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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 Mg²⁺) 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 (AmLac²⁺ and ThAc³⁺) 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 WPSNONPA_CMSROOT:[FMT].

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 $\log(\beta_{101}) = 4.41 \pm 0.02$, while Moore et al. (1999) report $\log(\beta_{101}) = 3.73 \pm 0.02$. 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 apparent 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+} , $\text{ThEDTA}_{(\text{aq})}$, MgAc^{2+} , $\text{MgOx}_{(\text{aq})}$, MgCit^- , and MgEDTA^{2-} . Parameter sets (μ^0/RT and appropriate Pitzer parameters) for each of these species were calculated using NONLIN version 2.0² 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 $\log \beta_{101}$ versus NaCl molality data. In the second (or verification) calculation the newly determined parameter values are used to predict $\log \beta_{101}$ 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 $\log \beta_{101}$ 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 WPSNONPA\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. $\text{ThEDTA}_{(\text{aq})}$

Choppin et al. (2001), concerned that Th hydrolysis species and Na-EDTA complexes were affecting their measurements of $\text{ThEDTA}_{(\text{aq})}$ complexation, expressed the opinion that more data should be collected before calculation of μ^0/RT and Pitzer parameters for $\text{ThEDTA}_{(\text{aq})}$. They recommended, however, that their β_{101} values for $\text{ThEDTA}_{(\text{aq})}$ 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 $\text{ThEDTA}_{(\text{aq})}$ 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+} , $\text{MgOx}_{(\text{aq})}$, MgCit^- , and MgEDTA^{2-} , although they did provide values for $\log \beta_{101}$ 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 $\text{NpO}_2\text{H}_2\text{EDTA}^-$, $\text{NpO}_2\text{HEDTA}^{2-}$, 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 $C^\phi(\text{ThAc}_2^{2+}-\text{Cl}^-)$ that Moore et al. (1999) listed for $C^\phi(\text{ThLac}_2^{2+}-\text{Cl}^-)$, 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 $C^\phi(\text{ThAc}_2^{2+}-\text{Cl}^-)$ and $C^\phi(\text{ThLac}_2^{2+}-\text{Cl}^-)$ 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.

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7. LIST OF FIGURES

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Figure 2. Log β_{101} versus NaCl molality for $\text{ThEDTA}_{(\text{aq})}$. 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 $\text{MgOx}_{(\text{aq})}$. 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:

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- 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.

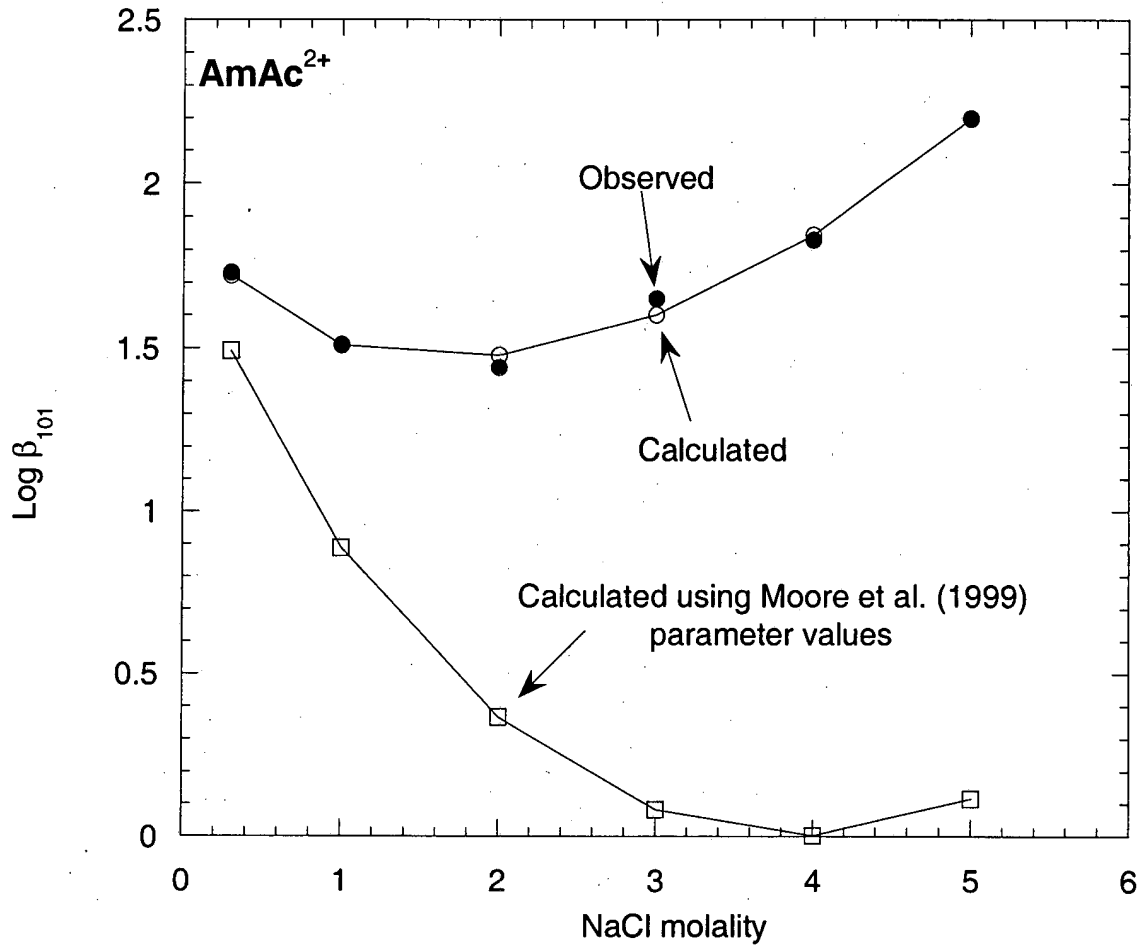


Figure 1. Log β_{101} versus NaCl molality for AmAc²⁺. Filled circles: values from Choppin et al. (2001); open squares: model prediction calculated using parameters listed in Choppin et al. (2001) and Moore et al. (1999); open circles: model prediction calculated using parameters listed in Tables 1 and 3.

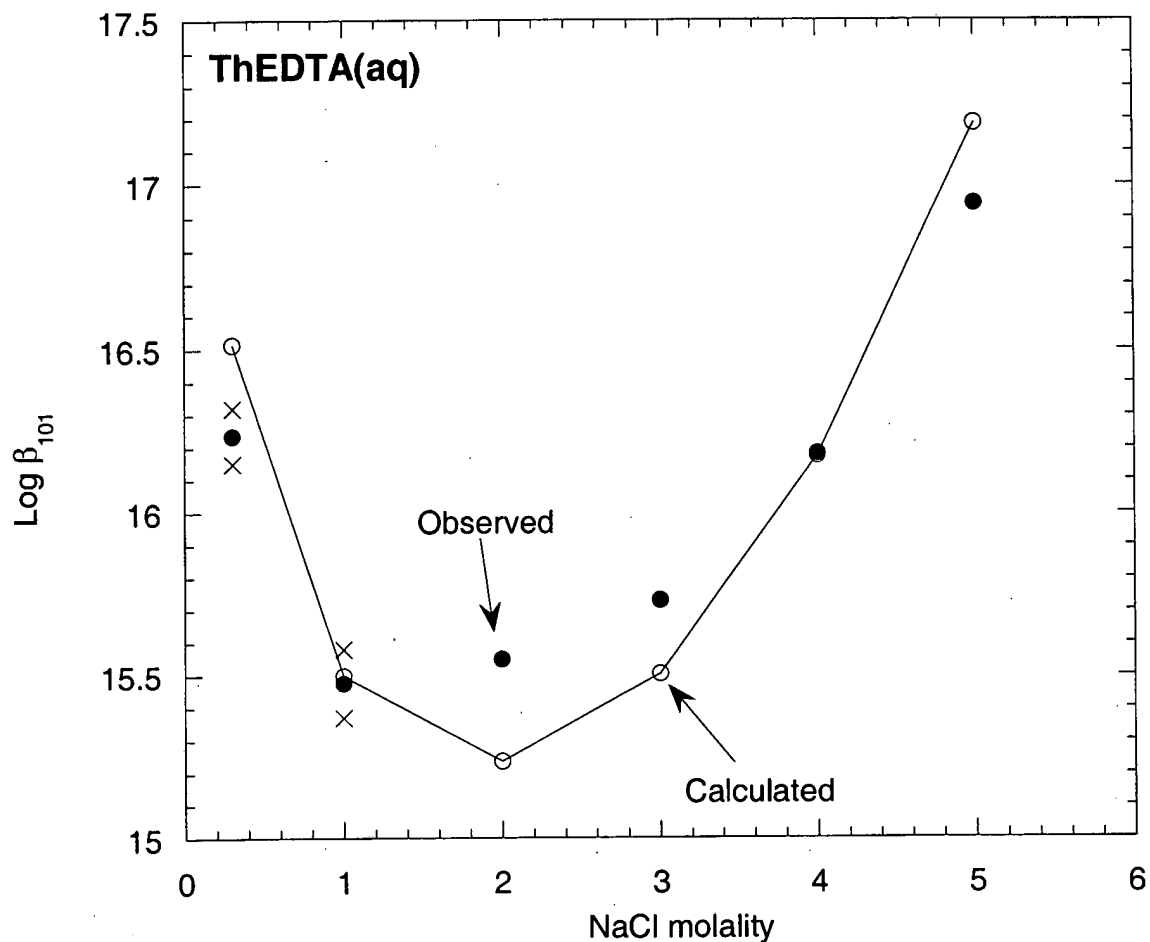


Figure 2. $\text{Log } \beta_{101}$ versus NaCl molality for ThEDTA_(aq). Filled circles: values from Choppin et al. (2001), points at 0.3 and 1 m NaCl are average values calculated from values plotted with X; open circles: model prediction calculated using parameters listed in Tables 1 and 3. Parameter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

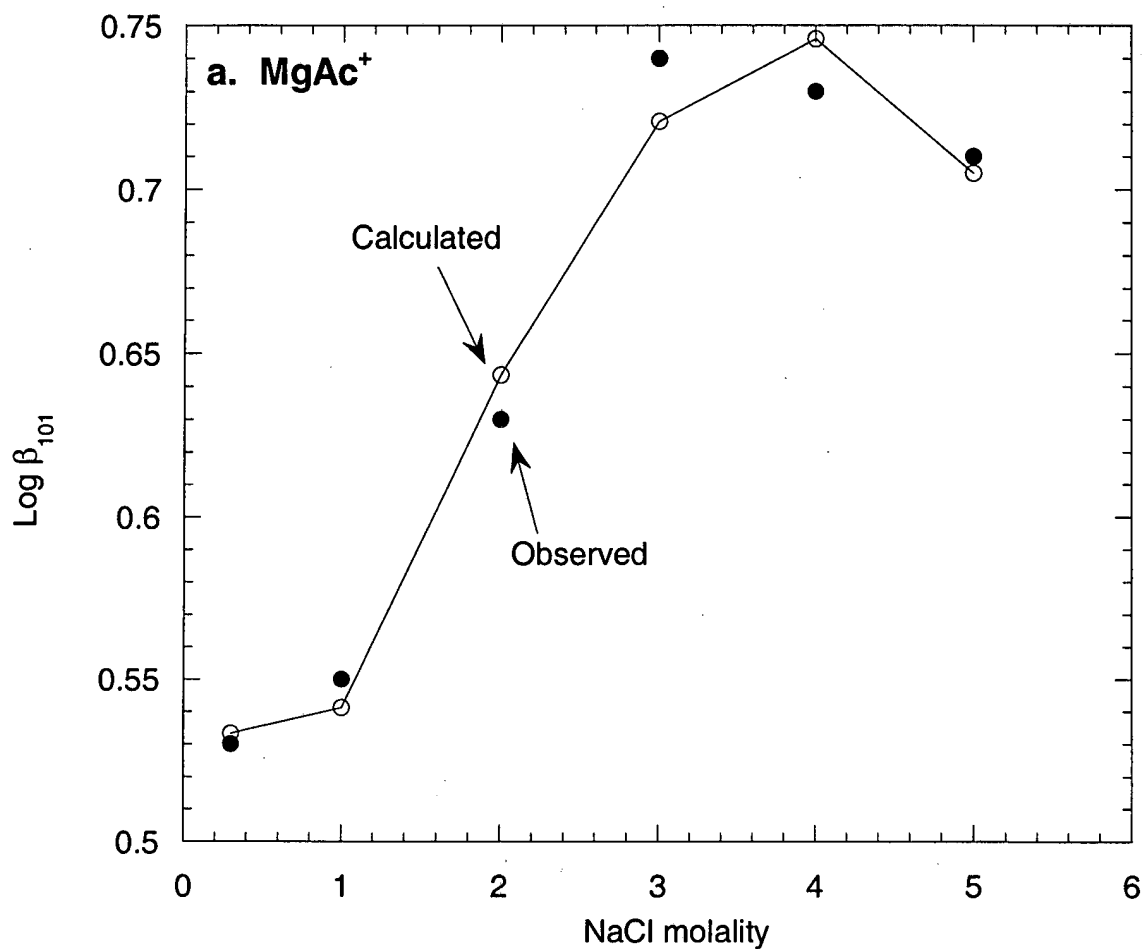


Figure 3a. Log β_{101} versus NaCl molality for MgAc⁺. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

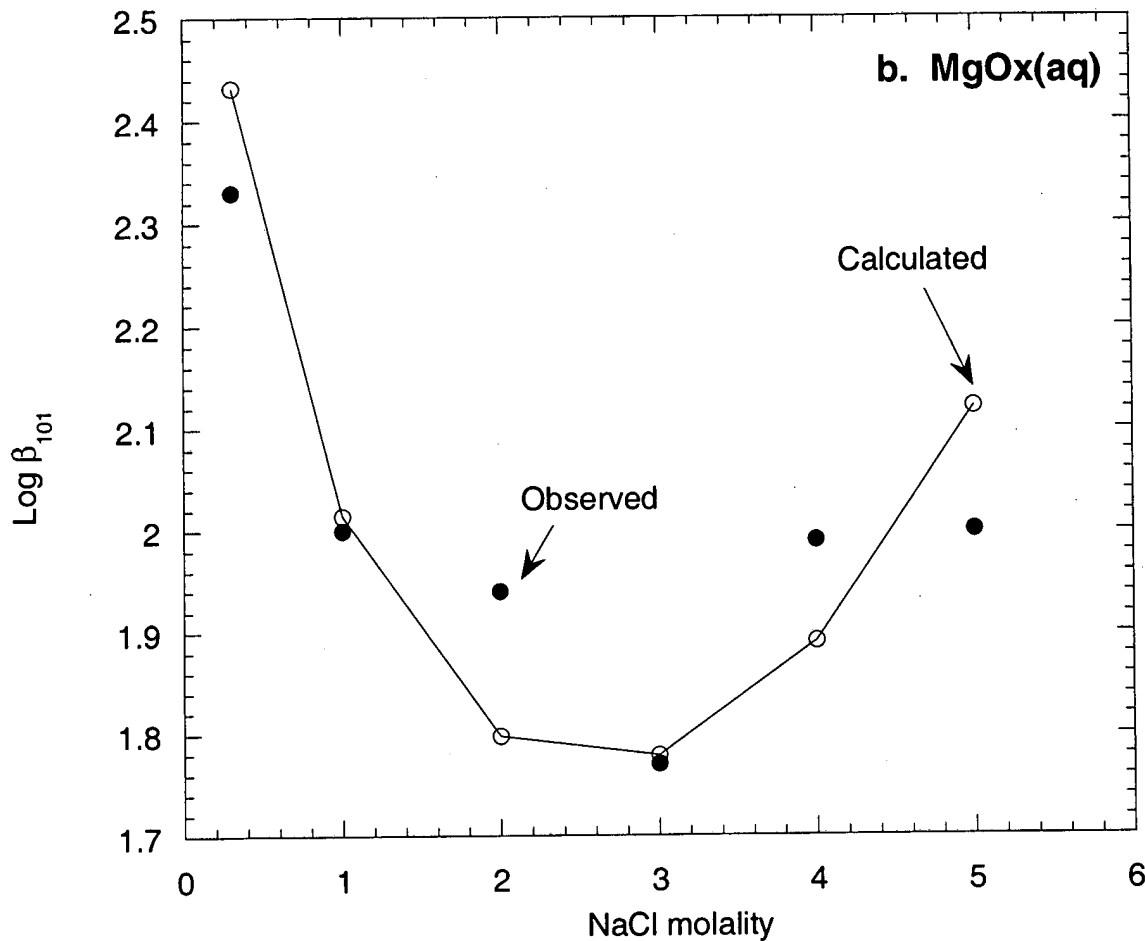


Figure 3b. $\text{Log } \beta_{101}$ versus NaCl molality for $\text{MgOx}_{(aq)}$. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

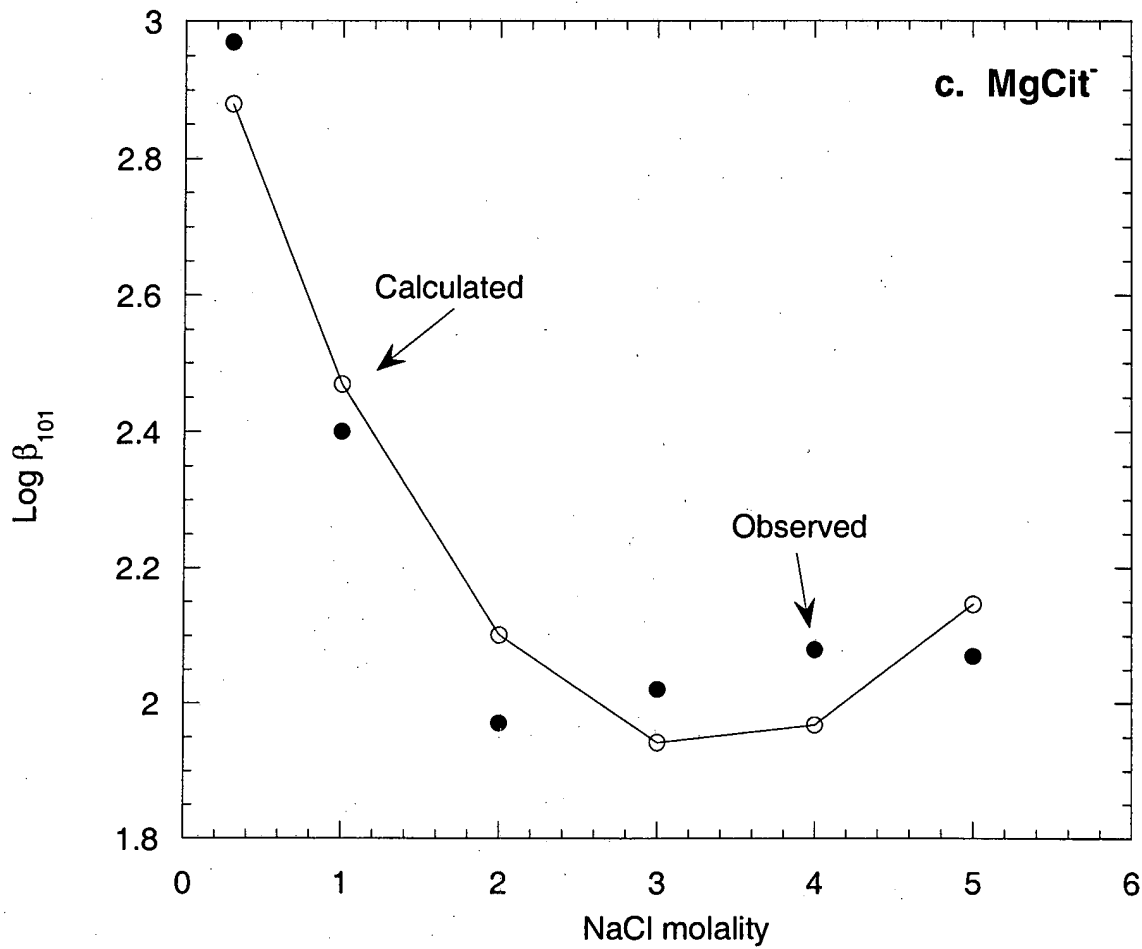


Figure 3c. $\text{Log } \beta_{101}$ versus NaCl molality for MgCit^- . Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

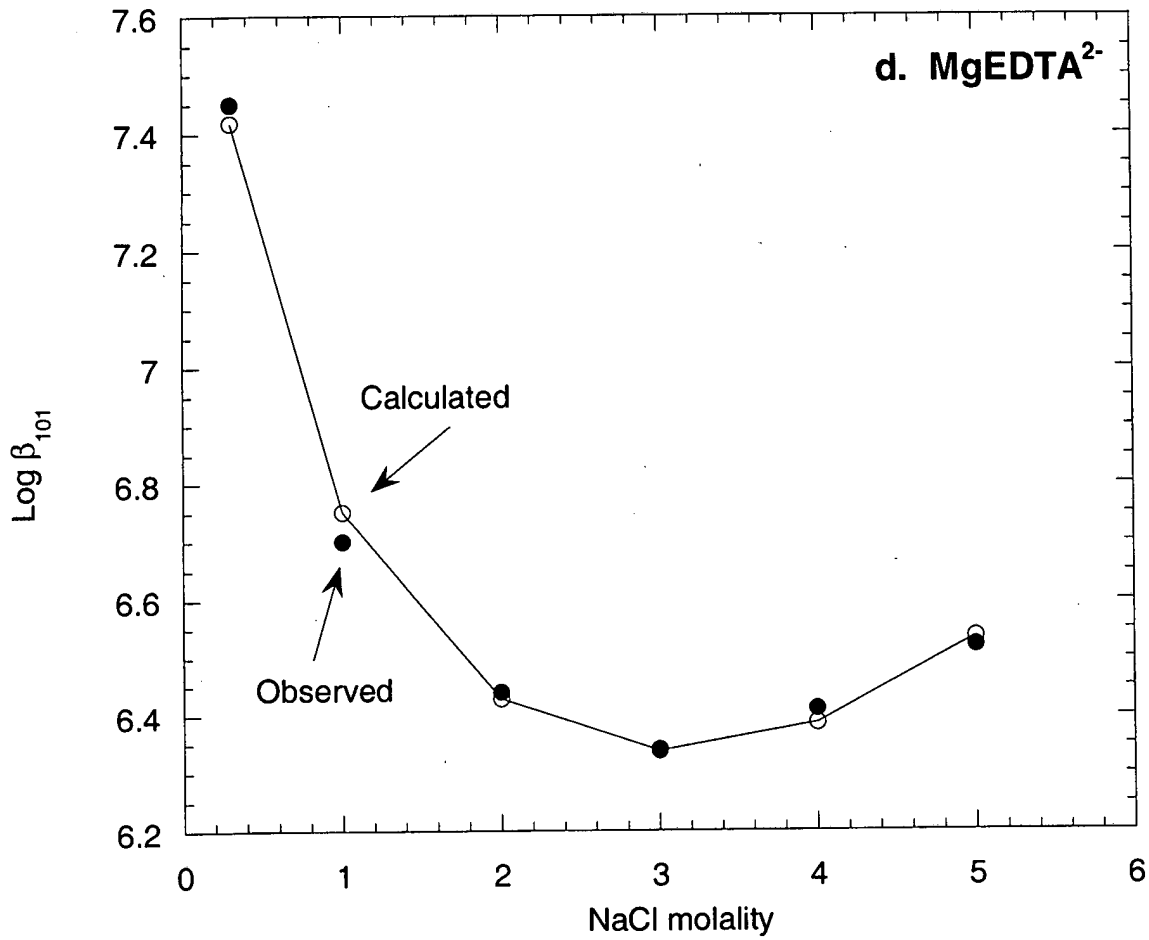


Figure 3d. Log β_{101} versus NaCl molality for MgEDTA²⁻. Filled circles: values from Choppin et al. (2001); open circles: model prediction calculated using parameters listed in Tables 1-5.

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 ₃ Cit _(aq)	0.000	0.000	Choppin et al. (2001); Mizera et al. (1999)
H ₂ Cit ⁻	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 ₄ EDTA _(aq)	0.000	0.000	Choppin et al. (2001); Mizera et al. (1999)
H ₃ EDTA ⁻	5.360	5.761	Choppin et al. (2001); Mizera et al. (1999)
H ₂ EDTA 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 ₂ Ox _(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 ₂ Ac _(aq)	-519.809	-526.061	Choppin et al. (2001)
NpO ₂ Cit ²⁻	-343.066	-343.747	Choppin et al. (2001)
NpO ₂ EDTA ³⁻	-337.030	-335.708	Choppin et al. (2001); Pokrovsky et al. (1998)
NpO ₂ Ox ⁻	-366.452	-365.851	Choppin et al. (2001); Borkowski et al. (2001)
NpO ₂ Lac _(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
<i>Species not in the PAVT database</i>			
NpO ₂ HEDTA ²⁻	xx	-351.852	Choppin et al. (2001); Pokrovsky et al. (1998)
NpO ₂ H ₂ EDTA ⁻	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

^aAc = Acetate; Cit = Citrate; Ox = Oxalate; Lac = Lactate

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

^cChoppin 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)

Cation	Anion	PAVT				Recommended				Source of Recommended Value
		$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	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 ₂ Cit ⁻	-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 ₃ EDTA ⁻	-0.0908	0.0825	0	0	-0.2345	0.29	0	0.059	Choppin et al. (2001); Mizera et al. (1999)
Na ⁺	H ₂ EDTA 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 ₂ Cit ²⁻	-0.4092	1.221	0	0.213	-0.4226	1.75	0	0.142	Choppin et al. (2001)
Na ⁺	NpO ₂ EDTA ³⁻	0.5067	7.738	0	0	0.683	5.911	0	0	Choppin et al. (2001); Pokrovsky et al. (1998)
Na ⁺	NpO ₂ Ox ⁻	-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)

Cation	Anion	PAVT				Recommended				Source of Recommended Value
		$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	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
<i>Species not in the PAVT database</i>										
Na ⁺	NpO ₂ HEDTA ²⁻	xx	xx	xx	xx	0.4733	-1.504	0	0	Pokrovsky et al. (1998) ^a
Na ⁺	NpO ₂ H ₂ EDTA ⁻	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

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

^bChoppin 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 ₃ Cit _(aq)	Cl ⁻	0	0	Choppin et al. (2001); Mizera et al. (1999)
H ₄ EDTA _(aq)	Cl ⁻	0	0	Choppin et al. (2001); Mizera et al. (1999)
H ₂ Ox _(aq)	Cl ⁻	0.035	0	Choppin et al. (2001); Mizera et al. (1999)
H ₂ Ox _(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 ₂ Ac _(aq)	Cl ⁻	0	0	Choppin et al. (2001); Novak et al. (1996)
NpO ₂ Lac _(aq)	Cl ⁻	-0.1853	0.015	Choppin et al. (2001); Moore et al. (1999)
MgOx _(aq)	Cl ⁻	-0.00514	0.0189	This work.

^aNovak 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.

^bSource 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
$\text{NpO}_2\text{Lac}_{(\text{aq})}$	Na^+	Cl^-	0.059	0	Choppin et al. (2001); Moore et al. (1999)

^aI assumed that Choppin et al. (2001) and Moore et al. (1999) set ζ values to zero because neither explicitly listed them.

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Table 5. Ternary Pitzer Parameters (θ , ψ)

Anion <i>i</i>	Anion <i>j</i>	Cation <i>k</i>	PAVT		Recommended		Source for Recommended Value
			θ_{ij}	$\psi_{ij,k}$	θ_{ij}	$\psi_{ij,k}$	
Ac ⁻	Cl ⁻	Na ⁺	-0.09	0.01029	-0.09	0.01029	Novak et al. (1996); Moore et al. (1999) ^a

^aChoppin 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 to the Equation A1.

Each set of calculated $\log \beta_{101}$ 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 nonexistent 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

Information Only

Cit=- SAND99/Mizera

References:

- HMW84 = Harvie, Moller, and Weare, 1984. *Geochimica et Cosmochimica Acta* 48:723-728.
- 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 Media*, 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* 48:723-724.
 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 Media* 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++++	FH+	theta	Cl-	psi	
Th++++	Na+	theta	Cl-	psi	RFSMMN
Th++++	FNa+	theta	Cl-	psi	

References:

- RFSMMN = Rai et al., 1997. Radiochimica Acta 79:239-247.
HMW84 = Harvie, Moller, and Weare, 1984. Geochimica et Cosmochimica Acta 48:723-733.
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

Information Only

```

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				

Information Only

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

Table with 5 columns: ID, NAME, MOLES, Z, u0rt. Rows include 1080H2O, 11000Na+, 1000H+, 95001Am+++F, 95891AmAc++F, 170Cl-, 891Ac-F.

SOLID PHASES

Table with 5 columns: ID, NAME, MOLES, Z, u0rt. Row includes 195890AmAc/Am/Ac(s).

CONSTRAINT EQUATIONS

Table with 10 columns: Species (H2O, Na+, H+, Am+++F, AmAc++F, Cl-, Ac-F, AmAc/Am/Ac(s)) and 10 constraint indices (0, 1, 8, 11, 95, 72, 89, 73, 17).

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

Table with 6 columns: Species pair (Na+ Cl-, Na+ Ac-F, H+ Cl-, H+ Ac-F, Am+++F Cl-, Am+++F Ac-F, AmAc++F Cl-, AmAc++F Ac-F) and 4 parameter values.

ternary electrolyte parameters

Table with 5 columns: Species pair (Na+ H+, Na+ Am+++F, Na+ AmAc++F, H+ Am+++F, H+ AmAc++F, Am+++F AmAc++F) and 3 parameter values.

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
0.0000000000000000E+00	-1.660113707291089E-002	
0.0000000000000000E+00	-1.717283835233729E-003	
0.0000000000000000E+00	8.852777900085584E-002	
0.0000000000000000E+00	-0.110911777906608	
0.0000000000000000E+00	4.113469835297678E-002	
0.0000000000000000E+00	-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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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

Information Only

-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

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

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

Information Only

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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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
0.0000000000000000E+000		0.0000000000000000E+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
0.0000000000000000E+000		0.0000000000000000E+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
0.0000000000000000E+000		0.0000000000000000E+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
0.0000000000000000E+000		0.0000000000000000E+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
0.0000000000000000E+000		0.0000000000000000E+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
1080H2O		0.000000000000	0.	-95.663
11000Na+		0.000000000000	1.	-105.651
1000H+		0.000000000000	1.	0.000
95000Am+++		0.000000000000	3.	-241.694
95892AmAc++moore		0.000000000000	2.	-395.239
170Cl-		0.000000000000	-1.	-52.955
890Ac-		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
Na+	Am+++	0.00000	0.00000
Na+	AmAc++moore	0.00000	0.00000
H+	Am+++	0.00000	0.00000
H+	AmAc++moore	0.00000	0.00000
Am+++	AmAc++moore	0.00000	0.00000

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

Information Only

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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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	0.4955	-1.7303	0.6915	-0.0678	-0.1559

SOLID PHASE NOW IN EQUILIBRIUM



projected hessian indefinite
projected hessian indefinite
projected hessian indefinite
0.0000000000000000E+000 0.0000000000000000E+000

AVERAGE DEVIATION = 0.0000E+00

STANDARD DEVIATION = 0.0000E+00

FINAL MOLALITIES

Table with 6 columns: Na+, H+, Am+++ (Am+++), AmAc++moore Cl-, Cl-, Ac-. Rows show values in scientific notation for each ion.

FINAL LOG ACTIVITIES

Table with 6 columns: Na+, H+, Am+++ (Am+++), AmAc++moore Cl-, Cl-, Ac-. Rows show log activity values in scientific notation for each ion.

Calculated Log Activity Coefficients

Table with 6 columns: Na+, H+, Am+++ (Am+++), AmAc++moore Cl-, Cl-, Ac-. Rows consist of asterisks representing coefficients.

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

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

neutral ion parameters
 ThEDTAF

Na+ 0.0000

Information Only

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

higher order lambdas

ThEDTAF Na+ Cl- EDTA==F 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
0.0000000000000000E+000 0.642008119066638
0.0000000000000000E+000 5.188313108466856E-002
0.0000000000000000E+000 -0.723811722606282
0.0000000000000000E+000 -0.519777812527454
0.0000000000000000E+000 -1.398043412079985E-002
0.0000000000000000E+000 0.563678498212074

AVERAGE DEVIATION = 4.1919E-01

STANDARD DEVIATION = 5.0446E-01

FINAL MOLALITIES

Information Only

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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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==	
---	---	-----	----	--------	--------	-----	--------	--

Information Only

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

Table with 5 columns: ID, NAME, MOLES, Z, u0rt. Rows include 1080H2O, 11000Na+, 1000H+, 90000Th++++, 90870ThEDTA, 170Cl-, 870EDTA==

SOLID PHASES

Table with 5 columns: ID, NAME, MOLES, Z, u0rt

CONSTRAINT EQUATIONS

Table with 8 columns: Species, 0, 1, 8, 11, 90, 87, 17. Rows include H2O, Na+, H+, Th++++, ThEDTA, Cl-, EDTA==

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

Table with 6 columns: Ion, Counterion, Parameter 1, Parameter 2, Parameter 3, Parameter 4. Rows include Na+ Cl-, Na+ EDTA==, H+ Cl-, H+ EDTA==, Th++++ Cl-, Th++++ EDTA==

ternary electrolyte parameters

Table with 6 columns: Ion 1, Ion 2, Parameter 1, Parameter 2, Parameter 3, Parameter 4. Rows include Na+ H+, Na+ Th++++, H+ Th++++, Cl- EDTA==, Cl- Na+, Cl- H+, Cl- Th++++

neutral ion parameters

Table with 2 columns: Ion, Parameter. Rows include ThEDTA, Na+, H+, Th++++

Information Only

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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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	-1.265E+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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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

Information Only

Information Only

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				

Information Only

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

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
112890MgAc/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

Information Only

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

Table with 6 columns: Na+, H+, Mg++F, MgAc+F, Cl-, Ac-F. Rows show values from 3.000E-01 to 5.000E+00.

-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)

Table with 3 columns: input, calc, diff. Rows show numerical values for each column.

AVERAGE DEVIATION = 2.5146E-02

STANDARD DEVIATION = 2.8330E-02

FINAL MOLALITIES

Table with 6 columns: Na+, H+, Mg++F, MgAc+F, Cl-, Ac-F. Rows show final molality values.

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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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

0	0	6	-1	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-

Information Only

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
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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
Na+	Mg++	0.07000	-0.01200
Na+	MgAc+	0.00000	0.00000
H+	Mg++	0.10000	-0.01100
H+	MgAc+	0.00000	0.00000
Mg++	MgAc+	0.00000	0.00000

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

Information Only

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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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

Table with 5 columns: ID, NAME, MOLES, Z, u0rt. Rows include 1080H2O, 11000Na+, 1000H+, 12001Mg++F, 12991MgOxF, 170Cl-, 991Ox=F.

SOLID PHASES

Table with 5 columns: ID, NAME, MOLES, Z, u0rt. Row: 112990MgOx/Mg/Ox(s).

CONSTRAINT EQUATIONS

Table with 10 columns (0-9) and 10 rows (H2O, Na+, H+, Mg++F, MgOxF, Cl-, Ox=F, MgOx/Mg/Ox(s)).

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

Table with 5 columns: Ion, Counterion, and four numerical values. Rows include Na+ Cl-, Na+ Ox=F, H+ Cl-, H+ Ox=F, Mg++F Cl-, Mg++F Ox=F.

ternary electrolyte parameters

Table with 5 columns: Ion 1, Ion 2, Ion 3, and three numerical values. Rows include Na+ H+, Na+ Mg++F, H+ Mg++F, Cl- Ox=F.

neutral ion parameters

Table with 2 columns: Ion, Value. Row: Na+ MgOxF 0.0000.

Information Only

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
0.0000000000000000E+000	0.216000391161975	
0.0000000000000000E+000	3.201168474836891E-002	
0.0000000000000000E+000	-0.319433996061528	
0.0000000000000000E+000	1.994774472088956E-002	
0.0000000000000000E+000	-0.224842078702181	
0.0000000000000000E+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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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
---	---	-----	----	------	------	-----	----

Information Only

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

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

neutral ion parameters

Na+	MgOx	0.0000
H+		0.0000
Mg++		0.0000

Information Only

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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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

Information Only

Information Only

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

SOLID PHASES

ID	NAME	MOLES	Z	u0rt
112860MgCit/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

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

Table with 6 columns: Na+, H+, Mg++F, Cl-, Cit=-F, MgCit-F. Rows show values from 3.000E-01 to 5.000E+00.

-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)

Table with 3 columns: input, calc, diff. Rows show numerical values for each column.

AVERAGE DEVIATION = 2.0258E-01

STANDARD DEVIATION = 2.0875E-01

FINAL MOLALITIES

Table with 6 columns: Na+, H+, Mg++F, Cl-, Cit=-F, MgCit-F. Rows show final molality values.

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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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

Information Only

-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-
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Information Only

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				

Information Only

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
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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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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				

Information Only

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

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
Cl-	EDTA==F	0.00000	0.00000	0.00000	0.00000
Cl-	MgEDTA=F	0.00000	0.00000	0.00000	0.00000

Information Only

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

Table with 6 columns: Na+, H+, Mg++F, Cl-, EDTA==F, MgEDTA=F. Rows show molality values for each species.

-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

Table with 4 columns: parameter name (u0rt, b0, cmx), species (Na+), parameter name (MgEDTA=F), and value.

DATA SET(1)

Table with 3 columns: input, calc, diff. Rows show calculated values and differences for each species.

AVERAGE DEVIATION = 5.1237E-02

STANDARD DEVIATION = 6.3713E-02

FINAL MOLALITIES

Table with 6 columns: Na+, H+, Mg++F, Cl-, EDTA==F, MgEDTA=F. Rows show final molality values for each species.

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
0.0000000000000000E+000	0.0000000000000000E+000	
0.0000000000000000E+000	0.0000000000000000E+000	
0.0000000000000000E+000	0.0000000000000000E+000	
0.0000000000000000E+000	0.0000000000000000E+000	
0.0000000000000000E+000	0.0000000000000000E+000	
0.0000000000000000E+000	0.0000000000000000E+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

Information Only

-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=	
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Information Only

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
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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

Information Only

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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+000
0.0000000000000000E+000	0.0000000000000000E+000	0.0000000000000000E+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