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Sandia National Laboratories
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Carlsbad Programs Group
4100 National Parks Highway
Carlsbad, NM 88220

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to: Larry Brush
Repository Performance Dept. 6712 (MS 1395)
Carlsbad Programs Group

from: Yongliang Xiong
Repository Performance Dept. 6712 (MS 1395)
Carlsbad Programs Group

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_2 by calcite ($CaCO_3$) precipitation on the excess factor calculated for the MgO engineered barrier that the U.S Department of Energy (DOE) is emplacing in the Waste Isolation Pilot Plant.

In the previous, modified version of the EQ3/6 database (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 ($Ca_3(C_6H_5O_7)_2 \bullet 4H_2O$) AND WHEWELLITE ($CaC_2O_4 \bullet H_2O$) into EQ3/6 HMP

Ciavatta et al. (2001) determined the solubility of earlandite in $NaClO_4$ solutions from 0 m to 3.5 m at 25 °C. In their experiments using $NaClO_4$ as an ionic strength-supporting medium, the solubility reaction of earlandite is expressed as:

$$Ca_3(C_6H_5O_7)_2 \bullet 4H_2O(\text{earlandite}) = 3Ca^{2+} + 2C_6H_5O_7^{3-} + 4H_2O(l) \quad (1)$$

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,

$$CaC_2O_4 \bullet H_2O(\text{whewellite}) = Ca^{2+} + C_2O_4^{2-} + H_2O(\ \ l) \quad (2)$$

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:

$$H_3C_6H_5O_7 = H^+ + H_2C_6H_5O_7^- \quad (3)$$

$$H_2C_6H_5O_7^- = H^+ + HC_6H_5O_7^{2-} \quad (4)$$

$$HC_6H_5O_7^{2-} = H^+ + C_6H_5O_7^{3-} \quad (5)$$

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 cal mol^{-1} K^{-1}), and T is absolute temperature in K (T = 298.15 K at 25 °C). The free energy change for a chemical reaction is expressed in the following general equation:

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

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:

$$H_2C_2O_4 = H^+ + HC_2O_4^- \quad (8)$$

$$HC_2O_4^- = H^+ + C_2O_4^{2-} \quad (9)$$

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 $\Delta_f G^o$ data converted from μ^o/RT of FMT_050405.CHEMDAT (see Table 2)
Reaction 4	–4.8397	Calculated from the $\Delta_f G^o$ data converted from μ^o/RT of FMT_050405.CHEMDAT (see Table 2)
Reaction 5	–6.4232	Calculated from the $\Delta_f G^o$ data converted from μ^o/RT of FMT_050405.CHEMDAT (see Table 2)
Reaction 8	–1.3936	Calculated from the $\Delta_f G^o$ data converted from μ^o/RT of FMT_050405.CHEMDAT (see Table 2)
Reaction 9	–4.2595	Calculated from the $\Delta_f G^o$ data converted from μ^o/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	μ°/RT in FMT_050405.CHEMDAT	$\Delta_f G^\circ$, cal mol^{-1}
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).

		Binary Interaction Parameters		
i	j	$\beta^{(0)}$, kg mol^{-1}	$\beta^{(1)}$, kg mol^{-1}	C^{ϕ}, kg^2 mol^{-2}
Na^+	$H_2C_6H_5O_7^-$	–0.1296	0.29	0.013
Na^+	$HC_6H_5O_7^{2-}$	–0.0989	1.74	0.027
Na^+	$C_6H_5O_7^{3-}$	0.0887	5.22	0.047
Na^+	$HC_2O_4^-$	–0.2448	0.29	0.068
Na^+	$C_2O_4^{2-}$	–0.2176	1.74	0.122
K^+	$H_2C_6H_5O_7^-$	–0.1296	0.29	0.013
K^+	$HC_6H_5O_7^{2-}$	–0.0989	1.74	0.027
K^+	$C_6H_5O_7^{3-}$	0.0887	5.22	0.047
K^+	$HC_2O_4^-$	–0.2448	0.29	0.068
K^+	$C_2O_4^{2-}$	–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
Cl-                           1    0
***** DATA1F.HMY
     1.0000  Ca
Citrate---                    1    0
         189.100  -3.
     1.0000  Citrate
Cl-                           1    0
*****

***** data1f.hmp
     1.0000  Na
SO4--                         2    0
***** DATA1F.HMY
     1.0000  Na
Oxalate--                     1    0
          88.020  -2.
     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.
     1.0000  Citrate      3.0000  H
    -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.
     1.0000  Citrate      2.0000  H
    -1.0000  H2Citrate-                  1.0000  Citrate---
```

```
     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+                          HCO3-
   lambda0 =   0.02960   lambda1 =  -0.01300   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
***** DATA1F.HMY
+------------------------------------------------------------------------
K+                          H2Citrate-
   lambda0 =  -0.12960   lambda1 =   0.29000   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
*****

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

```
   lambda0 =  -0.09890   lambda1 =   1.74000   lambda2 =   0.00000
                         alpha1 =   2.0        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
    dl0/dt =  0.000E+00  d2l0/dt2 =  0.000E+00
***** DATA1F.HMY
+---------------------------------------------------------------------
K+                        OH-
   lambda0 =   0.12980   lambda1 =   0.32000   lambda2 =   0.00000
                         alpha1 =   2.0        alpha2 =  12.0
    dl0/dt =  0.000E+00  d2l0/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
                         alpha1 =   2.0       alpha2 =  12.0
    dI0/dt =  0.000E+00  d2I0/dt2 =  0.000E+00
***** DATA1F.HMY
+----------------------------------------------------------------------
Mg++                        CO3--
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =   1.4       alpha2 =  12.0
    dI0/dt =  0.000E+00  d2I0/dt2 =  0.000E+00
*****

***** data1f.hmp
+----------------------------------------------------------------------
Mg++                        SO4--
   lambda0 =   0.22100   lambda1 =   3.34300   lambda2 = -37.23000
                         alpha1 =   1.4       alpha2 =  12.0
    dI0/dt =  0.000E+00  d2I0/dt2 =  0.000E+00
***** DATA1F.HMY
+----------------------------------------------------------------------
Mg++                        Cl-
   lambda0 =   0.35235   lambda1 =   1.68150   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
    dI0/dt =  0.000E+00  d2I0/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
```

```
                          alpha1 =   2.0       alpha2 =  12.0
    dl0/dt =  0.000E+00   d2l0/dt2 =  0.000E+00
***** DATA1F.HMY
+---------------------------------------------------------------------
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.hmp
+---------------------------------------------------------------------
MgOH+                      HSO4-
   lambda0 =   0.00000    lambda1 =   0.00000   lambda2 =   0.00000
***** DATA1F.HMY
+---------------------------------------------------------------------
CO2(aq)                    MgOH+
   lambda0 =   0.00000    lambda1 =   0.00000   lambda2 =   0.00000
*****

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

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

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

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

***** data1f.hmp
+---------------------------------------------------------------------
Na+                        Cl-
   lambda0 =   0.07650    lambda1 =   0.26640   lambda2 =   0.00000
                          alpha1 =   2.0       alpha2 =  12.0
***** DATA1F.HMY
+---------------------------------------------------------------------
MgOH+                      OH-
   lambda0 =   0.00000    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
    dl0/dt =  0.000E+00  d2l0/dt2 =  0.000E+00
***** DATA1F.HMY
+----------------------------------------------------------------------
Na+                          Cl-
   lambda0 =   0.07650   lambda1 =   0.26640   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
    dl0/dt =  0.000E+00  d2l0/dt2 =  0.000E+00
*****

***** data1f.hmp
+----------------------------------------------------------------------
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.HMY
+----------------------------------------------------------------------
Na+                          H2Citrate-
   lambda0 =  -0.12960   lambda1 =   0.29000   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
    dl0/dt =  0.000E+00  d2l0/dt2 =  0.000E+00
*****

***** data1f.hmp
+----------------------------------------------------------------------
Ca++                         Mg++
```

```
   lambda0 =   0.00700   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
***** DATA1F.HMY
+---------------------------------------------------------------------
Na+                       HCitrate--
   lambda0 =  -0.09890   lambda1 =   1.74000   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
*****

***** data1f.hmp
+---------------------------------------------------------------------
Ca++                      MgOH+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
***** DATA1F.HMY
+---------------------------------------------------------------------
Na+                       HCO3-
   lambda0 =   0.02770   lambda1 =   0.04110   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
*****

***** data1f.hmp
+---------------------------------------------------------------------
CO3--                     Cl-
   lambda0 =  -0.02000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
***** DATA1F.HMY
+---------------------------------------------------------------------
Na+                       HOxalate-
   lambda0 =  -0.24480   lambda1 =   0.29000   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
*****

***** data1f.hmp
+---------------------------------------------------------------------
Cl-                       HCO3-
   lambda0 =   0.03000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
***** DATA1F.HMY
+---------------------------------------------------------------------
Na+                       HSO4-
   lambda0 =   0.04540   lambda1 =   0.39800   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
*****

***** data1f.hmp
+---------------------------------------------------------------------
Cl-                       HSO4-
   lambda0 =  -0.00600   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
***** DATA1F.HMY
+---------------------------------------------------------------------
Na+                       OH-
   lambda0 =   0.08640   lambda1 =   0.25300   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
*****

***** data1f.hmp
+---------------------------------------------------------------------
Cl-                       OH-
   lambda0 =  -0.05000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
***** DATA1F.HMY
+---------------------------------------------------------------------
Na+                       Oxalate--
   lambda0 =  -0.21760   lambda1 =   1.74000   lambda2 =   0.00000
                         alpha1 =   2.0       alpha2 =  12.0
    dlO/dt =  0.000E+00  d2lO/dt2 =  0.000E+00
```

```
*****

***** data1f.hmp
+---------------------------------------------------------------------
Cl-                          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
***** DATA1F.HMY
+---------------------------------------------------------------------
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.hmp
+---------------------------------------------------------------------
CO3--                        HCO3-
   lambda0 =  -0.04000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
    dl0/dt =  0.000E+00  d2l0/dt2 =  0.000E+00
***** DATA1F.HMY
+---------------------------------------------------------------------
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.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+                          K+
   lambda0 =   0.00500   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMY
+-------------------------------------------------------------------
Cl-                         HCO3-
   lambda0 =   0.03000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmp
+-------------------------------------------------------------------
K+                          Mg++
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMY
+-------------------------------------------------------------------
Cl-                         HSO4-
   lambda0 =  -0.00600   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmp
+-------------------------------------------------------------------
K+                          MgOH+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMY
+-------------------------------------------------------------------
Cl-                         OH-
   lambda0 =  -0.05000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmp
+-------------------------------------------------------------------
H+                          Mg++
   lambda0 =   0.10000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMY
+-------------------------------------------------------------------
Cl-                         SO4--
   lambda0 =   0.02000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmp
+-------------------------------------------------------------------
Mg++                        MgOH+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMY
+-------------------------------------------------------------------
CO3--                       HCO3-
   lambda0 =  -0.04000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****

***** data1f.hmp
+-------------------------------------------------------------------
H+                          MgOH+
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
***** DATA1F.HMY
+-------------------------------------------------------------------
CO3--                       HSO4-
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
*****

***** data1f.hmp
+-------------------------------------------------------------------
Ca++                        Na+
   lambda0 =   0.07000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
***** DATA1F.HMY
+-------------------------------------------------------------------
HCO3-                       HSO4-
   lambda0 =   0.00000   lambda1 =   0.00000   lambda2 =   0.00000
                         alpha1 =  99.0       alpha2 =  99.0
*****
```

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

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

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

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

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

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

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

```
   lambda0 =   0.00000   lambda1 =   0.00000   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
                         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.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  d2mmx/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  d2mmx/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  d2mmx/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  d2mmx/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  d2mmx/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 Mercallite
    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 Mercallite
    38 Mirabilite
    39 Misenite
    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/tprn2) 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/tprca) 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/tprnn) 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---, HCitrate--
         Citrate---, HOxalate-
         Citrate---, HSO4-
         Citrate---, OH-
         Cl-, Oxalate--
         Cl-, H2Citrate-
         Cl-, HCitrate--
         Cl-, HOxalate-
         HCO3-, Oxalate--
         H2Citrate-, HCO3-
         HCO3-, HCitrate--
         HCO3-, HOxalate-
         Oxalate--, SO4--
         CO3--, Oxalate--

         plus 20 others

*****

***** output.hmp

 * warning - (eqpt/tprnc) 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/tprn2) 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/tprna) 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--

CaCO3(aq), CO3--
CaCO3(aq), HSO4-
CaCO3(aq), OH-
MgCO3(aq), Cl-
MgCO3(aq), HCO3-
MgCO3(aq), SO4--
MgCO3(aq), CO3--
MgCO3(aq), HSO4-
MgCO3(aq), OH-

***** OUTPUT.HMY

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

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

*****

***** output.hmp

* warning - (eqpt/tprn2n) 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/tprnc) 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+
H3Citrate(aq), Ca++
H3Citrate(aq), H+
H3Citrate(aq), K+
H3Citrate(aq), Mg++
H3Citrate(aq), Na+
H3Citrate(aq), MgOH+
H2Oxalate(aq), Ca++
H2Oxalate(aq), H+
H2Oxalate(aq), K+
H2Oxalate(aq), Mg++
H2Oxalate(aq), Na+
H2Oxalate(aq), MgOH+
MgCO3(aq), Ca++
MgCO3(aq), K+
MgCO3(aq), Mg++

plus 2 others

*****

***** output.hmp

* warning - (eqpt/tprnca) 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--

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

        plus 32 others

*****

***** output.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/tprcca) 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+, HCitrate--
        Ca++, H+, HOxalate-
        Ca++, K+, Citrate---
        Ca++, K+, Oxalate--
        Ca++, K+, H2Citrate-
        Ca++, K+, HCitrate--
        Ca++, K+, HOxalate-
        Ca++, Mg++, Citrate---
        Ca++, Mg++, Oxalate--
        Ca++, Mg++, H2Citrate-
        Ca++, Mg++, HCitrate--
        Ca++, Mg++, HOxalate-
        Ca++, Na+, Citrate---
```

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

        plus 55 others

*****

***** output.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/tpraac) 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/tprn2n) 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
```

```
    Coverage is 0.00 per cent

***** OUTPUT.HMY

 * warning - (eqpt/tprnca) 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
```

```
  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

*****
```

```
***** 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

*****
```