E-15	4.001E+00	7.000E-15
5.000E+00	1.000E-03	8.710E-04	7.000E-15	5.003E+00	7.000E-15

FINAL LOG ACTIVITIES

Na+	H+	Th++++	ThEDTA	Cl-	EDTA==
-6.741E-01	-3.112E+00	-8.010E+00	-1.413E+01	-6.723E-01	-1.691E+01
-1.839E-01	-3.060E+00	-8.952E+00	-1.406E+01	-1.835E-01	-1.769E+01
1.248E-01	-2.937E+00	-8.562E+00	-1.396E+01	1.251E-01	-1.817E+01
3.297E-01	-2.797E+00	-7.778E+00	-1.387E+01	3.300E-01	-1.841E+01
4.947E-01	-2.651E+00	-6.473E+00	-1.377E+01	4.952E-01	-1.850E+01
6.392E-01	-2.501E+00	-4.628E+00	-1.367E+01	6.413E-01	-1.848E+01

Calculated Log Activity Coefficients

Na+	H+	Th++++	ThEDTA	Cl-	EDTA==
-0.1512	-0.1120	-4.2451	0.0290	-0.1504	-2.7561
-0.1839	-0.0596	-4.4267	0.0965	-0.1836	-3.5361
-0.1762	0.0635	-4.1122	0.1930	-0.1759	-4.0163
-0.1475	0.2026	-3.5079	0.2896	-0.1472	-4.2556
-0.1074	0.3487	-2.6536	0.3861	-0.1069	-4.3443
-0.0597	0.4988	-1.5682	0.4829	-0.0580	-4.3262

FINAL L2 NORM OF THE RESIDUALS 0.0000000E+00

EXIT PARAMETER 0

FINAL APPROXIMATE SOLUTION

```
000005 -300.0          u0 MgAc+F
010401  0.1            b0 MgAc+F Cl-
040401  0.1            cMX MgAc+F Cl-
-1
    6   -1
0  0  0.3000  1.000E-07  7.8430E-04  1.965E-04  0.30000  0.07395
0  0  1.0000  1.000E-07  7.3170E-04  1.909E-04  1.00000  0.07353
0  0  2.0000  1.000E-07  6.9660E-04  2.171E-04  2.00000  0.07305
0  0  3.0000  1.000E-07  7.3170E-04  2.957E-04  3.00000  0.07353
0  0  4.0000  1.000E-07  6.6840E-04  2.494E-04  4.00000  0.06948
0  0  5.0000  1.000E-07  6.6540E-04  2.336E-04  5.00000  0.06846
-1

0  0  Na+      H+         Mg2+        MgAc+   Cl-      Ac-
```

```
     0     0     0     0
0.
001080      0.00000000      1  0 H2O
011000      0.00000000      2  1 Na+
001000      0.00000000      3  2 H+
012001      0.00000000      4  3 Mg++F
012891      0.00000000      5  4 MgAc+F
000170      0.00000000      6  1 Cl-
000891      0.00000000      7  2 Ac-F
000000
112890      0.00000000      8   MgAc/Mg/Ac(s)
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGAC.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGAC.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGAC.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
12001	Mg++F	0.000000000000	2.	-183.468
12891	MgAc+F	0.000000000000	1.	999.999
170	Cl-	0.000000000000	-1.	-52.955
891	Ac-F	0.000000000000	-1.	-147.347

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
112890	MgAc/Mg/Ac(s	0.000000000000	0.	0.000

CONSTRAINT EQUATIONS

	0	1	8	11	12	72	89	73	17
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mg++F	2.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
MgAc+F	1.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
Ac-F	-1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
MgAc/Mg/Ac(s	0.0	0.0	0.0	0.0	0.0	-1.0	0.0	1.0	0.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	Ac-F	0.14260	0.22000	0.00000	-0.00629
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	Ac-F	0.00000	0.00000	0.00000	0.00000
Mg++F	Cl-	0.35235	1.68150	0.00000	0.00519
Mg++F	Ac-F	0.00000	0.00000	0.00000	0.00000
MgAc+F	Cl-	0.00000	0.29000	0.00000	0.00000
MgAc+F	Ac-F	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	Ac-F
Na+	H+	0.03600	-0.00400	0.00000
Na+	Mg++F	0.07000	-0.01200	0.00000
Na+	MgAc+F	0.00000	0.00000	0.00000
H+	Mg++F	0.10000	-0.01100	0.00000
H+	MgAc+F	0.00000	0.00000	0.00000
Mg++F	MgAc+F	0.00000	0.00000	0.00000

	Na+	H+	Mg++F	MgAc

Cl- Ac-F -0.09000 0.01029 0.00000 0.00000 0.00

TOTAL NUMBER OF SPECIES = 8
NUMBER OF COMPONENTS = 10
INDEPENDENT CONSTRAINTS = 7

SOLUBILITY DATA

input molalities

Na+	H+	Mg++F	MgAc+F	Cl-	Ac-F
3.000E-01	1.000E-07	7.843E-04	1.965E-04	3.000E-01	7.395E-02
1.000E+00	1.000E-07	7.317E-04	1.909E-04	1.000E+00	7.353E-02
2.000E+00	1.000E-07	6.966E-04	2.171E-04	2.000E+00	7.305E-02
3.000E+00	1.000E-07	7.317E-04	2.957E-04	3.000E+00	7.353E-02
4.000E+00	1.000E-07	6.684E-04	2.494E-04	4.000E+00	6.948E-02
5.000E+00	1.000E-07	6.654E-04	2.336E-04	5.000E+00	6.846E-02

-3.0000E+02 1.0000E-01 1.0000E-01
L2 NORM OF THE RESIDUALS 8.6427743E+01

-3.3338E+02 -8.3263E-02 4.9350E-02
L2 NORM OF THE RESIDUALS 6.9394186E-02

-3.3338E+02 -8.3263E-02 4.9350E-02
L2 NORM OF THE RESIDUALS 6.9394186E-02

ADJUSTED PARAMETERS

u0rt(MgAc+F) -3.3337828E+02
b0(MgAc+F Cl-) -8.3262806E-02
cmx(MgAc+F Cl-) 4.9349535E-02

DATA SET(1)

input	calc	diff
0.000000000000000E+000		8.019122212175486E-003
0.000000000000000E+000		-1.971810947335938E-002
0.000000000000000E+000		3.089164532823928E-002
0.000000000000000E+000		-4.400949785417650E-002
0.000000000000000E+000		3.652662329258759E-002
0.000000000000000E+000		-1.170978350555174E-002

AVERAGE DEVIATION = 2.5146E-02

STANDARD DEVIATION = 2.8330E-02

FINAL MOLALITIES

Na+	H+	Mg++F	MgAc+F	Cl-	Ac-F
3.000E-01	1.000E-07	7.843E-04	1.965E-04	3.000E-01	7.395E-02
1.000E+00	1.000E-07	7.317E-04	1.909E-04	1.000E+00	7.353E-02
2.000E+00	1.000E-07	6.966E-04	2.171E-04	2.000E+00	7.305E-02
3.000E+00	1.000E-07	7.317E-04	2.957E-04	3.000E+00	7.353E-02
4.000E+00	1.000E-07	6.684E-04	2.494E-04	4.000E+00	6.948E-02
5.000E+00	1.000E-07	6.654E-04	2.336E-04	5.000E+00	6.846E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++F	MgAc+F	Cl-	Ac-F
-6.686E-01	-7.123E+00	-3.708E+00	-3.903E+00	-6.894E-01	-1.305E+00
-1.759E-01	-7.065E+00	-3.765E+00	-3.997E+00	-1.941E-01	-1.354E+00
1.333E-01	-6.940E+00	-3.672E+00	-3.940E+00	1.168E-01	-1.368E+00
3.385E-01	-6.800E+00	-3.481E+00	-3.701E+00	3.226E-01	-1.353E+00
5.032E-01	-6.654E+00	-3.322E+00	-3.575E+00	4.888E-01	-1.350E+00
6.479E-01	-6.504E+00	-3.111E+00	-3.312E+00	6.341E-01	-1.319E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++F	MgAc+F	Cl-	Ac-F
-0.1458	-0.1227	-0.6024	-0.1962	-0.1665	-0.1736
-0.1759	-0.0651	-0.6293	-0.2782	-0.1941	-0.2206
-0.1677	0.0599	-0.5147	-0.2770	-0.1843	-0.2320
-0.1387	0.1998	-0.3452	-0.1721	-0.1545	-0.2193
-0.0989	0.3465	-0.1475	0.0277	-0.1133	-0.1922
-0.0511	0.4964	0.0661	0.3195	-0.0649	-0.1549

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++F	MgAc+F	Cl-	Ac-F
3.000E-01	1.000E-07	7.843E-04	1.965E-04	3.000E-01	7.395E-02
1.000E+00	1.000E-07	7.317E-04	1.909E-04	1.000E+00	7.353E-02
2.000E+00	1.000E-07	6.966E-04	2.171E-04	2.000E+00	7.305E-02
3.000E+00	1.000E-07	7.317E-04	2.957E-04	3.000E+00	7.353E-02
4.000E+00	1.000E-07	6.684E-04	2.494E-04	4.000E+00	6.948E-02
5.000E+00	1.000E-07	6.654E-04	2.336E-04	5.000E+00	6.846E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++F	MgAc+F	Cl-	Ac-F
-6.686E-01	-7.123E+00	-3.708E+00	-3.903E+00	-6.894E-01	-1.305E+00
-1.759E-01	-7.065E+00	-3.765E+00	-3.997E+00	-1.941E-01	-1.354E+00
1.333E-01	-6.940E+00	-3.672E+00	-3.940E+00	1.168E-01	-1.368E+00
3.385E-01	-6.800E+00	-3.481E+00	-3.701E+00	3.226E-01	-1.353E+00
5.032E-01	-6.654E+00	-3.322E+00	-3.575E+00	4.888E-01	-1.350E+00
6.479E-01	-6.504E+00	-3.111E+00	-3.312E+00	6.341E-01	-1.319E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++F	MgAc+F	Cl-	Ac-F
-0.1458	-0.1227	-0.6024	-0.1962	-0.1665	-0.1736
-0.1759	-0.0651	-0.6293	-0.2782	-0.1941	-0.2206
-0.1677	0.0599	-0.5147	-0.2770	-0.1843	-0.2320
-0.1387	0.1998	-0.3452	-0.1721	-0.1545	-0.2193
-0.0989	0.3465	-0.1475	0.0277	-0.1133	-0.1922
-0.0511	0.4964	0.0661	0.3195	-0.0649	-0.1549

FINAL L2 NORM OF THE RESIDUALS 6.9394186E-02

EXIT PARAMETER 3

FINAL APPROXIMATE SOLUTION

0	0	5	-3.3337828E+02
1	4	1	-8.3262806E-02
4	4	1	4.9349535E-02

```
-1
     6   -1
0   0   0.3000   1.000E-07   7.8430E-04   1.965E-04   0.30000   0.07395
0   0   1.0000   1.000E-07   7.3170E-04   1.909E-04   1.00000   0.07353
0   0   2.0000   1.000E-07   6.9660E-04   2.171E-04   2.00000   0.07305
0   0   3.0000   1.000E-07   7.3170E-04   2.957E-04   3.00000   0.07353
0   0   4.0000   1.000E-07   6.6840E-04   2.494E-04   4.00000   0.06948
0   0   5.0000   1.000E-07   6.6540E-04   2.336E-04   5.00000   0.06846
-1

0   0   Na+       H+          Mg2+         MgAc+    Cl-       Ac-
```

```
     0    0    0    0
0
001080      0.00000000       1  0 H2O
011000      0.00000000       2  1 Na+
001000      0.00000000       3  2 H+
012000      0.00000000       4  3 Mg++
012890      0.00000000       5  4 MgAc+
000170      0.00000000       6  1 Cl-
000890      0.00000000       7  2 Ac-
000000
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGAC.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGAC.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGAC.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
12000	Mg++	0.000000000000	2.	-183.468
12890	MgAc+	0.000000000000	1.	-333.378
170	Cl-	0.000000000000	-1.	-52.955
890	Ac-	0.000000000000	-1.	-147.347

SOLID PHASES

ID	NAME	MOLES	Z	u0rt

CONSTRAINT EQUATIONS

	0	1	8	11	12	89	17
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Mg++	2.0	0.0	0.0	0.0	1.0	0.0	0.0
MgAc+	1.0	0.0	0.0	0.0	1.0	1.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	1.0
Ac-	-1.0	0.0	0.0	0.0	0.0	1.0	0.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	Ac-	0.14260	0.22000	0.00000	-0.00629
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	Ac-	0.00000	0.00000	0.00000	0.00000
Mg++	Cl-	0.35235	1.68150	0.00000	0.00519
Mg++	Ac-	0.00000	0.00000	0.00000	0.00000
MgAc+	Cl-	-0.08330	0.29000	0.00000	0.09870
MgAc+	Ac-	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	Ac-
Na+	H+	0.03600	-0.00400	0.00000
Na+	Mg++	0.07000	-0.01200	0.00000
Na+	MgAc+	0.00000	0.00000	0.00000
H+	Mg++	0.10000	-0.01100	0.00000
H+	MgAc+	0.00000	0.00000	0.00000
Mg++	MgAc+	0.00000	0.00000	0.00000

			Na+	H+	Mg++	MgAc
Cl-	Ac-	-0.09000	0.01029	0.00000	0.00000	0.00

TOTAL NUMBER OF SPECIES = 7
NUMBER OF COMPONENTS = 7
INDEPENDENT CONSTRAINTS = 6

SOLUBILITY DATA

input molalities

Na+	H+	Mg++	MgAc+	Cl-	Ac-
3.000E-01	1.000E-07	7.843E-04	1.965E-04	3.000E-01	7.395E-02
1.000E+00	1.000E-07	7.317E-04	1.909E-04	1.000E+00	7.353E-02
2.000E+00	1.000E-07	6.966E-04	2.171E-04	2.000E+00	7.305E-02
3.000E+00	1.000E-07	7.317E-04	2.957E-04	3.000E+00	7.353E-02
4.000E+00	1.000E-07	6.684E-04	2.494E-04	4.000E+00	6.948E-02
5.000E+00	1.000E-07	6.654E-04	2.336E-04	5.000E+00	6.846E-02

ADJUSTED PARAMETERS

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++	MgAc+	Cl-	Ac-
3.000E-01	1.000E-07	7.831E-04	1.977E-04	3.000E-01	7.395E-02
1.000E+00	1.000E-07	7.347E-04	1.879E-04	1.000E+00	7.353E-02
2.000E+00	1.000E-07	6.915E-04	2.222E-04	2.000E+00	7.304E-02
3.000E+00	1.000E-07	7.409E-04	2.865E-04	3.000E+00	7.354E-02
4.000E+00	1.000E-07	6.617E-04	2.561E-04	4.000E+00	6.947E-02
5.000E+00	1.000E-07	6.674E-04	2.316E-04	5.000E+00	6.846E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++	MgAc+	Cl-	Ac-
-6.686E-01	-7.123E+00	-3.709E+00	-3.900E+00	-6.894E-01	-1.305E+00
-1.759E-01	-7.065E+00	-3.763E+00	-4.004E+00	-1.941E-01	-1.354E+00
1.333E-01	-6.940E+00	-3.675E+00	-3.930E+00	1.168E-01	-1.368E+00
3.385E-01	-6.800E+00	-3.475E+00	-3.715E+00	3.226E-01	-1.353E+00
5.032E-01	-6.654E+00	-3.327E+00	-3.564E+00	4.888E-01	-1.350E+00
6.479E-01	-6.504E+00	-3.110E+00	-3.316E+00	6.341E-01	-1.319E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++	MgAc+	Cl-	Ac-
-0.1458	-0.1227	-0.6024	-0.1962	-0.1665	-0.1736
-0.1759	-0.0651	-0.6293	-0.2782	-0.1941	-0.2206
-0.1677	0.0599	-0.5147	-0.2770	-0.1843	-0.2320
-0.1387	0.1998	-0.3452	-0.1722	-0.1545	-0.2193
-0.0989	0.3465	-0.1475	0.0276	-0.1133	-0.1922
-0.0511	0.4964	0.0661	0.3194	-0.0649	-0.1549

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++	MgAc+	Cl-	Ac-
3.000E-01	4.624E+00	8.968E-04	8.401E-05	4.924E+00	7.406E-02
1.000E+00	4.195E+00	8.382E-04	8.443E-05	5.195E+00	7.364E-02
2.000E+00	3.598E+00	8.244E-04	8.926E-05	5.598E+00	7.318E-02
3.000E+00	3.025E+00	9.233E-04	1.041E-04	6.025E+00	7.372E-02
4.000E+00	2.480E+00	8.309E-04	8.690E-05	6.480E+00	6.964E-02
5.000E+00	1.971E+00	8.213E-04	7.769E-05	6.971E+00	6.862E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++	MgAc+	Cl-	Ac-
-4.457E-01	1.086E+00	-2.818E+00	-3.696E+00	1.071E+00	-1.991E+00
7.722E-02	1.095E+00	-2.801E+00	-3.601E+00	1.060E+00	-1.913E+00
3.810E-01	1.102E+00	-2.738E+00	-3.427E+00	1.049E+00	-1.802E+00
5.633E-01	1.102E+00	-2.613E+00	-3.188E+00	1.045E+00	-1.688E+00
6.977E-01	1.094E+00	-2.574E+00	-3.067E+00	1.048E+00	-1.606E+00
8.091E-01	1.077E+00	-2.485E+00	-2.881E+00	1.060E+00	-1.509E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++	MgAc+	Cl-	Ac-
0.0772	0.4215	0.2298	0.3798	0.3785	-0.8610
0.0772	0.4722	0.2755	0.4728	0.3441	-0.7797
0.0799	0.5458	0.3454	0.6222	0.3008	-0.6662
0.0862	0.6214	0.4216	0.7944	0.2646	-0.5560
0.0956	0.6999	0.5060	0.9936	0.2365	-0.4489
0.1101	0.7822	0.6003	1.2286	0.2169	-0.3453

FINAL L2 NORM OF THE RESIDUALS 0.0000000E+00

EXIT PARAMETER 0

FINAL APPROXIMATE SOLUTION

```
000005 -300.0          u0 MgOxF
100101  0.1            lambda MgOxF Cl-
-1
    6   -1
0  0  0.3000  1.000E-07  0.01000000  0.02138    0.30000  0.01000
0  0  1.0000  1.000E-07  0.01000000  0.01000    1.00000  0.01000
0  0  2.0000  1.000E-07  0.01000000  0.00871    2.00000  0.01000
0  0  3.0000  1.000E-07  0.01000000  0.00589    3.00000  0.01000
0  0  4.0000  1.000E-07  0.01000000  0.00977    4.00000  0.01000
0  0  5.0000  1.000E-07  0.01000000  0.01000    5.00000  0.01000
-1

0  0  Na+      H+         Mg2+        MgOx    Cl-      Ox
```

```
     0    0    0    0
0
001080      0.00000000       1  0 H2O
011000      0.00000000       2  1 Na+
001000      0.00000000       3  2 H+
012001      0.00000000       4  3 Mg++F
012991      0.00000000       5  1 MgOxF
000170      0.00000000       6  1 Cl-
000991      0.00000000       7  2 Ox=F
000000
112990      0.00000000       8   MgOx/Mg/Ox(s)
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGOX.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGOX.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGOX.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
12001	Mg++F	0.000000000000	2.	-183.468
12991	MgOxF	0.000000000000	0.	999.990
170	Cl-	0.000000000000	-1.	-52.955
991	Ox=F	0.000000000000	-2.	13.017

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
112990	MgOx/Mg/Ox(s	0.000000000000	0.	0.000

CONSTRAINT EQUATIONS

	0	1	8	11	12	72	99	73	17
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mg++F	2.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
MgOxF	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
Ox=F	-2.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
MgOx/Mg/Ox(s	0.0	0.0	0.0	0.0	0.0	-1.0	0.0	1.0	0.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	Ox=F	-0.21760	1.74000	0.00000	0.12200
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	Ox=F	0.00000	0.00000	0.00000	0.00000
Mg++F	Cl-	0.35235	1.68150	0.00000	0.00519
Mg++F	Ox=F	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	Ox=F	
Na+	H+	0.03600	-0.00400	0.00000	
Na+	Mg++F	0.07000	-0.01200	0.00000	
H+	Mg++F	0.10000	-0.01100	0.00000	

			Na+	H+	Mg++F
Cl-	Ox=F	0.00000	0.00000	0.00000	0.00000

neutral ion parameters

	MgOxF
Na+	0.0000

```
H+              0.0000
Mg++F           0.0000
Cl-             0.0000
Ox=F            0.0000
MgOxF           0.0000

        higher order lambdas

                        Cl-          Ox=F
MgOxF       Na+          0.00000      0.00000
MgOxF       H+           0.00000      0.00000
MgOxF       Mg++F        0.00000      0.00000

 TOTAL NUMBER OF SPECIES =  8
 NUMBER OF COMPONENTS    = 10
 INDEPENDENT CONSTRAINTS =  7

          SOLUBILITY DATA

          input molalities


   Na+          H+           Mg++F        MgOxF        Cl-          Ox=F
   3.000E-01    1.000E-07    1.000E-02    2.138E-02    3.000E-01    1.000E-02
   1.000E+00    1.000E-07    1.000E-02    1.000E-02    1.000E+00    1.000E-02
   2.000E+00    1.000E-07    1.000E-02    8.710E-03    2.000E+00    1.000E-02
   3.000E+00    1.000E-07    1.000E-02    5.890E-03    3.000E+00    1.000E-02
   4.000E+00    1.000E-07    1.000E-02    9.770E-03    4.000E+00    1.000E-02
   5.000E+00    1.000E-07    1.000E-02    1.000E-02    5.000E+00    1.000E-02

  -3.0000E+02  1.0000E-01
           L2 NORM OF THE RESIDUALS  2.9492205E+02


  -1.7919E+02  1.8850E-02
           L2 NORM OF THE RESIDUALS  5.2632836E-01


  -1.7919E+02  1.8850E-02
           L2 NORM OF THE RESIDUALS  5.2632836E-01


          ADJUSTED PARAMETERS
   u0rt(                        MgOxF       )  -1.7918520E+02
 lambda(            MgOxF       Cl-         )   1.8850447E-02

  DATA SET( 1)

   input    calc      diff
  0.000000000000000E+000  0.216000391161975
  0.000000000000000E+000  3.201168474836891E-002
  0.000000000000000E+000 -0.319433996061528
  0.000000000000000E+000  1.994774472088956E-002
  0.000000000000000E+000 -0.224842078702181
  0.000000000000000E+000  0.276316254132572

  AVERAGE DEVIATION   =  1.8143E-01

  STANDARD DEVIATION =  2.1487E-01

 FINAL MOLALITIES
```

Na+	H+	Mg++F	MgOxF	Cl-	Ox=F
3.000E-01	1.000E-07	1.000E-02	2.138E-02	3.000E-01	1.000E-02
1.000E+00	1.000E-07	1.000E-02	1.000E-02	1.000E+00	1.000E-02
2.000E+00	1.000E-07	1.000E-02	8.710E-03	2.000E+00	1.000E-02
3.000E+00	1.000E-07	1.000E-02	5.890E-03	3.000E+00	1.000E-02
4.000E+00	1.000E-07	1.000E-02	9.770E-03	4.000E+00	1.000E-02
5.000E+00	1.000E-07	1.000E-02	1.000E-02	5.000E+00	1.000E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++F	MgOxF	Cl-	Ox=F
-6.810E-01	-7.124E+00	-2.604E+00	-1.665E+00	-6.767E-01	-2.760E+00
-1.875E-01	-7.066E+00	-2.632E+00	-1.984E+00	-1.835E-01	-3.131E+00
1.227E-01	-6.940E+00	-2.516E+00	-2.027E+00	1.263E-01	-3.443E+00
3.284E-01	-6.800E+00	-2.346E+00	-2.181E+00	3.317E-01	-3.620E+00
4.942E-01	-6.653E+00	-2.148E+00	-1.945E+00	4.972E-01	-3.688E+00
6.397E-01	-6.503E+00	-1.933E+00	-1.918E+00	6.423E-01	-3.658E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++F	MgOxF	Cl-	Ox=F
-0.1581	-0.1243	-0.6045	0.0049	-0.1538	-0.7600
-0.1875	-0.0659	-0.6318	0.0164	-0.1835	-1.1311
-0.1784	0.0597	-0.5163	0.0328	-0.1747	-1.4429
-0.1487	0.2001	-0.3456	0.0491	-0.1454	-1.6197
-0.1078	0.3471	-0.1476	0.0655	-0.1048	-1.6879
-0.0593	0.4974	0.0668	0.0819	-0.0567	-1.6581

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++F	MgOxF	Cl-	Ox=F
3.000E-01	1.000E-07	1.000E-02	2.138E-02	3.000E-01	1.000E-02
1.000E+00	1.000E-07	1.000E-02	1.000E-02	1.000E+00	1.000E-02
2.000E+00	1.000E-07	1.000E-02	8.710E-03	2.000E+00	1.000E-02
3.000E+00	1.000E-07	1.000E-02	5.890E-03	3.000E+00	1.000E-02
4.000E+00	1.000E-07	1.000E-02	9.770E-03	4.000E+00	1.000E-02
5.000E+00	1.000E-07	1.000E-02	1.000E-02	5.000E+00	1.000E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++F	MgOxF	Cl-	Ox=F
-6.810E-01	-7.124E+00	-2.604E+00	-1.665E+00	-6.767E-01	-2.760E+00
-1.875E-01	-7.066E+00	-2.632E+00	-1.984E+00	-1.835E-01	-3.131E+00
1.227E-01	-6.940E+00	-2.516E+00	-2.027E+00	1.263E-01	-3.443E+00
3.284E-01	-6.800E+00	-2.346E+00	-2.181E+00	3.317E-01	-3.620E+00
4.942E-01	-6.653E+00	-2.148E+00	-1.945E+00	4.972E-01	-3.688E+00
6.397E-01	-6.503E+00	-1.933E+00	-1.918E+00	6.423E-01	-3.658E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++F	MgOxF	Cl-	Ox=F
-0.1581	-0.1243	-0.6045	0.0049	-0.1538	-0.7600
-0.1875	-0.0659	-0.6318	0.0164	-0.1835	-1.1311
-0.1784	0.0597	-0.5163	0.0328	-0.1747	-1.4429
-0.1487	0.2001	-0.3456	0.0491	-0.1454	-1.6197
-0.1078	0.3471	-0.1476	0.0655	-0.1048	-1.6879
-0.0593	0.4974	0.0668	0.0819	-0.0567	-1.6581

FINAL L2 NORM OF THE RESIDUALS 5.2632836E-01

EXIT PARAMETER 3

FINAL APPROXIMATE SOLUTION

0 0 5 -1.7918520E+02
10 1 1 1.8850447E-02

```
-1
     6   -1
0   0   0.3000   1.000E-07   0.01000000   0.02138    0.30000   0.01000
0   0   1.0000   1.000E-07   0.01000000   0.01000    1.00000   0.01000
0   0   2.0000   1.000E-07   0.01000000   0.00871    2.00000   0.01000
0   0   3.0000   1.000E-07   0.01000000   0.00589    3.00000   0.01000
0   0   4.0000   1.000E-07   0.01000000   0.00977    4.00000   0.01000
0   0   5.0000   1.000E-07   0.01000000   0.01000    5.00000   0.01000
-1

0   0   Na+      H+          Mg2+         MgOx    Cl-      Ox
```

```
     0     0     0     0
0
001080      0.00000000      1  0 H2O
011000      0.00000000      2  1 Na+
001000      0.00000000      3  2 H+
012000      0.00000000      4  3 Mg++
012990      0.00000000      5  1 MgOx
000170      0.00000000      6  1 Cl-
000990      0.00000000      7  2 Ox=
000000
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGOX.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGOX.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGOX.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
12000	Mg++	0.000000000000	2.	-183.468
12990	MgOx	0.000000000000	0.	-179.185
170	Cl-	0.000000000000	-1.	-52.955
990	Ox=	0.000000000000	-2.	13.017

SOLID PHASES

ID	NAME	MOLES	Z	u0rt

CONSTRAINT EQUATIONS

	0	1	8	11	12	99	17
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Mg++	2.0	0.0	0.0	0.0	1.0	0.0	0.0
MgOx	0.0	0.0	0.0	0.0	1.0	1.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	1.0
Ox=	-2.0	0.0	0.0	0.0	0.0	1.0	0.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	Ox=	-0.21760	1.74000	0.00000	0.12200
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	Ox=	0.00000	0.00000	0.00000	0.00000
Mg++	Cl-	0.35235	1.68150	0.00000	0.00519
Mg++	Ox=	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	Ox=
Na+	H+	0.03600	-0.00400	0.00000
Na+	Mg++	0.07000	-0.01200	0.00000
H+	Mg++	0.10000	-0.01100	0.00000

			Na+	H+	Mg++
Cl-	Ox=	0.00000	0.00000	0.00000	0.00000

neutral ion parameters

	MgOx
Na+	0.0000
H+	0.0000
Mg++	0.0000

Cl-	0.0189
Ox=	0.0000
MgOx	0.0000

higher order lambdas

		Cl-	Ox=
MgOx	Na+	0.00000	0.00000
MgOx	H+	0.00000	0.00000
MgOx	Mg++	0.00000	0.00000

TOTAL NUMBER OF SPECIES = 7
NUMBER OF COMPONENTS = 7
INDEPENDENT CONSTRAINTS = 6

SOLUBILITY DATA

input molalities

Na+	H+	Mg++	MgOx	Cl-	Ox=
3.000E-01	1.000E-07	1.000E-02	2.138E-02	3.000E-01	1.000E-02
1.000E+00	1.000E-07	1.000E-02	1.000E-02	1.000E+00	1.000E-02
2.000E+00	1.000E-07	1.000E-02	8.710E-03	2.000E+00	1.000E-02
3.000E+00	1.000E-07	1.000E-02	5.890E-03	3.000E+00	1.000E-02
4.000E+00	1.000E-07	1.000E-02	9.770E-03	4.000E+00	1.000E-02
5.000E+00	1.000E-07	1.000E-02	1.000E-02	5.000E+00	1.000E-02

ADJUSTED PARAMETERS

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++	MgOx	Cl-	Ox=
3.000E-01	1.000E-07	9.084E-03	2.230E-02	3.000E-01	9.084E-03
1.000E+00	1.000E-07	9.890E-03	1.011E-02	1.000E+00	9.890E-03
2.000E+00	1.000E-07	1.105E-02	7.663E-03	2.000E+00	1.105E-02
3.000E+00	1.000E-07	9.947E-03	5.943E-03	3.000E+00	9.947E-03
4.000E+00	1.000E-07	1.076E-02	9.008E-03	4.000E+00	1.076E-02
5.000E+00	1.000E-07	9.091E-03	1.091E-02	5.000E+00	9.091E-03

FINAL LOG ACTIVITIES

Na+	H+	Mg++	MgOx	Cl-	Ox=
-6.803E-01	-7.123E+00	-2.642E+00	-1.647E+00	-6.764E-01	-2.798E+00
-1.874E-01	-7.066E+00	-2.636E+00	-1.979E+00	-1.835E-01	-3.136E+00
1.224E-01	-6.941E+00	-2.475E+00	-2.083E+00	1.264E-01	-3.401E+00
3.284E-01	-6.800E+00	-2.348E+00	-2.177E+00	3.317E-01	-3.622E+00
4.942E-01	-6.653E+00	-2.116E+00	-1.980E+00	4.974E-01	-3.656E+00
6.396E-01	-6.503E+00	-1.974E+00	-1.880E+00	6.421E-01	-3.699E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++	MgOx	Cl-	Ox=
-0.1575	-0.1232	-0.6005	0.0049	-0.1535	-0.7560
-0.1874	-0.0659	-0.6316	0.0164	-0.1835	-1.1308
-0.1786	0.0593	-0.5180	0.0328	-0.1746	-1.4444
-0.1487	0.2001	-0.3456	0.0493	-0.1454	-1.6196
-0.1078	0.3469	-0.1482	0.0657	-0.1046	-1.6883
-0.0593	0.4975	0.0674	0.0821	-0.0569	-1.6579

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++	MgOx	Cl-	Ox=
3.000E-01	4.603E+00	1.850E-02	1.288E-02	4.903E+00	1.850E-02
1.000E+00	4.176E+00	1.236E-02	7.641E-03	5.176E+00	1.236E-02
2.000E+00	3.580E+00	1.039E-02	8.317E-03	5.580E+00	1.039E-02
3.000E+00	3.008E+00	7.968E-03	7.922E-03	6.008E+00	7.968E-03
4.000E+00	2.464E+00	7.543E-03	1.223E-02	6.464E+00	7.543E-03
5.000E+00	1.958E+00	5.926E-03	1.407E-02	6.958E+00	5.926E-03

FINAL LOG ACTIVITIES

Na+	H+	Mg++	MgOx	Cl-	Ox=
-4.578E-01	1.080E+00	-1.515E+00	-1.788E+00	1.077E+00	-4.066E+00
6.565E-02	1.090E+00	-1.640E+00	-2.012E+00	1.065E+00	-4.165E+00
3.699E-01	1.097E+00	-1.643E+00	-1.971E+00	1.054E+00	-4.121E+00
5.525E-01	1.098E+00	-1.680E+00	-1.988E+00	1.049E+00	-4.101E+00
6.879E-01	1.090E+00	-1.619E+00	-1.794E+00	1.052E+00	-3.969E+00
7.997E-01	1.073E+00	-1.628E+00	-1.728E+00	1.064E+00	-3.893E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++	MgOx	Cl-	Ox=
0.0651	0.4171	0.2181	0.1024	0.3868	-2.3332
0.0656	0.4691	0.2683	0.1049	0.3510	-2.2572
0.0689	0.5434	0.3401	0.1089	0.3071	-2.1378
0.0754	0.6197	0.4185	0.1133	0.2703	-2.0021
0.0858	0.6986	0.5036	0.1183	0.2419	-1.8463
0.1007	0.7815	0.5994	0.1240	0.2219	-1.6656

FINAL L2 NORM OF THE RESIDUALS 0.0000000E+00

EXIT PARAMETER 0

FINAL APPROXIMATE SOLUTION

```
000007 -300.0          u0 MgCit-F
010103  0.1            b0 MgCit-F Na+
040103  0.1            cMX MgCit-F Na+
-1
    6   -1
0  0  0.3000  1.000E-07  0.01000000  0.30000  0.01000  0.09333
0  0  1.0000  1.000E-07  0.01000000  1.00000  0.01000  0.02512
0  0  2.0000  1.000E-07  0.01000000  2.00000  0.01000  0.00933
0  0  3.0000  1.000E-07  0.01000000  3.00000  0.01000  0.01047
0  0  4.0000  1.000E-07  0.01000000  4.00000  0.01000  0.01202
0  0  5.0000  1.000E-07  0.01000000  5.00000  0.01000  0.01175
-1

0  0  Na+      H+         Mg2+       Cl-      Cit=-    MgCit-
```

```
     0    0    0    0
0
001080      0.00000000      1  0 H2O
011000      0.00000000      2  1 Na+
001000      0.00000000      3  2 H+
012001      0.00000000      4  3 Mg++F
000170      0.00000000      5  1 Cl-
000861      0.00000000      6  2 Cit=-F
012861      0.00000000      7  3 MgCit-F
000000
112860      0.00000000      8   MgCit/Mg/Cit
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGCIT.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGCIT.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGCIT.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
12001	Mg++F	0.000000000000	2.	-183.468
170	Cl-	0.000000000000	-1.	-52.955
861	Cit=-F	0.000000000000	-3.	33.410
12861	MgCit-F	0.000000000000	-1.	999.999

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
112860	MgCit/Mg/Cit	0.000000000000	0.	0.000

CONSTRAINT EQUATIONS

	0	1	8	11	12	72	17	86	71
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mg++F	2.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Cit=-F	-3.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0
MgCit-F	-1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0
MgCit/Mg/Cit	0.0	0.0	0.0	0.0	0.0	-1.0	0.0	0.0	-1.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	Cit=-F	0.08870	5.22000	0.00000	0.04700
Na+	MgCit-F	0.00000	0.29000	0.00000	0.00000
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	Cit=-F	0.00000	0.00000	0.00000	0.00000
H+	MgCit-F	0.00000	0.00000	0.00000	0.00000
Mg++F	Cl-	0.35235	1.68150	0.00000	0.00519
Mg++F	Cit=-F	0.00000	0.00000	0.00000	0.00000
Mg++F	MgCit-F	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	Cit=-F	MgCit-F
Na+	H+	0.03600	-0.00400	0.00000	0.00000
Na+	Mg++F	0.07000	-0.01200	0.00000	0.00000
H+	Mg++F	0.10000	-0.01100	0.00000	0.00000

			Na+	H+	Mg++F
Cl-	Cit=-F	0.00000	0.00000	0.00000	0.00000
Cl-	MgCit-F	0.00000	0.00000	0.00000	0.00000

Cit=-F MgCit-F 0.00000 0.00000 0.00000 0.00000

TOTAL NUMBER OF SPECIES = 8
NUMBER OF COMPONENTS = 10
INDEPENDENT CONSTRAINTS = 7

SOLUBILITY DATA

input molalities

Na+	H+	Mg++F	Cl-	Cit=-F	MgCit-F
3.000E-01	1.000E-07	1.000E-02	3.000E-01	1.000E-02	9.333E-02
1.000E+00	1.000E-07	1.000E-02	1.000E+00	1.000E-02	2.512E-02
2.000E+00	1.000E-07	1.000E-02	2.000E+00	1.000E-02	9.330E-03
3.000E+00	1.000E-07	1.000E-02	3.000E+00	1.000E-02	1.047E-02
4.000E+00	1.000E-07	1.000E-02	4.000E+00	1.000E-02	1.202E-02
5.000E+00	1.000E-07	1.000E-02	5.000E+00	1.000E-02	1.175E-02

-3.0000E+02 1.0000E-01 1.0000E-01
L2 NORM OF THE RESIDUALS 3.3229697E+02

-1.6226E+02 1.7421E-01 -3.4617E-02
L2 NORM OF THE RESIDUALS 5.1133329E-01

-1.6226E+02 1.7421E-01 -3.4617E-02
L2 NORM OF THE RESIDUALS 5.1133329E-01

ADJUSTED PARAMETERS

u0rt(		MgCit-F	)	-1.6226115E+02
b0(	Na+	MgCit-F	)	1.7421114E-01
cmx(	Na+	MgCit-F	)	-3.4616671E-02

DATA SET(1)

input	calc	diff
0.000000000000000E+000	-0.180806412201548	
0.000000000000000E+000	0.146393049359972	
0.000000000000000E+000	0.288356409902661	
0.000000000000000E+000	-0.173917402691416	
0.000000000000000E+000	-0.253016484457021	
0.000000000000000E+000	0.172990840087266	

AVERAGE DEVIATION = 2.0258E-01

STANDARD DEVIATION = 2.0875E-01

FINAL MOLALITIES

Na+	H+	Mg++F	Cl-	Cit=-F	MgCit-F
3.000E-01	1.000E-07	1.000E-02	3.000E-01	1.000E-02	9.333E-02
1.000E+00	1.000E-07	1.000E-02	1.000E+00	1.000E-02	2.512E-02
2.000E+00	1.000E-07	1.000E-02	2.000E+00	1.000E-02	9.330E-03
3.000E+00	1.000E-07	1.000E-02	3.000E+00	1.000E-02	1.047E-02
4.000E+00	1.000E-07	1.000E-02	4.000E+00	1.000E-02	1.202E-02
5.000E+00	1.000E-07	1.000E-02	5.000E+00	1.000E-02	1.175E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++F	Cl-	Cit=-F	MgCit-F
-6.591E-01	-7.142E+00	-2.673E+00	-7.045E-01	-3.902E+00	-1.196E+00
-1.774E-01	-7.072E+00	-2.655E+00	-1.955E-01	-4.325E+00	-1.744E+00
1.284E-01	-6.944E+00	-2.529E+00	1.184E-01	-4.810E+00	-2.165E+00
3.326E-01	-6.803E+00	-2.357E+00	3.249E-01	-5.171E+00	-2.152E+00
4.970E-01	-6.656E+00	-2.158E+00	4.909E-01	-5.433E+00	-2.181E+00
6.412E-01	-6.506E+00	-1.942E+00	6.364E-01	-5.615E+00	-2.333E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++F	Cl-	Cit=-F	MgCit-F
-0.1362	-0.1418	-0.6731	-0.1817	-1.9016	-0.1664
-0.1774	-0.0717	-0.6545	-0.1955	-2.3254	-0.1438
-0.1726	0.0563	-0.5294	-0.1826	-2.8104	-0.1352
-0.1446	0.1970	-0.3567	-0.1522	-3.1709	-0.1723
-0.1051	0.3440	-0.1576	-0.1111	-3.4328	-0.2607
-0.0578	0.4944	0.0576	-0.0626	-3.6154	-0.4032

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++F	Cl-	Cit=-F	MgCit-F
3.000E-01	1.000E-07	1.000E-02	3.000E-01	1.000E-02	9.333E-02
1.000E+00	1.000E-07	1.000E-02	1.000E+00	1.000E-02	2.512E-02
2.000E+00	1.000E-07	1.000E-02	2.000E+00	1.000E-02	9.330E-03
3.000E+00	1.000E-07	1.000E-02	3.000E+00	1.000E-02	1.047E-02
4.000E+00	1.000E-07	1.000E-02	4.000E+00	1.000E-02	1.202E-02
5.000E+00	1.000E-07	1.000E-02	5.000E+00	1.000E-02	1.175E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++F	Cl-	Cit=-F	MgCit-F
-6.591E-01	-7.142E+00	-2.673E+00	-7.045E-01	-3.902E+00	-1.196E+00
-1.774E-01	-7.072E+00	-2.655E+00	-1.955E-01	-4.325E+00	-1.744E+00
1.284E-01	-6.944E+00	-2.529E+00	1.184E-01	-4.810E+00	-2.165E+00
3.326E-01	-6.803E+00	-2.357E+00	3.249E-01	-5.171E+00	-2.152E+00
4.970E-01	-6.656E+00	-2.158E+00	4.909E-01	-5.433E+00	-2.181E+00
6.412E-01	-6.506E+00	-1.942E+00	6.364E-01	-5.615E+00	-2.333E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++F	Cl-	Cit=-F	MgCit-F
-0.1362	-0.1418	-0.6731	-0.1817	-1.9016	-0.1664
-0.1774	-0.0717	-0.6545	-0.1955	-2.3254	-0.1438
-0.1726	0.0563	-0.5294	-0.1826	-2.8104	-0.1352
-0.1446	0.1970	-0.3567	-0.1522	-3.1709	-0.1723
-0.1051	0.3440	-0.1576	-0.1111	-3.4328	-0.2607
-0.0578	0.4944	0.0576	-0.0626	-3.6154	-0.4032

FINAL L2 NORM OF THE RESIDUALS 5.1133329E-01

EXIT PARAMETER 3

FINAL APPROXIMATE SOLUTION

```
0 0 7  -1.6226115E+02
1 1 3   1.7421114E-01
4 1 3  -3.4616671E-02
```

```
-1
     6   -1
0   0   0.3000   1.000E-07  0.01000000  0.30000  0.01000  0.09333
0   0   1.0000   1.000E-07  0.01000000  1.00000  0.01000  0.02512
0   0   2.0000   1.000E-07  0.01000000  2.00000  0.01000  0.00933
0   0   3.0000   1.000E-07  0.01000000  3.00000  0.01000  0.01047
0   0   4.0000   1.000E-07  0.01000000  4.00000  0.01000  0.01202
0   0   5.0000   1.000E-07  0.01000000  5.00000  0.01000  0.01175
-1

0   0   Na+      H+         Mg2+        Cl-      Cit=-    MgCit-
```

```
     0     0     0     0
0
001080      0.00000000       1  0 H2O
011000      0.00000000       2  1 Na+
001000      0.00000000       3  2 H+
012000      0.00000000       4  3 Mg++
000170      0.00000000       5  1 Cl-
000860      0.00000000       6  2 Cit=-
012860      0.00000000       7  3 MgCit
000000
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGCIT.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGCIT.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGCIT.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
12000	Mg++	0.000000000000	2.	-183.468
170	Cl-	0.000000000000	-1.	-52.955
860	Cit=-	0.000000000000	-3.	33.410
12860	MgCit-	0.000000000000	-1.	-162.261

SOLID PHASES

ID	NAME	MOLES	Z	u0rt

CONSTRAINT EQUATIONS

	0	1	8	11	12	17	86
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Mg++	2.0	0.0	0.0	0.0	1.0	0.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	1.0	0.0
Cit=-	-3.0	0.0	0.0	0.0	0.0	0.0	1.0
MgCit-	-1.0	0.0	0.0	0.0	1.0	0.0	1.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	Cit=-	0.08870	5.22000	0.00000	0.04700
Na+	MgCit-	0.17420	0.29000	0.00000	-0.06923
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	Cit=-	0.00000	0.00000	0.00000	0.00000
H+	MgCit-	0.00000	0.00000	0.00000	0.00000
Mg++	Cl-	0.35235	1.68150	0.00000	0.00519
Mg++	Cit=-	0.00000	0.00000	0.00000	0.00000
Mg++	MgCit-	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	Cit=-	MgCit-
Na+	H+	0.03600	-0.00400	0.00000	0.00000
Na+	Mg++	0.07000	-0.01200	0.00000	0.00000
H+	Mg++	0.10000	-0.01100	0.00000	0.00000

			Na+	H+	Mg++
Cl-	Cit=-	0.00000	0.00000	0.00000	0.00000
Cl-	MgCit-	0.00000	0.00000	0.00000	0.00000
Cit=-	MgCit-	0.00000	0.00000	0.00000	0.00000

TOTAL NUMBER OF SPECIES = 7
NUMBER OF COMPONENTS = 7
INDEPENDENT CONSTRAINTS = 6

SOLUBILITY DATA

input molalities

Na+	H+	Mg++	Cl-	Cit=-	MgCit-
3.000E-01	1.000E-07	1.000E-02	3.000E-01	1.000E-02	9.333E-02
1.000E+00	1.000E-07	1.000E-02	1.000E+00	1.000E-02	2.512E-02
2.000E+00	1.000E-07	1.000E-02	2.000E+00	1.000E-02	9.330E-03
3.000E+00	1.000E-07	1.000E-02	3.000E+00	1.000E-02	1.047E-02
4.000E+00	1.000E-07	1.000E-02	4.000E+00	1.000E-02	1.202E-02
5.000E+00	1.000E-07	1.000E-02	5.000E+00	1.000E-02	1.175E-02

ADJUSTED PARAMETERS

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++	Cl-	Cit=-	MgCit-
3.000E-01	1.000E-07	1.104E-02	3.000E-01	1.104E-02	9.229E-02
1.000E+00	1.000E-07	9.353E-03	1.000E+00	9.353E-03	2.577E-02
2.000E+00	1.000E-07	9.034E-03	2.000E+00	9.034E-03	1.030E-02
3.000E+00	1.000E-07	1.062E-02	3.000E+00	1.062E-02	9.854E-03
4.000E+00	1.000E-07	1.093E-02	4.000E+00	1.093E-02	1.109E-02
5.000E+00	1.000E-07	9.392E-03	5.000E+00	9.392E-03	1.236E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++	Cl-	Cit=-	MgCit-
-6.589E-01	-7.143E+00	-2.635E+00	-7.061E-01	-3.868E+00	-1.204E+00
-1.776E-01	-7.071E+00	-2.681E+00	-1.950E-01	-4.350E+00	-1.732E+00
1.282E-01	-6.943E+00	-2.571E+00	1.189E-01	-4.850E+00	-2.121E+00
3.327E-01	-6.803E+00	-2.332E+00	3.248E-01	-5.147E+00	-2.179E+00
4.972E-01	-6.656E+00	-2.120E+00	4.908E-01	-5.396E+00	-2.217E+00
6.410E-01	-6.506E+00	-1.969E+00	6.364E-01	-5.641E+00	-2.311E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++	Cl-	Cit=-	MgCit-
-0.1360	-0.1433	-0.6786	-0.1832	-1.9112	-0.1690
-0.1776	-0.0712	-0.6523	-0.1950	-2.3210	-0.1427
-0.1728	0.0568	-0.5271	-0.1822	-2.8058	-0.1341
-0.1444	0.1968	-0.3577	-0.1524	-3.1731	-0.1729
-0.1048	0.3438	-0.1588	-0.1113	-3.4353	-0.2616
-0.0580	0.4945	0.0582	-0.0625	-3.6142	-0.4027

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

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++	Cl-	Cit=-	MgCit-
3.000E-01	7.000E-15	1.104E-02	3.000E-01	1.104E-02	9.229E-02
1.000E+00	7.000E-15	9.353E-03	1.000E+00	9.353E-03	2.577E-02
2.000E+00	7.000E-15	9.034E-03	2.000E+00	9.034E-03	1.030E-02
3.000E+00	7.000E-15	1.062E-02	3.000E+00	1.062E-02	9.854E-03
4.000E+00	7.000E-15	1.094E-02	4.000E+00	1.093E-02	1.108E-02
5.000E+00	7.000E-15	9.392E-03	5.000E+00	9.392E-03	1.236E-02

FINAL LOG ACTIVITIES

Na+	H+	Mg++	Cl-	Cit=-	MgCit-
-6.589E-01	-1.430E+01	-2.635E+00	-7.061E-01	-3.868E+00	-1.204E+00
-1.776E-01	-1.423E+01	-2.681E+00	-1.950E-01	-4.350E+00	-1.732E+00
1.282E-01	-1.410E+01	-2.571E+00	1.189E-01	-4.850E+00	-2.121E+00
3.327E-01	-1.396E+01	-2.332E+00	3.248E-01	-5.147E+00	-2.179E+00
4.972E-01	-1.381E+01	-2.120E+00	4.908E-01	-5.396E+00	-2.217E+00
6.410E-01	-1.366E+01	-1.969E+00	6.364E-01	-5.641E+00	-2.311E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++	Cl-	Cit=-	MgCit-
-0.1360	-0.1432	-0.6786	-0.1832	-1.9112	-0.1690
-0.1776	-0.0712	-0.6523	-0.1950	-2.3209	-0.1427
-0.1728	0.0568	-0.5271	-0.1822	-2.8058	-0.1341
-0.1444	0.1968	-0.3577	-0.1524	-3.1731	-0.1729
-0.1048	0.3438	-0.1588	-0.1113	-3.4353	-0.2616
-0.0580	0.4945	0.0582	-0.0625	-3.6142	-0.4027

FINAL L2 NORM OF THE RESIDUALS 0.0000000E+00

EXIT PARAMETER 0

FINAL APPROXIMATE SOLUTION

```
000007 -300.0          u0 MgEDTA=F
010103  0.1            b0 MgEDTA=F Na+
040103  0.1            cMX MgEDTA=F Na+
-1
    6   -1
0   0  0.3000  1.000E-07  1.0000E-06  0.30000  1.0E-06  2.818e-05
0   0  1.0000  1.000E-07  1.0000E-06  1.00000  1.0E-06  5.012e-06
0   0  2.0000  1.000E-07  1.0000E-06  2.00000  1.0E-06  2.754e-06
0   0  3.0000  1.000E-07  1.0000E-06  3.00000  1.0E-06  2.178e-06
0   0  4.0000  1.000E-07  1.0000E-06  4.00000  1.0E-06  2.570e-06
0   0  5.0000  1.000E-07  1.0000E-06  5.00000  1.0E-06  3.311e-06
-1

0   0  Na+      H+         Mg2+       Cl-      EDTA==    MgEDTA=
```

```
     0    0    0    0
0
001080      0.00000000       1  0 H2O
011000      0.00000000       2  1 Na+
001000      0.00000000       3  2 H+
012001      0.00000000       4  3 Mg++F
000170      0.00000000       5  1 Cl-
000871      0.00000000       6  2 EDTA==F
012871      0.00000000       7  3 MgEDTA==F
000000
112870      0.00000000       8   MgEDTA/Mg/EDTA
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGEDTA.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGEDTA.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]MGEDTA.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
12001	Mg++F	0.000000000000	2.	-183.468
170	Cl-	0.000000000000	-1.	-52.955
871	EDTA==F	0.000000000000	-4.	53.050
12871	MgEDTA=F	0.000000000000	-2.	999.999

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
112870	MgEDTA/Mg/ED	0.000000000000	0.	0.000

CONSTRAINT EQUATIONS

	0	1	8	11	12	72	17	87	71
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mg++F	2.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
EDTA==F	-4.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0
MgEDTA=F	-2.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0
MgEDTA/Mg/ED	0.0	0.0	0.0	0.0	0.0	-1.0	0.0	0.0	-1.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	EDTA==F	1.01600	11.60000	0.00000	0.00100
Na+	MgEDTA=F	0.00000	1.74000	0.00000	0.00000
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	EDTA==F	0.00000	0.00000	0.00000	0.00000
H+	MgEDTA=F	0.00000	0.00000	0.00000	0.00000
Mg++F	Cl-	0.35235	1.68150	0.00000	0.00519
Mg++F	EDTA==F	0.00000	0.00000	0.00000	0.00000
Mg++F	MgEDTA=F	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	EDTA==F	MgEDTA=F
Na+	H+	0.03600	-0.00400	0.00000	0.00000
Na+	Mg++F	0.07000	-0.01200	0.00000	0.00000
H+	Mg++F	0.10000	-0.01100	0.00000	0.00000

			Na+	H+	Mg++F
Cl-	EDTA==F	0.00000	0.00000	0.00000	0.00000
Cl-	MgEDTA=F	0.00000	0.00000	0.00000	0.00000

EDTA==F MgEDTA=F 0.00000 0.00000 0.00000 0.00000

TOTAL NUMBER OF SPECIES = 8
NUMBER OF COMPONENTS = 10
INDEPENDENT CONSTRAINTS = 7

SOLUBILITY DATA

input molalities

Na+	H+	Mg++F	Cl-	EDTA==F	MgEDTA=F
3.000E-01	1.000E-07	1.000E-06	3.000E-01	1.000E-06	2.818E-05
1.000E+00	1.000E-07	1.000E-06	1.000E+00	1.000E-06	5.012E-06
2.000E+00	1.000E-07	1.000E-06	2.000E+00	1.000E-06	2.754E-06
3.000E+00	1.000E-07	1.000E-06	3.000E+00	1.000E-06	2.178E-06
4.000E+00	1.000E-07	1.000E-06	4.000E+00	1.000E-06	2.570E-06
5.000E+00	1.000E-07	1.000E-06	5.000E+00	1.000E-06	3.311E-06

-3.0000E+02 1.0000E-01 1.0000E-01
L2 NORM OF THE RESIDUALS 3.5534974E+02

-1.5373E+02 2.1345E-01 3.0732E-03
L2 NORM OF THE RESIDUALS 1.5606443E-01

-1.5373E+02 2.1345E-01 3.0732E-03
L2 NORM OF THE RESIDUALS 1.5606443E-01

ADJUSTED PARAMETERS

u0rt(		MgEDTA=F	)	-1.5373418E+02
b0(	Na+	MgEDTA=F	)	2.1344556E-01
cmx(	Na+	MgEDTA=F	)	3.0731940E-03

DATA SET(1)

input	calc	diff
0.000000000000000E+000		-7.343657190935461E-002
0.000000000000000E+000		0.118923257709582
0.000000000000000E+000		-2.474180417223693E-002
0.000000000000000E+000		-7.832177896318628E-004
0.000000000000000E+000		-5.474929482136305E-002
0.000000000000000E+000		3.478763098306104E-002

AVERAGE DEVIATION = 5.1237E-02

STANDARD DEVIATION = 6.3713E-02

FINAL MOLALITIES

Na+	H+	Mg++F	Cl-	EDTA==F	MgEDTA=F
3.000E-01	1.000E-07	1.000E-06	3.000E-01	1.000E-06	2.818E-05
1.000E+00	1.000E-07	1.000E-06	1.000E+00	1.000E-06	5.012E-06
2.000E+00	1.000E-07	1.000E-06	2.000E+00	1.000E-06	2.754E-06
3.000E+00	1.000E-07	1.000E-06	3.000E+00	1.000E-06	2.178E-06
4.000E+00	1.000E-07	1.000E-06	4.000E+00	1.000E-06	2.570E-06
5.000E+00	1.000E-07	1.000E-06	5.000E+00	1.000E-06	3.311E-06

FINAL LOG ACTIVITIES

Na+	H+	Mg++F	Cl-	EDTA==F	MgEDTA=F
-6.735E-01	-7.112E+00	-6.559E+00	-6.736E-01	-8.754E+00	-5.155E+00
-1.838E-01	-7.059E+00	-6.607E+00	-1.838E-01	-9.534E+00	-6.067E+00
1.249E-01	-6.936E+00	-6.500E+00	1.249E-01	-1.001E+01	-6.378E+00
3.297E-01	-6.797E+00	-6.334E+00	3.297E-01	-1.025E+01	-6.462E+00
4.947E-01	-6.651E+00	-6.139E+00	4.947E-01	-1.034E+01	-6.331E+00
6.394E-01	-6.502E+00	-5.927E+00	6.394E-01	-1.032E+01	-6.133E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++F	Cl-	EDTA==F	MgEDTA=F
-0.1507	-0.1115	-0.5591	-0.1507	-2.7543	-0.6054
-0.1838	-0.0595	-0.6068	-0.1838	-3.5345	-0.7669
-0.1761	0.0635	-0.5000	-0.1761	-4.0149	-0.8181
-0.1474	0.2026	-0.3339	-0.1474	-4.2543	-0.7998
-0.1073	0.3487	-0.1389	-0.1073	-4.3420	-0.7410
-0.0595	0.4984	0.0733	-0.0595	-4.3173	-0.6530

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	

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++F	Cl-	EDTA==F	MgEDTA=F
3.000E-01	1.000E-07	1.000E-06	3.000E-01	1.000E-06	2.818E-05
1.000E+00	1.000E-07	1.000E-06	1.000E+00	1.000E-06	5.012E-06
2.000E+00	1.000E-07	1.000E-06	2.000E+00	1.000E-06	2.754E-06
3.000E+00	1.000E-07	1.000E-06	3.000E+00	1.000E-06	2.178E-06
4.000E+00	1.000E-07	1.000E-06	4.000E+00	1.000E-06	2.570E-06
5.000E+00	1.000E-07	1.000E-06	5.000E+00	1.000E-06	3.311E-06

FINAL LOG ACTIVITIES

Na+	H+	Mg++F	Cl-	EDTA==F	MgEDTA=F
-6.735E-01	-7.112E+00	-6.559E+00	-6.736E-01	-8.754E+00	-5.155E+00
-1.838E-01	-7.059E+00	-6.607E+00	-1.838E-01	-9.534E+00	-6.067E+00
1.249E-01	-6.936E+00	-6.500E+00	1.249E-01	-1.001E+01	-6.378E+00
3.297E-01	-6.797E+00	-6.334E+00	3.297E-01	-1.025E+01	-6.462E+00
4.947E-01	-6.651E+00	-6.139E+00	4.947E-01	-1.034E+01	-6.331E+00
6.394E-01	-6.502E+00	-5.927E+00	6.394E-01	-1.032E+01	-6.133E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++F	Cl-	EDTA==F	MgEDTA=F
-0.1507	-0.1115	-0.5591	-0.1507	-2.7543	-0.6054
-0.1838	-0.0595	-0.6068	-0.1838	-3.5345	-0.7669
-0.1761	0.0635	-0.5000	-0.1761	-4.0149	-0.8181
-0.1474	0.2026	-0.3339	-0.1474	-4.2543	-0.7998
-0.1073	0.3487	-0.1389	-0.1073	-4.3420	-0.7410
-0.0595	0.4984	0.0733	-0.0595	-4.3173	-0.6530

FINAL L2 NORM OF THE RESIDUALS 1.5606443E-01

EXIT PARAMETER 3

FINAL APPROXIMATE SOLUTION

0	0	7	-1.5373418E+02
1	1	3	2.1344556E-01
4	1	3	3.0731940E-03

```
-1
     6   -1
0   0   0.3000   1.000E-07   1.0000E-06   0.30000   1.0E-06   2.818e-05
0   0   1.0000   1.000E-07   1.0000E-06   1.00000   1.0E-06   5.012e-06
0   0   2.0000   1.000E-07   1.0000E-06   2.00000   1.0E-06   2.754e-06
0   0   3.0000   1.000E-07   1.0000E-06   3.00000   1.0E-06   2.178e-06
0   0   4.0000   1.000E-07   1.0000E-06   4.00000   1.0E-06   2.570e-06
0   0   5.0000   1.000E-07   1.0000E-06   5.00000   1.0E-06   3.311e-06
-1

0   0   Na+      H+          Mg2+        Cl-       EDTA==    MgEDTA=
```

```
     0    0    0    0
0
001080      0.00000000       1  0 H2O
011000      0.00000000       2  1 Na+
001000      0.00000000       3  2 H+
012000      0.00000000       4  3 Mg++
000170      0.00000000       5  1 Cl-
000870      0.00000000       6  2 EDTA==
012870      0.00000000       7  3 MgEDTA==
000000
-1
-1
```

NONLIN V2.0

NONLIN was developed by A.R. Felmy

INPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGEDTA.IN;1
GMIN file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGEDTA.GMIN;1
OUTPUT file name is U1:[ERGIAMB.NONLIN.ORG_MEMO]REV_MGEDTA.OUT;1

AQUEOUS SPECIES

ID	NAME	MOLES	Z	u0rt
1080	H2O	0.000000000000	0.	-95.663
11000	Na+	0.000000000000	1.	-105.651
1000	H+	0.000000000000	1.	0.000
12000	Mg++	0.000000000000	2.	-183.468
170	Cl-	0.000000000000	-1.	-52.955
870	EDTA==	0.000000000000	-4.	53.050
12870	MgEDTA=	0.000000000000	-2.	-153.734

SOLID PHASES

ID	NAME	MOLES	Z	u0rt

CONSTRAINT EQUATIONS

	0	1	8	11	12	17	87
H2O	0.0	2.0	1.0	0.0	0.0	0.0	0.0
Na+	1.0	0.0	0.0	1.0	0.0	0.0	0.0
H+	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Mg++	2.0	0.0	0.0	0.0	1.0	0.0	0.0
Cl-	-1.0	0.0	0.0	0.0	0.0	1.0	0.0
EDTA==	-4.0	0.0	0.0	0.0	0.0	0.0	1.0
MgEDTA=	-2.0	0.0	0.0	0.0	1.0	0.0	1.0

Closed input files GMIN and COMP

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

non-ideal electrolyte parameters

single electrolyte parameters

Na+	Cl-	0.07650	0.26640	0.00000	0.00127
Na+	EDTA==	1.01600	11.60000	0.00000	0.00100
Na+	MgEDTA=	0.21340	1.74000	0.00000	0.00869
H+	Cl-	0.17750	0.29450	0.00000	0.00080
H+	EDTA==	0.00000	0.00000	0.00000	0.00000
H+	MgEDTA=	0.00000	0.00000	0.00000	0.00000
Mg++	Cl-	0.35235	1.68150	0.00000	0.00519
Mg++	EDTA==	0.00000	0.00000	0.00000	0.00000
Mg++	MgEDTA=	0.00000	0.00000	0.00000	0.00000

ternary electrolyte parameters

			Cl-	EDTA==	MgEDTA=
Na+	H+	0.03600	-0.00400	0.00000	0.00000
Na+	Mg++	0.07000	-0.01200	0.00000	0.00000
H+	Mg++	0.10000	-0.01100	0.00000	0.00000

			Na+	H+	Mg++
Cl-	EDTA==	0.00000	0.00000	0.00000	0.00000
Cl-	MgEDTA=	0.00000	0.00000	0.00000	0.00000
EDTA==	MgEDTA=	0.00000	0.00000	0.00000	0.00000

TOTAL NUMBER OF SPECIES = 7
NUMBER OF COMPONENTS = 7
INDEPENDENT CONSTRAINTS = 6

SOLUBILITY DATA

input molalities

Na+	H+	Mg++	Cl-	EDTA==	MgEDTA=
3.000E-01	1.000E-07	1.000E-06	3.000E-01	1.000E-06	2.818E-05
1.000E+00	1.000E-07	1.000E-06	1.000E+00	1.000E-06	5.012E-06
2.000E+00	1.000E-07	1.000E-06	2.000E+00	1.000E-06	2.754E-06
3.000E+00	1.000E-07	1.000E-06	3.000E+00	1.000E-06	2.178E-06
4.000E+00	1.000E-07	1.000E-06	4.000E+00	1.000E-06	2.570E-06
5.000E+00	1.000E-07	1.000E-06	5.000E+00	1.000E-06	3.311E-06

ADJUSTED PARAMETERS

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

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++	Cl-	EDTA==	MgEDTA=
3.000E-01	1.000E-07	1.037E-06	3.000E-01	1.037E-06	2.814E-05
1.000E+00	1.000E-07	9.473E-07	1.000E+00	9.473E-07	5.065E-06
2.000E+00	1.000E-07	1.011E-06	2.000E+00	1.011E-06	2.743E-06
3.000E+00	1.000E-07	1.000E-06	3.000E+00	1.000E-06	2.178E-06
4.000E+00	1.000E-07	1.023E-06	4.000E+00	1.023E-06	2.547E-06
5.000E+00	1.000E-07	9.848E-07	5.000E+00	9.848E-07	3.326E-06

FINAL LOG ACTIVITIES

Na+	H+	Mg++	Cl-	EDTA==	MgEDTA=
-6.735E-01	-7.112E+00	-6.543E+00	-6.736E-01	-8.739E+00	-5.156E+00
-1.838E-01	-7.059E+00	-6.630E+00	-1.838E-01	-9.558E+00	-6.062E+00
1.249E-01	-6.936E+00	-6.495E+00	1.249E-01	-1.001E+01	-6.380E+00
3.297E-01	-6.797E+00	-6.334E+00	3.297E-01	-1.025E+01	-6.462E+00
4.947E-01	-6.651E+00	-6.129E+00	4.947E-01	-1.033E+01	-6.335E+00
6.394E-01	-6.502E+00	-5.933E+00	6.394E-01	-1.032E+01	-6.131E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++	Cl-	EDTA==	MgEDTA=
-0.1507	-0.1115	-0.5591	-0.1507	-2.7543	-0.6054
-0.1838	-0.0595	-0.6068	-0.1838	-3.5345	-0.7670
-0.1761	0.0635	-0.5000	-0.1761	-4.0149	-0.8182
-0.1474	0.2026	-0.3339	-0.1474	-4.2543	-0.8000
-0.1073	0.3487	-0.1389	-0.1073	-4.3420	-0.7412
-0.0595	0.4984	0.0733	-0.0595	-4.3173	-0.6532

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

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Na+	H+	Mg++	Cl-	EDTA==	MgEDTA=
3.000E-01	7.000E-15	1.049E-06	3.000E-01	1.024E-06	2.813E-05
1.000E+00	7.000E-15	9.588E-07	1.000E+00	9.338E-07	5.053E-06
2.000E+00	7.000E-15	1.021E-06	2.000E+00	9.961E-07	2.733E-06
3.000E+00	7.000E-15	1.011E-06	3.000E+00	9.855E-07	2.167E-06
4.000E+00	7.000E-15	1.034E-06	4.000E+00	1.009E-06	2.536E-06
5.000E+00	7.000E-15	9.958E-07	5.000E+00	9.708E-07	3.315E-06

FINAL LOG ACTIVITIES

Na+	H+	Mg++	Cl-	EDTA==	MgEDTA=
-6.735E-01	-1.427E+01	-6.538E+00	-6.736E-01	-8.744E+00	-5.156E+00
-1.838E-01	-1.421E+01	-6.625E+00	-1.838E-01	-9.564E+00	-6.063E+00
1.249E-01	-1.409E+01	-6.491E+00	1.249E-01	-1.002E+01	-6.382E+00
3.297E-01	-1.395E+01	-6.329E+00	3.297E-01	-1.026E+01	-6.464E+00
4.947E-01	-1.381E+01	-6.125E+00	4.947E-01	-1.034E+01	-6.337E+00
6.394E-01	-1.366E+01	-5.929E+00	6.394E-01	-1.033E+01	-6.133E+00

Calculated Log Activity Coefficients

Na+	H+	Mg++	Cl-	EDTA==	MgEDTA=
-0.1507	-0.1115	-0.5591	-0.1507	-2.7543	-0.6054
-0.1838	-0.0595	-0.6068	-0.1838	-3.5345	-0.7670
-0.1761	0.0636	-0.5000	-0.1761	-4.0149	-0.8182
-0.1474	0.2026	-0.3339	-0.1474	-4.2543	-0.8000
-0.1073	0.3487	-0.1389	-0.1073	-4.3420	-0.7412
-0.0595	0.4984	0.0733	-0.0595	-4.3173	-0.6532

FINAL L2 NORM OF THE RESIDUALS 0.0000000E+00

EXIT PARAMETER 0

FINAL APPROXIMATE SOLUTION