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Sandia Corporation

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date: April 14, 2008

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subject: HMI—An EQ3/6 Database with Iron Species

The objective of this memorandum is to document the incorporation of solubility constant and Pitzer parameters concerning iron species (metallic Fe or Fe(0), hereafter referred to as "Fe"; and the dissolved species Fe^{2+}) from the literature into a modified EQ3/6 database named HMI and its release to support the performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP). Specifically, the introduction of Fe and Fe^{2+} is necessary to rerun the simulations of calcite precipitation during the microbial degradation of CPR by SO_4^{2-} reduction in Brush et al. (2006) by using the special reactants containing iron. In the simulations of Brush et al. (2006), the microbial degradation of CPR by SO_4^{2-} reduction was simply treated as removal of $2H^+$ and SO_4^{2-} from, and titration of $CO_2(g)$ into, the system.

In the previous, modified version of the EQ3/6 database (HMO) that supports the Pitzer activity-coefficient option, aqueous complexes of Mg^{2+} and Ca^{2+} with acetate, citrate, EDTA and oxalate, and aqueous species of acetate and EDTA were incorporated (Xiong, 2007).

1 INCORPORATION OF Fe AND Fe^{2+} INTO THE EQ3/6 HMI DATABASE

The thermodynamic properties of Fe and Fe^{2+} at reference state (25 °C and 1 bar) are listed in Table 1. For the dissolution of Fe, the reaction can be expressed as:

$$Fe + 2H^+ + 0.5O_2(g) = Fe^{2+} + H_2O(l) \quad (1)$$

It should be noted that Reaction (1) is used to calculate a log K for the database, and that it is expected that this reaction would not occur in the WIPP because there will be essentially no free O_2. Based on the Gibbs free energy changes for Reaction (1), the log K can be calculated according to the following equation:

$$\log K = -\Delta_r G^\circ/(2.3026 \times R \times T), \quad (2)$$

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 a chemical reaction is expressed in the following general equation:

$$\Delta_r G = \sum_j \Delta_f G_{j,product} - \sum_i \Delta_f G_{i,reac.} \quad (3)$$

Therefore, according to the Gibbs free energies of formation of iron species listed in Table 1, and of auxiliary species listed in Table 2, the equilibrium constant for Reaction (1) is calculated as 57.5768.

2 INCORPORATION OF PITZER INTERACTION PARAMETERS INTO THE EQ3/6 HMI DATABASE

The binary, neutral-ion, and ternary, Pitzer interaction parameters involving Fe^{2+} are primarily taken from the compilation of Marion et al. (2003), and are listed in Tables 4, 5, and 6, respectively. It should be mentioned that although there are $\zeta_{CO_2,\ Fe^{2+},\ Cl^-}$ and $\zeta_{CO_2,\ Fe^{2+},\ SO_4^{2-}}$ in the compilation of Marion et al. (2003), they are not incorporated into the EQ3/6 HMI database, because EQ3/6 does not use ζ_{MNX}.

3 HMI DATABASE

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

REFERENCES

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Wolery, T.J. 1992. *EQ3NR, A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: Theoretical Manual, User's Guide, and Related Documentation (Version 7.0).* UCRL-MA-110662 PT III. Livermore, CA: Lawrence Livermore National Laboratory.

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Table 1. Thermodynamic Properties of Fe and Fe^{2+} at Reference State (298.15 K and 1 bar).

Species	$\Delta_f G^o$, kcal mol^{-1}	$\Delta_f H^o$, kcal mol^{-1}	S^o, cal mol^{-1} K^{-1}	Reference
Fe	0	0	6.52	Lide (2008)
Fe^{2+}	–21.870	–22.050	–25.300	SUP (Wolery, 1992)

Table 2. Standard Free Energies of Formation for Auxiliary Species at Reference State (298.15 K and 1 bar).

Species	$\Delta_f G^\circ$, kcal mol^{-1}	Reference
$H_2O(l)$	–56.679	HMO database
H^+	0	HMO database
$O_2(g)$	0	HMO database

Table 3. Equilibrium Constants at Infinite Dilution for Dissolution Reactions Involving Iron Species at 298.15 K and 1 bar.

Reaction	log K
$Fe + 2H^+ + 0.5O_2(g) = Fe^{2+} + H_2O(l)$	57.5768

Table 4. Binary Pitzer Interaction Parameters Involving Fe^{2+} Taken from Marion et al. (2003).

i	j	$\beta^{(0)}$, kg mol^{-1}	$\beta^{(1)}$, kg mol^{-1}	$\beta^{(2)}$, kg mol^{-1}	C^{ϕ}, kg^2 mol^{-2}
Fe^{2+}	Cl^-	0.33592*	1.53225*	0	–0.00861*
Fe^{2+}	HCO_3^-	–0.00930**	0.80281**	0	0
Fe^{2+}	SO_4^{2-}	0.25687	3.08794	–42.0	0.02090
Fe^{2+}	HSO_4^-	0.43379	3.48000	0	0

* From Pitzer (1991).
**According to the analog of Mg^{2+}–HCO_3^- interaction.

Table 5. Neutral-Ion Pitzer Interaction Parameter (λ) Involving Fe^{2+} Taken from Marion et al. (2003).

Neutral Species	Ion	λ
CO_2(aq)	Fe^{2+}	0.14473*

*Based on the analog of CO_2(aq)–Mg^{2+} interaction.

Table 6. Ternary Pitzer Interaction Parameters (θ_{ij} and Ψ_{ijk}) Involving Fe^{2+} Taken from Marion et al. (2003).

i	j	k	θ_{ij}, kg mol^{-1}	Ψ_{ijk}, kg mol^{-1}
Fe^{2+}	H^+		0	
Fe^{2+}	Na^+		0.08000	
Fe^{2+}	K^+		0.11670	
Fe^{2+}	Ca^{2+}		0.12437	
Fe^{2+}	Mg^{2+}		0	
Fe^{2+}	H^+	Cl^-		0.01198
Fe^{2+}	H^+	SO_4^{2-}		0
Fe^{2+}	H^+	HSO_4^-		0.01123
Fe^{2+}	Na^+	Cl^-		–0.01400
Fe^{2+}	Na^+	SO_4^{2-}		–0.00991
Fe^{2+}	K^+	Cl^-		–0.04948
Fe^{2+}	K^+	SO_4^{2-}		–0.12436
Fe^{2+}	Mg^{2+}	Cl^-		0
Fe^{2+}	Mg^{2+}	SO_4^{2-}		0
Fe^{2+}	Ca^{2+}	Cl^-		–0.02381
Fe^{2+}	Ca^{2+}	SO_4^{2-}		0.02400
Fe^{2+}	Cl^-	SO_4^{2-}		–0.01833
Fe^{2+}	Cl^-	HCO_3^-		–0.09600
Fe^{2+}	SO_4^{2-}	HSO_4^-		0
Fe^{2+}	SO_4^{2-}	HCO_3^-		–0.16100

Information Only

```
Comparing files output.hmo and OUTPUT.HMI
***** output.hmo

 Run  10:39:57  07Feb2007

***** OUTPUT.HMI

 Run  15:50:49  26Mar2008

*****

***** 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.HMI

           no. of elements on the data file =    14
              the dimensioned limit =   110
           no. of aqueous species in the master set =    15
              the dimensioned limit =   500
*****

***** output.hmo

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

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

***** output.hmo
 Output package:  eq3
 Data set:        hmo
 +------------------------------------------------------------------------
***** OUTPUT.HMI
 Output package:  eq3
 Data set:        hmi
 +------------------------------------------------------------------------
*****

***** output.hmo
 element = Edtacid , atwt =  292.24500
 element = H       , atwt =    1.00794
***** OUTPUT.HMI
 element = Edtacid , atwt =  292.24500
 element = Fe      , atwt =   55.84700
 element = H       , atwt =    1.00794
*****

***** output.hmo
     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.HMI
     6 EDTA----
     7 Fe++
     8 H+
     9 HCO3-
    10 K+
    11 Mg++
    12 Na+
    13 Oxalate--
    14 SO4--
    15 O2(g)
    16 Acetic_acid(aq)
    17 CO2(aq)
    18 CO3--
    19 CaAc+
    20 CaCit-
    21 CaCO3(aq)
    22 CaEDTA--
    23 CaOx(aq)
    24 H3Citrate(aq)
    25 H2Citrate-
    26 HCitrate--
    27 H4EDTA(aq)
    28 H3EDTA-
    29 H2EDTA--
    30 HEDTA---
    31 H2Oxalate(aq)
    32 HOxalate-
    33 HSO4-
    34 MgAc+
```

```
    35 MgCit-
    36 MgCO3(aq)
    37 MgEDTA--
    38 MgOH+
    39 MgOx(aq)
    40 OH-

*****

***** output.hmo
    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.HMI
    28 Hydromagne4323
    29 Iron
    30 K2CO3:1.5H2O
    31 K3H(SO4)2
    32 K8H4(CO3)6:3H2O
    33 KNaCO3:6H2O
    34 Kainite
    35 Kalicinite
    36 Kieserite
    37 Leonite
    38 Lime
    39 Magnesite
    40 Mercallite
    41 Mirabilite
    42 Misenite
```

```
    43 Na2CO3:7H2O
    44 Na3H(SO4)2
    45 Na4Ca(SO4)3:2H2O
    46 Nahcolite
    47 Natron
    48 Nesquehonite
    49 Oxychloride-Mg
    50 Periclase
    51 Picromerite
    52 Pirssonite
    53 Polyhalite
    54 Portlandite
    55 Sylvite
    56 Syngenite
    57 Tachyhydrite
    58 Thenardite
    59 Thermonatrite
    60 Trona
    61 Trona-K
    62 Whewellite

*****

***** output.hmo
         Ca++, MgEDTA--
         H+, Acetate-
         H+, Citrate---
         H+, EDTA----
         H+, Oxalate--
         H+, CaCit-
         H+, CaEDTA--

         plus 75 others

***** OUTPUT.HMI
         Ca++, MgEDTA--
         Fe++, Acetate-
         Fe++, Citrate---
         Fe++, EDTA----
         Fe++, Oxalate--
         Fe++, CO3--
         Fe++, CaCit-

         plus 91 others

*****

***** output.hmo
         Ca++, MgAc+
         CaAc+, H+
***** OUTPUT.HMI
         Ca++, MgAc+
         CaAc+, Fe++
         Fe++, MgAc+
         Fe++, MgOH+
         CaAc+, H+
*****

***** output.hmo
         Acetic_acid(aq), Ca++
         Acetic_acid(aq), H+
```

```
***** OUTPUT.HMI
         Acetic_acid(aq), Ca++
         Acetic_acid(aq), Fe++
         Acetic_acid(aq), H+
*****

***** output.hmo
         CaCO3(aq), Ca++
         CaCO3(aq), K+
***** OUTPUT.HMI
         CaCO3(aq), Ca++
         CaCO3(aq), Fe++
         CaCO3(aq), K+
*****

***** output.hmo
         CaOx(aq), Ca++
         CaOx(aq), H+
         CaOx(aq), K+

         plus 44 others

***** OUTPUT.HMI
         CaOx(aq), Ca++

         plus 52 others

*****

***** output.hmo

         Ca++, H+, Acetate-
***** OUTPUT.HMI

         Ca++, Fe++, Acetate-
         Ca++, Fe++, Citrate---
         Ca++, Fe++, EDTA----
         Ca++, Fe++, Oxalate--
         Ca++, Fe++, CO3--
         Ca++, Fe++, CaCit-
         Ca++, Fe++, CaEDTA--
         Ca++, Fe++, H2Citrate-
         Ca++, Fe++, HCitrate--
         Ca++, Fe++, H3EDTA-
         Ca++, Fe++, H2EDTA--
         Ca++, Fe++, HEDTA---
         Ca++, Fe++, HOxalate-
         Ca++, Fe++, MgCit-
         Ca++, Fe++, MgEDTA--
         Ca++, Fe++, OH-
         Ca++, H+, Acetate-
*****

***** output.hmo
         Ca++, H+, Oxalate--
         Ca++, H+, CaCit-
         Ca++, H+, CaEDTA--
         Ca++, H+, H2Citrate-
         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.HMI
         Ca++, H+, Oxalate--

         plus 595 others

*****

***** output.hmo
         Acetate-, Citrate---, Ca++
         Acetate-, Citrate---, H+
***** OUTPUT.HMI
         Acetate-, Citrate---, Ca++
         Acetate-, Citrate---, Fe++
         Acetate-, Citrate---, H+
*****

***** output.hmo
         Acetate-, Cl-, Ca++
         Acetate-, Cl-, H+
***** OUTPUT.HMI
         Acetate-, Cl-, Ca++
         Acetate-, Cl-, Fe++
         Acetate-, Cl-, H+
*****

***** output.hmo
         Acetate-, EDTA----, Ca++
         Acetate-, EDTA----, H+
         Acetate-, EDTA----, K+
         Acetate-, EDTA----, Mg++

         plus 1410 others

***** OUTPUT.HMI
         Acetate-, EDTA----, Ca++
         Acetate-, EDTA----, Fe++

         plus 1596 others

*****

***** output.hmo

         plus 1420 others

***** OUTPUT.HMI

         plus 1600 others
```

```
*****

***** 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.HMI

       69 pairs have Pitzer parameters specified on the DATA0 file
      180 pairs can be constructed from the species present on this file
    Coverage is 38.33 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.HMI

       20 pairs have Pitzer parameters specified on the DATA0 file
       36 pairs can be constructed from the species present on this file
    Coverage is 55.56 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.HMI

        9 pairs have Pitzer parameters specified on the DATA0 file
       81 pairs can be constructed from the species present on this file
    Coverage is 11.11 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.HMI

      105 triplets have Pitzer parameters specified on the DATA0 file
      720 triplets can be constructed from the species present on this
file
    Coverage is 14.58 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.HMI

       94 triplets have Pitzer parameters specified on the DATA0 file
     1710 triplets can be constructed from the species present on this
file
    Coverage is 5.50 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.HMI
        0 triplets have Pitzer parameters specified on the DATA0 file
     1620 triplets can be constructed from the species present on this
file
    Coverage is 0.00 per cent
*****

***** output.hmo

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

***** OUTPUT.HMI

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

*****

***** output.hmo

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

           run time =  0.200     seconds

***** OUTPUT.HMI

          Start time = 15:50:49  26Mar2008
            End time = 15:50:50  26Mar2008

           run time =  0.550     seconds

*****
```

```
Comparing files data1f.hmo and DATA1F.HMI
***** data1f.hmo
stpitz
   13   14
data0.hmo.V8.R6
CII: GEMBOCHS.V2-EQ8-data0.hmo.V8.R6
THERMODYNAMIC DATABASE
***** DATA1F.HMI
stpitz
   14   15
data0.hmi.V8.R6
CII: GEMBOCHS.V2-EQ8-data0.hmi.V8.R6
THERMODYNAMIC DATABASE
*****

***** data1f.hmo
Output package:  eq3
Data set:        hmo
+------------------------------------------------------------------------
***** DATA1F.HMI
Output package:  eq3
Data set:        hmi
+------------------------------------------------------------------------
*****

***** data1f.hmo
Edtacid  292.24500                      0.00000
H          1.00794                      0.00000
***** DATA1F.HMI
Edtacid  292.24500                      0.00000
Fe        55.84700                      0.00000
H          1.00794                      0.00000
*****

***** data1f.hmo
     1.0000  Edtacid
H+                              1    0
***** DATA1F.HMI
     1.0000  Edtacid
Fe++                            1    0
         55.847   2.
     1.0000  Fe
H+                              1    0
*****

***** data1f.hmo
 9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00
0.000000000E+00
K2CO3:1.5H2O                    4    5
***** DATA1F.HMI
 9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00
0.000000000E+00
Iron                            1    5
         55.847   0.    7.092
     1.0000  Fe
    -1.0000  Iron                          -2.0000  H+
    -0.5000  O2(g)                          1.0000  Fe++
     1.0000  H2O
 5.757680000E+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
K2CO3:1.5H2O                    4     5
*****

***** data1f.hmo
+---------------------------------------------------------------------------
CO2(aq)                          H+
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =    2.0        alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
Fe++                             Cl-
   lambda0 =    0.33592    lambda1 =    1.53225    lambda2 =    0.00000
                           alpha1 =    2.0        alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------------
H+                               CO3--
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =    2.0        alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
Fe++                             HCO3-
   lambda0 =   -0.00930    lambda1 =    0.80281    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
    dl0/dt =  0.000E+00    d2l0/dt2 =   0.000E+00
***** DATA1F.HMI
+---------------------------------------------------------------------------
Fe++                             SO4--
   lambda0 =    0.25687    lambda1 =    3.08794    lambda2 =  -42.00000
                           alpha1 =    1.4        alpha2 =   12.0
    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
***** DATA1F.HMI
+---------------------------------------------------------------------------
Fe++                             HSO4-
   lambda0 =    0.43379    lambda1 =    3.48000    lambda2 =    0.00000
                           alpha1 =    2.0        alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------------
H+                               HCO3-
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =    2.0        alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
```

```
CO2(aq)                    Fe++
   lambda0 =   0.14473   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.HMI
+---------------------------------------------------------------------
CO2(aq)                    H+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------
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.HMI
+---------------------------------------------------------------------
H+                         CO3--
   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
+---------------------------------------------------------------------
H+                         OH-
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
***** DATA1F.HMI
+---------------------------------------------------------------------
CaCO3(aq)                  H+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
*****

***** data1f.hmo
+---------------------------------------------------------------------
H+                         SO4--
   lambda0 =   0.02980   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
***** DATA1F.HMI
+---------------------------------------------------------------------
H+                         Cl-
   lambda0 =   0.17750   lambda1 =   0.29450   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*****

***** 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.HMI
+---------------------------------------------------------------------
```

```
H+                          HCO3-
   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
+---------------------------------------------------------------------------
K+                          Acetate-
   lambda0 =    0.15870    lambda1 =    0.32510    lambda2 =    0.00000
                           alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
H+                          HSO4-
   lambda0 =    0.20650    lambda1 =    0.55560    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
    dl0/dt =  0.000E+00    d2l0/dt2 =   0.000E+00
***** DATA1F.HMI
+---------------------------------------------------------------------------
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
+---------------------------------------------------------------------------
K+                          CO3--
   lambda0 =    0.14880    lambda1 =    1.43000    lambda2 =    0.00000
                           alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
H+                          OH-
   lambda0 =    0.00000    lambda1 =    0.00000    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.HMI
+---------------------------------------------------------------------------
H+                          SO4--
   lambda0 =    0.02980    lambda1 =    0.00000    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
```

```
    dl0/dt =  0.000E+00  d2l0/dt2 =  0.000E+00
***** DATA1F.HMI
+---------------------------------------------------------------------
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.hmo
+---------------------------------------------------------------------
K+                           Cl-
   lambda0 =   0.04835    lambda1 =   0.21220   lambda2 =   0.00000
                          alpha1 =   2.0       alpha2 =  12.0
***** DATA1F.HMI
+---------------------------------------------------------------------
K+                           Acetate-
   lambda0 =   0.15870    lambda1 =   0.32510   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.HMI
+---------------------------------------------------------------------
CO2(aq)                      K+
   lambda0 =   0.05100    lambda1 =   0.00000   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.HMI
+---------------------------------------------------------------------
K+                           CO3--
   lambda0 =   0.14880    lambda1 =   1.43000   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.HMI
+---------------------------------------------------------------------
K+                           CaCit-
   lambda0 =   0.17420    lambda1 =   0.29000   lambda2 =   0.00000
                          alpha1 =   2.0       alpha2 =  12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------
K+                           HCO3-
   lambda0 =   0.02960    lambda1 =  -0.01300   lambda2 =   0.00000
```

```
                          alpha1 =   2.0       alpha2 =  12.0
***** DATA1F.HMI
+---------------------------------------------------------------------
K+                         CaEDTA--
   lambda0 =   0.21340   lambda1 =   1.74000   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.HMI
+---------------------------------------------------------------------
K+                         Cl-
   lambda0 =   0.04835   lambda1 =   0.21220   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.HMI
+---------------------------------------------------------------------
K+                         EDTA----
   lambda0 =   1.01600   lambda1 =  11.60000   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.HMI
+---------------------------------------------------------------------
K+                         H2Citrate-
   lambda0 =  -0.12960   lambda1 =   0.29000   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.HMI
+---------------------------------------------------------------------
K+                         HCitrate--
   lambda0 =  -0.09890   lambda1 =   1.74000   lambda2 =   0.00000
                          alpha1 =   2.0       alpha2 =  12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------
K+                         HSO4-
   lambda0 =  -0.00030   lambda1 =   0.17350   lambda2 =   0.00000
                          alpha1 =   2.0       alpha2 =  12.0
```

```
***** DATA1F.HMI
+--------------------------------------------------------------------------
K+                          HCO3-
   lambda0 =    0.02960    lambda1 =  -0.01300   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.HMI
+--------------------------------------------------------------------------
K+                          H3EDTA-
   lambda0 =   -0.23460    lambda1 =   0.29000   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.HMI
+--------------------------------------------------------------------------
K+                          H2EDTA--
   lambda0 =   -0.12620    lambda1 =   1.74000   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.HMI
+--------------------------------------------------------------------------
K+                          HEDTA---
   lambda0 =    0.54580    lambda1 =   5.22000   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.HMI
+--------------------------------------------------------------------------
K+                          HOxalate-
   lambda0 =   -0.24480    lambda1 =   0.29000   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.HMI
```

```
+------------------------------------------------------------------------
K+                          HSO4-
   lambda0 =  -0.00030   lambda1 =   0.17350   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.HMI
+------------------------------------------------------------------------
K+                          MgCit-
   lambda0 =   0.17420   lambda1 =   0.29000   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*****

***** 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.HMI
+------------------------------------------------------------------------
K+                          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.hmo
+------------------------------------------------------------------------
Mg++                        Cl-
   lambda0 =   0.35235   lambda1 =   1.68150   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
***** DATA1F.HMI
+------------------------------------------------------------------------
K+                          OH-
   lambda0 =   0.12980   lambda1 =   0.32000   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.HMI
+------------------------------------------------------------------------
K+                          Oxalate--
   lambda0 =  -0.21760   lambda1 =   1.74000   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.HMI
+--------------------------------------------------------------------------
K+                          SO4--
   lambda0 =    0.04995    lambda1 =    0.77930    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.HMI
+--------------------------------------------------------------------------
CO2(aq)                     Mg++
   lambda0 =    0.18300    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
Mg++                        SO4--
   lambda0 =    0.22100    lambda1 =    3.34300    lambda2 = -37.23000
                           alpha1 =    1.4         alpha2 =   12.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Mg++                        CO3--
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =    1.4         alpha2 =   12.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
CO2(aq)                     MgOH+
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Mg++                        Cl-
   lambda0 =    0.35235    lambda1 =    1.68150    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.HMI
+--------------------------------------------------------------------------
Mg++                        HCO3-
   lambda0 =    0.32900    lambda1 =    0.60720    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.HMI
```

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

***** data1f.hmo
+----------------------------------------------------------------------
MgOH+                         HCO3-
   lambda0 =    0.00000   lambda1 =   0.00000   lambda2 =   0.00000
***** DATA1F.HMI
+----------------------------------------------------------------------
Mg++                          OH-
   lambda0 =    0.00000   lambda1 =   0.00000   lambda2 =   0.00000
*****

***** data1f.hmo
+----------------------------------------------------------------------
MgOH+                         HSO4-
   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.HMI
+----------------------------------------------------------------------
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
+----------------------------------------------------------------------
MgOH+                         OH-
   lambda0 =    0.00000   lambda1 =   0.00000   lambda2 =   0.00000
***** DATA1F.HMI
+----------------------------------------------------------------------
CO2(aq)                       MgOH+
   lambda0 =    0.00000   lambda1 =   0.00000   lambda2 =   0.00000
*****

***** data1f.hmo
+----------------------------------------------------------------------
MgOH+                         SO4--
   lambda0 =    0.00000   lambda1 =   0.00000   lambda2 =   0.00000
***** DATA1F.HMI
+----------------------------------------------------------------------
MgOH+                         CO3--
   lambda0 =    0.00000   lambda1 =   0.00000   lambda2 =   0.00000
*****

***** data1f.hmo
+----------------------------------------------------------------------
MgAc+                         Cl-
   lambda0 =   -0.08330   lambda1 =   0.29000   lambda2 =   0.00000
                          alpha1 =   2.0       alpha2 =  12.0
***** DATA1F.HMI
+----------------------------------------------------------------------
MgOH+                         Cl-
   lambda0 =   -0.10000   lambda1 =   1.65800   lambda2 =   0.00000
                          alpha1 =   2.0       alpha2 =  12.0
*****
```

```
***** data1f.hmo
+---------------------------------------------------------------------------
Na+                          Acetate-
   lambda0 =    0.14260     lambda1 =    0.22000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
MgOH+                        HCO3-
   lambda0 =    0.00000     lambda1 =    0.00000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------------
Na+                          Citrate---
   lambda0 =    0.08870     lambda1 =    5.22000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
MgOH+                        HSO4-
   lambda0 =    0.00000     lambda1 =    0.00000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------------
CO2(aq)                      Na+
   lambda0 =    0.10000     lambda1 =    0.00000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
MgOH+                        OH-
   lambda0 =    0.00000     lambda1 =    0.00000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------------
Na+                          CO3--
   lambda0 =    0.03990     lambda1 =    1.38900    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
MgOH+                        SO4--
   lambda0 =    0.00000     lambda1 =    0.00000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------------
Na+                          CaCit-
   lambda0 =    0.17420     lambda1 =    0.29000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
MgAc+                        Cl-
   lambda0 =   -0.08330     lambda1 =    0.29000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****
```

```
***** data1f.hmo
+---------------------------------------------------------------------
Na+                          CaEDTA--
   lambda0 =    0.21340     lambda1 =    1.74000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------
Na+                          Acetate-
   lambda0 =    0.14260     lambda1 =    0.22000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------
Na+                          Cl-
   lambda0 =    0.07650     lambda1 =    0.26640    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------
Na+                          Citrate---
   lambda0 =    0.08870     lambda1 =    5.22000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------
Na+                          EDTA----
   lambda0 =    1.01600     lambda1 =   11.60000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------
CO2(aq)                      Na+
   lambda0 =    0.10000     lambda1 =    0.00000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------
Na+                          H2Citrate-
   lambda0 =   -0.12960     lambda1 =    0.29000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------
Na+                          CO3--
   lambda0 =    0.03990     lambda1 =    1.38900    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+---------------------------------------------------------------------
Na+                          HCitrate--
   lambda0 =   -0.09890     lambda1 =    1.74000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+---------------------------------------------------------------------
Na+                          CaCit-
   lambda0 =    0.17420     lambda1 =    0.29000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
```

```
+----------------------------------------------------------------------
Na+                          HCO3-
   lambda0 =    0.02770     lambda1 =    0.04110    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+----------------------------------------------------------------------
Na+                          CaEDTA--
   lambda0 =    0.21340     lambda1 =    1.74000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+----------------------------------------------------------------------
Na+                          H3EDTA-
   lambda0 =   -0.23450     lambda1 =    0.29000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+----------------------------------------------------------------------
Na+                          Cl-
   lambda0 =    0.07650     lambda1 =    0.26640    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+----------------------------------------------------------------------
Na+                          H2EDTA--
   lambda0 =   -0.12620     lambda1 =    1.74000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+----------------------------------------------------------------------
Na+                          EDTA----
   lambda0 =    1.01600     lambda1 =   11.60000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+----------------------------------------------------------------------
Na+                          HEDTA---
   lambda0 =    0.54580     lambda1 =    5.22000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+----------------------------------------------------------------------
Na+                          H2Citrate-
   lambda0 =   -0.12960     lambda1 =    0.29000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+----------------------------------------------------------------------
Na+                          HOxalate-
   lambda0 =   -0.24480     lambda1 =    0.29000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
***** DATA1F.HMI
+----------------------------------------------------------------------
Na+                          HCitrate--
   lambda0 =   -0.09890     lambda1 =    1.74000    lambda2 =    0.00000
                            alpha1 =    2.0         alpha2 =   12.0
*****

***** data1f.hmo
+----------------------------------------------------------------------
```

```
Na+                          HSO4-
   lambda0 =    0.04540   lambda1 =    0.39800   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Na+                          HCO3-
   lambda0 =    0.02770   lambda1 =    0.04110   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
Na+                          MgCit-
   lambda0 =    0.17420   lambda1 =    0.29000   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Na+                          H3EDTA-
   lambda0 =   -0.23450   lambda1 =    0.29000   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
Na+                          MgEDTA--
   lambda0 =    0.21340   lambda1 =    1.74000   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Na+                          H2EDTA--
   lambda0 =   -0.12620   lambda1 =    1.74000   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
Na+                          OH-
   lambda0 =    0.08640   lambda1 =    0.25300   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Na+                          HEDTA---
   lambda0 =    0.54580   lambda1 =    5.22000   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
Na+                          Oxalate--
   lambda0 =   -0.21760   lambda1 =    1.74000   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Na+                          HOxalate-
   lambda0 =   -0.24480   lambda1 =    0.29000   lambda2 =    0.00000
                          alpha1 =    2.0        alpha2 =   12.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
Na+                          SO4--
```

```
   lambda0 =   0.01958   lambda1 =   1.11300   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
***** DATA1F.HMI
+---------------------------------------------------------------------
Na+                       HSO4-
   lambda0 =   0.04540   lambda1 =   0.39800   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*****

***** 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.HMI
+---------------------------------------------------------------------
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.hmo
+---------------------------------------------------------------------
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.HMI
+---------------------------------------------------------------------
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.hmo
+---------------------------------------------------------------------
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.HMI
+---------------------------------------------------------------------
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.hmo
+---------------------------------------------------------------------
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.HMI
+---------------------------------------------------------------------
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.hmo
+---------------------------------------------------------------------------
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.HMI
+---------------------------------------------------------------------------
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.hmo
+---------------------------------------------------------------------------
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.HMI
+---------------------------------------------------------------------------
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
+---------------------------------------------------------------------------
Cl-                       HSO4-
   lambda0 =  -0.00600   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
endit.
Ca++                      H+
   lambda0 =   0.09200   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.HMI
+---------------------------------------------------------------------------
Ca++                      Fe++
   lambda0 =   0.12437   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
***** DATA1F.HMI
+--------------------------------------------------------------------------
Ca++                      Mg++
   lambda0 =   0.00700   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
CO3--                     HCO3-
   lambda0 =  -0.04000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Ca++                      MgOH+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
CO3--                     HSO4-
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
CO3--                     Cl-
   lambda0 =  -0.02000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
HCO3-                     HSO4-
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Cl-                       HCO3-
   lambda0 =   0.03000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
HSO4-                     OH-
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Cl-                       HSO4-
   lambda0 =  -0.00600   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
Ca++                      K+
   lambda0 =   0.03200   lambda1 =   0.00000   lambda2 =   0.00000
```

```
                          alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Cl-                        OH-
   lambda0 =  -0.05000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
H+                         K+
   lambda0 =   0.00500   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Cl-                        SO4--
   lambda0 =   0.02000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
K+                         Mg++
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
***** DATA1F.HMI
+--------------------------------------------------------------------------
Fe++                       H+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
*****

***** data1f.hmo
+--------------------------------------------------------------------------
K+                         MgOH+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
CO3--                      HCO3-
   lambda0 =  -0.04000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
H+                         Mg++
   lambda0 =   0.10000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
CO3--                      HSO4-
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
Mg++                       MgOH+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
***** DATA1F.HMI
+--------------------------------------------------------------------------
HCO3-                      HSO4-
```

```
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
*****

***** data1f.hmo
+---------------------------------------------------------------------------
H+                          MgOH+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
***** DATA1F.HMI
+---------------------------------------------------------------------------
HSO4-                       OH-
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
*****

***** data1f.hmo
+---------------------------------------------------------------------------
Ca++                        Na+
   lambda0 =   0.07000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
Ca++                        K+
   lambda0 =   0.03200   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+---------------------------------------------------------------------------
H+                          Na+
   lambda0 =   0.03600   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
Fe++                        K+
   lambda0 =   0.11670   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+---------------------------------------------------------------------------
K+                          Na+
   lambda0 =  -0.01200   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
H+                          K+
   lambda0 =   0.00500   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmo
+---------------------------------------------------------------------------
Mg++                        Na+
   lambda0 =   0.07000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMI
+---------------------------------------------------------------------------
K+                          Mg++
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****
```

```
***** data1f.hmo
+--------------------------------------------------------------------------
MgOH+                          Na+
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
***** DATA1F.HMI
+--------------------------------------------------------------------------
K+                             MgOH+
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
*****

***** data1f.hmo
+--------------------------------------------------------------------------
CO3--                          OH-
   lambda0 =    0.10000    lambda1 =    0.00000    lambda2 =    0.00000
***** DATA1F.HMI
+--------------------------------------------------------------------------
H+                             Mg++
   lambda0 =    0.10000    lambda1 =    0.00000    lambda2 =    0.00000
*****

***** data1f.hmo
+--------------------------------------------------------------------------
HCO3-                          OH-
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
***** DATA1F.HMI
+--------------------------------------------------------------------------
Mg++                           MgOH+
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
*****

***** data1f.hmo
+--------------------------------------------------------------------------
CO3--                          SO4--
   lambda0 =    0.02000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =   99.0         alpha2 =   99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Fe++                           Mg++
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =   99.0         alpha2 =   99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
HCO3-                          SO4--
   lambda0 =    0.01000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =   99.0         alpha2 =   99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
H+                             MgOH+
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =   99.0         alpha2 =   99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
HSO4-                          SO4--
   lambda0 =    0.00000    lambda1 =    0.00000    lambda2 =    0.00000
                           alpha1 =   99.0         alpha2 =   99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
```

```
Ca++                          Na+
   lambda0 =    0.07000   lambda1 =    0.00000   lambda2 =    0.00000
                          alpha1 =  99.0        alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
OH-                           SO4--
   lambda0 =   -0.01300   lambda1 =    0.00000   lambda2 =    0.00000
                          alpha1 =  99.0        alpha2 =  99.0
***** DATA1F.HMI
+--------------------------------------------------------------------------
Fe++                          Na+
   lambda0 =    0.08000   lambda1 =    0.00000   lambda2 =    0.00000
                          alpha1 =  99.0        alpha2 =  99.0
*****

***** data1f.hmo
+--------------------------------------------------------------------------
endit.
***** DATA1F.HMI
+--------------------------------------------------------------------------
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+
   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
+--------------------------------------------------------------------------
MgOH+                         Na+
   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
+--------------------------------------------------------------------------
CO3--                         OH-
   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
+--------------------------------------------------------------------------
HCO3-                         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
+---------------------------------------------------------------------
CO3--                        SO4--
   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
    dl1/dt =  0.000E+00  d2l1/dt2 =  0.000E+00
    dl2/dt =  0.000E+00  d2l2/dt2 =  0.000E+00
+---------------------------------------------------------------------
HCO3-                        SO4--
   lambda0 =   0.01000   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-                        SO4--
   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
+---------------------------------------------------------------------
OH-                          SO4--
   lambda0 =  -0.01300   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
+---------------------------------------------------------------------
endit.
*****

***** data1f.hmo
+---------------------------------------------------------------------
H+                           H+                          CO3--
        mu =   0.00000  dmmx/dt =  0.000E+00  d2mmx/dt2 =  0.000E+00
***** DATA1F.HMI
+---------------------------------------------------------------------
Fe++                         Fe++                        Cl-
        mu =  -0.00203  dmmx/dt =  0.000E+00  d2mmx/dt2 =  0.000E+00
+---------------------------------------------------------------------
Fe++                         Cl-                         Cl-
        mu =  -0.00101  dmxx/dt =  0.000E+00  d2mxx/dt2 =  0.000E+00
+---------------------------------------------------------------------
Fe++                         Fe++                        HCO3-
        mu =   0.00000  dmmx/dt =  0.000E+00  d2mmx/dt2 =  0.000E+00
*****

***** data1f.hmo
+---------------------------------------------------------------------
H+                           CO3--                       CO3--
        mu =   0.00000  dmxx/dt =  0.000E+00  d2mxx/dt2 =  0.000E+00
***** DATA1F.HMI
+---------------------------------------------------------------------
Fe++                         HCO3-                       HCO3-
        mu =   0.00000  dmxx/dt =  0.000E+00  d2mxx/dt2 =  0.000E+00
*****

***** data1f.hmo
```

```
+----------------------------------------------------------------------
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
***** DATA1F.HMI
+----------------------------------------------------------------------
Fe++                        Fe++                        SO4--
        mu =   0.00000  dmmx/dt =  0.000E+00  d2mmx/dt2 =  0.000E+00
*****

***** data1f.hmo
+----------------------------------------------------------------------
H+                          HCO3-                       HCO3-
        mu =   0.00000  dmxx/dt =  0.000E+00  d2mxx/dt2 =  0.000E+00
***** DATA1F.HMI
+----------------------------------------------------------------------
Fe++                        SO4--                       SO4--
        mu =   0.00000  dmxx/dt =  0.000E+00  d2mxx/dt2 =  0.000E+00
*****

***** data1f.hmo
+----------------------------------------------------------------------
H+                          H+                          HSO4-
        mu =   0.00000  dmmx/dt =  0.000E+00  d2mmx/dt2 =  0.000E+00
***** DATA1F.HMI
+----------------------------------------------------------------------
Fe++                        Fe++                        HSO4-
        mu =   0.00000  dmmx/dt =  0.000E+00  d2mmx/dt2 =  0.000E+00
*****

***** data1f.hmo
+----------------------------------------------------------------------
H+                          HSO4-                       HSO4-
        mu =   0.00000  dmxx/dt =  0.000E+00  d2mxx/dt2 =  0.000E+00
***** DATA1F.HMI
+----------------------------------------------------------------------
Fe++                        HSO4-                       HSO4-
        mu =   0.00000  dmxx/dt =  0.000E+00  d2mxx/dt2 =  0.000E+00
*****

***** data1f.hmo
+----------------------------------------------------------------------
H+                          H+                          OH-
        mu =   0.00000  dmmx/dt =  0.000E+00  d2mmx/dt2 =  0.000E+00
***** DATA1F.HMI
+----------------------------------------------------------------------
H+                          H+                          CO3--
        mu =   0.00000  dmmx/dt =  0.000E+00  d2mmx/dt2 =  0.000E+00
*****

***** data1f.hmo
+----------------------------------------------------------------------
H+                          OH-                         OH-
        mu =   0.00000  dmxx/dt =  0.000E+00  d2mxx/dt2 =  0.000E+00
***** DATA1F.HMI
+----------------------------------------------------------------------
```

```
H+                          CO3--                       CO3--
        mu =   0.00000  dmxx/dt =  0.000E+00  d2mxx/dt2 =  0.000E+00
*****

***** data1f.hmo
+------------------------------------------------------------------------
H+                          H+                          SO4--
***** DATA1F.HMI
+------------------------------------------------------------------------
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--
*****

***** data1f.hmo
+------------------------------------------------------------------------
Ca++                        H+                          Cl-
***** DATA1F.HMI
+------------------------------------------------------------------------
Ca++                        Fe++                        Cl-
        mu =  -0.00502   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+------------------------------------------------------------------------
Ca++                        H+                          Cl-
*****

***** data1f.hmo
+------------------------------------------------------------------------
Ca++                        H+                          SO4--
***** DATA1F.HMI
+------------------------------------------------------------------------
Ca++                        Fe++                        SO4--
        mu =   0.00400   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+------------------------------------------------------------------------
Ca++                        H+                          SO4--
*****

***** data1f.hmo
+------------------------------------------------------------------------
H+                          K+                          CO3--
```

```
***** DATA1F.HMI
+-------------------------------------------------------------------------
Fe++                          H+                            Cl-
       mu =   0.00162   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
Fe++                          K+                            Cl-
       mu =  -0.00889   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
Fe++                          Mg++                          Cl-
       mu =  -0.00040   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
Fe++                          Na+                           Cl-
       mu =  -0.00263   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
Fe++                          H+                            SO4--
       mu =   0.00516   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
Fe++                          K+                            SO4--
       mu =  -0.02073   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
Fe++                          Mg++                          SO4--
       mu =   0.00208   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
Fe++                          Na+                           SO4--
       mu =  -0.00107   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
Fe++                          H+                            HSO4-
       mu =   0.00187   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
H+                            K+                            CO3--
*****

***** data1f.hmo
+-------------------------------------------------------------------------
CO3--                         Cl-                           H+
***** DATA1F.HMI
+-------------------------------------------------------------------------
Cl-                           HCO3-                         Fe++
       mu =  -0.01651   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
Cl-                           SO4--                         Fe++
       mu =  -0.00407   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
HCO3-                         SO4--                         Fe++
       mu =  -0.02683   dmu/dt =  0.000E+00   d2mu/dt2 =  0.000E+00
+-------------------------------------------------------------------------
CO3--                         Cl-                           H+
*****
```

Information Only