



545276

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to: Larry Brush, Repository Performance Dept. 6712 (MS 1395)

from: Yongliang Xiong/Repository Performance Dept. 6712 (MS 1395)

subject: Incorporation of Amorphous Calcium Carbonate with Higher Solubility ($\text{CaCO}_3(\text{am-cpa})$), Aqueous Complexes of Magnesium and Calcium with Acetate, Citrate, EDTA and Oxalate, and Aqueous Species of Acetate and EDTA into the EQ3/6 HML Database and Its Modified Version HMO

The objective of this memorandum is to document the release of a modified EQ3/6 database to support the analysis of the effects of the consumption of CO_2 by calcite (CaCO_3) precipitation on the excess factor calculated for the MgO engineered barrier that the U.S Department of Energy (DOE) is emplacing in the Waste Isolation Pilot Plant.

In the previous, modified version of the EQ3/6 database (HML) that supports the Pitzer activity-coefficient option, amorphous calcium carbonate ($\text{CaCO}_3(\text{am})$) was incorporated (Xiong, 2006b). That database, HML, was modified from the EQ3/6 HMY database (Xiong, 2006a). In the HML database, the solubility constant selected for $\text{CaCO}_3(\text{am})$ is from Brečević and Nielsen (1989). That solubility constant was adopted in the critical review of Gal et al. (1996). In order that the amounts of calcite precipitated in the analysis report may be more conservative, the higher solubility constant of the amorphous calcium carbonate from Clarkson et al. (1992) will be incorporated into the modified database, HMO. This phase is labeled as $\text{CaCO}_3(\text{am-cpa})$ (cpa stands for Clarkson, Price and Adams, who are the authors of Clarkson et al. (1992)). Aqueous complexes of magnesium and calcium with acetate, citrate, EDTA and oxalate, and aqueous species of acetate and EDTA will also be incorporated.

1 INCORPORATION OF CaCO₃(am-cpa) INTO EQ3/6 HMO

The dissolution of the CaCO₃(am-cpa) can be expressed as:



In the study of Clarkson et al. (1992), the equation for the temperature dependence of log K_{sp} from 16 to 60 °C is:

$$\log K_{sp} = 1247.0/T - 10.224, \quad (2)$$

in which T is the temperature in Kelvin, and K_{sp} is solubility product constant. According to Eq. (2), the log K_{sp} at 25 °C (298.15 K) is calculated to be -6.042.

Based on the log K_{sp} of Clarkson et al. (1992), the free energy change for Reaction (1) is calculated according to the following equation:

$$\log K_{sp} = -\Delta_r G^\circ / (2.3026 \times R \times T), \quad (3)$$

in which R is the gas constant (1.98719 cal mol⁻¹ K⁻¹), and T is absolute temperature (T = 298.15 K at 25 °C). The free energy change for Reaction 1 at 25 °C is listed in Table 1.

The free energy change for a chemical reaction is expressed in the following general equation:

$$\Delta_r G = \sum_j \Delta_f G_{j, \text{product}} - \sum_i \Delta_f G_{i, \text{react}} \quad (4)$$

According to Eq. 4, and based on Δ_rG⁰ listed in Table 1 and Δ_fG⁰ for Ca²⁺ and CO₃²⁻ listed in Table 2, the free energy of formation for CaCO₃(am-cpa) is derived from Reaction (1) and listed in Table 2.

In the HML database, the association reaction for CO₃²⁻ is given as:



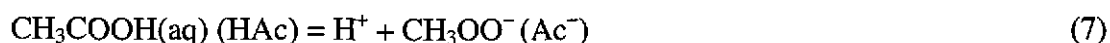
which has a log K of 10.3392 (Table 3). The combination of Reaction (1) with Reaction (5) yields the following dissolution reaction:



The equilibrium constant for Reaction (6) is 4.297 (see Table 3), which is calculated as the difference between the equilibrium constants for Reactions (5) and (1) (10.3392 - 6.042). This value is used in the modified database.

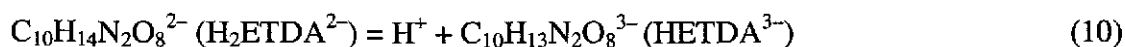
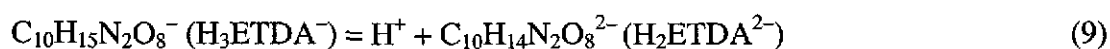
2 INCORPORATION OF AQUEOUS SPECIES OF ACETATE AND EDTA, AND AQUEOUS COMPLEXES OF MAGNESIUM AND CALCIUM WITH ACETATE, CITRATE, EDTA, AND OXALATE INTO THE EQ3/6 HMO DATABASE

Regarding aqueous acetate species, the following dissociation reaction is incorporated into the new database:



The dissociation constant for the above reaction listed in Table 4 is calculated from the above general equations in the form of Eq. (3) and (4) by employing the free energy data listed in Table 5.

Similarly, the following dissociation reactions for the EDTA aqueous species are incorporated into the new database:



Again, the dissociation constants for Reactions (8)—(11) are calculated from the Eq. (3) by utilizing the respective free energy data in Table 5.

Regarding the aqueous complexes of magnesium and calcium with acetate, citrate, EDTA and oxalate, the following formation reactions apply:



The formation constants for the above complexes are calculated from the free energies of formation listed in Table 5.

3 INCORPORATION OF PITZER INTERACTION PARAMETERS INTO THE EQ3/6 HMP DATABASE

Regarding the interaction parameters in the Pitzer formalism involving Mg and Ca complexes mentioned above, and aqueous acetate and EDTA species, the interaction parameters from the FMT_050405.CHEMDAT (Xiong, 2005) were incorporated into the new EQ3/6 database and are listed in Tables 6-7.

4 HMO DATABASE

Using the equilibrium constants listed in Tables 3-4 and the Pitzer interaction parameters tabulated in Tables 6-7 to modify HML, the HMO database is formally established. This database has been successfully run by EQPT, an executable with EQ3/6 package (Wolery, 1992), and files of "output.hmo" and "data1f.hmo" (a formatted data file) have been generated. File comparisons between "output.hmo" and "output.html", and between "data1f.hmo" and "data1f.html" indicate that the only differences between HMO and HML are those of entries of the above species and the Pitzer interaction parameters (see attached files).

REFERENCES

- Brečević, L., A.E. Nielsen. 1989. "Solubility of Amorphous Calcium Carbonate," *Journal of Crystal Growth*. Vol. 98, 504-510.
- Clarkson, J.R., T.J. Price, C.J. Adams. 1992. "Role of Metastable Phases in the Spontaneous Precipitation of Calcium Carbonate," *Journal of Chemical Society Faraday Transactions*. Vol. 88, no. 2, 504-510.
- Gal, J.-Y., J.-C. Bollinger, H. Tolosa, N. Gache. 1996. "Calcium Carbonate Solubility: A Reappraisal of Scale Formation and Inhibition," *Talanta*. Vol. 43, 504-510.
- Wolery, T.J. 1992. *EQ3/6, A Software Package for Geochemical Modeling of Aqueous Systems: Package Overview and Installation Guide (Version 7.0)*. UCRL-MA-110662 PT I. Livermore, CA: Lawrence Livermore National Laboratory.
- Xiong, Y.-L. 2005. "Release of FMT_050405.CHEMDAT." E-mail to J.F. Kanney and J.J. Long, April 5, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS 539304.
- Xiong, Y.-L. 2006a. "Incorporation of Calcium Citrate Hydrate, Earlandite; Calcium Oxalate Monohydrate, Whewellite; and Aqueous Species of Citrate and Oxalate into the EQ3/6 HMP Database and Its Modified Version HMY." Memorandum to L.H. Brush, October 18, 2006. Carlsbad, NM: Sandia National Laboratories. ERMS 544529.

Xiong, Y.-L. 2006b. "Incorporation of Amorphous Calcium Carbonate into the EQ3/6 HMY Database and Its Modified Version HML." Memorandum to L.H. Brush, October 26, 2006. Carlsbad, NM: Sandia National Laboratories. ERMS 544629.

Information Only

Table 1. The Free Energy Change at Reference State (298.15 K and 1 bar) Calculated in This Memorandum.

Reaction	$\Delta_r G^\circ$, cal mol ⁻¹	Reference
Reaction (1)	8,243	Calculated from log K_{sp} from Clarkson et al. (1992)

Table 2. Standard Free Energies of Formation for Ca²⁺, CO₃²⁻ and CaCO₃(am-cpa) at Reference State (298.15 K and 1 bar).

Species	$\Delta_f G^\circ$, cal mol ⁻¹	References
Ca ²⁺	-132,302	HML database (Xiong, 2006b)
CO ₃ ²⁻	-126,166	HML database (Xiong, 2006b)
CaCO ₃ (am-cpa)	-266,711	This memorandum

Table 3. Dissolution Constant of CaCO₃(am-cpa) at Reference State (298.15 K and 1 bar) Used in the Modified EQ3/6 Database.

Reaction	log K	References
Reaction (5)	10.3392	HML database (Xiong, 2006b)
Reaction (6)	4.297	This memorandum, based on log K_{sp} for Reaction 1 from Clarkson et al. (1992), and log K for Reaction 5 from HML (Xiong, 2006b)

Table 4. Equilibrium Constants at Infinite Dilution for Reactions Investigated in This Memorandum (298.15 K and 1 bar).

Reactions	log K	References
Reaction (7)	-4.7568	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (8)	-2.5020	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (9)	-3.0874	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (10)	-6.8792	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (11)	-10.5707	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (12)	1.1131	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (13)	5.2997	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (14)	10.1259	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (15)	3.7931	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (16)	1.1131	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (17)	5.2997	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (18)	10.1259	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)
Reaction (19)	3.7931	Calculated from the $\Delta_f G^\circ$ data converted from μ°/RT of FMT_050405.CHEMDAT (see Table 5)

Table 5. Dimensionless Standard Chemical Potentials and Corresponding Standard Free Energies of Formation for H⁺, Acetate and EDTA Aqueous Species at Reference State (298.15 K and 1 bar).

Species	μ°/RT in FMT_050405.CHEMDAT	$\Delta_f G^\circ$, cal mol ⁻¹
H ⁺	0	0
CH ₃ COOH(aq)	-158.300	-93,785
CH ₃ COO ⁻	-147.347	-87,296
C ₁₀ H ₁₆ N ₂ O ₈ (aq)	0	0
C ₁₀ H ₁₅ N ₂ O ₈ ⁻	5.761	3,413
C ₁₀ H ₁₄ N ₂ O ₈ ²⁻	12.870	7,625
C ₁₀ H ₁₃ N ₂ O ₈ ³⁻	28.710	17,009
C ₁₀ H ₁₂ N ₂ O ₈ ⁴⁻	53.050	31,430
C ₆ H ₅ O ₇ ³⁻ (Cit ³⁻)	33.41	19,794
C ₂ O ₄ ²⁻ (Ox ²⁻)	13.017	7,712
Mg ²⁺	-183.468	-108,696
MgAc ⁺	-333.378	-197,510
MgCit ⁻	-162.261	-96,132
MgEDTA ²⁻	-153.734	-91,080
MgOx(aq)	-179.185	-106,159
Ca ²⁺	-223.300	-132,295
CaAc ⁺	-373.210	-221,109
CaCit ⁻	-202.093	-119,730
CaEDTA ²⁻	-193.566	-114,676
CaOx(aq)	-219.017	-129,757

Table 6. Binary Pitzer Interaction Parameters Involving Mg, Ca Complexes, Acetate and EDTA Aqueous Species Taken from FMT_050405.CHEMDAT (Xiong, 2005).

i	j	Binary Interaction Parameters		
		$\beta^{(0)}$, kg mol ⁻¹	$\beta^{(1)}$, kg mol ⁻¹	C^ϕ , kg ² mol ⁻²
Na ⁺	CH ₃ OO ⁻	0.1426	0.22	-0.00629
Na ⁺	C ₁₀ H ₁₅ N ₂ O ₈ ⁻	-0.2345	0.29	0.059
Na ⁺	C ₁₀ H ₁₄ N ₂ O ₈ ²⁻	-0.1262	1.74	0.054
Na ⁺	C ₁₀ H ₁₃ N ₂ O ₈ ³⁻	0.5458	5.22	-0.048
Na ⁺	C ₁₀ H ₁₂ N ₂ O ₈ ⁴⁻	1.016	11.6	0.001
Na ⁺	MgCit ⁻	0.1742	0.29	-0.06923
Na ⁺	MgEDTA ²⁻	0.2134	1.74	0.00869
Na ⁺	CaCit ⁻	0.1742	0.29	-0.06923
Na ⁺	CaEDTA ²⁻	0.2134	1.74	0.00869
K ⁺	CH ₃ OO ⁻	0.1587	0.3251	-0.0066
K ⁺	C ₁₀ H ₁₅ N ₂ O ₈ ⁻	-0.2345	0.29	0.059
K ⁺	C ₁₀ H ₁₄ N ₂ O ₈ ²⁻	-0.1262	1.74	0.054
K ⁺	C ₁₀ H ₁₃ N ₂ O ₈ ³⁻	0.5458	5.22	-0.048
K ⁺	C ₁₀ H ₁₂ N ₂ O ₈ ⁴⁻	1.016	11.6	0.001
K ⁺	MgCit ⁻	0.1742	0.29	-0.06923
K ⁺	MgEDTA ²⁻	0.2134	1.74	0.00869
K ⁺	CaCit ⁻	0.1742	0.29	-0.06923
K ⁺	CaEDTA ²⁻	0.2134	1.74	0.00869
MgAc ⁺	Cl ⁻	-0.0833	0.29	0.0987

Table 6. Binary Pitzer Interaction Parameters Involving Mg, Ca Complexes, Acetate and EDTA Aqueous Species Taken from FMT_050405.CHEMDAT (Xiong, 2005) (cont.).

		Binary Interaction Parameters		
i	j	$\beta^{(0)}$, kg mol ⁻¹	$\beta^{(1)}$, kg mol ⁻¹	C^ϕ , kg ² mol ⁻²
CaAc ⁺	Cl ⁻	-0.0833	0.29	0.0987

Table 7. Neutral-Ion Pitzer Interaction Parameter (λ) Involving Mg, and Ca Complexes Taken from FMT_050405.CHEMDAT (Xiong, 2005).

Neutral Species	Ion	λ , kg mol ⁻¹
MgOx(aq)	Cl ⁻	0.0189
CaOx(aq)	Cl ⁻	0.0189

Distribution:

MS 1395 M.J. Chavez (Org. 6710)

MS 1395 J.R. Trone (Org. 6710)

MS 1395 M. Lee (Org. 6711)

MS 1395 J.W. Garner (Org. 6711)

MS 1395 M.B. Nemer (Org. 6711)

MS 1395 E.D. Vugrin (Org. 6711)

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MS 1395 S.L. Casey (Org. 6712), for the SNL/WIPP Records Center, WIPP:1.4.2.2:SFT:QA-L:519559
(2 copies)

Information Only

Comparing files output.html and OUTPUT.HMO

***** output.html

Run 16:51:44 26Oct2006

***** OUTPUT.HMO

Run 10:39:57 07Feb2007

***** output.html

no. of elements on the data file = 11
the dimensioned limit = 110
no. of aqueous species in the master set = 12
the dimensioned limit = 500

***** OUTPUT.HMO

no. of elements on the data file = 13
the dimensioned limit = 110
no. of aqueous species in the master set = 14
the dimensioned limit = 500

***** output.html

data0.html.V8.R6
CII: GEMBOCHS.V2-EQ8-data0.html.V8.R6
THERMODYNAMIC DATABASE

***** OUTPUT.HMO

data0.hmo.V8.R6
CII: GEMBOCHS.V2-EQ8-data0.hmo.V8.R6
THERMODYNAMIC DATABASE

***** output.html

Output package: eq3
Data set: hml

***** OUTPUT.HMO

Output package: eq3
Data set: hmo

***** output.html

element = O , atwt = 15.99940
element = Ca , atwt = 40.07800

***** OUTPUT.HMO

element = O , atwt = 15.99940
element = Acetate , atwt = 59.04400
element = Ca , atwt = 40.07800

***** output.html

element = Cl , atwt = 35.45270
element = H , atwt = 1.00794

***** OUTPUT.HMO

element = Cl , atwt = 35.45270
element = Edtacid , atwt = 292.24500
element = H , atwt = 1.00794

***** output.html

Information Only

1 H2O
2 Ca++
3 Citrate---
4 Cl-
5 H+
6 HCO3-
7 K+
8 Mg++
9 Na+
10 Oxalate--
11 SO4--
12 O2(g)
13 CO2(aq)
14 CO3--
15 CaCO3(aq)
16 H3Citrate(aq)
17 H2Citrate-
18 HCitrate--
19 H2Oxalate(aq)
20 HOxalate-
21 HSO4-
22 MgCO3(aq)
23 MgOH+
24 OH-

***** OUTPUT.HMO

1 H2O
2 Acetate-
3 Ca++
4 Citrate---
5 Cl-
6 EDTA----
7 H+
8 HCO3-
9 K+
10 Mg++
11 Na+
12 Oxalate--
13 SO4--
14 O2(g)
15 Acetic_acid(aq)
16 CO2(aq)
17 CO3--
18 CaAc+
19 CaCit-
20 CaCO3(aq)
21 CaEDTA--
22 CaOx(aq)
23 H3Citrate(aq)
24 H2Citrate-
25 HCitrate--
26 H4EDTA(aq)
27 H3EDTA-
28 H2EDTA--
29 HEDTA---
30 H2Oxalate(aq)
31 HOxalate-
32 HSO4-
33 MgAc+
34 MgCit-
35 MgCO3(aq)
36 MgEDTA--
37 MgOH+
38 MgOx(aq)
39 OH-

Information Only

***** output.html

14 CaCO3(am)
15 Calcite
16 Carnallite
17 Chloromagnesite
18 Dolomite
19 Earlandite
20 Epsomite
21 Gaylussite
22 Glauberite
23 Gypsum
24 Halite
25 Hexahydrate
26 Hydromagne5424
27 Hydromagne4323
28 K2CO3:1.5H2O
29 K3H(SO4)2
30 K8H4(CO3)6:3H2O
31 KNaCO3:6H2O
32 Kainite
33 Kalicinite
34 Kieserite
35 Leonite
36 Lime
37 Magnesite
38 Mercallite
39 Mirabilite
40 Misenite
41 Na2CO3:7H2O
42 Na3H(SO4)2
43 Na4Ca(SO4)3:2H2O
44 Nahcolite
45 Natron
46 Nesquehonite
47 Oxychloride-Mg
48 Periclase
49 Picromerite
50 Pirssonite
51 Polyhalite
52 Portlandite
53 Sylvite
54 Syngenite
55 Tachyhydrite
56 Thenardite
57 Thermonatrite
58 Trona
59 Trona-K
60 Whewellite

***** OUTPUT.HMO

14 CaCO3(am)
15 CaCO3(am-cpa)
16 Calcite
17 Carnallite
18 Chloromagnesite
19 Dolomite
20 Earlandite
21 Epsomite
22 Gaylussite
23 Glauberite
24 Gypsum
25 Halite
26 Hexahydrate
27 Hydromagne5424

Information Only

28 Hydromagne4323
29 K2CO3:1.5H2O
30 K3H(SO4)2
31 K8H4(CO3)6:3H2O
32 KNaCO3:6H2O
33 Kainite
34 Kalicinite
35 Kieserite
36 Leonite
37 Lime
38 Magnesite
39 Mercurite
40 Mirabilite
41 Misenite
42 Na2CO3:7H2O
43 Na3H(SO4)2
44 Na4Ca(SO4)3:2H2O
45 Nahcolite
46 Natron
47 Nesquehonite
48 Oxychloride-Mg
49 Periclase
50 Picromerite
51 Pirssonite
52 Polyhalite
53 Portlandite
54 Sylvite
55 Syngenite
56 Tachyhydrite
57 Thenardite
58 Thermonatrite
59 Trona
60 Trona-K
61 Whewellite

***** output.html

Ca++, Citrate---
Ca++, Oxalate--
Ca++, H2Citrate-

***** OUTPUT.HMO

Ca++, Acetate-
Ca++, Citrate---
Ca++, EDTA----
Ca++, Oxalate--
Ca++, CaCit-
Ca++, CaEDTA--
Ca++, H2Citrate-

***** output.html

Ca++, HCitrate--
Ca++, HOxalate-
H+, Citrate---
H+, Oxalate--
H+, H2Citrate-
H+, HCitrate--
H+, HOxalate-
K+, Citrate---
Mg++, Citrate---
Mg++, Oxalate--
Mg++, H2Citrate-
Mg++, HCitrate--

Information Only

Mg++, HOxalate-
MgOH+, Citrate---
MgOH+, Oxalate--
MgOH+, H2Citrate-
MgOH+, HCitrate--

plus 1 others

***** OUTPUT.HMO

Ca++, HCitrate--
Ca++, H3EDTA-
Ca++, H2EDTA--
Ca++, HEDTA---
Ca++, HOxalate-
Ca++, MgCit-
Ca++, MgEDTA--
H+, Acetate-
H+, Citrate---
H+, EDTA----
H+, Oxalate--
H+, CaCit-
H+, CaEDTA--

plus 75 others

***** output.html

* warning - (eqpt/tpraa) Did not find a data block on the DATA0 file
***** OUTPUT.HMO

* warning - (eqpt/tprcc) Did not find a data block on the DATA0 file
for any of the following cc' pairs:

Ca++, CaAc+
Ca++, MgAc+
CaAc+, H+
H+, MgAc+
CaAc+, K+
K+, MgAc+
CaAc+, Mg++
Mg++, MgAc+
CaAc+, Na+
MgAc+, Na+
CaAc+, MgAc+
CaAc+, MgOH+
MgAc+, MgOH+

* warning - (eqpt/tpraa) Did not find a data block on the DATA0 file

***** output.html

Citrate---, Cl-
Citrate---, HCO3-
Citrate---, Oxalate--
Citrate---, SO4--
CO3--, Citrate---
Citrate---, H2Citrate-
Citrate---, HCitrate--
Citrate---, HOxalate-
Citrate---, HSO4-
Citrate---, OH-
Cl-, Oxalate--

Information Only

Cl-, H2Citrate-
Cl-, HCitrate--
Cl-, HOxalate-
HCO3-, Oxalate--
H2Citrate-, HCO3-
HCO3-, HCitrate--
HCO3-, HOxalate-
Oxalate--, SO4--
CO3--, Oxalate--

plus 20 others

***** OUTPUT.HMO

Acetate-, Citrate---
Acetate-, Cl-
Acetate-, EDTA----
Acetate-, HCO3-
Acetate-, Oxalate--
Acetate-, SO4--
Acetate-, CO3--
Acetate-, CaCit-
Acetate-, CaEDTA--
Acetate-, H2Citrate-
Acetate-, HCitrate--
Acetate-, H3EDTA-
Acetate-, H2EDTA--
Acetate-, HEDTA---
Acetate-, HOxalate-
Acetate-, HSO4-
Acetate-, MgCit-
Acetate-, MgEDTA--
Acetate-, OH-
Citrate---, Cl-

plus 155 others

***** output.html

CO2(aq), CO2(aq)

***** OUTPUT.HMO

Acetic_acid(aq), Acetic_acid(aq)
CO2(aq), CO2(aq)

***** output.html

CaCO3(aq), CaCO3(aq)
H3Citrate(aq), H3Citrate(aq)
H2Oxalate(aq), H2Oxalate(aq)

***** OUTPUT.HMO

CaCO3(aq), CaCO3(aq)
CaOx(aq), CaOx(aq)
H3Citrate(aq), H3Citrate(aq)
H4EDTA(aq), H4EDTA(aq)
H2Oxalate(aq), H2Oxalate(aq)

***** output.html

MgCO3(aq), MgCO3(aq)

***** OUTPUT.HMO

MgCO3(aq), MgCO3(aq)
MgOx(aq), MgOx(aq)

Information Only

***** output.html

CO2(aq), CaCO3(aq)
CO2(aq), H3Citrate(aq)
CO2(aq), H2Oxalate(aq)

***** OUTPUT.HMO

Acetic_acid(aq), CO2(aq)
Acetic_acid(aq), CaCO3(aq)
Acetic_acid(aq), CaOx(aq)
Acetic_acid(aq), H3Citrate(aq)
Acetic_acid(aq), H4EDTA(aq)
Acetic_acid(aq), H2Oxalate(aq)
Acetic_acid(aq), MgCO3(aq)
Acetic_acid(aq), MgOx(aq)
CO2(aq), CaCO3(aq)
CO2(aq), CaOx(aq)
CO2(aq), H3Citrate(aq)
CO2(aq), H4EDTA(aq)
CO2(aq), H2Oxalate(aq)

***** output.html

CO2(aq), MgCO3(aq)
CaCO3(aq), H3Citrate(aq)
CaCO3(aq), H2Oxalate(aq)

***** OUTPUT.HMO

CO2(aq), MgCO3(aq)
CO2(aq), MgOx(aq)
CaCO3(aq), CaOx(aq)
CaCO3(aq), H3Citrate(aq)
CaCO3(aq), H4EDTA(aq)
CaCO3(aq), H2Oxalate(aq)

***** output.html

CaCO3(aq), MgCO3(aq)
H2Oxalate(aq), H3Citrate(aq)
H3Citrate(aq), MgCO3(aq)
H2Oxalate(aq), MgCO3(aq)

***** OUTPUT.HMO

CaCO3(aq), MgCO3(aq)

plus 16 others

***** output.html

CaCO3(aq), Ca++

***** OUTPUT.HMO

Acetic_acid(aq), Ca++
Acetic_acid(aq), H+
Acetic_acid(aq), K+
Acetic_acid(aq), Mg++
Acetic_acid(aq), Na+
Acetic_acid(aq), CaAc+
Acetic_acid(aq), MgAc+
Acetic_acid(aq), MgOH+
CO2(aq), CaAc+
CO2(aq), MgAc+

Information Only

```

CaCO3(aq), Ca++
*****

***** output.html
CaCO3(aq), Na+
CaCO3(aq), MgOH+
H3Citrate(aq), Ca++
H3Citrate(aq), H+
H3Citrate(aq), K+
H3Citrate(aq), Mg++
H3Citrate(aq), Na+
H3Citrate(aq), MgOH+
H2Oxalate(aq), Ca++
H2Oxalate(aq), H+
H2Oxalate(aq), K+
H2Oxalate(aq), Mg++
H2Oxalate(aq), Na+
H2Oxalate(aq), MgOH+
MgCO3(aq), Ca++
MgCO3(aq), K+
MgCO3(aq), Mg++

plus 2 others

***** OUTPUT.HMO
CaCO3(aq), Na+
CaCO3(aq), CaAc+
CaCO3(aq), MgAc+
CaCO3(aq), MgOH+
CaOx(aq), Ca++
CaOx(aq), H+
CaOx(aq), K+

plus 44 others

*****

***** output.html

CO2(aq), Citrate---
CO2(aq), HCO3-
CO2(aq), Oxalate--
CO2(aq), CO3--
CO2(aq), H2Citrate-
CO2(aq), HCitrate--
CO2(aq), HOxalate-
CO2(aq), OH-
CaCO3(aq), Citrate---
CaCO3(aq), Cl-
CaCO3(aq), HCO3-
CaCO3(aq), Oxalate--
CaCO3(aq), SO4--
CaCO3(aq), CO3--
CaCO3(aq), H2Citrate-
CaCO3(aq), HCitrate--
CaCO3(aq), HOxalate-
CaCO3(aq), HSO4-
CaCO3(aq), OH-
H3Citrate(aq), Citrate---

plus 32 others

***** OUTPUT.HMO

Acetic_acid(aq), Acetate-
Acetic_acid(aq), Citrate---

```

Acetic_acid(aq), Cl-
Acetic_acid(aq), EDTA----
Acetic_acid(aq), HCO3-
Acetic_acid(aq), Oxalate--
Acetic_acid(aq), SO4--
Acetic_acid(aq), CO3--
Acetic_acid(aq), CaCit-
Acetic_acid(aq), CaEDTA--
Acetic_acid(aq), H2Citrate-
Acetic_acid(aq), HCitrate--
Acetic_acid(aq), H3EDTA-
Acetic_acid(aq), H2EDTA--
Acetic_acid(aq), HEDTA---
Acetic_acid(aq), HOxalate-
Acetic_acid(aq), HSO4-
Acetic_acid(aq), MgCit-
Acetic_acid(aq), MgEDTA--
Acetic_acid(aq), OH-

plus 155 others

***** output.html

Ca++, H+, Citrate---
Ca++, H+, Oxalate--
Ca++, H+, H2Citrate-

***** OUTPUT.HMO

Ca++, H+, Acetate-
Ca++, H+, Citrate---
Ca++, H+, EDTA----
Ca++, H+, Oxalate--
Ca++, H+, CaCit-
Ca++, H+, CaEDTA--
Ca++, H+, H2Citrate-

***** output.html

Ca++, H+, HCitrate--
Ca++, H+, HOxalate-
Ca++, K+, Citrate---
Ca++, K+, Oxalate--
Ca++, K+, H2Citrate-
Ca++, K+, HCitrate--
Ca++, K+, HOxalate-
Ca++, Mg++, Citrate---
Ca++, Mg++, Oxalate--
Ca++, Mg++, H2Citrate-
Ca++, Mg++, HCitrate--
Ca++, Mg++, HOxalate-
Ca++, Na+, Citrate---
Ca++, Na+, Oxalate--
Ca++, Na+, H2Citrate-
Ca++, Na+, HCitrate--
Ca++, Na+, HOxalate-

plus 55 others

***** OUTPUT.HMO

Ca++, H+, HCitrate--
Ca++, H+, H3EDTA-
Ca++, H+, H2EDTA--
Ca++, H+, HEDTA---
Ca++, H+, HOxalate-

Information Only

Ca++, H+, MgCit-
Ca++, H+, MgEDTA--
Ca++, K+, Acetate-
Ca++, K+, Citrate---
Ca++, K+, EDTA----
Ca++, K+, Oxalate--
Ca++, K+, CaCit-
Ca++, K+, CaEDTA--

plus 450 others

***** output.html

Citrate---, Cl-, Ca++
Citrate---, Cl-, H+
Citrate---, Cl-, K+
Citrate---, Cl-, Mg++
Citrate---, Cl-, Na+
Citrate---, Cl-, MgOH+
Citrate---, HCO3-, Ca++
Citrate---, HCO3-, H+
Citrate---, HCO3-, K+
Citrate---, HCO3-, Mg++
Citrate---, HCO3-, Na+
Citrate---, HCO3-, MgOH+
Citrate---, Oxalate--, Ca++
Citrate---, Oxalate--, H+
Citrate---, Oxalate--, K+
Citrate---, Oxalate--, Mg++
Citrate---, Oxalate--, Na+
Citrate---, Oxalate--, MgOH+
Citrate---, SO4--, Ca++
Citrate---, SO4--, H+

plus 220 others

***** OUTPUT.HMO

Acetate-, Citrate---, Ca++
Acetate-, Citrate---, H+
Acetate-, Citrate---, K+
Acetate-, Citrate---, Mg++
Acetate-, Citrate---, Na+
Acetate-, Citrate---, CaAc+
Acetate-, Citrate---, MgAc+
Acetate-, Citrate---, MgOH+
Acetate-, Cl-, Ca++
Acetate-, Cl-, H+
Acetate-, Cl-, K+
Acetate-, Cl-, Mg++
Acetate-, Cl-, Na+
Acetate-, Cl-, CaAc+
Acetate-, Cl-, MgAc+
Acetate-, Cl-, MgOH+
Acetate-, EDTA----, Ca++
Acetate-, EDTA----, H+
Acetate-, EDTA----, K+
Acetate-, EDTA----, Mg++

plus 1410 others

***** output.html

Information Only

CO2(aq), CO2(aq), CaCO3(aq)
***** OUTPUT.HMO

Acetic_acid(aq), Acetic_acid(aq), CO2(aq)
CO2(aq), CO2(aq), Acetic_acid(aq)
Acetic_acid(aq), Acetic_acid(aq), CaCO3(aq)
CaCO3(aq), CaCO3(aq), Acetic_acid(aq)
Acetic_acid(aq), Acetic_acid(aq), CaOx(aq)
CaOx(aq), CaOx(aq), Acetic_acid(aq)
Acetic_acid(aq), Acetic_acid(aq), H3Citrate(aq)
H3Citrate(aq), H3Citrate(aq), Acetic_acid(aq)
Acetic_acid(aq), Acetic_acid(aq), H4EDTA(aq)
H4EDTA(aq), H4EDTA(aq), Acetic_acid(aq)
Acetic_acid(aq), Acetic_acid(aq), H2Oxalate(aq)
H2Oxalate(aq), H2Oxalate(aq), Acetic_acid(aq)
Acetic_acid(aq), Acetic_acid(aq), MgCO3(aq)
MgCO3(aq), MgCO3(aq), Acetic_acid(aq)
Acetic_acid(aq), Acetic_acid(aq), MgOx(aq)
MgOx(aq), MgOx(aq), Acetic_acid(aq)
CO2(aq), CO2(aq), CaCO3(aq)

***** output.html

CaCO3(aq), CaCO3(aq), CO2(aq)
CO2(aq), CO2(aq), H3Citrate(aq)
H3Citrate(aq), H3Citrate(aq), CO2(aq)
CO2(aq), CO2(aq), H2Oxalate(aq)
H2Oxalate(aq), H2Oxalate(aq), CO2(aq)
CO2(aq), CO2(aq), MgCO3(aq)
MgCO3(aq), MgCO3(aq), CO2(aq)
CaCO3(aq), CaCO3(aq), H3Citrate(aq)
H3Citrate(aq), H3Citrate(aq), CaCO3(aq)

***** OUTPUT.HMO

CaCO3(aq), CaCO3(aq), CO2(aq)

***** output.html

CO2(aq), Ca++, Citrate---
CO2(aq), Ca++, Cl-
CO2(aq), Ca++, HCO3-
CO2(aq), Ca++, Oxalate--
CO2(aq), Ca++, SO4--
CO2(aq), Ca++, CO3--
CO2(aq), Ca++, H2Citrate-
CO2(aq), Ca++, HCitrate--
CO2(aq), Ca++, HOxalate-
CO2(aq), Ca++, HSO4-
CO2(aq), Ca++, OH-
CO2(aq), H+, Citrate---
CO2(aq), H+, Cl-
CO2(aq), H+, HCO3-
CO2(aq), H+, Oxalate--
CO2(aq), H+, SO4--
CO2(aq), H+, CO3--
CO2(aq), H+, H2Citrate-
CO2(aq), H+, HCitrate--
CO2(aq), H+, HOxalate-

plus 310 others

***** OUTPUT.HMO

Information Only

Acetic_acid(aq), Ca++, Acetate-
Acetic_acid(aq), Ca++, Citrate---
Acetic_acid(aq), Ca++, Cl-
Acetic_acid(aq), Ca++, EDTA----
Acetic_acid(aq), Ca++, HCO3-
Acetic_acid(aq), Ca++, Oxalate--
Acetic_acid(aq), Ca++, SO4--
Acetic_acid(aq), Ca++, CO3--
Acetic_acid(aq), Ca++, CaCit-
Acetic_acid(aq), Ca++, CaEDTA--
Acetic_acid(aq), Ca++, H2Citrate-
Acetic_acid(aq), Ca++, HCitrate--
Acetic_acid(aq), Ca++, H3EDTA-
Acetic_acid(aq), Ca++, H2EDTA--
Acetic_acid(aq), Ca++, HEDTA---
Acetic_acid(aq), Ca++, HOxalate-
Acetic_acid(aq), Ca++, HSO4-
Acetic_acid(aq), Ca++, MgCit-
Acetic_acid(aq), Ca++, MgEDTA--
Acetic_acid(aq), Ca++, OH-

plus 1420 others

***** output.html

45 pairs have Pitzer parameters specified on the DATA0 file
66 pairs can be constructed from the species present on this file
Coverage is 68.18 per cent

***** OUTPUT.HMO

65 pairs have Pitzer parameters specified on the DATA0 file
160 pairs can be constructed from the species present on this file
Coverage is 40.63 per cent

***** output.html

15 pairs have Pitzer parameters specified on the DATA0 file
15 pairs can be constructed from the species present on this file
Coverage is 100.00 per cent

***** OUTPUT.HMO

15 pairs have Pitzer parameters specified on the DATA0 file
28 pairs can be constructed from the species present on this file
Coverage is 53.57 per cent

***** output.html

15 pairs have Pitzer parameters specified on the DATA0 file
55 pairs can be constructed from the species present on this file
Coverage is 27.27 per cent

***** OUTPUT.HMO

15 pairs have Pitzer parameters specified on the DATA0 file
190 pairs can be constructed from the species present on this file
Coverage is 7.89 per cent

***** output.html

0 pairs have Pitzer parameters specified on the DATA0 file
5 pairs can be constructed from the species present on this file

Coverage is 0.00 per cent
***** OUTPUT.HMO
 0 pairs have Pitzer parameters specified on the DATA0 file
 9 pairs can be constructed from the species present on this file
 Coverage is 0.00 per cent

***** output.html
 0 pairs have Pitzer parameters specified on the DATA0 file
 10 pairs can be constructed from the species present on this file
 Coverage is 0.00 per cent
***** OUTPUT.HMO
 0 pairs have Pitzer parameters specified on the DATA0 file
 36 pairs can be constructed from the species present on this file
 Coverage is 0.00 per cent

***** output.html
 8 pairs have Pitzer parameters specified on the DATA0 file
 30 pairs can be constructed from the species present on this file
 Coverage is 26.67 per cent

***** OUTPUT.HMO
 8 pairs have Pitzer parameters specified on the DATA0 file
 72 pairs can be constructed from the species present on this file
 Coverage is 11.11 per cent

***** output.html
 3 pairs have Pitzer parameters specified on the DATA0 file
 55 pairs can be constructed from the species present on this file
 Coverage is 5.45 per cent

***** OUTPUT.HMO
 5 pairs have Pitzer parameters specified on the DATA0 file
 180 pairs can be constructed from the species present on this file
 Coverage is 2.78 per cent

***** output.html
 90 triplets have Pitzer parameters specified on the DATA0 file
 165 triplets can be constructed from the species present on this file
 Coverage is 54.55 per cent

***** OUTPUT.HMO
 90 triplets have Pitzer parameters specified on the DATA0 file
 560 triplets can be constructed from the species present on this file
 Coverage is 16.07 per cent

***** output.html
 90 triplets have Pitzer parameters specified on the DATA0 file
 330 triplets can be constructed from the species present on this file
 Coverage is 27.27 per cent

***** OUTPUT.HMO
 90 triplets have Pitzer parameters specified on the DATA0 file
 1520 triplets can be constructed from the species present on this file
 Coverage is 5.92 per cent

Information Only


```
***** output.html
      0 triplets have Pitzer parameters specified on the DATA0 file
      10 triplets can be constructed from the species present on this file
      Coverage is 0.00 per cent
***** OUTPUT.HMO
      0 triplets have Pitzer parameters specified on the DATA0 file
      18 triplets can be constructed from the species present on this file
      Coverage is 0.00 per cent
*****

***** output.html
      0 triplets have Pitzer parameters specified on the DATA0 file
      330 triplets can be constructed from the species present on this file
      Coverage is 0.00 per cent
***** OUTPUT.HMO
      0 triplets have Pitzer parameters specified on the DATA0 file
      1440 triplets can be constructed from the species present on this file
      Coverage is 0.00 per cent
*****

***** output.html

      Completed processing the pitzer data file data0.html.V8.R6.
***** OUTPUT.HMO

      Completed processing the pitzer data file data0.hmo.V8.R6.
*****

***** output.html

      10 warning(s) were encountered.
***** OUTPUT.HMO

      11 warning(s) were encountered.
*****

***** output.html

      Start time = 16:51:44 26Oct2006
      End time   = 16:51:45 26Oct2006

      run time  = 0.440    seconds
***** OUTPUT.HMO

      Start time = 10:39:57 07Feb2007
      End time   = 10:39:57 07Feb2007

      run time  = 0.200    seconds
*****
```

Information Only

Comparing files data1f.hml and DATA1F.HMO

***** data1f.hml

stpitzz

11 12

data0.hml.V8.R6

CII: GEMBOCHS.V2-EQ8-data0.hml.V8.R6

THERMODYNAMIC DATABASE

***** DATA1F.HMO

stpitzz

13 14

data0.hmo.V8.R6

CII: GEMBOCHS.V2-EQ8-data0.hmo.V8.R6

THERMODYNAMIC DATABASE

***** data1f.hml

Output package: eq3

Data set: hml

+-----

***** DATA1F.HMO

Output package: eq3

Data set: hmo

+-----

***** data1f.hml

O 15.99940 0.00000

Ca 40.07800 0.00000

***** DATA1F.HMO

O 15.99940 0.00000

Acetate 59.04400 0.00000

Ca 40.07800 0.00000

***** data1f.hml

Cl 35.45270 0.00000

H 1.00794 0.00000

***** DATA1F.HMO

Cl 35.45270 0.00000

Edtacid 292.24500 0.00000

H 1.00794 0.00000

***** data1f.hml

2.0000 H 1.0000 O

Ca++ 1 0

***** DATA1F.HMO

2.0000 H 1.0000 O

Acetate- 1 0

59.044 -1.

1.0000 Acetate 1 0

Ca++ 1 0

***** data1f.hml

1.0000 Cl 1 0

H+ 1 0

***** DATA1F.HMO

1.0000 Cl 1 0

EDTA----- 1 0

292.245 -4.

1.0000 Edtacid 1 0

H+ 1 0

***** data1f.hml

Information Only

```

2.0000 O
CO2(aq)                2    4
***** DATA1F.HMO
2.0000 O
Acetic_acid(aq)        2    3
60.052  0.
1.0000 Acetate         1.0000 H
-1.0000 Acetic_acid(aq)          1.0000 Acetate-
1.0000 H+
-4.756800000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
CO2(aq)                2    4
*****

***** data1f.hml
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
CaCO3(aq)              3    4
***** DATA1F.HMO
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
CaAc+                  2    3
99.122  1.
1.0000 Acetate         1.0000 Ca
-1.0000 CaAc+          1.0000 Acetate-
1.0000 Ca++
-1.113100000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
CaCit-                 2    3
229.178 -1.
1.0000 Citrate         1.0000 Ca
-1.0000 CaCit-        1.0000 Citrate---
1.0000 Ca++
-5.299700000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
CaCO3(aq)              3    4
*****

***** data1f.hml
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
H3Citrate(aq)         2    3
***** DATA1F.HMO
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
CaEDTA--              2    3
332.323 -2.
1.0000 Edtacid         1.0000 Ca
-1.0000 CaEDTA--      1.0000 EDTA----
1.0000 Ca++
-1.012590000E+01 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
CaOx(aq)               2    3
128.098  0.
1.0000 Oxalate         1.0000 Ca
-1.0000 CaOx(aq)      1.0000 Oxalate--
1.0000 Ca++
-3.793100000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
H3Citrate(aq)         2    3
*****

***** data1f.hml
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
H2Oxalate(aq)         2    3
***** DATA1F.HMO
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
H4EDTA(aq)            2    3
296.277  0.
1.0000 Edtacid         4.0000 H

```

```

-1.0000 H4EDTA(aq) 1.0000 EDTA----
  4.0000 H+
-2.303920000E+01 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
H3EDTA- 2 3
  295.269 -1.
  1.0000 Edtacid 3.0000 H
-1.0000 H3EDTA- 1.0000 EDTA----
  3.0000 H+
-2.053720000E+01 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
H2EDTA-- 2 3
  294.261 -2.
  1.0000 Edtacid 2.0000 H
-1.0000 H2EDTA-- 1.0000 EDTA----
  2.0000 H+
-1.744980000E+01 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
HEDTA--- 2 3
  293.253 -3.
  1.0000 Edtacid 1.0000 H
-1.0000 HEDTA--- 1.0000 EDTA----
  1.0000 H+
-1.057070000E+01 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
H2Oxalate(aq) 2 3

```

```

***** data1f.hml
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
MgCO3(aq) 3 4
***** DATA1F.HMO
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
MgAc+ 2 3
  83.349 1.
  1.0000 Acetate 1.0000 Mg
-1.0000 MgAc+ 1.0000 Acetate-
  1.0000 Mg++
-1.113100000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
MgCit- 2 3
  213.405 -1.
  1.0000 Citrate 1.0000 Mg
-1.0000 MgCit- 1.0000 Citrate---
  1.0000 Mg++
-5.299700000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
MgCO3(aq) 3 4

```

```

***** data1f.hml
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
MgOH+ 3 4
***** DATA1F.HMO
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
MgEDTA-- 2 3
  316.550 -2.
  1.0000 Edtacid 1.0000 Mg
-1.0000 MgEDTA-- 1.0000 EDTA----
  1.0000 Mg++
-1.012590000E+01 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
  9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
MgOH+ 3 4

```

***** data1f.hml

Information Only

9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
OH- 2 3

***** DATA1F.HMO

9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
MgOx(aq) 2 3

112.325 0.
1.0000 Oxalate 1.0000 Mg
-1.0000 MgOx(aq) 1.0000 Oxalate--
1.0000 Mg++

-3.793100000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
OH- 2 3

***** data1f.hml

9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
Calcite 3 4

100.087 0. 36.934

***** DATA1F.HMO

9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
CaCO3(am-cpa) 3 4

100.087 0. 36.934

***** data1f.hml

3.0000 O
-1.0000 Calcite -1.0000 H+

***** DATA1F.HMO

3.0000 O
-1.0000 CaCO3(am-cpa) -1.0000 H+
1.0000 Ca++ 1.0000 HCO3-

4.297000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
Calcite 3 4

100.087 0. 36.934
1.0000 C 1.0000 Ca
3.0000 O
-1.0000 Calcite -1.0000 H+

***** data1f.hml

+-----+
CO2(aq) Cl-
lambda0 = -0.00500 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
CaAc+ Cl-
lambda0 = -0.08330 lambda1 = 0.29000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
CO2(aq) H+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
CaOx(aq) Cl-
lambda0 = 0.01890 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+

H+ CO3--
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

CO2(aq) Cl-
lambda0 = -0.00500 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

CaCO3(aq) H+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

MgOx(aq) Cl-
lambda0 = 0.01890 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

H+ Cl-
lambda0 = 0.17750 lambda1 = 0.29450 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

CO2(aq) H+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

H+ HCO3-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000

***** DATA1F.HMO

H+ CO3--
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000

***** data1f.hml

H+ HSO4-
lambda0 = 0.20650 lambda1 = 0.55560 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

CaCO3(aq) H+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

MgCO3(aq) H+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 0.0 alpha2 = 0.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00

***** DATA1F.HMO

H+ Cl-
lambda0 = 0.17750 lambda1 = 0.29450 lambda2 = 0.00000

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alpha1 = 2.0 alpha2 = 12.0
dI0/dt = 0.000E+00 d2I0/dt2 = 0.000E+00

***** data1f.hml

+-----+
H+ OH-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
***** DATA1F.HMO

+-----+
H+ HCO3-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000

***** data1f.hml

+-----+
H+ SO4--
lambda0 = 0.02980 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
***** DATA1F.HMO

+-----+
H+ HSO4-
lambda0 = 0.20650 lambda1 = 0.55560 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
CO2(aq) HSO4-
lambda0 = -0.00300 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 0.0 alpha2 = 0.0
***** DATA1F.HMO

+-----+
MgCO3(aq) H+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 0.0 alpha2 = 0.0

***** data1f.hml

+-----+
CO2(aq) K+
lambda0 = 0.05100 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
***** DATA1F.HMO

+-----+
H+ OH-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
K+ CO3--
lambda0 = 0.14880 lambda1 = 1.43000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
***** DATA1F.HMO

+-----+
H+ SO4--
lambda0 = 0.02980 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
K+ Cl-
lambda0 = 0.04835 lambda1 = 0.21220 lambda2 = 0.00000

alpha1 = 2.0 alpha2 = 12.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00
***** DATA1F.HMO

+-----+
CO2(aq) HSO4-
lambda0 = -0.00300 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 0.0 alpha2 = 0.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00

***** data1f.hml

+-----+
K+ H2Citrate-
lambda0 = -0.12960 lambda1 = 0.29000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ Acetate-
lambda0 = 0.15870 lambda1 = 0.32510 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
K+ HCitrate--
lambda0 = -0.09890 lambda1 = 1.74000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
CO2(aq) K+
lambda0 = 0.05100 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
K+ HCO3-
lambda0 = 0.02960 lambda1 = -0.01300 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ CO3--
lambda0 = 0.14880 lambda1 = 1.43000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
K+ HOxalate-
lambda0 = -0.24480 lambda1 = 0.29000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ CaCit-
lambda0 = 0.17420 lambda1 = 0.29000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
K+ HSO4-
lambda0 = -0.00030 lambda1 = 0.17350 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ CaEDTA-

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lambda0 = 0.21340 lambda1 = 1.74000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
K+ OH-
lambda0 = 0.12980 lambda1 = 0.32000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ Cl-
lambda0 = 0.04835 lambda1 = 0.21220 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
K+ Oxalate--
lambda0 = -0.21760 lambda1 = 1.74000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ EDTA----
lambda0 = 1.01600 lambda1 = 11.60000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
K+ SO4--
lambda0 = 0.04995 lambda1 = 0.77930 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ H2Citrate-
lambda0 = -0.12960 lambda1 = 0.29000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
CO2 (aq) Mg++
lambda0 = 0.18300 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ HCitrate--
lambda0 = -0.09890 lambda1 = 1.74000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
Mg++ CO3--
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 1.4 alpha2 = 12.0
dI0/dt = 0.000E+00 d2I0/dt2 = 0.000E+00

***** DATA1F.HMO

+-----+
K+ HCO3-
lambda0 = 0.02960 lambda1 = -0.01300 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

dI0/dt = 0.000E+00 d2I0/dt2 = 0.000E+00

Information Only

***** data1f.hml

+-----+
Mg++ Cl-
 lambda0 = 0.35235 lambda1 = 1.68150 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ H3EDTA-
 lambda0 = -0.23460 lambda1 = 0.29000 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
Mg++ HCO3-
 lambda0 = 0.32900 lambda1 = 0.60720 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ H2EDTA--
 lambda0 = -0.12620 lambda1 = 1.74000 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
Mg++ HSO4-
 lambda0 = 0.47460 lambda1 = 1.72900 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ HEDTA---
 lambda0 = 0.54580 lambda1 = 5.22000 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
Mg++ OH-
 lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
K+ HOxalate-
 lambda0 = -0.24480 lambda1 = 0.29000 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
Mg++ SO4--
 lambda0 = 0.22100 lambda1 = 3.34300 lambda2 = -37.23000
 alpha1 = 1.4 alpha2 = 12.0
 d10/dt = 0.000E+00 d210/dt2 = 0.000E+00

***** DATA1F.HMO

+-----+
K+ HSO4-
 lambda0 = -0.00030 lambda1 = 0.17350 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0
 d10/dt = 0.000E+00 d210/dt2 = 0.000E+00

***** data1f.hml

+-----+
CO2(aq) MgOH+
 lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000

```

alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMO
+-----+
K+      MgCit-
lambda0 = 0.17420  lambda1 = 0.29000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
*****

***** data1f.hml
+-----+
MgOH+   CO3--
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMO
+-----+
K+      MgEDTA--
lambda0 = 0.21340  lambda1 = 1.74000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
*****

***** data1f.hml
+-----+
MgOH+   Cl-
lambda0 = -0.10000  lambda1 = 1.65800  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMO
+-----+
K+      OH-
lambda0 = 0.12980  lambda1 = 0.32000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
*****

***** data1f.hml
+-----+
MgOH+   HCO3-
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMO
+-----+
K+      Oxalate--
lambda0 = -0.21760  lambda1 = 1.74000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
*****

***** data1f.hml
+-----+
MgOH+   HSO4-
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMO
+-----+
K+      SO4--
lambda0 = 0.04995  lambda1 = 0.77930  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
*****

***** data1f.hml
+-----+
MgOH+   OH-
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMO
+-----+
CO2(aq) Mg++
lambda0 = 0.18300  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0

```

***** data1f.hml

+-----+
MgOH+ SO4--
 lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0
 d10/dt = 0.000E+00 d210/dt2 = 0.000E+00

***** DATA1F.HMO

+-----+
Mg++ CO3--
 lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 1.4 alpha2 = 12.0
 d10/dt = 0.000E+00 d210/dt2 = 0.000E+00

***** data1f.hml

+-----+
Na+ Citrate---
 lambda0 = 0.08870 lambda1 = 5.22000 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
Mg++ Cl-
 lambda0 = 0.35235 lambda1 = 1.68150 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
CO2(aq) Na+
 lambda0 = 0.10000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
Mg++ HCO3~
 lambda0 = 0.32900 lambda1 = 0.60720 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
Na+ CO3--
 lambda0 = 0.03990 lambda1 = 1.38900 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
Mg++ HSO4-
 lambda0 = 0.47460 lambda1 = 1.72900 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
Na+ Cl-
 lambda0 = 0.07650 lambda1 = 0.26640 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

+-----+
Mg++ OH-
 lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

+-----+
Information Only

Na+ H2Citrate-
lambda0 = -0.12960 lambda1 = 0.29000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00

***** DATA1F.HMO

Mg++ SO4--
lambda0 = 0.22100 lambda1 = 3.34300 lambda2 = -37.23000
alpha1 = 1.4 alpha2 = 12.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00

***** data1f.hml

Na+ HCitrate--
lambda0 = -0.09890 lambda1 = 1.74000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

CO2(aq) MgOH+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

Na+ HCO3-
lambda0 = 0.02770 lambda1 = 0.04110 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

MgOH+ CO3--
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

Na+ HOxalate-
lambda0 = -0.24480 lambda1 = 0.29000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

MgOH+ Cl-
lambda0 = -0.10000 lambda1 = 1.65800 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

Na+ HSO4-
lambda0 = 0.04540 lambda1 = 0.39800 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

MgOH+ HCO3-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** data1f.hml

Na+ OH-
lambda0 = 0.08640 lambda1 = 0.25300 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0

***** DATA1F.HMO

```

+-----+
MgOH+          HSO4-
  lambda0 =    0.00000  lambda1 =    0.00000  lambda2 =    0.00000
                    alpha1 =     2.0      alpha2 =    12.0
*****

***** data1f.hml
+-----+
Na+            Oxalate--
  lambda0 =   -0.21760  lambda1 =    1.74000  lambda2 =    0.00000
                    alpha1 =     2.0      alpha2 =    12.0
***** DATA1F.HMO
+-----+
MgOH+          OH-
  lambda0 =    0.00000  lambda1 =    0.00000  lambda2 =    0.00000
                    alpha1 =     2.0      alpha2 =    12.0
*****

***** data1f.hml
+-----+
Na+            SO4--
  lambda0 =    0.01958  lambda1 =    1.11300  lambda2 =    0.00000
                    alpha1 =     2.0      alpha2 =    12.0
***** DATA1F.HMO
+-----+
MgOH+          SO4--
  lambda0 =    0.00000  lambda1 =    0.00000  lambda2 =    0.00000
                    alpha1 =     2.0      alpha2 =    12.0
*****

***** data1f.hml
+-----+
CO2 (aq)       SO4--
  lambda0 =    0.09700  lambda1 =    0.00000  lambda2 =    0.00000
                    alpha1 =     0.0      alpha2 =     0.0
  d10/dt =  0.000E+00  d210/dt2 =  0.000E+00
***** DATA1F.HMO
+-----+
MgAc+          Cl-
  lambda0 =   -0.08330  lambda1 =    0.29000  lambda2 =    0.00000
                    alpha1 =     2.0      alpha2 =    12.0
  d10/dt =  0.000E+00  d210/dt2 =  0.000E+00
*****

***** data1f.hml
+-----+
endit.
Ca++           H+
  lambda0 =    0.09200  lambda1 =    0.00000  lambda2 =    0.00000
                    alpha1 =    99.0     alpha2 =    99.0
  d10/dt =  0.000E+00  d210/dt2 =  0.000E+00
***** DATA1F.HMO
+-----+
Na+            Acetate-
  lambda0 =    0.14260  lambda1 =    0.22000  lambda2 =    0.00000
                    alpha1 =     2.0      alpha2 =    12.0
  d10/dt =  0.000E+00  d210/dt2 =  0.000E+00
*****

***** data1f.hml
+-----+
Ca++           Mg++
  lambda0 =    0.00700  lambda1 =    0.00000  lambda2 =    0.00000
                    alpha1 =    99.0     alpha2 =    99.0
  d10/dt =  0.000E+00  d210/dt2 =  0.000E+00
***** DATA1F.HMO

```

```

+-----+
Na+          Citrate---
  lambda0 = 0.08870  lambda1 = 5.22000  lambda2 = 0.00000
              alpha1 = 2.0          alpha2 = 12.0
  dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
Ca++         MgOH+
  lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
              alpha1 = 99.0         alpha2 = 99.0
  dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
CO2(aq)      Na+
  lambda0 = 0.10000  lambda1 = 0.00000  lambda2 = 0.00000
              alpha1 = 2.0          alpha2 = 12.0
  dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
CO3---       Cl-
  lambda0 = -0.02000  lambda1 = 0.00000  lambda2 = 0.00000
              alpha1 = 99.0         alpha2 = 99.0
  dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
Na+          CO3---
  lambda0 = 0.03990  lambda1 = 1.38900  lambda2 = 0.00000
              alpha1 = 2.0          alpha2 = 12.0
  dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
Cl-          HCO3-
  lambda0 = 0.03000  lambda1 = 0.00000  lambda2 = 0.00000
              alpha1 = 99.0         alpha2 = 99.0
  dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
Na+          CaCit-
  lambda0 = 0.17420  lambda1 = 0.29000  lambda2 = 0.00000
              alpha1 = 2.0          alpha2 = 12.0
  dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
Cl-          HSO4-
  lambda0 = -0.00600  lambda1 = 0.00000  lambda2 = 0.00000
              alpha1 = 99.0         alpha2 = 99.0
  dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
Na+          CaEDTA--
  lambda0 = 0.21340  lambda1 = 1.74000  lambda2 = 0.00000
              alpha1 = 2.0          alpha2 = 12.0
  dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
Cl-          OH-

```

```

lambda0 = -0.05000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
Na+ Cl-
lambda0 = 0.07650 lambda1 = 0.26640 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
Cl- SO4--
lambda0 = 0.02000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
Na+ EDTA----
lambda0 = 1.01600 lambda1 = 11.60000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
CO3-- HCO3-
lambda0 = -0.04000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
Na+ H2Citrate-
lambda0 = -0.12960 lambda1 = 0.29000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
CO3-- HSO4-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
Na+ HCitrate--
lambda0 = -0.09890 lambda1 = 1.74000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
HCO3- HSO4-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
Na+ HCO3-
lambda0 = 0.02770 lambda1 = 0.04110 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
*****

```


lambda0 = 0.04540 lambda1 = 0.39800 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00

***** data1f.hml

+-----+
H+ Mg++
lambda0 = 0.10000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00
***** DATA1F.HMO

***** DATA1F.HMO

+-----+
Na+ MgCit-
lambda0 = 0.17420 lambda1 = 0.29000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00

***** data1f.hml

+-----+
Mg++ MgOH+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00
***** DATA1F.HMO

***** DATA1F.HMO

+-----+
Na+ MgEDTA--
lambda0 = 0.21340 lambda1 = 1.74000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00

***** data1f.hml

+-----+
H+ MgOH+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00
***** DATA1F.HMO

***** DATA1F.HMO

+-----+
Na+ OH-
lambda0 = 0.08640 lambda1 = 0.25300 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00

***** data1f.hml

+-----+
Ca++ Na+
lambda0 = 0.07000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00
***** DATA1F.HMO

***** DATA1F.HMO

+-----+
Na+ Oxalate--
lambda0 = -0.21760 lambda1 = 1.74000 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
dl0/dt = 0.000E+00 d2l0/dt2 = 0.000E+00

***** data1f.hml

+-----+
H+ Na+
lambda0 = 0.03600 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0

```

      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
Na+                SO4--
  lambda0 = 0.01958  lambda1 = 1.11300  lambda2 = 0.00000
                    alpha1 = 2.0      alpha2 = 12.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
K+                Na+
  lambda0 = -0.01200  lambda1 = 0.00000  lambda2 = 0.00000
                    alpha1 = 99.0     alpha2 = 99.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
CO2(aq)           SO4--
  lambda0 = 0.09700  lambda1 = 0.00000  lambda2 = 0.00000
                    alpha1 = 0.0      alpha2 = 0.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
*****

***** data1f.hml
+-----+
Mg++             Na+
  lambda0 = 0.07000  lambda1 = 0.00000  lambda2 = 0.00000
                    alpha1 = 99.0     alpha2 = 99.0
***** DATA1F.HMO
+-----+
endit.
Ca++            H+
  lambda0 = 0.09200  lambda1 = 0.00000  lambda2 = 0.00000
                    alpha1 = 99.0     alpha2 = 99.0
*****

***** data1f.hml
+-----+
MgOH+           Na+
  lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
                    alpha1 = 99.0     alpha2 = 99.0
***** DATA1F.HMO
+-----+
Ca++            Mg++
  lambda0 = 0.00700  lambda1 = 0.00000  lambda2 = 0.00000
                    alpha1 = 99.0     alpha2 = 99.0
*****

***** data1f.hml
+-----+
CO3--           OH-
  lambda0 = 0.10000  lambda1 = 0.00000  lambda2 = 0.00000
                    alpha1 = 99.0     alpha2 = 99.0
***** DATA1F.HMO
+-----+
Ca++            MgOH+
  lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
                    alpha1 = 99.0     alpha2 = 99.0
*****

***** data1f.hml
+-----+
HCO3-           OH-
  lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
                    alpha1 = 99.0     alpha2 = 99.0
***** DATA1F.HMO

```

+-----+
CO3-- Cl-
 lambda0 = -0.02000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 99.0 alpha2 = 99.0

***** data1f.hml

+-----+
CO3-- SO4--
 lambda0 = 0.02000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 99.0 alpha2 = 99.0
***** DATA1F.HMO

+-----+
Cl- HCO3-
 lambda0 = 0.03000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 99.0 alpha2 = 99.0

***** data1f.hml

+-----+
HCO3- SO4--
 lambda0 = 0.01000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 99.0 alpha2 = 99.0
***** DATA1F.HMO

+-----+
Cl- HSO4-
 lambda0 = -0.00600 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 99.0 alpha2 = 99.0

***** data1f.hml

+-----+
HSO4- SO4--
 lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 99.0 alpha2 = 99.0
***** DATA1F.HMO

+-----+
Cl- OH-
 lambda0 = -0.05000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 99.0 alpha2 = 99.0

***** data1f.hml

+-----+
OH- SO4--
 lambda0 = -0.01300 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 99.0 alpha2 = 99.0
***** DATA1F.HMO

+-----+
Cl- SO4--
 lambda0 = 0.02000 lambda1 = 0.00000 lambda2 = 0.00000
 alpha1 = 99.0 alpha2 = 99.0

Resync Failed. Files are too different.

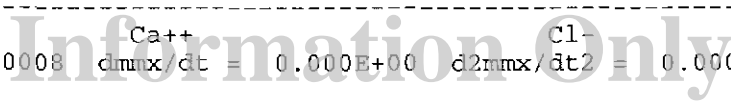
***** data1f.hml

+-----+
endit.

Ca++ Ca++ CO3--
 mu = 0.00000 dmmx/dt = 0.000E+00 d2mmx/dt2 = 0.000E+00

+-----+
Ca++ CO3-- CO3--
 mu = 0.00000 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00

+-----+
Ca++ Ca++ Cl-
 mu = -0.00008 dmmx/dt = 0.000E+00 d2mmx/dt2 = 0.000E+00



Ca++	mu = -0.00004	Cl-	dmxx/dt = 0.000E+00	Cl-	d2mxx/dt2 = 0.000E+00
Ca++	mu = 0.00000	Ca++	dmxx/dt = 0.000E+00	HCO3-	d2mxx/dt2 = 0.000E+00
Ca++	mu = 0.00000	HCO3-	dmxx/dt = 0.000E+00	HCO3-	d2mxx/dt2 = 0.000E+00
Ca++	mu = 0.00000	Ca++	dmxx/dt = 0.000E+00	HSO4-	d2mxx/dt2 = 0.000E+00
Ca++	mu = 0.00000	HSO4-	dmxx/dt = 0.000E+00	HSO4-	d2mxx/dt2 = 0.000E+00
Ca++	mu = 0.00000	Ca++	dmxx/dt = 0.000E+00	OH-	d2mxx/dt2 = 0.000E+00
Ca++	mu = 0.00000	OH-	dmxx/dt = 0.000E+00	OH-	d2mxx/dt2 = 0.000E+00
Ca++	mu = 0.00000	Ca++	dmxx/dt = 0.000E+00	SO4--	d2mxx/dt2 = 0.000E+00
Ca++	mu = 0.00000	SO4--	dmxx/dt = 0.000E+00	SO4--	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00000	H+	dmxx/dt = 0.000E+00	CO3--	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00000	CO3--	dmxx/dt = 0.000E+00	CO3--	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00013	H+	dmxx/dt = 0.000E+00	Cl-	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00013	Cl-	dmxx/dt = 0.000E+00	Cl-	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00000	H+	dmxx/dt = 0.000E+00	HCO3-	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00000	HCO3-	dmxx/dt = 0.000E+00	HCO3-	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00000	H+	dmxx/dt = 0.000E+00	HSO4-	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00000	HSO4-	dmxx/dt = 0.000E+00	HSO4-	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00000	H+	dmxx/dt = 0.000E+00	OH-	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00000	OH-	dmxx/dt = 0.000E+00	OH-	d2mxx/dt2 = 0.000E+00
H+	mu = 0.00516	H+	dmxx/dt = 0.000E+00	SO4--	d2mxx/dt2 = 0.000E+00
H+	mu = 0.01032	SO4--	dmxx/dt = 0.000E+00	SO4--	d2mxx/dt2 = 0.000E+00
K+	mu = -0.00018	K+	dmxx/dt = 0.000E+00	CO3--	d2mxx/dt2 = 0.000E+00

```

+-----+
K+          CO3--          CO3--
mu = -0.00035 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
K+          K+          Cl-
mu = -0.00014 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
K+          Cl-          Cl-
mu = -0.00014 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
K+          K+          H2Citrate-
mu = 0.00217 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
K+          H2Citrate-          H2Citrate-
mu = 0.00217 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
K+          K+          HCitrate--
mu = 0.00318 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
K+          HCitrate--          HCitrate--
mu = 0.00636 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
K+          K+          HCO3-
mu = -0.00133 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
***** DATA1F.HMO
+-----+
CO3--          HCO3-
lambda0 = -0.04000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00
+-----+
CO3--          HSO4-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00
+-----+
HCO3-          HSO4-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00
+-----+
HSO4-          OH-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00
+-----+
Ca++          K+
lambda0 = 0.03200 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00
+-----+
H+          K+
lambda0 = 0.00500 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00

```

```

      dl2/dt = 0.000E+00  d2l2/dt2 = 0.000E+00
+-----+
K+      Mg++
      lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
      alpha1 = 99.0      alpha2 = 99.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
      dl1/dt = 0.000E+00  d2l1/dt2 = 0.000E+00
      dl2/dt = 0.000E+00  d2l2/dt2 = 0.000E+00
+-----+
K+      MgOH+
      lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
      alpha1 = 99.0      alpha2 = 99.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
      dl1/dt = 0.000E+00  d2l1/dt2 = 0.000E+00
      dl2/dt = 0.000E+00  d2l2/dt2 = 0.000E+00
+-----+
H+      Mg++
      lambda0 = 0.10000  lambda1 = 0.00000  lambda2 = 0.00000
      alpha1 = 99.0      alpha2 = 99.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
      dl1/dt = 0.000E+00  d2l1/dt2 = 0.000E+00
      dl2/dt = 0.000E+00  d2l2/dt2 = 0.000E+00
+-----+
Mg++     MgOH+
      lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
      alpha1 = 99.0      alpha2 = 99.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
      dl1/dt = 0.000E+00  d2l1/dt2 = 0.000E+00
      dl2/dt = 0.000E+00  d2l2/dt2 = 0.000E+00
+-----+
H+      MgOH+
      lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
      alpha1 = 99.0      alpha2 = 99.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
      dl1/dt = 0.000E+00  d2l1/dt2 = 0.000E+00
      dl2/dt = 0.000E+00  d2l2/dt2 = 0.000E+00
+-----+
Ca++     Na+
      lambda0 = 0.07000  lambda1 = 0.00000  lambda2 = 0.00000
      alpha1 = 99.0      alpha2 = 99.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
      dl1/dt = 0.000E+00  d2l1/dt2 = 0.000E+00
      dl2/dt = 0.000E+00  d2l2/dt2 = 0.000E+00
+-----+
H+      Na+
      lambda0 = 0.03600  lambda1 = 0.00000  lambda2 = 0.00000
      alpha1 = 99.0      alpha2 = 99.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
      dl1/dt = 0.000E+00  d2l1/dt2 = 0.000E+00
      dl2/dt = 0.000E+00  d2l2/dt2 = 0.000E+00
+-----+
K+      Na+
      lambda0 = -0.01200  lambda1 = 0.00000  lambda2 = 0.00000
      alpha1 = 99.0      alpha2 = 99.0
      dl0/dt = 0.000E+00  d2l0/dt2 = 0.000E+00
      dl1/dt = 0.000E+00  d2l1/dt2 = 0.000E+00
      dl2/dt = 0.000E+00  d2l2/dt2 = 0.000E+00
+-----+
Mg++     Na+
*****

```

Information Only