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

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

Yongliang Xiong

subject: Incorporation of Amorphous Calcium Carbonate with Higher Solubility ($CaCO_3$(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 ($CaCO_3$(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 $CaCO_3$(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 $CaCO_3$(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 $CaCO_3$(am-cpa) INTO EQ3/6 HMO

The dissolution of the $CaCO_3$(am-cpa) can be expressed as:

$$CaCO_3(am\text{-}cpa) = Ca^{2+} + CO_3^{2-} \quad (1)$$

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:

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

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:

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

According to Eq. 4, and based on $\Delta_r G^o$ listed in Table 1 and $\Delta_f G^o$ for Ca^{2+} and CO_3^{2-} listed in Table 2, the free energy of formation for $CaCO_3$(am-cpa) is derived from Reaction (1) and listed in Table 2.

In the HML database, the association reaction for CO_3^{2-} is given as:

$$CO_3^{2-} + H^+ = HCO_3^-, \quad (5)$$

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

$$CaCO_3(am\text{-}cpa) + H^+ = Ca^{2+} + HCO_3^- \quad (6)$$

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:

$$CH_3COOH(aq)\ (HAc) = H^+ + CH_3OO^-\ (Ac^-) \quad (7)$$

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:

$$C_{10}H_{16}N_2O_8(aq)\ (H_4ETDA) = H^+ + C_{10}H_{15}N_2O_8^-\ (H_3ETDA^-) \quad (8)$$

$$C_{10}H_{15}N_2O_8^-\ (H_3ETDA^-) = H^+ + C_{10}H_{14}N_2O_8^{2-}\ (H_2ETDA^{2-}) \quad (9)$$

$$C_{10}H_{14}N_2O_8^{2-}\ (H_2ETDA^{2-}) = H^+ + C_{10}H_{13}N_2O_8^{3-}\ (HETDA^{3-}) \quad (10)$$

$$C_{10}H_{13}N_2O_8^{3-}\ (HETDA^{3-}) = H^+ + C_{10}H_{12}N_2O_8^{4-}\ (ETDA^{4-}) \quad (11)$$

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:

$$Mg^{2+} + Ac^- = MgAc^+ \quad (12)$$

$$Mg^{2+} + Cit^{3-} = MgCit^- \quad (13)$$

$$Mg^{2+} + EDTA^{4-} = MgEDTA^{2-} \quad (14)$$

$$Mg^{2+} + Ox^{2-} = MgOx(aq) \quad (15)$$

$$Ca^{2+} + Ac^- = CaAc^+ \quad (16)$$

$$Ca^{2+} + Cit^{3-} = CaCit^- \quad (17)$$

$$Ca^{2+} + EDTA^{4-} = CaEDTA^{2-} \quad (18)$$

$$Ca^{2+} + Ox^{2-} = CaOx(aq) \quad (19)$$

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.hml", and between "data1f.hmo" and "data1f.hml" 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.

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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.

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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.

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

Reaction	$\Delta_r G^o$, 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 Ca^{2+}, CO_3^{2-} and $CaCO_3$(am-cpa) at Reference State (298.15 K and 1 bar).

Species	$\Delta_f G^o$, 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 $CaCO_3$(am-cpa) at Reference Sate (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
$CH_3COOH(aq)$	–158.300	–93,785
CH_3OO^-	–147.347	–87,296
$C_{10}H_{16}N_2O_8(aq)$	0	0
$C_{10}H_{15}N_2O_8^-$	5.761	3,413
$C_{10}H_{14}N_2O_8^{2-}$	12.870	7,625
$C_{10}H_{13}N_2O_8^{3-}$	28.710	17,009
$C_{10}H_{12}N_2O_8^{4-}$	53.050	31,430
$C_6H_5O_7^{3-}$ (Cit^{3-})	33.41	19,794
$C_2O_4^{2-}$ (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).

		Binary Interaction Parameters		
i	j	$\beta^{(0)}$, kg mol^{-1}	$\beta^{(1)}$, kg mol^{-1}	C^{ϕ}, kg^2 mol^{-2}
Na^+	CH_3OO^-	0.1426	0.22	–0.00629
Na^+	$C_{10}H_{15}N_2O_8^-$	–0.2345	0.29	0.059
Na^+	$C_{10}H_{14}N_2O_8^{2-}$	–0.1262	1.74	0.054
Na^+	$C_{10}H_{13}N_2O_8^{3-}$	0.5458	5.22	–0.048
Na^+	$C_{10}H_{12}N_2O_8^{4-}$	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_3OO^-	0.1587	0.3251	–0.0066
K^+	$C_{10}H_{15}N_2O_8^-$	–0.2345	0.29	0.059
K^+	$C_{10}H_{14}N_2O_8^{2-}$	–0.1262	1.74	0.054
K^+	$C_{10}H_{13}N_2O_8^{3-}$	0.5458	5.22	–0.048
K^+	$C_{10}H_{12}N_2O_8^{4-}$	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:

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```
Comparing files output.hml and OUTPUT.HMO
***** output.hml

 Run  16:51:44  26Oct2006

***** OUTPUT.HMO

 Run  10:39:57  07Feb2007

*****

***** output.hml

           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.hml

 data0.hml.V8.R6
 CII: GEMBOCHS.V2-EQ8-data0.hml.V8.R6
 THERMODYNAMIC DATABASE
***** OUTPUT.HMO

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

***** output.hml
 Output package:  eq3
 Data set:        hml
 +------------------------------------------------------------------------
***** OUTPUT.HMO
 Output package:  eq3
 Data set:        hmo
 +------------------------------------------------------------------------
*****

***** output.hml
 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.hml
 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.hml
```

```
      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-
```

```
*****

***** output.hml
    14 CaCO3(am)
    15 Calcite
    16 Carnallite
    17 Chloromagnesite
    18 Dolomite
    19 Earlandite
    20 Epsomite
    21 Gaylussite
    22 Glauberite
    23 Gypsum
    24 Halite
    25 Hexahydrite
    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 Hexahydrite
    27 Hydromagne5424
```

```
    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 Mercallite
    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.hml

         Ca++, Citrate---
         Ca++, Oxalate--
         Ca++, H2Citrate-
***** OUTPUT.HMO

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

***** output.hml
         Ca++, HCitrate--
         Ca++, HOxalate-
         H+, Citrate---
         H+, Oxalate--
         H+, H2Citrate-
         H+, HCitrate--
         H+, HOxalate-
         K+, Citrate---
         Mg++, Citrate---
         Mg++, Oxalate--
         Mg++, H2Citrate-
         Mg++, HCitrate--
```

```
         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.hml

 * 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.hml

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

```
         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.hml

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

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

***** output.hml
         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.hml
         MgCO3(aq), MgCO3(aq)

***** OUTPUT.HMO
         MgCO3(aq), MgCO3(aq)
         MgOx(aq), MgOx(aq)
```

```
*****

***** output.hml

         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.hml
         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.hml
         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.hml

         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+
```

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

***** output.hml
         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.hml

         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.hml

         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.hml
         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-
```

```
        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.hml

        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.hml
```

```
         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.hml
         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.hml

         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
```

```
          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.hml

       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.hml
       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.hml
       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.hml
        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.hml
        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.hml
        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.hml

        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.hml
       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.hml
       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

*****
```

```
***** output.hml
        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.hml
        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.hml

 Completed processing the pitzer data file data0.hml.V8.R6.

***** OUTPUT.HMO

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

*****

***** output.hml

 10 warning(s) were encountered.

***** OUTPUT.HMO

 11 warning(s) were encountered.

*****

***** output.hml

          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

*****
```

```
Comparing files data1f.hml and DATA1F.HMO
***** data1f.hml
stpitz
   11   12
data0.hml.V8.R6
CII: GEMBOCHS.V2-EQ8-data0.hml.V8.R6
THERMODYNAMIC DATABASE
***** DATA1F.HMO
stpitz
   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
Ca++                          1    0
*****

***** data1f.hml
     1.0000  Cl
H+                            1    0
***** DATA1F.HMO
     1.0000  Cl
EDTA----                      1    0
        292.245  -4.
     1.0000  Edtacid
H+                            1    0
*****

***** data1f.hml
```

```
     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
```

```
 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
    dl0/dt =  0.000E+00    d2l0/dt2 =  0.000E+00
***** DATA1F.HMO
+---------------------------------------------------------------------------
H+                          Cl-
   lambda0 =    0.17750    lambda1 =    0.29450    lambda2 =    0.00000
```

```
                          alpha1 =   2.0       alpha2 =  12.0
    dl0/dt =  0.000E+00  d2l0/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--
```

```
   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
    dl0/dt =  0.000E+00   d2l0/dt2 =  0.000E+00
***** DATA1F.HMO
+---------------------------------------------------------------------------
K+                         HCO3-
   lambda0 =    0.02960   lambda1 =   -0.01300   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
    dl0/dt =  0.000E+00   d2l0/dt2 =  0.000E+00
*****
```

```
***** 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
    dl0/dt =  0.000E+00  d2l0/dt2 =  0.000E+00
***** DATA1F.HMO
+---------------------------------------------------------------------------
K+                            HSO4-
   lambda0 =   -0.00030   lambda1 =    0.17350   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
    dl0/dt =  0.000E+00  d2l0/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
    dl0/dt =  0.000E+00   d2l0/dt2 =   0.000E+00
***** DATA1F.HMO
+---------------------------------------------------------------------
Mg++                           CO3--
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =    1.4        alpha2 =   12.0
    dl0/dt =  0.000E+00   d2l0/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
+---------------------------------------------------------------------
```

```
Na+                          H2Citrate-
   lambda0 =   -0.12960   lambda1 =    0.29000   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
    dl0/dt =   0.000E+00  dl2l0/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  dl2l0/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
    dl0/dt =  0.000E+00   d2l0/dt2 =  0.000E+00
***** DATA1F.HMO
+----------------------------------------------------------------------
MgAc+                          Cl-
   lambda0 =   -0.08330    lambda1 =    0.29000    lambda2 =    0.00000
                           alpha1 =    2.0         alpha2 =   12.0
    dl0/dt =  0.000E+00   d2l0/dt2 =  0.000E+00
*****

***** data1f.hml
+----------------------------------------------------------------------
endit.
Ca++                           H+
   lambda0 =    0.09200    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+                            Acetate-
   lambda0 =    0.14260    lambda1 =    0.22000    lambda2 =    0.00000
                           alpha1 =    2.0         alpha2 =   12.0
    dl0/dt =  0.000E+00   d2l0/dt2 =  0.000E+00
*****

***** data1f.hml
+----------------------------------------------------------------------
Ca++                           Mg++
   lambda0 =    0.00700    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+                          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
*****
```

```
***** data1f.hml
+---------------------------------------------------------------------------
HSO4-                          OH-
   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
+---------------------------------------------------------------------------
Na+                            H3EDTA-
   lambda0 =   -0.23450    lambda1 =    0.29000    lambda2 =    0.00000
                           alpha1 =    2.0        alpha2 =   12.0
    dl0/dt =   0.000E+00   d2l0/dt2 =   0.000E+00
*****

***** data1f.hml
+---------------------------------------------------------------------------
Ca++                           K+
   lambda0 =    0.03200    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+                            H2EDTA--
   lambda0 =   -0.12620    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+                             K+
   lambda0 =    0.00500    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+                            HEDTA---
   lambda0 =    0.54580    lambda1 =    5.22000    lambda2 =    0.00000
                           alpha1 =    2.0        alpha2 =   12.0
    dl0/dt =   0.000E+00   d2l0/dt2 =   0.000E+00
*****

***** data1f.hml
+---------------------------------------------------------------------------
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
***** DATA1F.HMO
+---------------------------------------------------------------------------
Na+                            HOxalate-
   lambda0 =   -0.24480    lambda1 =    0.29000    lambda2 =    0.00000
                           alpha1 =    2.0        alpha2 =   12.0
    dl0/dt =   0.000E+00   d2l0/dt2 =   0.000E+00
*****

***** data1f.hml
+---------------------------------------------------------------------------
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
***** DATA1F.HMO
+---------------------------------------------------------------------------
Na+                            HSO4-
```

```
   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
+---------------------------------------------------------------------------
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
+---------------------------------------------------------------------------
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
+---------------------------------------------------------------------------
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
+---------------------------------------------------------------------------
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++		Cl-		Cl-	
	mu = -0.00004	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
Ca++		Ca++		HCO3-	
	mu = 0.00000	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
Ca++		HCO3-		HCO3-	
	mu = 0.00000	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
Ca++		Ca++		HSO4-	
	mu = 0.00000	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
Ca++		HSO4-		HSO4-	
	mu = 0.00000	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
Ca++		Ca++		OH-	
	mu = 0.00000	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
Ca++		OH-		OH-	
	mu = 0.00000	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
Ca++		Ca++		SO4--	
	mu = 0.00000	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
Ca++		SO4--		SO4--	
	mu = 0.00000	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
H+		H+		CO3--	
	mu = 0.00000	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
H+		CO3--		CO3--	
	mu = 0.00000	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
H+		H+		Cl-	
	mu = 0.00013	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
H+		Cl-		Cl-	
	mu = 0.00013	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
H+		H+		HCO3-	
	mu = 0.00000	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
H+		HCO3-		HCO3-	
	mu = 0.00000	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
H+		H+		HSO4-	
	mu = 0.00000	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
H+		HSO4-		HSO4-	
	mu = 0.00000	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
H+		H+		OH-	
	mu = 0.00000	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
H+		OH-		OH-	
	mu = 0.00000	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
H+		H+		SO4--	
	mu = 0.00516	dmmx/dt =	0.000E+00	d2mmx/dt2 =	0.000E+00
H+		SO4--		SO4--	
	mu = 0.01032	dmxx/dt =	0.000E+00	d2mxx/dt2 =	0.000E+00
K+		K+		CO3--	
	mu = -0.00018	dmmx/dt =	0.000E+00	d2mmx/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  dmmx/dt =  0.000E+00  d2mmx/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  dmmx/dt =  0.000E+00  d2mmx/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  dmmx/dt =  0.000E+00  d2mmx/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  dmmx/dt =  0.000E+00  d2mmx/dt2 =  0.000E+00
***** DATA1F.HMO
+-----------------------------------------------------------------------
CO3--                       HCO3-
   lambda0 =  -0.04000   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
+-----------------------------------------------------------------------
CO3--                       HSO4-
   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
+-----------------------------------------------------------------------
HCO3-                       HSO4-
   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
+-----------------------------------------------------------------------
HSO4-                       OH-
   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++                        K+
   lambda0 =   0.03200   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+                          K+
   lambda0 =   0.00500   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+                          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+
*****
```