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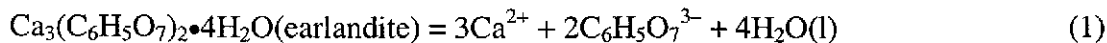
*subject:* Incorporation of Calcium Citrate Hydrate, Earlandite; Calcium Oxalate Monohydrate, Whewellite; and Aqueous Species of Citrate and Oxalate into the EQ3/6 HMP Database and Its Modified Version HMY

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<sub>2</sub> by calcite (CaCO<sub>3</sub>) 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 (HMP) that supports the Pitzer activity-coefficient option, six solid phases were incorporated (Xiong, 2004b). That database, HMP, was modified from the original EQ3/6 HMW database (Wolery, 1992). In turn, the HMP database will be modified to incorporate the following changes.

### **1 INCORPORATION OF EARLANDITE (Ca<sub>3</sub>(C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>)<sub>2</sub>•4H<sub>2</sub>O) AND WHEWELLITE (CaC<sub>2</sub>O<sub>4</sub>•H<sub>2</sub>O) into EQ3/6 HMP**

Ciavatta et al. (2001) determined the solubility of earlandite in NaClO<sub>4</sub> solutions from 0 m to 3.5 m at 25 °C. In their experiments using NaClO<sub>4</sub> as an ionic strength-supporting medium, the solubility reaction of earlandite is expressed as:

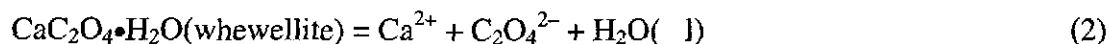


By using the specific interaction theory, they derived the equilibrium constant at infinite dilution for Reaction (1) as -17.81 in logarithmic units, and this value is adopted in the HMY database (Table 1).

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For the dissolution reaction of whewellite,



the solubility product constant at infinite dilution for Reaction 2 to be used in the HMY database is the same as that recommended by Xiong (2004a) and implemented in FMT\_050405.CHEMDAT (Xiong, 2005). That value is  $-8.75$  (Table 1).

## 2 INCORPORATION OF AQUEOUS SPECIES OF CITRATE AND OXALATE INTO THE EQ3/6 HMP DATABASE

Regarding aqueous citrate species, the following dissociation reactions are incorporated into the new database:



The dissociation constants for the above reactions are calculated from the following general equation by employing the free energy data listed in Table 2:

$$\log K = -\Delta_r G^\circ / (2.3026 \times R \times T) \quad (6)$$

in which  $R$  is the gas constant ( $1.98719 \text{ cal mol}^{-1} \text{ K}^{-1}$ ), and  $T$  is absolute temperature in K ( $T = 298.15 \text{ K}$  at  $25^\circ\text{C}$ ). The free energy change for a chemical reaction is expressed in the following general equation:

$$\Delta_r G = \sum_j \Delta_f G_{j,\text{product}} - \sum_i \Delta_f G_{i,\text{reactants}} \quad (7)$$

The equilibrium constants calculated for these reactions are tabulated in Table 1.

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



Again, the dissociation constants for Reactions (8) and (9) are calculated from the Eq. (6) by utilizing the respective free energy data in Table 2.

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

Regarding the interaction parameters in the Pitzer formalism involving aqueous citrate and oxalate species, the binary interaction parameters from the FMT\_050405.CHEMDAT (Xiong, 2005) were incorporated into the new EQ3/6 database and are listed in Table 3.

### 4 HMY DATABASE

Using the equilibrium constants listed in Table 1 and the Pitzer interaction parameters tabulated in Table 3 to modify HMP, the HMY database is formally established. This database has been successfully run by EQPT, an executable with EQ3/6 package (Wolery, 1992), and files of "output.hmy" and "data1f.hmy" (a formatted data file) have been generated. File comparisons between "output.hmy" and "output.hmp", and between "data1f.hmy" and "data1f.hmp" indicate that the only differences between HMY and HMP are those of entries of the above species and the Pitzer interaction parameters (see attached files).

### REFERENCES

- Ciavatta, L., G.D. Tommaso, and M. Iuliano. 2001. "The Solubility of Calcium Citrate Hydrate in Sodium Perchlorate Solutions," *Analytical Letters*, Vol. 34, no. 6, 1053-1062.
- 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. 2004a. "A Correction of the Molecular Weight of Oxalate in FMT\_021120.CHEMDAT, and Incorporation of Calcium Oxalate Monohydrate (Whewellite) into CHEMDAT with Its Recommended Dimensionless Standard Chemical Potential Value." Memorandum to L.H. Brush, June 8, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 535813.
- Xiong, Y.-L. 2004b. "Incorporation of Six Solid Phases Including Hydromagnesite (5424) and Hydromagnesite (4323) into EQ3/6 HMW Database and Its Modified Version HMP." Memorandum to L.H. Brush, August 4, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 536321.
- 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.

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

Reactions	log K	References
Reaction 1	-17.81	Ciavatta et al. (2001)
Reaction 2	-8.75	Xiong (2004a)
Reaction 3	-3.2468	Calculated from the $\Delta_f G^\circ$ data converted from $\mu^\circ/RT$ of FMT_050405.CHEMDAT (see Table 2)
Reaction 4	-4.8397	Calculated from the $\Delta_f G^\circ$ data converted from $\mu^\circ/RT$ of FMT_050405.CHEMDAT (see Table 2)
Reaction 5	-6.4232	Calculated from the $\Delta_f G^\circ$ data converted from $\mu^\circ/RT$ of FMT_050405.CHEMDAT (see Table 2)
Reaction 8	-1.3936	Calculated from the $\Delta_f G^\circ$ data converted from $\mu^\circ/RT$ of FMT_050405.CHEMDAT (see Table 2)
Reaction 9	-4.2595	Calculated from the $\Delta_f G^\circ$ data converted from $\mu^\circ/RT$ of FMT_050405.CHEMDAT (see Table 2)

Table 2. Dimensionless Standard Chemical Potentials and Corresponding Standard Free Energies of Formation for  $H^+$ , Citrate and Oxalate Aqueous Species at Reference State (298.15 K and 1 bar).

Species	$\mu^\circ/RT$ in FMT_050405.CHEMDAT	$\Delta_f G^\circ$ , cal mol <sup>-1</sup>
$H^+$	0	0
$H_3C_6H_5O_7(aq)$	0	0
$H_2C_6H_5O_7^-$	7.476	4429
$HC_6H_5O_7^{2-}$	18.62	11031
$C_6H_5O_7^{3-}$	33.41	19794
$H_2C_2O_4(aq)$	0	0
$HC_2O_4^-$	3.209	1901
$C_2O_4^{2-}$	13.017	7712

Table 3. Pitzer Interaction Parameters Involving Citrate and Oxalate Aqueous Species Taken from FMT\_050405.CHEMDAT (Xiong, 2005).

i	j	Binary Interaction Parameters		
		$\beta^{(0)}$ , kg mol <sup>-1</sup>	$\beta^{(1)}$ , kg mol <sup>-1</sup>	$C^\phi$ , kg <sup>2</sup> mol <sup>-2</sup>
Na <sup>+</sup>	H <sub>2</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> <sup>-</sup>	-0.1296	0.29	0.013
Na <sup>+</sup>	HC <sub>6</sub> H <sub>5</sub> O <sub>7</sub> <sup>2-</sup>	-0.0989	1.74	0.027
Na <sup>+</sup>	C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> <sup>3-</sup>	0.0887	5.22	0.047
Na <sup>+</sup>	HC <sub>2</sub> O <sub>4</sub> <sup>-</sup>	-0.2448	0.29	0.068
Na <sup>+</sup>	C <sub>2</sub> O <sub>4</sub> <sup>2-</sup>	-0.2176	1.74	0.122
K <sup>+</sup>	H <sub>2</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> <sup>-</sup>	-0.1296	0.29	0.013
K <sup>+</sup>	HC <sub>6</sub> H <sub>5</sub> O <sub>7</sub> <sup>2-</sup>	-0.0989	1.74	0.027
K <sup>+</sup>	C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> <sup>3-</sup>	0.0887	5.22	0.047
K <sup>+</sup>	HC <sub>2</sub> O <sub>4</sub> <sup>-</sup>	-0.2448	0.29	0.068
K <sup>+</sup>	C <sub>2</sub> O <sub>4</sub> <sup>2-</sup>	-0.2176	1.74	0.122

Comparing files data1f.hmp and DATA1F.HMY

\*\*\*\*\* data1f.hmp

stpitz  
9 10

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

\*\*\*\*\* DATA1F.HMY

stpitz  
11 12

data0.hmy.V8.R6  
CII: GEMBOCHS.V2-EQ8-data0.hmp.V8.R6

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

Output package: eq3  
Data set: hmp

+-----

\*\*\*\*\* DATA1F.HMY

Output package: eq3  
Data set: hmy

+-----

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

Ca 40.07800 0.00000  
Cl 35.45270 0.00000

\*\*\*\*\* DATA1F.HMY

Ca 40.07800 0.00000  
Citrate 189.10000 0.00000  
Cl 35.45270 0.00000

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

Na 22.98977 0.00000  
S 32.06600 0.00000

\*\*\*\*\* DATA1F.HMY

Na 22.98977 0.00000  
Oxalate 88.01960 0.00000  
S 32.06600 0.00000

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

1.0000 Ca 1 0  
Cl-

\*\*\*\*\* DATA1F.HMY

1.0000 Ca 1 0  
Citrate---

189.100 -3. 1 0  
1.0000 Citrate

Cl- 1 0  
\*\*\*\*\*

\*\*\*\*\* data1f.hmp

1.0000 Na 2 0  
SO4--

\*\*\*\*\* DATA1F.HMY

1.0000 Na 1 0  
Oxalate--

88.020 -2. 2 0  
1.0000 Oxalate

SO4-- 2 0  
\*\*\*\*\*

\*\*\*\*\* data1f.hmp

9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00  
HSO4- 3 3

\*\*\*\*\* DATA1F.HMY

9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00  
H3Citrate(aq) 2 3

192.124 0. 3.0000 H  
1.0000 Citrate  
-1.0000 H3Citrate(aq) 1.0000 Citrate---

3.0000 H+ -1.450970000E+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

H2Citrate- 2 3  
191.116 -1. 2.0000 H  
1.0000 Citrate  
-1.0000 H2Citrate- 1.0000 Citrate---

hmp\_hmy\_1f.txt

```

2.0000 H+
-1.126290000E+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
HCitrate-- 2 3
190.108 -2.
1.0000 Citrate 1.0000 H
-1.0000 HCitrate-- 1.0000 Citrate---
1.0000 H+
-6.423200000E+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
H2Oxalate(aq) 2 3
90.035 0.
1.0000 Oxalate 2.0000 H
-1.0000 H2Oxalate(aq) 1.0000 Oxalate--
2.0000 H+
-5.653200000E+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
HOxalate- 2 3
89.028 -1.
1.0000 Oxalate 1.0000 H
-1.0000 HOxalate- 1.0000 Oxalate--
1.0000 H+
-4.259500000E+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
HSO4- 3 3
*****

```

```

***** data1f.hmp
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
Epsomite 4 4
***** DATA1F.HMY
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
Earlandite 4 4
570.495 0. 0.000
2.0000 Citrate 8.0000 H
4.0000 O 3.0000 Ca
-1.0000 Earlandite 3.0000 Ca++
2.0000 Citrate--- 4.0000 H2O
-1.781000000E+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
Epsomite 4 4
*****

```

```

***** data1f.hmp
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
endit.
***** DATA1F.HMY
9.999999000E+06 0.000000000E+00 0.000000000E+00 0.000000000E+00 0.000000000E+00
Whewellite 4 4
146.113 0. 0.000
1.0000 Oxalate 2.0000 H
1.0000 O 1.0000 Ca
-1.0000 whewellite 1.0000 Ca++
1.0000 Oxalate-- 1.0000 H2O
-8.751700000E+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
endit.
*****

```

```

***** data1f.hmp
+-----
K+
lambda0 = 0.02960 HCO3-
lambda1 = -0.01300 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
***** DATA1F.HMY

```

```

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

```

```

***** data1f.hmp
+-----
K+
lambda0 = -0.00030 HSO4-
lambda1 = 0.17350 lambda2 = 0.00000
alpha1 = 2.0 alpha2 = 12.0
***** DATA1F.HMY

```

```

+-----
K+
HCitrate--

```



lambda0 = -0.09890    lambda1 = 1.74000    hmp\_hmy\_1f.txt  
                          alpha1 = 2.0            lambda2 = 0.00000  
  alpha2 = 12.0

\*\*\*\*\* data1f.hmp

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

\*\*\*\*\* DATA1F.HMY

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

\*\*\*\*\* data1f.hmp

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

\*\*\*\*\* DATA1F.HMY

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

\*\*\*\*\* data1f.hmp

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

\*\*\*\*\* DATA1F.HMY

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

\*\*\*\*\* data1f.hmp

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

\*\*\*\*\* DATA1F.HMY

+-----  
K+            OH-  
lambda0 = 0.12980    lambda1 = 0.32000    lambda2 = 0.00000  
                          alpha1 = 2.0            alpha2 = 12.0  
d10/dt = 0.000E+00    d210/dt2 = 0.000E+00

\*\*\*\*\* data1f.hmp

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

\*\*\*\*\* DATA1F.HMY

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

\*\*\*\*\* data1f.hmp

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

\*\*\*\*\* DATA1F.HMY

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

\*\*\*\*\* data1f.hmp

```

+-----+-----+-----+
Mg++      HSO4-
lambda0 = 0.47460  lambda1 = 1.72900  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
**** DATA1F.HMY
+-----+-----+-----+
CO2(aq)   Mg++
lambda0 = 0.18300  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
****
**** data1f.hmp
+-----+-----+-----+
Mg++      OH-
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
d10/dt = 0.000E+00  alpha1 = 2.0      alpha2 = 12.0
d210/dt2 = 0.000E+00
**** DATA1F.HMY
+-----+-----+-----+
Mg++      CO3--
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
d10/dt = 0.000E+00  alpha1 = 1.4      alpha2 = 12.0
d210/dt2 = 0.000E+00
****
**** data1f.hmp
+-----+-----+-----+
Mg++      SO4--
lambda0 = 0.22100  lambda1 = 3.34300  lambda2 = -37.23000
d10/dt = 0.000E+00  alpha1 = 1.4      alpha2 = 12.0
d210/dt2 = 0.000E+00
**** DATA1F.HMY
+-----+-----+-----+
Mg++      Cl-
lambda0 = 0.35235  lambda1 = 1.68150  lambda2 = 0.00000
d10/dt = 0.000E+00  alpha1 = 2.0      alpha2 = 12.0
d210/dt2 = 0.000E+00
****
**** data1f.hmp
+-----+-----+-----+
CO2(aq)   MgOH+
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
**** DATA1F.HMY
+-----+-----+-----+
Mg++      HCO3-
lambda0 = 0.32900  lambda1 = 0.60720  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
****
**** data1f.hmp
+-----+-----+-----+
MgOH+     CO3--
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
**** DATA1F.HMY
+-----+-----+-----+
Mg++      HSO4-
lambda0 = 0.47460  lambda1 = 1.72900  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
****
**** data1f.hmp
+-----+-----+-----+
MgOH+     Cl-
lambda0 = -0.10000  lambda1 = 1.65800  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
**** DATA1F.HMY
+-----+-----+-----+
Mg++      OH-
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
****
**** data1f.hmp
+-----+-----+-----+
MgOH+     HCO3-
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000

```

```

                                hmp_hmy_1f.txt
                                alpha2 = 12.0
                                alpha1 = 2.0
d10/dt = 0.000E+00      d210/dt2 = 0.000E+00
***** DATA1F.HMY
+-----+
Mg++
lambda0 = 0.22100      SO4--
lambda1 = 3.34300      lambda2 = -37.23000
alpha1 = 1.4           alpha2 = 12.0
d10/dt = 0.000E+00      d210/dt2 = 0.000E+00
*****

***** data1f.hmp
+-----+
MgOH+
lambda0 = 0.00000      HSO4-
lambda1 = 0.00000      lambda2 = 0.00000
***** DATA1F.HMY
+-----+
CO2(aq)
lambda0 = 0.00000      MgOH+
lambda1 = 0.00000      lambda2 = 0.00000
*****

***** data1f.hmp
+-----+
MgOH+
lambda0 = 0.00000      OH-
lambda1 = 0.00000      lambda2 = 0.00000
***** DATA1F.HMY
+-----+
MgOH+
lambda0 = 0.00000      CO3--
lambda1 = 0.00000      lambda2 = 0.00000
*****

***** data1f.hmp
+-----+
MgOH+
lambda0 = 0.00000      SO4--
lambda1 = 0.00000      lambda2 = 0.00000
alpha1 = 2.0           alpha2 = 12.0
***** DATA1F.HMY
+-----+
MgOH+
lambda0 = -0.10000     Cl-
lambda1 = 1.65800      lambda2 = 0.00000
alpha1 = 2.0           alpha2 = 12.0
*****

***** data1f.hmp
+-----+
CO2(aq)
lambda0 = 0.10000      Na+
lambda1 = 0.00000      lambda2 = 0.00000
alpha1 = 2.0           alpha2 = 12.0
***** DATA1F.HMY
+-----+
MgOH+
lambda0 = 0.00000      HCO3-
lambda1 = 0.00000      lambda2 = 0.00000
alpha1 = 2.0           alpha2 = 12.0
*****

***** data1f.hmp
+-----+
Na+
lambda0 = 0.03990      CO3--
lambda1 = 1.38900      lambda2 = 0.00000
alpha1 = 2.0           alpha2 = 12.0
***** DATA1F.HMY
+-----+
MgOH+
lambda0 = 0.00000      HSO4-
lambda1 = 0.00000      lambda2 = 0.00000
alpha1 = 2.0           alpha2 = 12.0
*****

***** data1f.hmp
+-----+
Na+
lambda0 = 0.07650      Cl-
lambda1 = 0.26640      lambda2 = 0.00000
alpha1 = 2.0           alpha2 = 12.0
***** DATA1F.HMY
+-----+
MgOH+
lambda0 = 0.00000      OH-
lambda1 = 0.00000      lambda2 = 0.00000
alpha1 = 2.0           alpha2 = 12.0
*****

***** data1f.hmp

```

```

+-----+-----+-----+
Na+      HCO3-
lambda0 = 0.02770  lambda1 = 0.04110  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMY
+-----+-----+-----+
MgOH+    SO4--
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
*****
***** data1f.hmp
+-----+-----+-----+
Na+      HSO4-
lambda0 = 0.04540  lambda1 = 0.39800  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMY
+-----+-----+-----+
Na+      Citrate---
lambda0 = 0.08870  lambda1 = 5.22000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
*****
***** data1f.hmp
+-----+-----+-----+
Na+      OH-
lambda0 = 0.08640  lambda1 = 0.25300  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMY
+-----+-----+-----+
CO2(aq)  Na+
lambda0 = 0.10000  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
*****
***** data1f.hmp
+-----+-----+-----+
Na+      SO4--
lambda0 = 0.01958  lambda1 = 1.11300  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
***** DATA1F.HMY
+-----+-----+-----+
Na+      CO3--
lambda0 = 0.03990  lambda1 = 1.38900  lambda2 = 0.00000
alpha1 = 2.0      alpha2 = 12.0
*****
***** data1f.hmp
+-----+-----+-----+
CO2(aq)  SO4--
lambda0 = 0.09700  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 0.0      alpha2 = 0.0
d10/dt = 0.000E+00  d210/dt2 = 0.000E+00
***** DATA1F.HMY
+-----+-----+-----+
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.hmp
+-----+-----+-----+
endit.
Ca++     H+
lambda0 = 0.09200  lambda1 = 0.00000  lambda2 = 0.00000
alpha1 = 99.0     alpha2 = 99.0
d10/dt = 0.000E+00  d210/dt2 = 0.000E+00
***** DATA1F.HMY
+-----+-----+-----+
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.hmp
+-----+-----+-----+
Ca++     Mg++

```

```

lambda0 = 0.00700 lambda1 = 0.00000 hmp_hmy_1f.txt
                    lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 99.0 alpha2 = 99.0
d210/dt2 = 0.000E+00
**** DATA1F.HMY

```

```

+-----+
Na+      Hcitrate--
lambda0 = -0.09890 lambda1 = 1.74000 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 2.0 alpha2 = 12.0
d210/dt2 = 0.000E+00
****

```

\*\*\*\* data1f.hmp

```

+-----+
Ca++     MgOH+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 99.0 alpha2 = 99.0
d210/dt2 = 0.000E+00
**** DATA1F.HMY

```

```

+-----+
Na+      HCO3-
lambda0 = 0.02770 lambda1 = 0.04110 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 2.0 alpha2 = 12.0
d210/dt2 = 0.000E+00
****

```

\*\*\*\* data1f.hmp

```

+-----+
CO3--    Cl-
lambda0 = -0.02000 lambda1 = 0.00000 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 99.0 alpha2 = 99.0
d210/dt2 = 0.000E+00
**** DATA1F.HMY

```

```

+-----+
Na+      HOxalate-
lambda0 = -0.24480 lambda1 = 0.29000 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 2.0 alpha2 = 12.0
d210/dt2 = 0.000E+00
****

```

\*\*\*\* data1f.hmp

```

+-----+
Cl-      HCO3-
lambda0 = 0.03000 lambda1 = 0.00000 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 99.0 alpha2 = 99.0
d210/dt2 = 0.000E+00
**** DATA1F.HMY

```

```

+-----+
Na+      HSO4-
lambda0 = 0.04540 lambda1 = 0.39800 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 2.0 alpha2 = 12.0
d210/dt2 = 0.000E+00
****

```

\*\*\*\* data1f.hmp

```

+-----+
Cl-      HSO4-
lambda0 = -0.00600 lambda1 = 0.00000 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 99.0 alpha2 = 99.0
d210/dt2 = 0.000E+00
**** DATA1F.HMY

```

```

+-----+
Na+      OH-
lambda0 = 0.08640 lambda1 = 0.25300 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 2.0 alpha2 = 12.0
d210/dt2 = 0.000E+00
****

```

\*\*\*\* data1f.hmp

```

+-----+
Cl-      OH-
lambda0 = -0.05000 lambda1 = 0.00000 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 99.0 alpha2 = 99.0
d210/dt2 = 0.000E+00
**** DATA1F.HMY

```

```

+-----+
Na+      Oxalate--
lambda0 = -0.21760 lambda1 = 1.74000 lambda2 = 0.00000
d10/dt = 0.000E+00 alpha1 = 2.0 alpha2 = 12.0
d210/dt2 = 0.000E+00

```

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

```

+-----+
Cl-      SO4--
lambda0 = 0.02000   lambda1 = 0.00000   lambda2 = 0.00000
alpha1 = 99.0      alpha2 = 99.0
dI0/dt = 0.000E+00 d2I0/dt2 = 0.000E+00
***** DATA1F.HMY

```

```

+-----+
Na+      SO4--
lambda0 = 0.01958   lambda1 = 1.11300   lambda2 = 0.00000
alpha1 = 2.0       alpha2 = 12.0
dI0/dt = 0.000E+00 d2I0/dt2 = 0.000E+00
*****

```

\*\*\*\*\* data1f.hmp

```

+-----+
CO3--    HCO3-
lambda0 = -0.04000   lambda1 = 0.00000   lambda2 = 0.00000
alpha1 = 99.0      alpha2 = 99.0
dI0/dt = 0.000E+00 d2I0/dt2 = 0.000E+00
***** DATA1F.HMY

```

```

+-----+
CO2(aq)  SO4--
lambda0 = 0.09700   lambda1 = 0.00000   lambda2 = 0.00000
alpha1 = 0.0       alpha2 = 0.0
dI0/dt = 0.000E+00 d2I0/dt2 = 0.000E+00
*****

```

\*\*\*\*\* data1f.hmp

```

+-----+
CO3--    HSO4-
lambda0 = 0.00000   lambda1 = 0.00000   lambda2 = 0.00000
alpha1 = 99.0      alpha2 = 99.0
***** DATA1F.HMY

```

endit.

```

+-----+
Ca++     H+
lambda0 = 0.09200   lambda1 = 0.00000   lambda2 = 0.00000
alpha1 = 99.0      alpha2 = 99.0
*****

```

\*\*\*\*\* data1f.hmp

```

+-----+
HCO3-    HSO4-
lambda0 = 0.00000   lambda1 = 0.00000   lambda2 = 0.00000
alpha1 = 99.0      alpha2 = 99.0
***** DATA1F.HMY

```

```

+-----+
Ca++     Mg++
lambda0 = 0.00700   lambda1 = 0.00000   lambda2 = 0.00000
alpha1 = 99.0      alpha2 = 99.0
*****

```

\*\*\*\*\* data1f.hmp

```

+-----+
HSO4-    OH-
lambda0 = 0.00000   lambda1 = 0.00000   lambda2 = 0.00000
***** DATA1F.HMY

```

```

+-----+
Ca++     MgOH+
lambda0 = 0.00000   lambda1 = 0.00000   lambda2 = 0.00000
*****

```

\*\*\*\*\* data1f.hmp

```

+-----+
Ca++     K+
lambda0 = 0.03200   lambda1 = 0.00000   lambda2 = 0.00000
alpha1 = 99.0      alpha2 = 99.0
***** DATA1F.HMY

```

```

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

```

\*\*\*\*\* data1f.hmp

H+      lambda0 = 0.00500      K+      lambda1 = 0.00000      lambda2 = 0.00000  
       alpha1 = 99.0           alpha2 = 99.0

\*\*\*\*\* DATA1F.HMY

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

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

+-----  
 K+      lambda0 = 0.00000      Mg++      lambda1 = 0.00000      lambda2 = 0.00000  
       alpha1 = 99.0           alpha2 = 99.0

\*\*\*\*\* DATA1F.HMY

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

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

+-----  
 K+      lambda0 = 0.00000      MgOH+      lambda1 = 0.00000      lambda2 = 0.00000  
       alpha1 = 99.0           alpha2 = 99.0

\*\*\*\*\* DATA1F.HMY

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

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

+-----  
 H+      lambda0 = 0.10000      Mg++      lambda1 = 0.00000      lambda2 = 0.00000  
       alpha1 = 99.0           alpha2 = 99.0

\*\*\*\*\* DATA1F.HMY

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

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

+-----  
 Mg++      lambda0 = 0.00000      MgOH+      lambda1 = 0.00000      lambda2 = 0.00000  
       alpha1 = 99.0           alpha2 = 99.0

\*\*\*\*\* DATA1F.HMY

+-----  
 CO3--      lambda0 = -0.04000      HCO3-      lambda1 = 0.00000      lambda2 = 0.00000  
       alpha1 = 99.0           alpha2 = 99.0

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

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

\*\*\*\*\* DATA1F.HMY

+-----  
 CO3--      lambda0 = 0.00000      HSO4-      lambda1 = 0.00000      lambda2 = 0.00000

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

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

\*\*\*\*\* DATA1F.HMY

+-----  
 HCO3-      lambda0 = 0.00000      HSO4-      lambda1 = 0.00000      lambda2 = 0.00000  
       alpha1 = 99.0           alpha2 = 99.0

\*\*\*\*\*

```

***** data1f.hmp
+-----+
H+      lambda0 = 0.03600   Na+      lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
***** DATA1F.HMY
+-----+
HSO4-   lambda0 = 0.00000   OH-      lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
*****

***** data1f.hmp
+-----+
K+      lambda0 = -0.01200  Na+      lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
***** DATA1F.HMY
+-----+
Ca++    lambda0 = 0.03200   K+       lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
*****

***** data1f.hmp
+-----+
Mg++    lambda0 = 0.07000   Na+      lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
***** DATA1F.HMY
+-----+
H+      lambda0 = 0.00500   K+       lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
*****

***** data1f.hmp
+-----+
MgOH+   lambda0 = 0.00000   Na+      lambda1 = 0.00000   lambda2 = 0.00000
***** DATA1F.HMY
+-----+
K+      lambda0 = 0.00000   Mg++     lambda1 = 0.00000   lambda2 = 0.00000
*****

***** data1f.hmp
+-----+
CO3--   lambda0 = 0.10000   OH-      lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
***** DATA1F.HMY
+-----+
K+      lambda0 = 0.00000   MgOH+    lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
*****

***** data1f.hmp
+-----+
HCO3-   lambda0 = 0.00000   OH-      lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
***** DATA1F.HMY
+-----+
H+      lambda0 = 0.10000   Mg++     lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
*****

***** data1f.hmp
+-----+
CO3--   lambda0 = 0.02000   SO4--    lambda1 = 0.00000   lambda2 = 0.00000
      alpha1 = 99.0       alpha2 = 99.0
***** DATA1F.HMY
+-----+
Mg++    MgOH+

```



```

lambda0 = 0.00000 lambda1 = 0.00000 hmp_hmy_1f.txt
lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0

```

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

```

-----
HCO3-          SO4--
lambda0 = 0.01000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0

```

\*\*\*\*\* DATA1F.HMY

```

-----
H+          MgOH+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0

```

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

```

-----
HSO4-          SO4--
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0

```

\*\*\*\*\* DATA1F.HMY

```

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

```

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

```

-----
OH-          SO4--
lambda0 = -0.01300 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0

```

\*\*\*\*\* DATA1F.HMY

```

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

```

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

```

-----
endit.

```

\*\*\*\*\* DATA1F.HMY

```

-----
K+          Na+
lambda0 = -0.01200 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00

```

-----

```

Mg++          Na+
lambda0 = 0.07000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00

```

-----

```

MgOH+          Na+
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00

```

-----

```

CO3--          OH-
lambda0 = 0.10000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00

```

-----

```

HCO3-          OH-
lambda0 = 0.00000 lambda1 = 0.00000 lambda2 = 0.00000
alpha1 = 99.0 alpha2 = 99.0
d10/dt = 0.000E+00 d210/dt2 = 0.000E+00
d11/dt = 0.000E+00 d211/dt2 = 0.000E+00
d12/dt = 0.000E+00 d212/dt2 = 0.000E+00

```

```

+-----+
CO3--          SO4--
lambda0 = 0.02000  lambda1 = 0.00000  lambda2 = 0.00000
d10/dt = 0.000E+00  d210/dt2 = 0.000E+00
d11/dt = 0.000E+00  d211/dt2 = 0.000E+00
d12/dt = 0.000E+00  d212/dt2 = 0.000E+00
alpha1 = 99.0      alpha2 = 99.0
+-----+
HCO3-          SO4--
lambda0 = 0.01000  lambda1 = 0.00000  lambda2 = 0.00000
d10/dt = 0.000E+00  d210/dt2 = 0.000E+00
d11/dt = 0.000E+00  d211/dt2 = 0.000E+00
d12/dt = 0.000E+00  d212/dt2 = 0.000E+00
alpha1 = 99.0      alpha2 = 99.0
+-----+
HSO4-          SO4--
lambda0 = 0.00000  lambda1 = 0.00000  lambda2 = 0.00000
d10/dt = 0.000E+00  d210/dt2 = 0.000E+00
d11/dt = 0.000E+00  d211/dt2 = 0.000E+00
d12/dt = 0.000E+00  d212/dt2 = 0.000E+00
alpha1 = 99.0      alpha2 = 99.0
+-----+
OH-            SO4--
lambda0 = -0.01300  lambda1 = 0.00000  lambda2 = 0.00000
d10/dt = 0.000E+00  d210/dt2 = 0.000E+00
d11/dt = 0.000E+00  d211/dt2 = 0.000E+00
d12/dt = 0.000E+00  d212/dt2 = 0.000E+00
alpha1 = 99.0      alpha2 = 99.0
+-----+

```

endit.

\*\*\*\*\*

\*\*\*\*\* data1f.hmp

```

+-----+
K+            K+            HCO3-
***** DATA1F.HMY
+-----+
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-
*****

```

\*\*\*\*\* data1f.hmp

```

+-----+
K+            K+            HSO4-
***** DATA1F.HMY
+-----+
K+            K+            HOxalate-
mu = 0.01133  dmmx/dt = 0.000E+00  d2mmx/dt2 = 0.000E+00
+-----+
K+            HOxalate-      HOxalate-
mu = 0.01133  dmxx/dt = 0.000E+00  d2mxx/dt2 = 0.000E+00
+-----+
K+            K+            HSO4-
*****

```

\*\*\*\*\* data1f.hmp

```

+-----+
K+            K+            SO4--
***** DATA1F.HMY
+-----+
K+            K+            Oxalate--
mu = 0.01438  dmmx/dt = 0.000E+00  d2mmx/dt2 = 0.000E+00
+-----+
K+            Oxalate--      Oxalate--
mu = 0.02876  dmxx/dt = 0.000E+00  d2mxx/dt2 = 0.000E+00
+-----+
K+            K+            SO4--
*****

```

```

***** data1f.hmp
+-----+
Na+          Na+          CO3--
***** DATA1F.HMY
+-----+
Na+          Na+          Citrate--
mu = 0.00452 dmmx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          Citrate--   Citrate--
mu = 0.01357 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          Na+          CO3--
*****

```

```

***** data1f.hmp
+-----+
Na+          Na+          HCO3-
***** DATA1F.HMY
+-----+
Na+          Na+          H2Citrate-
mu = 0.00217 dmmx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          H2Citrate-   H2Citrate-
mu = 0.00217 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          Na+          HCitrate--
mu = 0.00318 dmmx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          HCitrate--   HCitrate--
mu = 0.00636 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          Na+          HCO3-
*****

```

```

***** data1f.hmp
+-----+
Na+          Na+          HSO4-
***** DATA1F.HMY
+-----+
Na+          Na+          HOxalate-
mu = 0.01133 dmmx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          HOxalate-   HOxalate-
mu = 0.01133 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          Na+          HSO4-
*****

```

```

***** data1f.hmp
+-----+
Na+          Na+          SO4--
***** DATA1F.HMY
+-----+
Na+          Na+          Oxalate--
mu = 0.01438 dmmx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          Oxalate--   Oxalate--
mu = 0.02876 dmxx/dt = 0.000E+00 d2mxx/dt2 = 0.000E+00
+-----+
Na+          Na+          SO4--
*****

```

Comparing files output.hmp and OUTPUT.HMY

\*\*\*\*\* output.hmp

Run 11:13:32 20Jul2004

\*\*\*\*\* OUTPUT.HMY

Run 09:53:06 18Oct2006

\*\*\*\*\*

\*\*\*\*\* output.hmp

no. of elements on the data file = 9  
 the dimensioned limit = 110  
 no. of aqueous species in the master set = 10  
 the dimensioned limit = 500

\*\*\*\*\* OUTPUT.HMY

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.hmp

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

\*\*\*\*\* OUTPUT.HMY

data0.hmy.V8.R6  
 CII: GEMBOCHS.V2-EQ8-data0.hmp.V8.R6

\*\*\*\*\*

\*\*\*\*\* output.hmp

Output package: eq3  
 Data set: hmp

\*\*\*\*\* OUTPUT.HMY

Output package: eq3  
 Data set: hmy

\*\*\*\*\*

\*\*\*\*\* output.hmp

element = Ca , atwt = 40.07800  
 element = Cl , atwt = 35.45270

\*\*\*\*\* OUTPUT.HMY

element = Ca , atwt = 40.07800  
 element = Citrate , atwt = 189.10000  
 element = Cl , atwt = 35.45270

\*\*\*\*\*

\*\*\*\*\* output.hmp

element = Na , atwt = 22.98977  
 element = S , atwt = 32.06600

\*\*\*\*\* OUTPUT.HMY

element = Na , atwt = 22.98977  
 element = Oxalate , atwt = 88.01960  
 element = S , atwt = 32.06600

\*\*\*\*\*

\*\*\*\*\* output.hmp

2 Ca++  
 3 Cl-  
 4 H+  
 5 HCO3-  
 6 K+  
 7 Mg++  
 8 Na+  
 9 SO4--  
 10 O2(g)  
 11 CO2(aq)  
 12 CO3--  
 13 CaCO3(aq)  
 14 HSO4-  
 15 MgCO3(aq)  
 16 MgOH+

17 OH-

```

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

```

```

***** OUTPUT.HMY
17 Dolomite
18 Earlandite
19 Epsomite
20 Gaylussite
21 Glauberite
22 Gypsum

```

23 Halite  
24 Hexahydrite  
25 Hydromagne5424  
26 Hydromagne4323  
27 K2CO3:1.5H2O  
28 K3H(SO4)2  
29 K8H4(CO3)6:3H2O  
30 KNaCO3:6H2O  
31 Kainite  
32 Kalicinite  
33 Kieserite  
34 Leonite  
35 Lime  
36 Magnesite  
37 Mercurite  
38 Mirabilite  
39 Misenerite  
40 Na2CO3:7H2O  
41 Na3H(SO4)2  
42 Na4Ca(SO4)3:2H2O  
43 Nahcolite  
44 Natron  
45 Nesquehonite  
46 Oxychloride-Mg  
47 Periclase  
48 Picromerite  
49 Pirssonite  
50 Polyhalite  
51 Portlandite  
52 Sylvite  
53 Syngenite  
54 Tachyhydrite  
55 Thenardite  
56 Thermonatrite  
57 Trona  
58 Trona-K  
59 whewellite

\*\*\*\*\*

\*\*\*\*\* output.hmp

\* warning - (eqpt/tpn2) Did not find a data block on the DATA0 file for any of the following nn pairs:

CO2(aq), CO2(aq)  
CaCO3(aq), CaCO3(aq)  
MgCO3(aq), MgCO3(aq)

\*\*\*\*\* OUTPUT.HMY

\* warning - (eqpt/tpnca) Did not find a data block on the DATA0 file for any of the following ca pairs:

Ca++, Citrate---  
Ca++, Oxalate--  
Ca++, H2Citrate-  
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.hmp

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

CO2(aq), CaCO3(aq)  
CO2(aq), MgCO3(aq)  
CaCO3(aq), MgCO3(aq)

\*\*\*\*\* OUTPUT.HMY

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

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

plus 20 others

\*\*\*\*\*

\*\*\*\*\* output.hmp

\* warning - (eqpt/tprrnc) Did not find a data block on the DATA0 file for any of the following nc pairs:

CaCO3(aq), Ca++  
CaCO3(aq), K+  
CaCO3(aq), Mg++  
CaCO3(aq), Na+  
CaCO3(aq), MgOH+  
MgCO3(aq), Ca++  
MgCO3(aq), K+  
MgCO3(aq), Mg++  
MgCO3(aq), Na+  
MgCO3(aq), MgOH+

\*\*\*\*\* OUTPUT.HMY

\* warning - (eqpt/tprrn2) Did not find a data block on the DATA0 file for any of the following nn pairs:

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

\*\*\*\*\*

\*\*\*\*\* output.hmp

\* warning - (eqpt/tprrna) Did not find a data block on the DATA0 file for any of the following na pairs:

CO2(aq), HCO3-  
CO2(aq), CO3--  
CO2(aq), OH-  
CaCO3(aq), Cl-  
CaCO3(aq), HCO3-  
CaCO3(aq), SO4--

hmp\_hmy\_out.txt

CaCO3(aq), CO3--  
CaCO3(aq), HS04-  
CaCO3(aq), OH-  
MgCO3(aq), Cl-  
MgCO3(aq), HCO3-  
MgCO3(aq), SO4--  
MgCO3(aq), CO3--  
MgCO3(aq), HS04-  
MgCO3(aq), OH-

\*\*\*\*\* OUTPUT.HMY

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

CO2(aq), CaCO3(aq)  
CO2(aq), H3Citr(aq)  
CO2(aq), H2Oxalate(aq)  
CO2(aq), MgCO3(aq)  
CaCO3(aq), H3Citr(aq)  
CaCO3(aq), H2Oxalate(aq)  
CaCO3(aq), MgCO3(aq)  
H2Oxalate(aq), H3Citr(aq)  
H3Citr(aq), MgCO3(aq)  
H2Oxalate(aq), MgCO3(aq)

\*\*\*\*\*

\*\*\*\*\* output.hmp

\* warning - (eqpt/tpn2n) Did not find a data block on the DATA0 file for any of the following nnn' triplets:

CO2(aq), CO2(aq), CaCO3(aq)  
CaCO3(aq), CaCO3(aq), CO2(aq)  
CO2(aq), CO2(aq), MgCO3(aq)  
MgCO3(aq), MgCO3(aq), CO2(aq)  
CaCO3(aq), CaCO3(aq), MgCO3(aq)  
MgCO3(aq), MgCO3(aq), CaCO3(aq)

\*\*\*\*\* OUTPUT.HMY

\* warning - (eqpt/tpnnc) Did not find a data block on the DATA0 file for any of the following nc pairs:

CaCO3(aq), Ca++  
CaCO3(aq), K+  
CaCO3(aq), Mg++  
CaCO3(aq), Na+  
CaCO3(aq), MgOH+  
H3Citr(aq), Ca++  
H3Citr(aq), H+  
H3Citr(aq), K+  
H3Citr(aq), Mg++  
H3Citr(aq), Na+  
H3Citr(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.hmp

\* warning - (eqpt/tpnca) Did not find a data block on the DATA0 file for any of the following nca triplets:

CO2(aq), Ca++, Cl-  
CO2(aq), Ca++, HCO3-  
CO2(aq), Ca++, SO4--  
CO2(aq), Ca++, CO3--



hmp\_hmy\_out.txt

CO2(aq), Ca++, HSO4-  
CO2(aq), Ca++, OH-  
CO2(aq), H+, Cl-  
CO2(aq), H+, HCO3-  
CO2(aq), H+, SO4--  
CO2(aq), H+, CO3--  
CO2(aq), H+, HSO4-  
CO2(aq), H+, OH-  
CO2(aq), K+, Cl-  
CO2(aq), K+, HCO3-  
CO2(aq), K+, SO4--  
CO2(aq), K+, CO3--  
CO2(aq), K+, HSO4-  
CO2(aq), K+, OH-  
CO2(aq), Mg++, Cl-  
CO2(aq), Mg++, HCO3-

plus 88 others

\*\*\*\*\* OUTPUT.HMY

\* warning - (eqpt/tprna) Did not find a data block on the DATA0 file  
for any of the following na pairs:

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

plus 32 others

\*\*\*\*\*

\*\*\*\*\* output.hmp

Cation-anion (ca) pair coverage:

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

\*\*\*\*\* OUTPUT.HMY

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

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

hmp\_hmy\_out.txt

Ca++, Na+, Oxalate--  
Ca++, Na+, H2Citrate-  
Ca++, Na+, HCitrate--  
Ca++, Na+, HOxalate-

plus 55 others

\*\*\*\*\*

\*\*\*\*\* output.hmp

Cation-distinct cation (cc') pair coverage:

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.HMY

\* warning - (eqpt/tpaac) Did not find a data block on the DATA0 file  
for any of the following aa'c triplets:

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.hmp

Anion-distinct anion (aa') pair coverage:

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.HMY

\* warning - (eqpt/tpn2n) Did not find a data block on the DATA0 file  
for any of the following nnn' triplets:

CO2(aq), CO2(aq), CaCO3(aq)  
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.hmp

Repeated-neutral (nn) pair coverage:

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

Page 7

Information Only

Coverage is 0.00 per cent

\*\*\*\*\* OUTPUT.HMY

\* warning - (eqpt/tpnrca) did not find a data block on the DATA0 file for any of the following nca triplets:

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.hmp

Neutral-distinct neutral (nn') pair coverage:

0 pairs have Pitzer parameters specified on the DATA0 file  
3 pairs can be constructed from the species present on this file  
Coverage is 0.00 per cent

\*\*\*\*\* OUTPUT.HMY

Cation-anion (ca) pair coverage:

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.hmp

Neutral-cation (nc) pair coverage:

8 pairs have Pitzer parameters specified on the DATA0 file  
18 pairs can be constructed from the species present on this file  
Coverage is 44.44 per cent

\*\*\*\*\* OUTPUT.HMY

Cation-distinct cation (cc') pair coverage:

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.hmp

Neutral-anion (na) pair coverage:

3 pairs have Pitzer parameters specified on the DATA0 file  
18 pairs can be constructed from the species present on this file  
Coverage is 16.67 per cent

\*\*\*\*\* OUTPUT.HMY

hmp\_hmy\_out.txt  
Anion-distinct anion (aa') pair coverage:  
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.hmp  
Cation-distinct cation-anion (cc'a) triplet coverage:  
90 triplets have Pitzer parameters specified on the DATA0 file  
90 triplets can be constructed from the species present on this file  
Coverage is 100.00 per cent  
\*\*\*\*\* OUTPUT.HMY  
Repeated-neutral (nn) pair coverage:  
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.hmp  
Anion-distinct anion-cation (aa'c) triplet coverage:  
90 triplets have Pitzer parameters specified on the DATA0 file  
90 triplets can be constructed from the species present on this file  
Coverage is 100.00 per cent  
\*\*\*\*\* OUTPUT.HMY  
Neutral-distinct neutral (nn') pair coverage:  
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.hmp  
Repeated neutral-distinct neutral (nnn') triplet coverage:  
0 triplets have Pitzer parameters specified on the DATA0 file  
6 triplets can be constructed from the species present on this file  
Coverage is 0.00 per cent  
\*\*\*\*\* OUTPUT.HMY  
Neutral-cation (nc) pair coverage:  
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.hmp  
Neutral-cation-anion (nca) triplet coverage:  
0 triplets have Pitzer parameters specified on the DATA0 file  
108 triplets can be constructed from the species present on this file  
Coverage is 0.00 per cent  
\*\*\*\*\* OUTPUT.HMY  
Neutral-anion (na) pair coverage:  
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  
\*\*\*\*\*

hmp\_hmy\_out.txt

\*\*\*\*\* output.hmp

Completed processing the pitzer data file data0.hmp.v8.R6.

\*\*\*\*\* OUTPUT.HMY

Cation-distinct cation-anion (cc'a) triplet coverage:

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.hmp

No errors were encountered.

6 warning(s) were encountered.

\*\*\*\*\* OUTPUT.HMY

Anion-distinct anion-cation (aa'c) triplet coverage:

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.hmp

Start time = 11:13:32 20Jul2004  
End time = 11:13:33 20Jul2004

run time = 0.390 seconds

\*\*\*\*\* OUTPUT.HMY

Repeated neutral-distinct neutral (nnn') triplet coverage:

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

Neutral-cation-anion (nca) triplet coverage:

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

Completed processing the pitzer data file data0.hmy.v8.R6.

No errors were encountered.

10 warning(s) were encountered.

Start time = 09:53:06 18Oct2006  
End time = 09:53:06 18Oct2006

run time = 0.400 seconds

\*\*\*\*\*