```
 EQ3NR, version 3245R110

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 Supported by EQLIB, version 3245R136

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 Run



 --- reading the input file ---
450 C & 10.0 kbar
 Data0 from DEW

 Revised antigorite volumes

 Atg1 fluid in equilibrium with:

 Antigorite
 Magnetite
 Diopside


 log fO2 in between QFM and HM




 endit.
       tempc=   .45000E+03
         rho=   .10234E+01    tdspkg=   .00000E+00     tdspl=   .
00000E+00
         fep=  -.26800E+02    uredox=
       tolbt=   .00000E+00     toldl=   .00000E+00    tolsat=   .
00000E+00
     itermx=  0
                  1    2    3    4    5    6    7    8    9   10
   iopt1-10=     0    0    0    0    0    0    0    0    0    0
   iopg1-10=     0   -1    0    0    1    0    0    0    0    0
   iopr1-10=     0    2    0    0    0    0    1    0    0    0
  iopr11-20=     0    0    0    0    0    0    0    0    0    0
   iodb1-10=     0    0    0    0    0    0    0    0    0    0
      uebal= NA+
     uacion= CL-
```

```
      nxmod=  5
    species= HEMATITE
       type=  1              option= -1             xlkmod=   .
00000E+00
    species= FORSTERITE
       type=  1              option= -1             xlkmod=   .
00000E+00
    species= FAYALITE
       type=  1              option= -1             xlkmod=   .
00000E+00
    species= ENSTATITE-CL
       type=  1              option= -1             xlkmod=   .
00000E+00
    species= PERICLASE
       type=  1              option= -1             xlkmod=   .
00000E+00
 data file master species= NA+
    switch with species=
    jflag=  0   csp=   .50000E+00
 data file master species= CL-
    switch with species=
    jflag=  0   csp=   .50000E+00
 data file master species= CA++
    switch with species=
    jflag=  0   csp=   .10000E-02
 data file master species= MG++
    switch with species=
    jflag= 19   csp=   .00000E+00
            uphas1= ANTIGORITE                uphas2=

 data file master species= FE++
    switch with species=
    jflag= 19   csp=   .00000E+00
            uphas1= MAGNETITE                 uphas2=

 data file master species= H4SIO4(AQ)
    switch with species=
    jflag= 19   csp=   .00000E+00
            uphas1= DIOPSIDE                  uphas2=

 data file master species= AL+++
    switch with species=
    jflag=  0   csp=   .10000E-05
 data file master species= H+
    switch with species=
    jflag= 16   csp=  -.66000E+01
endit.

 --- the input file has been successfuly read ---
```

```
--- reading the data1 file ---

--- the data1 file has been successfully read ---
the species HEMATITE                 has been user-suppressed

the species FORSTERITE               has been user-suppressed

the species FAYALITE                 has been user-suppressed

the species ENSTATITE-CL             has been user-suppressed

the species PERICLASE                has been user-suppressed




eeee   qqq   33333  n   n  rrrr
e     q   q      3  nn  n  r   r
eeee  q   q    33   n n n  rrrr
e     q q q      3  n  nn  r  r
eeee   qqq   3333   n   n  r   r
          q



eq3nr.3245R110
 supported by eqlib.3245R136


300 C & 10.0 kbar
Data0 from DEW

Revised antigorite volumes

Atg1 fluid in equilibrium with:

Antigorite
Magnetite
Diopside


log fO2 in between QFM and HM
```

```
 DATA FILE GENERATED WITH PROCESS REACTIONS PACKAGE THEN CONVERTED TO
HYDROUS, AQ
   log K DATA refer to the range of temperatures at the pressure
specified below
   LAST REVISED May, 2019


   the activity coefficients of aqueous solute species
 and the activity of water are calculated according to
 b-dot equation plus others



 temperature= 450.00 degrees celsius
 pressure=  500.0000 bars


         31 elements are in the data base
         70 elements can be loaded into memory
          9 elements are active in this problem


        117 aqueous species are in the data base
         87 aqueous species were loaded into memory
        750 aqueous species can be loaded into memory
         40 aqueous species are active in this problem

         85 aqueous reactions are in the data base
         55 aqueous reactions were loaded into memory
        679 aqueous reactions can be loaded into memory


              80 minerals are in the data base
              57 minerals were loaded into memory
             750 minerals can be loaded into memory
              51 minerals are active in this problem

              15 solid solutions are in the data base
              20 solid solutions can be loaded into memory

               7 gases are in the data base
               3 gases were loaded into memory
              15 gases can be loaded into memory
               3 gases are active in this problem




      iopt1  =  0 (redox option switch)
      iopt2  =  0 (automatic basis switching switch)
```

```
      iopt3  =  0 (interfacing output control switch)
      iopt4  =  0 (turn-on solid solutions switch)
      iopt5  =  0 (not used)
      iopt6  =  0 (conv. test criteria switch)
      iopt7  =  0 (0/1 3245/post-3245 pickup file)
      iopt8  =  0 (not used)
      iopt9  =  0 (not used)
      iopt10 =  0 (not used)


           iopg1  =  0 (act. coeff. choice)
           iopg2  = -1 (ph scale convention switch)
           iopg3  =  0 (iopg1=3 - 0/1 uelam= on/onplus)
           iopg4  =  0 (iopg1=3 or 4 - f switch - 0/1 dhoa/dhca)
           iopg5  =  1 (use bdot term instead of co2 polynomial)
           iopg6  =  0 (approx. of j(x) function)
           iopg7  =  0 (not used)
           iopg8  =  0 (not used)
           iopg9  =  0 (not used)
           iopg10 =  0 (not used)


                iopr1  =  0 (list loading of species)
                iopr2  =  2 (list reactions and log k values)
                iopr3  =  0 (aqueous species print order control)
                iopr4  =  0 (aqueous species print cut-off control)
                iopr5  =  0 (mass balance percentages print control)
                iopr6  =  0 (mean ionic act coeff print control)
                iopr7  =  1 (mineral affinity print control)
                iopr8  =  0 (ion size and hydr. no. print control)
                iopr9  =  0 (pitzer coefficients tabulation)
                iopr10 =  0 (print concbs array)
                iopr11 =  0 (not used)
                iopr12 =  0 (not used)
                iopr13 =  0 (not used)
                iopr14 =  0 (not used)
                iopr15 =  0 (not used)
                iopr16 =  0 (not used)
                iopr17 =  0 (not used)
                iopr18 =  0 (not used)
                iopr19 =  0 (not used)
                iopr20 =  0 (not used)


                     iodb1  =  0 (print info. messages switch)
                     iodb2  =  0 (print pre-newton-raphson
optimizations switch)
                     iodb3  =  0 (request iteration variables to kill)
                     iodb4  =  0 (print newton-raphson iterations
```

```
switch)
                     iodb5  =  0 (list stoichiometric equivalences)
                     iodb6  =  0 (controls iodb5 level of detail)
                     iodb7  =  0 (write reactions on file rlist
switch)
                     iodb8  =  0 (not used)
                     iodb9  =  0 (not used)
                     iodb10 =  0 (not used)


      the default redox state is constrained by log fo2 =     -26.8000
(log bars)


                solution density =  1.02336 g/ml

                total dissolved salts =        .00 mg/kg solution
                total dissolved salts =        .00 mg/l


           tolbt  =   .10000E-05 (convergence tolerance on residual
functions)
           toldl  =   .10000E-05 (convergence tolerance on correction
terms)
           tolsat =   .50000E+00 (phase saturation tolerance, does not
affect
                                  convergence)



                                    ----- input constraints -----

     species          csp       jflag  type of input      controlling
phase

   NA+                          .50000E+00    0   tot conc, molal
   CL-                          .50000E+00    0   tot conc, molal
   CA++                         .10000E-02    0   tot conc, molal
   MG++                         .00000E+00   19   mineral equilibrium
ANTIGORITE

                      1.000  ANTIGORITE
                   + 48.000  H+
                         ==
                      5.500  H2O
                   + 24.000  MG++
                   + 17.000  H4SIO4(AQ)
   FE++                         .00000E+00   19   mineral equilibrium
MAGNETITE
```

```
                        1.000  MAGNETITE
                     +  8.000  H+
                            ==
                        4.000  H2O
                     +  1.000  FE++
                     +  2.000  FE+++
   H4SIO4(AQ)                    .00000E+00   19   mineral equilibrium
DIOPSIDE

                        1.000  DIOPSIDE
                     +  2.000  H2O
                     +  4.000  H+
                            ==
                        1.000  CA++
                     +  1.000  MG++
                     +  2.000  H4SIO4(AQ)
   AL+++                         .10000E-05    0   tot conc, molal
   H+                           -.66000E+01   16   log activity


  the ion that defines equiv. stoich. ionic strength
    is CL-

  electrical balance will be achieved by adjusting
    the concentration of NA+


                      --- inactive aqueous species ---




                                 --- modified input constraints ---

     species          csp        jflag  type of input      controlling
phase

   NA+                           .50000E+00    0   tot conc, molal
   CA++                          .10000E-02    0   tot conc, molal
   MG++                          .00000E+00   19   mineral equilibrium
ANTIGORITE

                        1.000  ANTIGORITE
                     + 48.000  H+
                            ==
                        5.500  H2O
                     + 24.000  MG++
                     + 17.000  H4SIO4(AQ)
   AL+++                         .10000E-05    0   tot conc, molal
   H4SIO4(AQ)                    .00000E+00   19   mineral equilibrium
```

```
DIOPSIDE

                          1.000  DIOPSIDE
                       +  2.000  H2O
                       +  4.000  H+
                              ==
                          1.000  CA++
                       +  1.000  MG++
                       +  2.000  H4SIO4(AQ)
   H+                              -.66000E+01   16   log activity
   CL-                              .50000E+00    0   tot conc, molal
   FE++                             .00000E+00   19   mineral equilibrium
MAGNETITE

                          1.000  MAGNETITE
                       +  6.000  H+
                              ==
                          3.000  H2O
                       +  3.000  FE++
                       +   .500  O2(G)
   O2(AQ)                           .00000E+00   27   dependent species
   H2(AQ)                           .00000E+00   27   dependent species
   FE+++                            .00000E+00   30   eliminated species
   OH-                              .00000E+00   30   eliminated species
   H8SI3O10(AQ)                     .00000E+00   30   eliminated species
   H6SI2O7(AQ)                      .00000E+00   30   eliminated species



 ---listing of species and reactions ---

       temperature=    450.000 degrees celsius
       pressure=   500.000     bars

        --- strict basis species ---

                                 H2O
                                 NA+
                                 CA++
                                 MG++
                                 AL+++
                                 H4SIO4(AQ)
                                 H+
                                 CL-
                                 FE++


        --- aqueous species dissociation reactions ---
```

```
--------------------------------------------------

                      1.000  O2(AQ)
                          ==
                      1.000  O2(G)

         log k=       4.0749

--------------------------------------------------

                      2.000  H2(AQ)
                   +  1.000  O2(G)
                          ==
                      2.000  H2O

         log k=      29.7740

--------------------------------------------------

                      1.000  FE+++
                   +   .500  H2O
                          ==
                      1.000  H+
                   +  1.000  FE++
                   +   .250  O2(G)

         log k=       1.2974

--------------------------------------------------

                      1.000  OH-
                   +  1.000  H+
                          ==
                      1.000  H2O

         log k=       8.0712

--------------------------------------------------

                      1.000  H8SI3O10(AQ)
                   +  2.000  H2O
                          ==
                      3.000  H4SIO4(AQ)

         log k=       2.3076

--------------------------------------------------

                      1.000  H6SI2O7(AQ)
```

```
                 +  1.000  H2O
                        ==
                    2.000  H4SIO4(AQ)

         log k=     -.4251

--------------------------------------------------

                    1.000  AL(OH)3(AQ)
                 +  3.000  H+
                        ==
                    3.000  H2O
                 +  1.000  AL+++

         log k=     1.7476

--------------------------------------------------

                    1.000  AL(OH)4-
                 +  4.000  H+
                        ==
                    4.000  H2O
                 +  1.000  AL+++

         log k=     6.3031

--------------------------------------------------

                    1.000  AL(OH)SI(OH)-
                 +  4.000  H+
                        ==
                    3.000  H2O
                 +  1.000  AL+++
                 +  1.000  H4SIO4(AQ)

         log k=     4.0544

--------------------------------------------------

                    1.000  CACL+
                        ==
                    1.000  CA++
                 +  1.000  CL-

         log k=    -1.6501

--------------------------------------------------

                    1.000  CACL2(AQ)
                        ==
```

```
                  1.000  CA++
               +  2.000  CL-

         log k=          -.7441

--------------------------------------------------

                  1.000  CA(OH)+
               +  1.000  H+
                      ==
                  1.000  H2O
               +  1.000  CA++

         log k=          5.3633

--------------------------------------------------

                  1.000  CA(H3SIO4)+
               +  1.000  H+
                      ==
                  1.000  CA++
               +  1.000  H4SIO4(AQ)

         log k=          2.4563

--------------------------------------------------

                  1.000  FE(OH)+
               +  1.000  H+
                      ==
                  1.000  H2O
               +  1.000  FE++

         log k=          4.4058

--------------------------------------------------

                  1.000  FE(OH)2
               +  2.000  H+
                      ==
                  2.000  H2O
               +  1.000  FE++

         log k=          9.9116

--------------------------------------------------

                  1.000  FE(OH)3-
               +  3.000  H+
                      ==
```

```
                   3.000  H2O
                +  1.000  FE++

         log k=      15.7443

--------------------------------------------------

                   1.000  FECL+
                       ==
                   1.000  CL-
                +  1.000  FE++

         log k=      -1.3702

--------------------------------------------------

                   1.000  FECL2(AQ)
                       ==
                   2.000  CL-
                +  1.000  FE++

         log k=      -3.5721

--------------------------------------------------

                   1.000  FE(H3SIO4)+
                +  1.000  H+
                       ==
                   1.000  H4SIO4(AQ)
                +  1.000  FE++

         log k=      -1.6734

--------------------------------------------------

                   1.000  FECL++
                +   .500  H2O
                       ==
                   1.000  H+
                +  1.000  CL-
                +  1.000  FE++
                +   .250  O2(G)

         log k=      -3.3132

--------------------------------------------------

                   1.000  FECL2+
                +   .500  H2O
                       ==
```

```
                 1.000  H+
              +  2.000  CL-
              +  1.000  FE++
              +   .250  O2(G)

    log k=      -4.9444

--------------------------------------------------

                 1.000  FECL3
              +   .500  H2O
                     ==
                 1.000  H+
              +  3.000  CL-
              +  1.000  FE++
              +   .250  O2(G)

    log k=      25.0194

--------------------------------------------------

                 1.000  FECL4-
              +   .500  H2O
                     ==
                 1.000  H+
              +  4.000  CL-
              +  1.000  FE++
              +   .250  O2(G)

    log k=       -.1365

--------------------------------------------------

                 1.000  MGCL+
                     ==
                 1.000  MG++
              +  1.000  CL-

    log k=      -1.3244

--------------------------------------------------

                 1.000  MG(OH)+
              +  1.000  H+
                     ==
                 1.000  H2O
              +  1.000  MG++

    log k=       4.5117
```

```
--------------------------------------------------

                     1.000  MG(OH)2(AQ)
                  +  2.000  H+
                         ==
                     2.000  H2O
                  +  1.000  MG++

         log k=      6.0392

--------------------------------------------------

                     1.000  MG(H3SIO4)+
                  +  1.000  H+
                         ==
                     1.000  MG++
                  +  1.000  H4SIO4(AQ)

         log k=      4.9816

--------------------------------------------------

                     1.000  NACL(AQ)
                         ==
                     1.000  NA+
                  +  1.000  CL-

         log k=       .2557

--------------------------------------------------

                     1.000  NAOH(AQ)
                  +  1.000  H+
                         ==
                     1.000  H2O
                  +  1.000  NA+

         log k=      7.8363

--------------------------------------------------

                     1.000  H3SIO4-
                  +  1.000  H+
                         ==
                     1.000  H4SIO4(AQ)

         log k=      7.2069

--------------------------------------------------
```

```
                   1.000  HCL(AQ)
                       ==
                   1.000  H+
                +  1.000  CL-

      log k=       -.9347

--------------------------------------------------

       --- mineral dissolution reactions ----

--------------------------------------------------

                   1.000  MAGNETITE
                +  6.000  H+
                       ==
                   3.000  H2O
                +  3.000  FE++
                +   .500  O2(G)

      log k=      -2.3399

--------------------------------------------------

                   1.000  CORUNDUM
                +  6.000  H+
                       ==
                   3.000  H2O
                +  2.000  AL+++

      log k=      -4.2533

--------------------------------------------------

                   1.000  LIME
                +  2.000  H+
                       ==
                   1.000  H2O
                +  1.000  CA++

      log k=      13.8508

--------------------------------------------------

                   1.000  SPINEL
                +  8.000  H+
                       ==
                   4.000  H2O
                +  1.000  MG++
                +  2.000  AL+++
```

```
         log k=       1.4787

--------------------------------------------------

                      1.000  BRUCITE
                   +  2.000  H+
                          ==
                      2.000  H2O
                   +  1.000  MG++

         log k=       6.4000

--------------------------------------------------

                      1.000  DIASPORE
                   +  3.000  H+
                          ==
                      2.000  H2O
                   +  1.000  AL+++

         log k=      -2.2328

--------------------------------------------------

                      1.000  ANDALUSITE
                   +  6.000  H+
                          ==
                      1.000  H2O
                   +  2.000  AL+++
                   +  1.000  H4SIO4(AQ)

         log k=      -5.3248

--------------------------------------------------

                      1.000  KYANITE
                   +  6.000  H+
                          ==
                      1.000  H2O
                   +  2.000  AL+++
                   +  1.000  H4SIO4(AQ)

         log k=      -5.6932

--------------------------------------------------

                      1.000  SILLIMANITE
                   +  6.000  H+
                          ==
```

```
                  1.000  H2O
               +  2.000  AL+++
               +  1.000  H4SIO4(AQ)

      log k=      -5.3962

--------------------------------------------------

                  1.000  GLAUCOPHANE
               +  8.000  H2O
               + 14.000  H+
                      ==
                  2.000  NA+
               +  3.000  MG++
               +  2.000  AL+++
               +  8.000  H4SIO4(AQ)

      log k=       9.3871

--------------------------------------------------

                  1.000  LAWSONITE
               +  8.000  H+
                      ==
                  2.000  H2O
               +  1.000  CA++
               +  2.000  AL+++
               +  2.000  H4SIO4(AQ)

      log k=       -.9355

--------------------------------------------------

                  1.000  PUMPELLYITE
               + 25.000  H+
                      ==
                  4.000  H2O
               +  4.000  CA++
               +  1.000  MG++
               +  5.000  AL+++
               +  6.000  H4SIO4(AQ)

      log k=      11.0868

--------------------------------------------------

                  1.000  ZOISITE
               + 13.000  H+
                      ==
                  1.000  H2O
```

```
               +  2.000  CA++
               +  3.000  AL+++
               +  3.000  H4SIO4(AQ)

      log k=        1.4281

--------------------------------------------------

                  1.000  CLINOZOISITE
               + 13.000  H+
                      ==
                  1.000  H2O
               +  2.000  CA++
               +  3.000  AL+++
               +  3.000  H4SIO4(AQ)

      log k=        1.6428

--------------------------------------------------

                  1.000  MONTICELLITE
               +  4.000  H+
                      ==
                  2.000  CA++
               +  1.000  H4SIO4(AQ)

      log k=       21.6025

--------------------------------------------------

                  1.000  MERWINITE
               +  8.000  H+
                      ==
                  3.000  CA++
               +  1.000  MG++
               +  2.000  H4SIO4(AQ)

      log k=       29.7229

--------------------------------------------------

                  1.000  CHRYSOTILE
               +  6.000  H+
                      ==
                  1.000  H2O
               +  3.000  MG++
               +  2.000  H4SIO4(AQ)

      log k=       12.7828
```

```
--------------------------------------------------

                     1.000  ENSTATITE-OR
                  +  1.000  H2O
                  +  2.000  H+
                         ==
                     1.000  MG++
                  +  1.000  H4SIO4(AQ)

         log k=      3.9432

--------------------------------------------------

                     1.000  ENSTATITE-PR
                  +  1.000  H2O
                  +  2.000  H+
                         ==
                     1.000  MG++
                  +  1.000  H4SIO4(AQ)

         log k=      4.0657

--------------------------------------------------

                     1.000  DIOPSIDE
                  +  2.000  H2O
                  +  4.000  H+
                         ==
                     1.000  CA++
                  +  1.000  MG++
                  +  2.000  H4SIO4(AQ)

         log k=      8.6560

--------------------------------------------------

                     1.000  HEDENBERGITE
                  +  2.000  H2O
                  +  4.000  H+
                         ==
                     1.000  CA++
                  +  2.000  H4SIO4(AQ)
                  +  1.000  FE++

         log k=      7.4004

--------------------------------------------------

                     1.000  JADEITE
                  +  2.000  H2O
```

```
                    +  4.000  H+
                           ==
                       1.000  NA+
                    +  1.000  AL+++
                    +  2.000  H4SIO4(AQ)

          log k=         .1310

--------------------------------------------------

                       1.000  FERROSILITE
                    +  1.000  H2O
                    +  2.000  H+
                           ==
                       1.000  H4SIO4(AQ)
                    +  1.000  FE++

          log k=        2.2222

--------------------------------------------------

                       1.000  WOLLASTONITE
                    +  1.000  H2O
                    +  2.000  H+
                           ==
                       1.000  CA++
                    +  1.000  H4SIO4(AQ)

          log k=        6.4574

--------------------------------------------------

                       1.000  PSEUDOWOLLASTONITE
                    +  1.000  H2O
                    +  2.000  H+
                           ==
                       1.000  CA++
                    +  1.000  H4SIO4(AQ)

          log k=        6.6043

--------------------------------------------------

                       1.000  TREMOLITE
                    +  8.000  H2O
                    + 14.000  H+
                           ==
                       2.000  CA++
                    +  5.000  MG++
                    +  8.000  H4SIO4(AQ)
```

```
         log k=      25.8873

--------------------------------------------------

                      1.000  ANTHOPHYLLITE
                   +  8.000  H2O
                   + 14.000  H+
                          ==
                      7.000  MG++
                   +  8.000  H4SIO4(AQ)

         log k=      25.2586

--------------------------------------------------

                      1.000  CORDIERITE
                   +  2.000  H2O
                   + 16.000  H+
                          ==
                      2.000  MG++
                   +  4.000  AL+++
                   +  5.000  H4SIO4(AQ)

         log k=      -2.9564

--------------------------------------------------

                      1.000  ALBITE
                   +  4.000  H2O
                   +  4.000  H+
                          ==
                      1.000  NA+
                   +  1.000  AL+++
                   +  3.000  H4SIO4(AQ)

         log k=      -1.4177

--------------------------------------------------

                      1.000  ANORTHITE
                   +  8.000  H+
                          ==
                      1.000  CA++
                   +  2.000  AL+++
                   +  2.000  H4SIO4(AQ)

         log k=       -.1579

--------------------------------------------------
```

```
                 1.000  GEHLENITE
               + 10.000  H+
                      ==
                 3.000  H2O
               +  2.000  CA++
               +  2.000  AL+++
               +  1.000  H4SIO4(AQ)

      log k=      11.9193

--------------------------------------------------

                 1.000  KAOLINITE
               +  6.000  H+
                      ==
                 1.000  H2O
               +  2.000  AL+++
               +  2.000  H4SIO4(AQ)

      log k=      -6.4221

--------------------------------------------------

                 1.000  ANTIGORITE
               + 48.000  H+
                      ==
                 5.500  H2O
               + 24.000  MG++
               + 17.000  H4SIO4(AQ)

      log k=      97.9360

--------------------------------------------------

                 1.000  PYROPHYLLITE
               +  4.000  H2O
               +  6.000  H+
                      ==
                 2.000  AL+++
               +  4.000  H4SIO4(AQ)

      log k=      -8.9524

--------------------------------------------------

                 1.000  TALC
               +  4.000  H2O
               +  6.000  H+
                      ==
```

```
                  3.000  MG++
               +  4.000  H4SIO4(AQ)

     log k=       9.0499

--------------------------------------------------

                  1.000  PARAGONITE
               + 10.000  H+
                      ==
                  1.000  NA+
               +  3.000  AL+++
               +  3.000  H4SIO4(AQ)

     log k=      -6.9549

--------------------------------------------------

                  1.000  MARGARITE
               + 14.000  H+
                      ==
                  4.000  H2O
               +  1.000  CA++
               +  4.000  AL+++
               +  2.000  H4SIO4(AQ)

     log k=      -5.6067

--------------------------------------------------

                  1.000  PREHNITE
               + 10.000  H+
                      ==
                  2.000  CA++
               +  2.000  AL+++
               +  3.000  H4SIO4(AQ)

     log k=       4.9601

--------------------------------------------------

                  1.000  CLINOCHLORE
               +  3.200  H+
                      ==
                  1.200  H2O
               +  1.000  MG++
               +   .400  AL+++
               +   .600  H4SIO4(AQ)

     log k=       2.6783
```

```
--------------------------------------------------

                     1.000  CHAMOSITE
                  +  3.200  H+
                         ==
                     1.200  H2O
                  +   .400  AL+++
                  +   .600  H4SIO4(AQ)
                  +  1.000  FE++

         log k=      1.5495

--------------------------------------------------

                     1.000  PYROPE
                  +  4.000  H+
                         ==
                     1.001  MG++
                  +   .666  AL+++
                  +  1.000  H4SIO4(AQ)

         log k=      2.7045

--------------------------------------------------

                     1.000  ALMANDINE
                  +  4.000  H+
                         ==
                      .666  AL+++
                  +  1.000  H4SIO4(AQ)
                  +  1.001  FE++

         log k=       .3358

--------------------------------------------------

                     1.000  GROSSULAR
                  +  4.000  H+
                         ==
                     1.001  CA++
                  +   .666  AL+++
                  +  1.000  H4SIO4(AQ)

         log k=      3.8126

--------------------------------------------------

                     1.000  QUARTZ-ALPHA
                  +  2.000  H2O
```

```
                         ==
                     1.000  H4SIO4(AQ)

         log k=      -1.1065

--------------------------------------------------

                     1.000  QUARTZ-BETA
                  +  2.000  H2O
                         ==
                     1.000  H4SIO4(AQ)

         log k=      -1.0349

--------------------------------------------------

                     1.000  COESITE
                  +  2.000  H2O
                         ==
                     1.000  H4SIO4(AQ)

         log k=       -.9263

--------------------------------------------------

                     1.000  IRON-ALPHA
                  +  2.000  H+
                  +   .500  O2(G)
                         ==
                     1.000  H2O
                  +  1.000  FE++

         log k=      19.7037

--------------------------------------------------

                     1.000  IRON-GAMMA
                  +  2.000  H+
                  +   .500  O2(G)
                         ==
                     1.000  H2O
                  +  1.000  FE++

         log k=      19.4448

--------------------------------------------------

                     1.000  HALITE
                         ==
                     1.000  NA+
```

```
                  +  1.000  CL-

         log k=        1.8265

--------------------------------------------------

                     1.000  CRISTOBALITE-ALPHA
                  +  2.000  H2O
                         ==
                     1.000  H4SIO4(AQ)

         log k=        -.7179

--------------------------------------------------

                     1.000  CRISTOBALITE-BETA
                  +  2.000  H2O
                         ==
                     1.000  H4SIO4(AQ)

         log k=        -.5023

--------------------------------------------------

       --- gas dissolution reactions ---

--------------------------------------------------

                     1.000  O2(G)
                         ==
                     1.000  O2(G)

         log k=         .0000

--------------------------------------------------

                     1.000  H2(G)
                  +   .500  O2(G)
                         ==
                     1.000  H2O

         log k=       11.1151

--------------------------------------------------

                     1.000  H2O(G)
                         ==
                     1.000  H2O

         log k=       -3.8131
```

```
--------------------------------------------------
--- arrset - optimization ended within requested limits ---

iter=   0, delmax=  0.00000E+00 (unrelaxed)
       del(                 )=  0.00000E+00, delfnc =  0.00000E+00
      beta(CONC    CL-     )=  7.01313E-02, betfnc =  0.00000E+00
      no. of under-relaxation cycles=   0
       bbig=  7.01313E-02, ubbig= CL-
       bneg= -3.17462E-02, ubneg= NA+
      bgamx=  3.24529E-02, ubgamx= AL+++
        bxi=  5.93488E-02, bxistq=  7.16430E-02
iter=   1, delmax=  2.85382E-02 (unrelaxed)
       del(CONC    CL-     )= -2.85382E-02, delfnc =  0.00000E+00
      beta(CONC    AL+++   )=  2.13224E-02, betfnc =  6.95964E-01
      no. of under-relaxation cycles=   0
       bbig=  2.13224E-02, ubbig= AL+++
       bneg= -5.82458E-04, ubneg= NA+
      bgamx=  1.60556E-02, ubgamx= AL+++
        bxi= -2.81177E-02, bxistq= -6.41114E-02
iter=   2, delmax=  1.61665E-02 (unrelaxed)
       del(CONC    AL+++   )= -1.61665E-02, delfnc =  4.33515E-01
      beta(CONC    AL+++   )=  1.27666E-03, betfnc =  9.40126E-01
      no. of under-relaxation cycles=   0
       bbig=  1.27666E-03, ubbig= AL+++
       bneg=  0.00000E+00, ubneg= none
      bgamx=  8.52019E-04, ubgamx= AL+++
        bxi= -1.51249E-03, bxistq= -2.88901E-03
iter=   3, delmax=  9.26870E-04 (unrelaxed)
       del(CONC    AL+++   )= -9.26870E-04, delfnc =  9.42667E-01
      beta(CONC    AL+++   )=  2.04815E-05, betfnc =  9.83957E-01
      no. of under-relaxation cycles=   0
       bbig=  2.04815E-05, ubbig= AL+++
       bneg=  0.00000E+00, ubneg= none
      bgamx=  1.67263E-05, ubgamx= AL+++
        bxi= -2.97145E-05, bxistq= -4.02483E-05
iter=   4, delmax=  1.60330E-05 (unrelaxed)
       del(CONC    AL+++   )= -1.60330E-05, delfnc =  9.82702E-01
      beta(CONC    AL+++   )=  3.68849E-07, betfnc =  9.81991E-01
      no. of under-relaxation cycles=   0
       bbig=  3.68849E-07, ubbig= AL+++
       bneg=  0.00000E+00, ubneg= none
      bgamx=  3.16516E-07, ubgamx= AL+++
        bxi= -5.62303E-07, bxistq= -7.05113E-07
iter=   5, delmax=  2.94718E-07 (unrelaxed)
       del(CONC    AL+++   )= -2.94718E-07, delfnc =  9.81618E-01
      beta(CONC    AL+++   )=  7.00449E-09, betfnc =  9.81010E-01
      no. of under-relaxation cycles=   0
       bbig=  7.00449E-09, ubbig= AL+++
       bneg=  0.00000E+00, ubneg= none
```

```
          bgamx=  6.01873E-09, ubgamx= AL+++
            bxi= -1.06925E-08, bxistq= -1.33209E-08


 hybrid newton-raphson iteration converged in   5 steps
```

----- Summary of the Aqueous Phase -----

----- Elemental composition of the aqueous phase -----

element	mg/l	mg/kg	moles/kg
O	945595.2935	924010.4104	.5775281638E+02
NA	13516.2162	13207.6847	.5745026908E+00
CA	41.0163	40.0800	.1000000004E-02
MG	26835.4218	26222.8559	.1078907875E+01
AL	.0276	.0270	.1000000007E-05
SI	76.6980	74.9472	.2668538021E-02
H	116887.8676	114219.6955	.1133244325E+03
CL	18140.5910	17726.5000	.5000000001E+00
FE	9.1210	8.9128	.1595932989E-03

----- elemental composition as strict basis species -----

species	mg/l	mg/kg	moles/kg
H2O	1064732.9482	1040428.5376	.5775281638E+02
NA+	13516.2162	13207.6847	.5745026908E+00
CA++	41.0163	40.0800	.1000000004E-02
MG++	26835.4218	26222.8559	.1078907875E+01
AL+++	.0276	.0270	.1000000007E-05
H4SIO4	262.4772	256.4857	.2668538021E-02
H+	116887.8676	114219.6955	.1133244325E+03
CL-	18140.5910	17726.5000	.5000000001E+00
FE++	9.1210	8.9128	.1595932989E-03

--- equivalent composition of the aqueous phase (cte
balances) ---

```
            original basis                          existing basis

   species               moles/kg h2o   species               moles/kg
h2o
```

```
     H2O                .5000000000E+01     H2O                .
5775281638E+02
     NA+                .5000000000E+01     NA+                .
5745026908E+00
     CA++               .5000000000E+01     CA++               .
1000000004E-02
     MG++               .5000000000E+01     MG++               .
1078907875E+01
     AL+++              .5000000000E+01     AL+++              .
1000000007E-05
     H4SIO4(AQ)         .5000000000E+01     H4SIO4(AQ)         .
2668538021E-02
     H+                 .5000000000E+01     H+                 .
1133244325E+03
     CL-                .5000000000E+01     CL-                .
5000000001E+00
     FE++               .5000000000E+01     FE++               .
1595932989E-03


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                            ph           eh            pe


     internal ph scale               6.6000         .4547
3.1693E+00
     modified nbs ph scale           6.5872         .4566
3.1821E+00
     rational ph scale               6.3535         .4901
3.4158E+00

   phcl =      7.1859


                            activity of water =     .98384
                        log activity of water =    -.00707

                     true osmotic coefficient=     .41000
           stoichiometric osmotic coefficient=     .40219

                     sum of true molalities=    2.2050872587804
           sum of stoichiometric molalities=    2.2479475840349

                     true ionic strength=     .5170779555312
           stoichiometric ionic strength=    2.7267131246933
```

```
       equiv. stoich. ionic strength (CL-   ) =     .5000000001291

          ----- electrical balance totals -----


                                            equiv/kg

                        sigma(mz) cations =      .5169772066E+00
                        sigma(mz) anions  =     -.5169772064E+00
                             total charge =      .1033954413E+01
                              mean charge =      .5169772065E+00
                         charge imbalance =      .1736975008E-09

            total charge = sigma(mz) cations + abs ( sigma(mz)
anions )
            mean charge = 1/2 total charge


            the electrical imbalance is

                              .00 per cent of the total charge
                              .00 per cent of the mean charge
                              .00 per cent of sigma(mz) cations
                              .00 per cent of abs ( sigma(mz) anions )


          ----- electrical balancing on NA+    -----

                   mg/l           mg/kg           moles/kg

          input    11763.4055      11494.8850     .5000000000E+00
          final    13516.2162      13207.6847     .5745026908E+00
          adj       1752.8107       1712.7997     .7450269080E-01


                    ----- activity ratios of ions -----

          log ( act(NA+         ) / act(h+)xx 1 ) =      6.0659
          log ( act(CA++        ) / act(h+)xx 2 ) =      8.2140
          log ( act(MG++        ) / act(h+)xx 2 ) =      6.0863
          log ( act(AL+++       ) / act(h+)xx 3 ) =     -6.6196
          log ( act(H4SIO4(AQ)  )                 ) =     -2.8293
          log ( act(CL-         ) x act(h+)xx 1 ) =     -7.1859
          log ( act(FE++        ) / act(h+)xx 2 ) =      3.6938
          log ( act(O2(AQ)      )                 ) =    -30.8749
          log ( act(H2(AQ)      )                 ) =     -1.4941
          log ( act(FE+++       ) / act(h+)xx 3 ) =     -4.3001
          log ( act(OH-         ) x act(h+)xx 1 ) =     -8.0783
          log ( act(H8SI3O10(AQ))                 ) =    -10.7812
          log ( act(H6SI2O7(AQ) )                 ) =     -5.2263
```

----- distribution of aqueous species -----

species	molal conc	log conc	log g	activity	log act
MG(OH)2(AQ)	.1079E+01	.0330	.0000	.1079E+01	.0330
NA+	.5157E+00	-.2876	-.2465	.2924E+00	-.5341
CL-	.4577E+00	-.3394	-.2465	.2595E+00	-.5859
OH-	.5864E-01	-1.2318	-.2465	.3325E-01	-1.4783
NACL(AQ)	.4210E-01	-1.3757	.0000	.4210E-01	-1.3757
H2(AQ)	.3206E-01	-1.4941	.0000	.3206E-01	-1.4941
NAOH(AQ)	.1669E-01	-1.7774	.0000	.1669E-01	-1.7774
H4SIO4(AQ)	.1482E-02	-2.8293	.0000	.1482E-02	-2.8293
H3SIO4-	.6461E-03	-3.1897	-.2465	.3663E-03	-3.4362
CA(H3SIO4)+	.3758E-03	-3.4250	-.2465	.2130E-03	-3.6715
CA(OH)+	.3091E-03	-3.5099	-.2465	.1752E-03	-3.7564
CACL+	.2112E-03	-3.6753	-.2465	.1197E-03	-3.9218
FE(H3SIO4)+	.1529E-03	-3.8156	-.2465	.8667E-04	-4.0621
CA++	.1000E-03	-4.0000	-.9860	.1033E-04	-4.9860
MG(OH)+	.1637E-04	-4.7859	-.2465	.9281E-05	-5.0324
FE(OH)3-	.5953E-05	-5.2252	-.2465	.3375E-05	-5.4717
H6SI2O7(AQ)	.5938E-05	-5.2263	.0000	.5938E-05	-5.2263
CACL2(AQ)	.3857E-05	-5.4137	.0000	.3857E-05	-5.4137
AL(OH)4-	.7860E-06	-6.1046	-.2465	.4456E-06	-6.3511
MG++	.7453E-06	-6.1277	-.9860	.7697E-07	-7.1137
MGCL+	.7436E-06	-6.1287	-.2465	.4215E-06	-6.3752
FE(OH)2	.5862E-06	-6.2319	.0000	.5862E-06	

```
-6.2319
   HCL(AQ)              .5608E-06    -6.2512      .0000    .5608E-06
-6.2512
   H+                   .4431E-06    -6.3535     -.2465    .2512E-06
-6.6000
   AL(OH)SI(OH)-        .2099E-06    -6.6780     -.2465    .1190E-06
-6.9245
   FE(OH)+              .8461E-07    -7.0726     -.2465    .4797E-07
-7.3191
   FECL2(AQ)            .7835E-07    -7.1060      .0000    .7835E-07
-7.1060
   MG(H3SIO4)+          .8355E-08    -8.0781     -.2465    .4736E-08
-8.3245
   AL(OH)3(AQ)          .4088E-08    -8.3884      .0000    .4088E-08
-8.3884
   FECL+                .3346E-08    -8.4755     -.2465    .1897E-08
-8.7220
   FE++                 .3018E-08    -8.5202     -.9860    .3117E-09
-9.5062
   H8SI3O10(AQ)         .1655E-10   -10.7812      .0000    .1655E-10
-10.7812
   FECL2+               .1646E-18   -18.7837     -.2465    .9329E-19
-19.0302
   FECL++               .8138E-19   -19.0895     -.9860    .8406E-20
-20.0754
   FE+++                .1313E-21   -21.8816    -2.2185    .7942E-24
-24.1001
   AL+++                .6292E-24   -24.2012    -2.2185    .3805E-26
-26.4196
   FECL4-               .1724E-24   -24.7634     -.2465    .9775E-25
-25.0099
   O2(AQ)               .1334E-30   -30.8749      .0000    .1334E-30
-30.8749
   FECL3                .2631E-49   -49.5799      .0000    .2631E-49
-49.5799


           ----- major aqueous species contributing to mass balances
-----


 aqueous species accounting for 99% or more of NA+

    species            molal conc    per cent

   NA+                   .5157E+00    89.77
   NACL(AQ)              .4210E-01     7.33
   NAOH(AQ)              .1669E-01     2.91
 - - - - - - - - - - - - - - - - - - - - - - -
   total                              100.00
```

```
aqueous species accounting for 99% or more of CA++

    species            molal conc    per cent

  CA(H3SIO4)+            .3758E-03    37.58
  CA(OH)+                .3091E-03    30.91
  CACL+                  .2112E-03    21.12
  CA++                   .1000E-03    10.00
- - - - - - - - - - - - - - - - - - - - - - -
  total                               99.61


aqueous species accounting for 99% or more of MG++

    species            molal conc    per cent

  MG(OH)2(AQ)            .1079E+01   100.00
- - - - - - - - - - - - - - - - - - - - - - -
  total                              100.00


aqueous species accounting for 99% or more of AL+++

    species            molal conc    per cent

  AL(OH)4-               .7860E-06    78.60
  AL(OH)SI(OH)-          .2099E-06    20.99
- - - - - - - - - - - - - - - - - - - - - - -
  total                               99.59


aqueous species accounting for 99% or more of H4SIO4(AQ)

    species            molal conc    per cent

  H4SIO4(AQ)             .1482E-02    55.52
  H3SIO4-                .6461E-03    24.21
  CA(H3SIO4)+            .3758E-03    14.08
  FE(H3SIO4)+            .1529E-03     5.73
- - - - - - - - - - - - - - - - - - - - - - -
  total                               99.55


aqueous species accounting for 99% or more of CL-

    species            molal conc    per cent

  CL-                    .4577E+00    91.54
```

```
  NACL(AQ)               .4210E-01     8.42
- - - - - - - - - - - - - - - - - - - - - - -
  total                               99.96


 aqueous species accounting for 99% or more of FE++

    species           molal conc    per cent

  FE(H3SIO4)+            .1529E-03    95.80
  FE(OH)3-               .5953E-05     3.73
- - - - - - - - - - - - - - - - - - - - - - -
  total                               99.53



          ----- summary of aqueous redox reactions -----

     couple         eh, volts      pe-       log fo2     ah, kcal

  default               .455     .3169E+01    -26.800      10.487
  O2(AQ)  /H2O          .455     .3169E+01    -26.800      10.487
  H2(AQ)  /H2O          .455     .3169E+01    -26.800      10.487
  FE+++   /FE++         .455     .3169E+01    -26.800      10.487


          ----- summary of aqueous non-equilibrium non-redox
reactions -----

     couple       affinity, kcal

     none


          ----- summary of stoichiometric mineral saturation states
-----


  mineral       log q/k   aff, kcal  state           mineral
log q/k   aff, kcal  state

 MAGNETITE          .000       .000  satd          CORUNDUM
-9.007    -29.805
 LIME             -5.644    -18.676                SPINEL
-8.660    -28.656
 BRUCITE           -.328     -1.085                DIASPORE
-4.401    -14.563
 ANDALUSITE      -10.751    -35.575                KYANITE
-10.382    -34.356
 SILLIMANITE     -10.679    -35.338                GLAUCOPHANE
```

```
-14.813    -49.016
 LAWSONITE         -9.762    -32.304                  PUMPELLYITE
-22.246    -73.614
 ZOISITE          -13.354    -44.188                  CLINOZOISITE
-13.569    -44.898
 MONTICELLITE      -8.004    -26.484                  MERWINITE
-4.653    -15.397
 CHRYSOTILE         -.189      -.627                  ENSTATITE-OR
-.679     -2.247
 ENSTATITE-PR       -.802     -2.652
DIOPSIDE            .000       .000  satd
 HEDENBERGITE      -1.137     -3.762                  JADEITE
-6.329    -20.943
 FERROSILITE       -1.351     -4.469                  WOLLASTONITE
-1.066     -3.526
 PSEUDOWOLLAS      -1.212     -4.012                  TREMOLITE
-1.605     -5.311
 ANTHOPHYLLIT      -5.232    -17.312                  CORDIERITE
-25.482    -84.319
 ALBITE            -7.596    -25.134                  ANORTHITE
-10.526    -34.830
 GEHLENITE        -11.581    -38.322                  KAOLINITE
-12.483    -41.306
 ANTIGORITE          .000       .000  satd            PYROPHYLLITE
-15.576    -51.540
 TALC              -2.080     -6.881                  PARAGONITE
-15.326    -50.714
 MARGARITE        -18.345    -60.703                  PREHNITE
-10.259    -33.948
 CLINOCHLORE        -.946     -3.130                  CHAMOSITE
-2.210     -7.312
 PYROPE            -3.850    -12.740                  ALMANDINE
-3.876    -12.827
 GROSSULAR         -2.828     -9.359                  QUARTZ-ALPHA
-1.709     -5.654
 QUARTZ-BETA       -1.780     -5.891                  COESITE
-1.889     -6.250
 IRON-ALPHA        -2.617     -8.660                  IRON-GAMMA
-2.358     -7.803
 HALITE            -2.947     -9.750                  CRISTOBALITE
-2.097     -6.940
 CRISTOBALITE      -2.313     -7.653


     3 approx. saturated pure minerals
     0 approx. saturated end-members of specified solid solutions
     0 saturated end-members of hypothetical solid solutions


     0 supersaturated pure minerals
```

```
     0 supersatd. end-members of specified solid solutions
     0 supersatd. hypothetical solid solution phases



                    ----- summary of gases -----


     gas                    fugacity    log fugacity

   O2(G)                   .158489E-26    -26.80000
   H2(G)                   .189595E+03      2.27783
   H2O(G)                  .639774E+04      3.80603

 ----- end of output -----
 ----- pickup file successfully written -----

 --- reading the input file ---
```

```
EQ6, version 3245R100

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Run



--- reading the input file ---
This run calculates the reaction between serp fluid + oxide gabbro

Revised antigorite volumes

Reactant minerals present:

Chrysotile 1 mole

nxopt = all (suppress al mineral precipitation)

isothermal titration system model at 450 C, 10 kb



endit.
    nmodl1=  1              nmodl2=  0
    tempc0=  4.50000E+02     jtemp=  0
       tk1=  0.00000E+00       tk2=  0.00000E+00       tk3=
0.00000E+00
    zistrt=  0.00000E+00     zimax=  1.00000E+01
     tstrt=  0.00000E+00    timemx=  0.00000E+00
    kstpmx=        10000     cplim=  0.00000E+00
    dzprnt=  1.00000E+38    dzprlg=  2.00000E-01    ksppmx= 10000
    dzplot=  1.00000E+38    dzpllg=  1.00000E+04    ksplmx= 10000
     ifile= 16
                  1    2    3    4    5    6    7    8    9   10
  iopt1-10=     0    0    0    1    0    0    0    0    0    0
     11-20=     0    0    0    0    0    0    0    0    0    0
  iopr1-10=     0    0    0    0    1    0    0    1    0    0
 iopr11-20=     0    0    0    0    0    0    0    0    0    0
  iodb1-10=     0    0    0    0    0    0    0    0    0    0
     11-20=     0    0    0    0    0    0    0    0    0    0
     nxopt=  0
```

```
       nffg =  0
        nrct=     4
   reactant= PLAGIOCLASE(SS)
       jcode=  1               jreac=  0
        morr=  1.00000E+02      modr=  0.00000E+00
    ALBITE                6.00000E-01
    ANORTHITE             4.00000E-01
   endit.
         nsk=  0                  sk=  0.00000E+00         fk=
0.00000E+00
         nrk=  1                nrpk=  0
         rk1=  1.67530E+00       rk2=  0.00000E+00        rk3=
0.00000E+00
   reactant= CLINOPYROXENE(SS)
       jcode=  1               jreac=  0
        morr=  1.00000E+02      modr=  0.00000E+00
    DIOPSIDE              8.00000E-01
    HEDENBERGITE          2.00000E-01
   endit.
         nsk=  0                  sk=  0.00000E+00         fk=
0.00000E+00
         nrk=  1                nrpk=  0
         rk1=  2.01920E+00       rk2=  0.00000E+00        rk3=
0.00000E+00
   reactant= MAGNETITE
       jcode=  0               jreac=  0
        morr=  1.00000E+02      modr=  0.00000E+00
         nsk=  0                  sk=  0.00000E+00         fk=
0.00000E+00
         nrk=  1                nrpk=  0
         rk1=  2.16000E-01       rk2=  0.00000E+00        rk3=
0.00000E+00
   reactant= TREMOLITE
       jcode=  0               jreac=  0
        morr=  1.00000E+02      modr=  0.00000E+00
         nsk=  0                  sk=  0.00000E+00         fk=
0.00000E+00
         nrk=  1                nrpk=  0
         rk1=  1.83200E-01       rk2=  0.00000E+00        rk3=
0.00000E+00
      dlzidp=  0.00000E+00
       tolbt=  1.00000E-10     toldl=  1.00000E-10       tolx=
0.00000E+00
      tolsat=  0.00000E+00    tolsst=  0.00000E+00
      screw1=  0.00000E+00    screw2=  0.00000E+00     screw3=
0.00000E+00
      screw4=  0.00000E+00    screw5=  0.00000E+00     screw6=
0.00000E+00
      zklogu=         .000    zklogl=         .000      zkfac=          .
000
```

```
     dlzmx1=  0.00000E+00    dlzmx2=  0.00000E+00    nordlm=  0
     itermx=  0              ntrymx=  0
     npslmx=  0              nsslmx=  0              ioscan=  0
 300 C & 10.0 kbar
 Data0 from DEW

 Revised antigorite volumes

 Atg1 fluid in equilibrium with:

 Antigorite
 Magnetite
 Diopside


 log fO2 in between QFM and HM




 endit.
     uacion= CL-
     tempci=  4.50000E+02
      nxmod=  5
    species= HEMATITE
       type=  1              option= -1              xlkmod=
0.00000E+00
    species= FORSTERITE
       type=  1              option= -1              xlkmod=
0.00000E+00
    species= FAYALITE
       type=  1              option= -1              xlkmod=
0.00000E+00
    species= ENSTATITE-CL
       type=  1              option= -1              xlkmod=
0.00000E+00
    species= PERICLASE
       type=  1              option= -1              xlkmod=
0.00000E+00
      iopg1=  0               iopg2= -1               iopg3=  0
      iopg4=  0               iopg5=  1               iopg6=  0
      iopg7=  0               iopg8=  0               iopg9=  0
     iopg10=  0
        kct=  9                 ksq= 10                 kmt= 10
        kxt= 10                kdim= 10                kprs=  0
 component            moles              moles aqueous
    O                  5.775281637771040E+01
0.000000000000000E+00
    NA                 5.745026907971400E-01
0.000000000000000E+00
```

```
    CA                  1.000000003513890E-03
0.000000000000000E+00
    MG                  1.078907875205220E+00
0.000000000000000E+00
    AL                  1.000000007004490E-06
0.000000000000000E+00
    SI                  2.668538021482200E-03
0.000000000000000E+00
    H                   1.133244325036410E+02
0.000000000000000E+00
    CL                  5.000000001310330E-01
0.000000000000000E+00
    FE                  1.595932988871920E-04
0.000000000000000E+00
    electr              1.736975008270750E-10
    H2O                 H2O                  1.744360912091830E+00
    NA+                 NA+                 -2.875952658150730E-01
    CA++                CA++                -3.999996928119610E+00
    MG++                MG++                -6.127675197590440E+00
    AL+++               AL+++               -2.420118078219210E+01
    H4SIO4(AQ)          H4SIO4(AQ)          -2.829258412160970E+00
    H+                  H+                  -6.353505231877080E+00
    CL-                 CL-                 -3.394376202669030E-01
    FE++                FE++                -8.520247380000621E+00
    O2(G)               O2(G)               -2.680000000000000E+01

 --- the input file has been successfully read ---

 --- reading the data1 file ---


                     --- list of solid solutions ---

  1  K-FELDSPAR(SS)           no.components=   2
          model type=   0  (ideal solution                )
  2  PLAGIOCLASE(SS)          no.components=   2
          model type=   0  (ideal solution                )
  3  ORTHOPYROXENE(SS)        no.components=   2
          model type=   0  (ideal solution                )
  4  OLIVINE(SS)              no.components=   2
          model type=   0  (ideal solution                )
  5  BIOTITE(SS)              no.components=   2
          model type=   0  (ideal solution                )
  6  GARNET(SS)               no.components=   3
          model type=   0  (ideal solution                )
  7  TALC(SS)                 no.components=   2
          model type=   0  (ideal solution                )
  8  CLINOPYROXENE(SS)        no.components=   3
          model type=   0  (ideal solution                )
  9  CPX_SUBCALCIC(SS)        no.components=   3
```

```
         model type=   0  (ideal solution                )
10  CA-AMPHIBOLE(SS)          no.components=   2
         model type=   0  (ideal solution                )
11  CHLORITE(SS)              no.components=   2
         model type=   0  (ideal solution                )
12  MAGNETITE(SS)             no.components=   2
         model type=   0  (ideal solution                )
13  SPHALERITE(SS)            no.components=   2
         model type=   0  (ideal solution                )
14  CALCITE(SS)               no.components=   3
         model type=   0  (ideal solution                )
15  APATITE(SS)               no.components=   3
         model type=   0  (ideal solution                )

--- the data1 file has been successfully read ---
the species HEMATITE                 has been user-suppressed

the species FORSTERITE               has been user-suppressed

the species FAYALITE                 has been user-suppressed

the species ENSTATITE-CL             has been user-suppressed

the species PERICLASE                has been user-suppressed





eeeee  qqq   666
e     q   q 6
eeee  q   q 6666
e     q q q 6   6
eeeee  qqq   666
          q



eq6.3245R100
 supported by eqlib.3245R136


This run calculates the reaction between serp fluid + oxide gabbro

Revised antigorite volumes

Reactant minerals present:
```

Chrysotile 1 mole

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isothermal titration system model at 450 C, 10 kb

300 C & 10.0 kbar
Data0 from DEW

Revised antigorite volumes

Atg1 fluid in equilibrium with:

Antigorite
Magnetite
Diopside

log fO2 in between QFM and HM

DATA FILE GENERATED WITH PROCESS REACTIONS PACKAGE THEN CONVERTED TO HYDROUS, AQ
log K DATA refer to the range of temperatures at the pressure specified below
LAST REVISED May, 2019

the activity coefficients of aqueous solute species and the activity of water are calculated according to b-dot equation plus others

no. of elements in the data base = 31
no. of elements dimensioned for = 70
no. of active elements = 9

no. of aqueous species dimensioned for = 750
no. of aqueous species loaded = 87
no. of active aqueous species = 40

no. of aqueous reactions dimensioned for = 679
no. of aqueous reactions loaded = 55
no. of active aqueous reactions = 31

```
          no. of pure minerals dimensioned for = 750
          no. of pure minerals loaded =  57
          no. of active pure minerals =  39

          no. of gases dimensioned for =  15
          no. of gases loaded =   3
          no. of active gases =   3

             no. of solid solutions in the data base =  15
             no. of solid solutions dimensioned for =  20
             no. of active solid solutions =   6

 zistrt =  0.000000E+00 (initial value of zi)
 zimax  =  1.000000E+01 (maximum value of zi)
 timemx =  1.000000E+38 (maximum value of time, sec)
 kstpmx =         10000 (maximum number of steps this run)


    dzprnt =  1.000000E+38 (linear print interval)
    dzprlg =  2.000000E-01 (logarithmic print interval)
    dlzidp =  1.000000E+38 (p.r.s. transfer interval)

    maximum permitted step sizes.....
       dlzmx1 =  1.000000E-08 (nord=0)
       dlzmx2 =  1.000000E+38 (nord.ge.1)
    nordlm =  6 (maximum permitted order)


 temperature =    450.000 c


 nmodl1 =  1 (physical system switch)
   1 = titration, 2 = closed, 3 = flow-through)
 nmodl2 =  0 (economy mode permission switch)
   0 = normal, 1 = economy, 3 = super economy)

    iopt1  =  0 (kinetic mode switch)
    iopt2  =  0 (suppress phase boundary location)
    iopt3  =  0 (interfacing output switch)
    iopt4  =  1 (permit solid solutions switch)
    iopt5  =  0 (remove initial solids switch)
    iopt6  =  0 (clear p.r.s. at start switch)
    iopt7  =  0 (auto basis switch mode switch)
    iopt8  =  0 (linear vs. log taylor-s series)
    iopt9  =  0 (not used)
    iopt10 =  0 (not used)
    iopt11 =  0 (suppress all redox reactions switch)
    iopt12 =  0 (not used)
```

```
        iopt13 =  0 (tab file output switch)
        iopt14 =  0 (ahv input file access)
        iopt15 =  0 (not used)
        iopt16-20   (not used)
        ifile  = 16 (supplementary input file)

           iopg1  =  0 (choice of act. coeff. equations)
           iopg2  = -1 (choice of ph scale)
           iopg3  =  0 (e-lambda switch for hydration theory)
           iopg4  =  0 (not used)
           iopg5  =  1 (use bdot term instead of co2 polynomial)
           iopg6  =  0 (choice of pitzer j(x) approximation)
           iopg7  =  0 (not used)
           iopg8  =  0 (not used)
           iopg9  =  0 (not used)
           iopg10 =  0 (not used)

        iopr1  =  0 (print loading of species from data1)
        iopr2  =  0 (print derivatives of basis elements)
        iopr3  =  0 (print loaded species and log k values)
        iopr4  =  0 (print aqueous species distribution)
        iopr5  =  1 (print cation/h+ activity ratios)
        iopr6  =  0 (print element/oxide comp. of mineral assemblage)
        iopr7  =  0 (print mineral affinity summary)
        iopr8  =  1 (print gas fugacity summary)
        iopr9  =  0 (print mean molal activity coefficient)
        iopr10 =  0 (print tabulation of pitzer coefficients)
        iopr11 =  0 (print major species for each element)
        iopr12-20   (not used)

           iodb1  =  0 (enable comp. messages)
           iodb2  =  0 (print pre-newton-raphson optimization)
           iodb3  =  0 (print order/scaling info.)
           iodb4  =  0 (print newton iteration info.)
           iodb5  =  0 (print search iterations)
           iodb6  =  0 (print hpsatz iterations)
           iodb7  =  0 (print f.d. and t.s. calculations)
           iodb8  =  0 (turns iodb3 on and off)
           iodb9  =  0 (print kinetics info.)
           iodb10 =  0 (check basis var. f.d. and t.s.)
           iodb11 =  0 (check reac. rate f.d. and t.s.)
           iodb12 =  0 (iteration variable killer option)
           iodb13 =  0 (not used)
           iodb14 =  0 (not used)
           iodb15 =  0 (not used)
           iodb16 =  0 (turn on akmatr prints)
           iodb17-20   (not used)

        tolbt  =  1.000000E-10 (residual function convergence
tolerance)
```

```
       toldl  =  1.000000E-10 (correction term convergence tolerance)
       tolx   =  1.000000E-08 (sol-sol reactant/product identity
tolerance)
       tolsat =  5.000000E-03 (lower supersaturation tolerance)
       tolsst =  1.000000E-02 (upper supersaturation tolerance)


   screw1 =  1.000E-04 (primary step-size parameter for basis
variables)
   screw2 =     .00000 (not used)
   screw3 =  1.000E-04 (step size parameter for rate functions)
   screw4 =  1.000E-04 (corrector parameter for rate functions)
   screw5 =    4.00000 (under-relaxation control for n-r iteration)
   screw6 =    4.00000 (step size parameter for economy mode)

       zklogu =     -6.000 (threshhold log mass for solids)
       zklogl =      2.000 (log mass decrement for p.r.s shift)
        zkfac =       .980 (shift adjustment factor)
       zklgmn =     -6.009 (minimum log mass after a shift)


           itermx= 30 (newton-raphson iteration limit)
           ntrymx= 25 (phase assemblage try limit)
           npslmx=  8 (critical phase instability slide limit)
           nsslmx=  3 (critical redox instability slide limit)


      iacion = 16, CL-          (defines xisteq)



   --- inactive loaded aqueous species ---


     K+                      SR++                    ZN++
     PB++                    AG+                     BA++
     CO3--                   NH4+                    SO4--
     F-                      HG++                    MN++
     CU+                     AU+                     CS+
     CD++                    U++++                   HPO4--
     CR++                    TI(OH)4(AQ)             ZR(OH)4(AQ)
     EU++                    N2(AQ)                  HS-
     S3-                     HG2++                   CU++
     NO3-                    HCO3-                   HCOO-
     CH3COO-                 CH3CH2COO-              CN-
     CO(AQ)                  CH4(AQ)                 ETHANE(AQ)
     PROPANE(AQ)             METHANOL(AQ)            ETHANOL(AQ)
     PROPANOL                ETHYLENE(AQ)            GLYCINE,AQ
     DIGLYCINE,AQ            DKP,AQ                  GLUTAMATE
     UO2++
```

```
   --- inactive loaded minerals ---

     HEMATITE                 PERICLASE                FORSTERITE
     FAYALITE                 ENSTATITE-CL             ENSTATITE-OR
     DIOPSIDE                 HEDENBERGITE             JADEITE
     CA-AL-PYROXENE           FERROSILITE              ALBITE
     ANORTHITE                CLINOCHLORE              CHAMOSITE
     PYROPE                   ALMANDINE                GROSSULAR


                     --- reactants and rate coefficients ---

      forward/dissolution=

   PLAGIOCLASE(SS)           arbitrary relative rate
                    rk1=  1.67530E+00   rk2=  0.00000E+00   rk3=
0.00000E+00
   CLINOPYROXENE(SS)         arbitrary relative rate
                    rk1=  2.01920E+00   rk2=  0.00000E+00   rk3=
0.00000E+00
   MAGNETITE                 arbitrary relative rate
                    rk1=  2.16000E-01   rk2=  0.00000E+00   rk3=
0.00000E+00
   TREMOLITE                 arbitrary relative rate
                    rk1=  1.83200E-01   rk2=  0.00000E+00   rk3=
0.00000E+00

   reverse/precipitation=

   PLAGIOCLASE(SS)           no precipitation rate
   CLINOPYROXENE(SS)         no precipitation rate
   MAGNETITE                 no precipitation rate
   TREMOLITE                 no precipitation rate


           --- solid solution reactants ---


          PLAGIOCLASE(SS)
            mol. wt. =       268.618g/mol
            molar volume =       100.798 cc

                            composition

                                          mole fraction

                     ALBITE                 6.00000E-01
```

```
                    ANORTHITE            4.00000E-01

          CLINOPYROXENE(SS)
            mol. wt. =      222.861g/mol
            molar volume =       66.200 cc

                          composition

                                        mole fraction

                    DIOPSIDE             8.00000E-01
                    HEDENBERGITE         2.00000E-01
                    JADEITE              0.00000E+00

 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
-


 stepping to zi=  0.0000E+00, delzi=  0.0000E+00, nord= 0

   attempted species assemblage no.   1

              1      1  H2O
              2      2  NA+
              3      4  CA++
              4      5  MG++
              5      6  AL+++
              6      7  H4SIO4(AQ)
              7     13  H+
              8     16  CL-
              9     21  FE++
             10     32  O2(G)

               ncycle=  0
 iter =    5
       0 supersaturated pure minerals
       2 supersaturated solid solutions

                          the most supersaturated phases     affinity,
kcal

                            1   50800   CLINOPYROXENE(SS)        .
10118919
                            2   50900   CPX_SUBCALCIC(SS)        .
10118856


   attempted species assemblage no.   2

              1      1  H2O
```

```
              2      2  NA+
              3      4  CA++
              4      5  MG++
              5      6  AL+++
              6      7  H4SIO4(AQ)
              7     13  H+
              8     16  CL-
              9     21  FE++
             10     32  O2(G)
             11      1  CLINOPYRDIOPSIDE
             12      2  CLINOPYRHEDENBERGITE
             13      3  CLINOPYRJADEITE

 iter =    7
       1 supersaturated pure minerals
       0 supersaturated solid solutions

                         the most supersaturated phases     affinity,
kcal

                           1       1   MAGNETITE                .
02713454


   attempted species assemblage no.   3

              1      1  H2O
              2      2  NA+
              3      4  CA++
              4      5  MG++
              5      6  AL+++
              6      7  H4SIO4(AQ)
              7     13  H+
              8     16  CL-
              9     21  FE++
             10     32  O2(G)
             11      1  MAGNETITE
             12      1  CLINOPYRDIOPSIDE
             13      2  CLINOPYRHEDENBERGITE
             14      3  CLINOPYRJADEITE

 iter =    9

 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  0.00000000000000E+00
                    log of reaction progress =    -999.0000000
```

```
                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 change in the product phase assemblage

 start or re-start of run


                              --- reactant summary ---


     definitions and conventions

          delta x = x now - x at start
          affinity is + for forward direction (dissolution),
                      - for reverse direction (precipitation)
          rates are + for forward direction (dissolution),
                    - for reverse direction (precipitation)


         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        1.00000E+02    0.00000E+00    2.68618E+04
0.00000E+00
   CLINOPYROXENE(SS)      1.00000E+02    0.00000E+00    2.22861E+04
0.00000E+00
   MAGNETITE              1.00000E+02    0.00000E+00    2.31539E+04
0.00000E+00
   TREMOLITE              1.00000E+02    0.00000E+00    8.12370E+04
0.00000E+00


               current total mass =  1.53539E+05 grams
               delta total mass   =  0.00000E+00 grams
               delta total volume =       .00000 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           28.1324    1.67530E+00
   CLINOPYROXENE(SS)           .1345    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.6389    1.83200E-01

          affinity of the overall irreversible reaction=    48.163
kcal
```

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434542E+05	5.775244E+01	5.775261E+01
NA	1.205627E+04	5.745010E-01	5.745027E-01
CA	3.534963E+01	9.662060E-04	9.662089E-04
MG	2.393611E+04	1.078873E+00	1.078876E+00
AL	2.462897E-02	9.999817E-07	9.999848E-07
SI	6.668088E+01	2.600948E-03	2.600956E-03
H	1.042623E+05	1.133241E+02	1.133244E+02
CL	1.618114E+04	4.999985E-01	5.000000E-01
FE	7.970633E+00	1.563527E-04	1.563532E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.5998	.4548	3.1695E+00
modified nbs ph scale	6.3533	.4901	3.4160E+00
rational ph scale	6.3533	.4901	3.4160E+00

phcl = 7.1857

oxygen fugacity = 1.58487E-27
log oxygen fugacity = -26.80001

```
                         activity of water =    .98384
              log activity of water =   -.00707
              alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                   ionic strength =  5.170393E-01 molal
                sum of molalities =    2.2049456040005
              osmotic coefficient =     .41003
                   equiv. stoich. ionic strength =  4.999985E-01
molal

                        mass of solution =   1.095504 kg
                        mass of solvent  =   1.000003 kg
                        mass of solutes  =    .095501 kg
                        conc of solutes  =   8.717509 per cent (w/w)


   species               moles        grams         conc        log
conc      log g      log act

   H2O                 5.55088E+01   1.00000E+03
   NA+                 5.15714E-01   1.18561E+01   5.15712E-01     -.
28759     -.24649     -.53408
   CA++                9.74353E-05   3.90521E-03   9.74350E-05
-4.01129     -.98596    -4.99725
   MG++                7.45844E-07   1.81277E-05   7.45842E-07
-6.12735     -.98596    -7.11331
   AL+++               6.33075E-25   1.70813E-23   6.33073E-25
-24.19855    -2.21841   -26.41696
   H4SIO4(AQ)          1.44968E-03   1.39335E-01   1.44967E-03
-2.83873      .00000    -2.83873
   H+                  4.43271E-07   4.46772E-07   4.43269E-07
-6.35333     -.24649    -6.59982
   CL-                 4.57685E-01   1.62263E+01   4.57683E-01     -.
33944     -.24649     -.58593
   FE++                3.02059E-09   1.68691E-07   3.02058E-09
-8.51991     -.98596    -9.50587
   O2(AQ)              1.33381E-31   4.26805E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)              3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++               1.31478E-22   7.34267E-21   1.31478E-22
-21.88115    -2.21841   -24.09956
   OH-                 5.86193E-02   9.96956E-01   5.86191E-02
-1.23196     -.24649    -1.47845
   H8SI3O10(AQ)        1.55010E-11   3.91111E-09   1.55009E-11
-10.80964      .00000   -10.80964
   H6SI2O7(AQ)         5.68481E-06   9.90374E-04   5.68479E-06
-5.24529      .00000    -5.24529
```

```
   AL(OH)3(AQ)          4.10873E-09   3.20495E-07   4.10872E-09
-8.38629      .00000    -8.38629
   AL(OH)4-             7.89595E-07   7.50200E-05   7.89593E-07
-6.10260     -.24649    -6.34909
   AL(OH)SI(OH)-        2.06281E-07   3.57093E-05   2.06280E-07
-6.68554     -.24649    -6.93203
   CACL+                2.05788E-04   1.55438E-02   2.05787E-04
-3.68658     -.24649    -3.93307
   CACL2(AQ)            3.75863E-06   4.17156E-04   3.75862E-06
-5.42497      .00000    -5.42497
   CA(OH)+              3.01087E-04   1.71883E-02   3.01086E-04
-3.52131     -.24649    -3.76780
   CA(H3SIO4)+          3.58140E-04   4.84158E-02   3.58139E-04
-3.44595     -.24649    -3.69244
   FE(OH)+              8.46444E-08   6.16671E-06   8.46441E-08
-7.07240     -.24649    -7.31889
   FE(OH)2              5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.95083E-06   6.35958E-04   5.95081E-06
-5.22542     -.24649    -5.47191
   FECL+                3.34889E-09   3.05754E-07   3.34888E-09
-8.47510     -.24649    -8.72159
   FECL2(AQ)            7.84121E-08   9.93897E-06   7.84118E-08
-7.10562      .00000    -7.10562
   FE(H3SIO4)+          1.49647E-04   2.25897E-02   1.49646E-04
-3.82493     -.24649    -4.07142
   MGCL+                7.44151E-07   4.44690E-05   7.44149E-07
-6.12834     -.24649    -6.37483
   MG(OH)+              1.63773E-05   6.76582E-04   1.63772E-05
-4.78576     -.24649    -5.03225
   MG(OH)2(AQ)          1.07886E+00   6.29186E+01   1.07886E+00        .
03296      .00000      .03296
   MG(H3SIO4)+          8.17781E-09   9.76527E-07   8.17778E-09
-8.08736     -.24649    -8.33385
   NACL(AQ)             4.21007E-02   2.46048E+00   4.21006E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)             1.66880E-02   6.67472E-01   1.66880E-02
-1.77760      .00000    -1.77760
   H3SIO4-              6.31907E-04   6.00986E-02   6.31905E-04
-3.19935     -.24649    -3.44584
   HCL(AQ)              5.61022E-07   2.04554E-05   5.61020E-07
-6.25102      .00000    -6.25102

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657400
           log (CA++  /h+**0)            8.2023996
           log (MG++  /h+**0)            6.0863317
           log (AL+++ /h+**0)           -6.6174896
```

```
          log (FE++  /h+**0)           3.6937745
          log (FE+++ /h+**0)          -4.3000902


          --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE                -6.5028179    3.14183E-07    7.27454E-05
1.39874E-05

   CLINOPYROXENE(SS)        -4.4711971    3.37911E-05    7.39002E-03
2.23697E-03
   DIOPSIDE                 -4.5017780    3.14936E-05    6.82001E-03
2.08487E-03
   HEDENBERGITE             -5.6387352    2.29755E-06    5.70009E-04
1.52098E-04
   JADEITE                 -10.8172591    1.52314E-11    3.07886E-09
9.19065E-10


               --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

       phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                 2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)           2.0000000    1.00000E+02

   ALBITE                    1.7781513    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                 1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)         2.0000001    1.00000E+02

   DIOPSIDE                  1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE              1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                 -10.8172591    1.52314E-11    3.07886E-09
9.19065E-10
```

```
                     mass, grams        volume, cc

         created         7.462768E-03       2.250961E-03
         destroyed       0.000000E+00       0.000000E+00
         net             7.462768E-03       2.250961E-03

        warning-- these volume totals may be incomplete because
        of missing partial molar volume data in the data base



         --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3501
 PERICLASE              -4.8210                BRUCITE
-1.0847
 FORSTERITE              -.3962                FAYALITE
-1.7306
 CHRYSOTILE              -.6894                ENSTATITE-CL
-2.2002
 ENSTATITE-OR           -2.2783                ENSTATITE-PR
-2.6837
 DIOPSIDE                -.1012                HEDENBERGITE
-3.8634
 FERROSILITE            -4.5005                WOLLASTONITE
-3.5958
 PSEUDOWOLLASTONITE     -4.0819                TREMOLITE
-5.6389
 ANTIGORITE              -.5339                TALC
-7.0069
 CLINOCHLORE            -3.1458                CHAMOSITE
-7.3276
 GROSSULAR              -9.4240                QUARTZ-ALPHA
-5.6852
 QUARTZ-BETA            -5.9221                COESITE
-6.2814
 IRON-ALPHA             -8.6597                IRON-GAMMA
-7.8030
 HALITE                 -9.7500                CRISTOBALITE-ALPHA
-6.9710
 CRISTOBALITE-BETA      -7.6845
```

```
                   --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -25.2194
     ALBITE                    -25.21944     .9988270     1.00000
     ANORTHITE                 -25.21944     .0011730     1.00000

 ORTHOPYROXENE(SS)        -2.0008
     ENSTATITE-OR               -2.00080     .8243812     1.00000
     FERROSILITE                -2.00080     .1756188     1.00000

 GARNET(SS)               -9.1744
     PYROPE                     -9.17440     .0821270     1.00000
     ALMANDINE                  -9.17440     .0773101     1.00000
     GROSSULAR                  -9.17440     .8405628     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9320069     1.00000
     HEDENBERGITE                 .00000     .0679926     1.00000
     JADEITE                      .00000     .0000005     1.00000

 CPX_SUBCALCIC(SS)          .0000
     DIOPSIDE                     .00000     .9320073     1.00000
     HEDENBERGITE                 .00000     .0679927     1.00000

 CHLORITE(SS)             -3.0696
     CLINOCHLORE                -3.06961     .9483341     1.00000
     CHAMOSITE                  -3.06961     .0516659     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
              .0000    1.0000     .0000   -6.3461     .0000   -6.3461


           --- summary of gas species ---
```

```
          gas                  log fugacity         fugacity
partial pressure

   O2(G)                         -26.80001      1.58487E-27
   H2(G)                           2.27783      1.89596E+02
   H2O(G)                          3.80603      6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.0000E-08, delzi=  1.0000E-08, nord= 0
               ncycle=  0
 steps completed =     1, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =    -10.8067

 stepping to zi=  1.0000E-08, delzi=  6.0775E-17, nord= 0
               ncycle=  0
 steps completed =     2, iter =  1, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =    -10.8067
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  9.99999999999998E-09
                     log of reaction progress =      -8.0000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         1.00000E+02    1.67530E-08    2.68618E+04
4.50015E-06
   CLINOPYROXENE(SS)       1.00000E+02    2.01920E-08    2.22861E+04
4.50001E-06
```

```
   MAGNETITE              1.00000E+02    2.16000E-09    2.31539E+04
5.00123E-07
   TREMOLITE              1.00000E+02    1.83200E-09    8.12370E+04
1.48826E-06


                 current total mass =  1.53539E+05 grams
                 delta total mass   =  1.09885E-05 grams
                 delta total volume =       .00000 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           28.0857    1.67530E+00
   CLINOPYROXENE(SS)           .1345    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.6388    1.83200E-01

          affinity of the overall irreversible reaction=    48.085
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O         8.434542E+05        5.775244E+01        5.775261E+01
      NA        1.205627E+04        5.745010E-01        5.745027E-01
      CA        3.534927E+01        9.661959E-04        9.661989E-04
      MG        2.393610E+04        1.078873E+00        1.078876E+00
      AL        2.520662E-02        1.023436E-06        1.023439E-06
      SI        6.668132E+01        2.600965E-03        2.600973E-03
      H         1.042623E+05        1.133241E+02        1.133244E+02
      CL        1.618114E+04        4.999985E-01        5.000000E-01
      FE        7.970687E+00        1.563538E-04        1.563543E-04

      co3--                         0.000000E+00        0.000000E+00
      so4--                         0.000000E+00        0.000000E+00
      s--                           0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale
```

```
                                       ph            eh            pe

     internal ph scale               6.5998         .4548
3.1695E+00
     modified nbs ph scale           6.3533         .4901
3.4160E+00
     rational ph scale               6.3533         .4901
3.4160E+00

   phcl =      7.1857



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001



                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                           (not def. for t.gt.50 c)

                    ionic strength =  5.170393E-01 molal
                 sum of molalities =    2.2049456092512
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999985E-01
molal

                         mass of solution =   1.095504 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095501 kg
                         conc of solutes  =   8.717509 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15714E-01   1.18561E+01   5.15712E-01     -.
28759     -.24649     -.53408
   CA++                 9.74340E-05   3.90516E-03   9.74337E-05
-4.01129     -.98596    -4.99725
   MG++                 7.45845E-07   1.81278E-05   7.45843E-07
-6.12735     -.98596    -7.11331
   AL+++                6.47923E-25   1.74820E-23   6.47921E-25
-24.18848    -2.21841   -26.40689
```

```
   H4SIO4(AQ)              1.44969E-03   1.39336E-01   1.44968E-03
-2.83873      .00000    -2.83873
   H+                      4.43271E-07   4.46773E-07   4.43269E-07
-6.35333     -.24649    -6.59982
   CL-                     4.57685E-01   1.62263E+01   4.57683E-01      -.
33944     -.24649     -.58593
   FE++                    3.02059E-09   1.68691E-07   3.02058E-09
-8.51991     -.98596    -9.50587
   O2(AQ)                  1.33381E-31   4.26805E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)                  3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                   1.31479E-22   7.34268E-21   1.31478E-22
-21.88115    -2.21841   -24.09956
   OH-                     5.86192E-02   9.96955E-01   5.86191E-02
-1.23196     -.24649    -1.47845
   H8SI3O10(AQ)            1.55013E-11   3.91119E-09   1.55013E-11
-10.80963      .00000   -10.80963
   H6SI2O7(AQ)             5.68488E-06   9.90387E-04   5.68486E-06
-5.24528      .00000    -5.24528
   AL(OH)3(AQ)             4.20509E-09   3.28012E-07   4.20508E-09
-8.37623      .00000    -8.37623
   AL(OH)4-                8.08114E-07   7.67795E-05   8.08111E-07
-6.09253     -.24649    -6.33902
   AL(OH)SI(OH)-           2.11120E-07   3.65470E-05   2.11119E-07
-6.67547     -.24649    -6.92196
   CACL+                   2.05785E-04   1.55436E-02   2.05785E-04
-3.68659     -.24649    -3.93308
   CACL2(AQ)               3.75859E-06   4.17151E-04   3.75858E-06
-5.42498      .00000    -5.42498
   CA(OH)+                 3.01083E-04   1.71880E-02   3.01082E-04
-3.52131     -.24649    -3.76780
   CA(H3SIO4)+             3.58137E-04   4.84155E-02   3.58136E-04
-3.44595     -.24649    -3.69244
   FE(OH)+                 8.46444E-08   6.16671E-06   8.46442E-08
-7.07240     -.24649    -7.31889
   FE(OH)2                 5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-                5.95082E-06   6.35958E-04   5.95081E-06
-5.22542     -.24649    -5.47191
   FECL+                   3.34890E-09   3.05754E-07   3.34889E-09
-8.47510     -.24649    -8.72159
   FECL2(AQ)               7.84121E-08   9.93897E-06   7.84119E-08
-7.10562      .00000    -7.10562
   FE(H3SIO4)+             1.49648E-04   2.25899E-02   1.49647E-04
-3.82493     -.24649    -4.07142
   MGCL+                   7.44152E-07   4.44690E-05   7.44150E-07
-6.12834     -.24649    -6.37483
   MG(OH)+                 1.63773E-05   6.76582E-04   1.63772E-05
-4.78576     -.24649    -5.03225
```

```
   MG(OH)2(AQ)          1.07886E+00   6.29186E+01   1.07886E+00      .
03296      .00000      .03296
   MG(H3SIO4)+          8.17787E-09   9.76534E-07   8.17784E-09
-8.08736    -.24649    -8.33385
   NACL(AQ)             4.21007E-02   2.46048E+00   4.21006E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)             1.66880E-02   6.67472E-01   1.66880E-02
-1.77760      .00000    -1.77760
   H3SIO4-              6.31911E-04   6.00990E-02   6.31909E-04
-3.19935    -.24649    -3.44584
   HCL(AQ)              5.61022E-07   2.04554E-05   5.61020E-07
-6.25102      .00000    -6.25102

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657399
           log (CA++  /h+**0)            8.2023938
           log (MG++  /h+**0)            6.0863317
           log (AL+++ /h+**0)           -6.6074216
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE                -6.4997413    3.16416E-07    7.32626E-05
1.40869E-05

   CLINOPYROXENE(SS)        -4.4706760    3.38317E-05    7.39889E-03
2.23966E-03
   DIOPSIDE                 -4.5012569    3.15314E-05    6.82820E-03
2.08738E-03
   HEDENBERGITE             -5.6382142    2.30031E-06    5.70693E-04
1.52280E-04
   JADEITE                 -10.8066644    1.56076E-11    3.15490E-09
9.41761E-10


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 2.0000000    1.00000E+02    2.31539E+04
```

```
4.45200E+03
   TREMOLITE                  2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)            2.0000000    1.00000E+02

   ALBITE                     1.7781513    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                  1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)          2.0000001    1.00000E+02

   DIOPSIDE                   1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE               1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -10.8066644    1.56076E-11    3.15490E-09
9.41761E-10



                          mass, grams        volume, cc

           created        7.472157E-03       2.253746E-03
           destroyed      1.098854E-05       3.621092E-06
           net            7.461168E-03       2.250125E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3501
 PERICLASE              -4.8210                BRUCITE
-1.0847
 FORSTERITE              -.3962                FAYALITE
-1.7306
 CHRYSOTILE              -.6894                ENSTATITE-CL
-2.2002
 ENSTATITE-OR           -2.2783                ENSTATITE-PR
-2.6837
```

```
 DIOPSIDE                  -.1012                HEDENBERGITE
-3.8634
 FERROSILITE              -4.5005                WOLLASTONITE
-3.5958
 PSEUDOWOLLASTONITE       -4.0819                TREMOLITE
-5.6388
 ANTIGORITE                -.5337                TALC
-7.0069
 CLINOCHLORE              -3.1325                CHAMOSITE
-7.3143
 GROSSULAR                -9.4018                QUARTZ-ALPHA
-5.6852
 QUARTZ-BETA              -5.9221                COESITE
-6.2814
 IRON-ALPHA               -8.6597                IRON-GAMMA
-7.8030
 HALITE                   -9.7500                CRISTOBALITE-ALPHA
-6.9710
 CRISTOBALITE-BETA        -7.6845


                     --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -25.1861
     ALBITE                      -25.18606     .9987996     1.00000
     ANORTHITE                   -25.18606     .0012004     1.00000

 ORTHOPYROXENE(SS)          -2.0008
     ENSTATITE-OR                 -2.00079     .8243812     1.00000
     FERROSILITE                  -2.00079     .1756188     1.00000

 GARNET(SS)                 -9.1522
     PYROPE                       -9.15222     .0821280     1.00000
     ALMANDINE                    -9.15222     .0773110     1.00000
     GROSSULAR                    -9.15222     .8405610     1.00000

 CLINOPYROXENE(SS)            .0000
saturated
     DIOPSIDE                       .00000     .9320069     1.00000
     HEDENBERGITE                   .00000     .0679926     1.00000
     JADEITE                        .00000     .0000005     1.00000

 CPX_SUBCALCIC(SS)            .0000
     DIOPSIDE                       .00000     .9320073     1.00000
     HEDENBERGITE                   .00000     .0679927     1.00000

 CHLORITE(SS)               -3.0563
     CLINOCHLORE                  -3.05628     .9483341     1.00000
```

```
    CHAMOSITE                  -3.05628     .0516659     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0000    1.0000     .0000   -6.3360     .0000   -6.3360


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.80001       1.58487E-27
   H2(G)                          2.27783       1.89596E+02
   H2O(G)                         3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.5849E-08, delzi=  5.8489E-09, nord= 0
              ncycle=  0
 steps completed =     3, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =    -10.8006
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  1.58489319246111E-08
                    log of reaction progress =      -7.8000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000
```

step size is limited by the print requirement

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	1.00000E+02	2.65517E-08	2.68618E+04	7.13226E-06
CLINOPYROXENE(SS)	1.00000E+02	3.20022E-08	2.22861E+04	7.13203E-06
MAGNETITE	1.00000E+02	3.42337E-09	2.31539E+04	7.92642E-07
TREMOLITE	1.00000E+02	2.90352E-09	8.12370E+04	2.35874E-06

current total mass = 1.53539E+05 grams
delta total mass = 1.74157E-05 grams
delta total volume = .00001 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	28.0589	1.67530E+00
CLINOPYROXENE(SS)	.1345	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.6388	1.83200E-01

affinity of the overall irreversible reaction= 48.040 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434542E+05	5.775244E+01	5.775261E+01
NA	1.205627E+04	5.745010E-01	5.745027E-01
CA	3.534905E+01	9.661901E-04	9.661930E-04
MG	2.393610E+04	1.078873E+00	1.078876E+00
AL	2.554449E-02	1.037153E-06	1.037157E-06
SI	6.668158E+01	2.600976E-03	2.600983E-03

```
      H          1.042623E+05        1.133241E+02        1.133244E+02
      CL         1.618114E+04        4.999985E-01        5.000000E-01
      FE         7.970718E+00        1.563544E-04        1.563549E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                    ph           eh            pe

     internal ph scale            6.5998        .4548
3.1695E+00
     modified nbs ph scale        6.3533        .4901
3.4160E+00
     rational ph scale            6.3533        .4901
3.4160E+00

   phcl =      7.1857



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001



                       activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  5.170393E-01 molal
                 sum of molalities =    2.2049456123224
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999985E-01
molal

                         mass of solution =   1.095504 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095501 kg
```

conc of solutes = 8.717509 per cent (w/w)

species	moles	grams	conc	log conc	log g	log act
H2O	5.55088E+01	1.00000E+03				
NA+	5.15714E-01	1.18561E+01	5.15712E-01	-.28759	-.24649	-.53408
CA++	9.74333E-05	3.90513E-03	9.74330E-05	-4.01129	-.98596	-4.99725
MG++	7.45845E-07	1.81278E-05	7.45843E-07	-6.12735	-.98596	-7.11331
AL+++	6.56608E-25	1.77163E-23	6.56606E-25	-24.18270	-2.21841	-26.40111
H4SIO4(AQ)	1.44969E-03	1.39337E-01	1.44969E-03	-2.83872	.00000	-2.83872
H+	4.43271E-07	4.46773E-07	4.43269E-07	-6.35333	-.24649	-6.59982
CL-	4.57685E-01	1.62263E+01	4.57683E-01	-.33944	-.24649	-.58593
FE++	3.02059E-09	1.68691E-07	3.02058E-09	-8.51991	-.98596	-9.50587
O2(AQ)	1.33381E-31	4.26805E-30	1.33381E-31	-30.87491	.00000	-30.87491
H2(AQ)	3.20576E-02	6.46217E-02	3.20575E-02	-1.49407	.00000	-1.49407
FE+++	1.31479E-22	7.34269E-21	1.31478E-22	-21.88115	-2.21841	-24.09956
OH-	5.86192E-02	9.96955E-01	5.86191E-02	-1.23196	-.24649	-1.47845
H8SI3O10(AQ)	1.55015E-11	3.91124E-09	1.55014E-11	-10.80963	.00000	-10.80963
H6SI2O7(AQ)	5.68493E-06	9.90395E-04	5.68491E-06	-5.24528	.00000	-5.24528
AL(OH)3(AQ)	4.26145E-09	3.32408E-07	4.26144E-09	-8.37044	.00000	-8.37044
AL(OH)4-	8.18945E-07	7.78085E-05	8.18942E-07	-6.08675	-.24649	-6.33324
AL(OH)SI(OH)-	2.13950E-07	3.70370E-05	2.13950E-07	-6.66969	-.24649	-6.91618
CACL+	2.05784E-04	1.55435E-02	2.05783E-04	-3.68659	-.24649	-3.93308
CACL2(AQ)	3.75856E-06	4.17147E-04	3.75855E-06	-5.42498	.00000	-5.42498
CA(OH)+	3.01081E-04	1.71879E-02	3.01080E-04	-3.52132	-.24649	-3.76781
CA(H3SIO4)+	3.58136E-04	4.84153E-02	3.58135E-04	-3.44595	-.24649	-3.69244
FE(OH)+	8.46444E-08	6.16671E-06	8.46442E-08			

```
-7.07240     -.24649    -7.31889
   FE(OH)2                5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-               5.95082E-06   6.35958E-04   5.95080E-06
-5.22542     -.24649    -5.47191
   FECL+                  3.34890E-09   3.05754E-07   3.34889E-09
-8.47510     -.24649    -8.72159
   FECL2(AQ)              7.84122E-08   9.93898E-06   7.84119E-08
-7.10562      .00000    -7.10562
   FE(H3SIO4)+            1.49648E-04   2.25900E-02   1.49648E-04
-3.82493     -.24649    -4.07142
   MGCL+                  7.44152E-07   4.44690E-05   7.44150E-07
-6.12834     -.24649    -6.37483
   MG(OH)+                1.63773E-05   6.76583E-04   1.63772E-05
-4.78576     -.24649    -5.03225
   MG(OH)2(AQ)            1.07886E+00   6.29186E+01   1.07886E+00      .
03296      .00000      .03296
   MG(H3SIO4)+            8.17790E-09   9.76538E-07   8.17788E-09
-8.08736     -.24649    -8.33385
   NACL(AQ)               4.21007E-02   2.46048E+00   4.21006E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)               1.66880E-02   6.67472E-01   1.66880E-02
-1.77760      .00000    -1.77760
   H3SIO4-                6.31913E-04   6.00992E-02   6.31911E-04
-3.19934     -.24649    -3.44583
   HCL(AQ)                5.61022E-07   2.04554E-05   5.61021E-07
-6.25102      .00000    -6.25102

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657398
           log (CA++  /h+**0)            8.2023904
           log (MG++  /h+**0)            6.0863317
           log (AL+++ /h+**0)           -6.6016393
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE               -6.4979518    3.17723E-07    7.35651E-05
1.41450E-05

   CLINOPYROXENE(SS)       -4.4703716    3.38554E-05    7.40408E-03
2.24123E-03
```

```
   DIOPSIDE                  -4.5009524    3.15535E-05    6.83299E-03
2.08884E-03
   HEDENBERGITE              -5.6379097    2.30192E-06    5.71094E-04
1.52387E-04
   JADEITE                  -10.8005744    1.58280E-11    3.19945E-09
9.55061E-10


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                  2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)            2.0000000    1.00000E+02

   ALBITE                     1.7781513    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                  1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)          2.0000001    1.00000E+02

   DIOPSIDE                   1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE               1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -10.8005744    1.58280E-11    3.19945E-09
9.55061E-10



                         mass, grams        volume, cc

           created       7.477648E-03       2.255375E-03
           destroyed     1.741566E-05       5.739044E-06
           net           7.460233E-03       2.249636E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---
```

mineral	affinity, kcal	state	mineral	affinity, kcal	state
MAGNETITE	.0000	satd	HEMATITE	-3.3501	
PERICLASE	-4.8210		BRUCITE	-1.0847	
FORSTERITE	-.3962		FAYALITE	-1.7306	
CHRYSOTILE	-.6894		ENSTATITE-CL	-2.2002	
ENSTATITE-OR	-2.2783		ENSTATITE-PR	-2.6837	
DIOPSIDE	-.1012		HEDENBERGITE	-3.8634	
FERROSILITE	-4.5005		WOLLASTONITE	-3.5958	
PSEUDOWOLLASTONITE	-4.0819		TREMOLITE	-5.6388	
ANTIGORITE	-.5336		TALC	-7.0069	
CLINOCHLORE	-3.1249		CHAMOSITE	-7.3067	
GROSSULAR	-9.3891		QUARTZ-ALPHA	-5.6851	
QUARTZ-BETA	-5.9221		COESITE	-6.2814	
IRON-ALPHA	-8.6597		IRON-GAMMA	-7.8030	
HALITE	-9.7500		CRISTOBALITE-ALPHA	-6.9710	
CRISTOBALITE-BETA	-7.6845				

--- summary of solid solutions ---

mineral	aff. kcal/mol	mole frac.	lambda	state
PLAGIOCLASE(SS)	-25.1669			
ALBITE	-25.16689	.9987835	1.00000	
ANORTHITE	-25.16689	.0012165	1.00000	
ORTHOPYROXENE(SS)	-2.0008			
ENSTATITE-OR	-2.00079	.8243812	1.00000	
FERROSILITE	-2.00079	.1756188	1.00000	
GARNET(SS)	-9.1395			
PYROPE	-9.13948	.0821285	1.00000	

```
    ALMANDINE                    -9.13948     .0773115     1.00000
    GROSSULAR                    -9.13948     .8405600     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
    DIOPSIDE                       .00000     .9320069     1.00000
    HEDENBERGITE                   .00000     .0679926     1.00000
    JADEITE                        .00000     .0000005     1.00000

 CPX_SUBCALCIC(SS)          .0000
    DIOPSIDE                       .00000     .9320073     1.00000
    HEDENBERGITE                   .00000     .0679927     1.00000

 CHLORITE(SS)             -3.0486
    CLINOCHLORE                  -3.04862     .9483341     1.00000
    CHAMOSITE                    -3.04862     .0516659     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0000    1.0000     .0000   -6.3302     .0000   -6.3302


           --- summary of gas species ---

           gas               log fugacity         fugacity
partial pressure

   O2(G)                         -26.80001       1.58487E-27
   H2(G)                           2.27783       1.89596E+02
   H2O(G)                          3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  2.5119E-08, delzi=  9.2699E-09, nord= 0
```

```
                ncycle=  0
 steps completed =     4, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =    -10.7911
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                      reaction progress        =  2.51188643150958E-08
                      log of reaction progress =      -7.6000000

                      temperature    =    450.000 degrees c
                      total pressure =    500.000 bars

                      computing units remaining =       .000


 step size is limited by the print requirement


                                --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         1.00000E+02    4.20816E-08    2.68618E+04
1.13039E-05
   CLINOPYROXENE(SS)       1.00000E+02    5.07200E-08    2.22861E+04
1.13035E-05
   MAGNETITE               1.00000E+02    5.42567E-09    2.31539E+04
1.25625E-06
   TREMOLITE               1.00000E+02    4.60178E-09    8.12370E+04
3.73835E-06


                 current total mass =  1.53539E+05 grams
                 delta total mass   =  2.76020E-05 grams
                 delta total volume =       .00001 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)          28.0172    1.67530E+00
   CLINOPYROXENE(SS)          .1345    0.00000E+00
   MAGNETITE                  .0000    0.00000E+00
   TREMOLITE                 5.6388    1.83200E-01

          affinity of the overall irreversible reaction=    47.970
kcal
```

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434542E+05	5.775244E+01	5.775261E+01
NA	1.205627E+04	5.745010E-01	5.745027E-01
CA	3.534871E+01	9.661808E-04	9.661837E-04
MG	2.393610E+04	1.078873E+00	1.078876E+00
AL	2.607997E-02	1.058895E-06	1.058898E-06
SI	6.668200E+01	2.600992E-03	2.601000E-03
H	1.042623E+05	1.133241E+02	1.133244E+02
CL	1.618114E+04	4.999985E-01	5.000000E-01
FE	7.970768E+00	1.563554E-04	1.563559E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.5998	.4548	3.1695E+00
modified nbs ph scale	6.3533	.4901	3.4160E+00
rational ph scale	6.3533	.4901	3.4160E+00

phcl = 7.1857

oxygen fugacity = 1.58487E-27
log oxygen fugacity = -26.80001

```
                           activity of water =    .98384
              log activity of water =   -.00707
              alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  5.170393E-01 molal
                sum of molalities =    2.2049456171903
              osmotic coefficient =     .41003
                   equiv. stoich. ionic strength =  4.999985E-01
molal

                         mass of solution =   1.095504 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095501 kg
                         conc of solutes  =   8.717509 per cent (w/w)


   species                moles         grams          conc         log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15714E-01   1.18561E+01   5.15712E-01     -.
28759     -.24649     -.53408
   CA++                 9.74322E-05   3.90508E-03   9.74319E-05
-4.01130     -.98596    -4.99726
   MG++                 7.45846E-07   1.81278E-05   7.45844E-07
-6.12735     -.98596    -7.11331
   AL+++                6.70372E-25   1.80877E-23   6.70370E-25
-24.17369    -2.21841   -26.39210
   H4SIO4(AQ)           1.44970E-03   1.39338E-01   1.44970E-03
-2.83872      .00000    -2.83872
   H+                   4.43271E-07   4.46773E-07   4.43270E-07
-6.35333     -.24649    -6.59982
   CL-                  4.57685E-01   1.62263E+01   4.57683E-01     -.
33944     -.24649     -.58593
   FE++                 3.02059E-09   1.68691E-07   3.02058E-09
-8.51991     -.98596    -9.50587
   O2(AQ)               1.33381E-31   4.26805E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)               3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                1.31479E-22   7.34269E-21   1.31478E-22
-21.88115    -2.21841   -24.09956
   OH-                  5.86192E-02   9.96955E-01   5.86190E-02
-1.23196     -.24649    -1.47845
   H8SI3O10(AQ)         1.55018E-11   3.91131E-09   1.55017E-11
-10.80962      .00000   -10.80962
   H6SI2O7(AQ)          5.68500E-06   9.90407E-04   5.68498E-06
-5.24527      .00000    -5.24527
```

```
   AL(OH)3(AQ)          4.35078E-09   3.39376E-07   4.35077E-09
-8.36143      .00000    -8.36143
   AL(OH)4-             8.36111E-07   7.94395E-05   8.36108E-07
-6.07774     -.24649    -6.32423
   AL(OH)SI(OH)-        2.18436E-07   3.78136E-05   2.18436E-07
-6.66068     -.24649    -6.90717
   CACL+                2.05782E-04   1.55433E-02   2.05781E-04
-3.68659     -.24649    -3.93308
   CACL2(AQ)            3.75852E-06   4.17143E-04   3.75850E-06
-5.42498      .00000    -5.42498
   CA(OH)+              3.01077E-04   1.71877E-02   3.01076E-04
-3.52132     -.24649    -3.76781
   CA(H3SIO4)+          3.58134E-04   4.84150E-02   3.58133E-04
-3.44596     -.24649    -3.69245
   FE(OH)+              8.46445E-08   6.16671E-06   8.46442E-08
-7.07240     -.24649    -7.31889
   FE(OH)2              5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.95082E-06   6.35958E-04   5.95080E-06
-5.22542     -.24649    -5.47191
   FECL+                3.34890E-09   3.05755E-07   3.34889E-09
-8.47510     -.24649    -8.72159
   FECL2(AQ)            7.84122E-08   9.93899E-06   7.84120E-08
-7.10562      .00000    -7.10562
   FE(H3SIO4)+          1.49649E-04   2.25901E-02   1.49649E-04
-3.82493     -.24649    -4.07142
   MGCL+                7.44153E-07   4.44691E-05   7.44150E-07
-6.12834     -.24649    -6.37483
   MG(OH)+              1.63773E-05   6.76583E-04   1.63772E-05
-4.78576     -.24649    -5.03225
   MG(OH)2(AQ)          1.07886E+00   6.29186E+01   1.07886E+00       .
03296      .00000      .03296
   MG(H3SIO4)+          8.17795E-09   9.76544E-07   8.17793E-09
-8.08736     -.24649    -8.33385
   NACL(AQ)             4.21007E-02   2.46048E+00   4.21006E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)             1.66880E-02   6.67472E-01   1.66880E-02
-1.77760      .00000    -1.77760
   H3SIO4-              6.31917E-04   6.00996E-02   6.31915E-04
-3.19934     -.24649    -3.44583
   HCL(AQ)              5.61022E-07   2.04554E-05   5.61021E-07
-6.25102      .00000    -6.25102

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657396
           log (CA++  /h+**0)            8.2023850
           log (MG++  /h+**0)            6.0863317
           log (AL+++ /h+**0)           -6.5926299
```

```
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                       log moles        moles        grams
volume, cc

   MAGNETITE                   -6.4951307    3.19793E-07    7.40445E-05
1.42372E-05

   CLINOPYROXENE(SS)           -4.4698894    3.38930E-05    7.41231E-03
2.24372E-03
   DIOPSIDE                    -4.5004703    3.15885E-05    6.84058E-03
2.09116E-03
   HEDENBERGITE                -5.6374276    2.30448E-06    5.71728E-04
1.52556E-04
   JADEITE                    -10.7910775    1.61779E-11    3.27018E-09
9.76175E-10


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member          log moles        moles        grams
volume, cc

   MAGNETITE                    2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                    2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)              2.0000000    1.00000E+02

   ALBITE                       1.7781513    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                    1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)            2.0000001    1.00000E+02

   DIOPSIDE                     1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE                 1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                    -10.7910775    1.61779E-11    3.27018E-09
9.76175E-10
```

```
                      mass, grams        volume, cc

           created         7.486352E-03       2.257957E-03
           destroyed       2.760197E-05       9.095773E-06
           net             7.458750E-03       2.248861E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                 .0000  satd          HEMATITE
-3.3501
 PERICLASE               -4.8210                BRUCITE
-1.0847
 FORSTERITE               -.3962                FAYALITE
-1.7306
 CHRYSOTILE               -.6893                ENSTATITE-CL
-2.2002
 ENSTATITE-OR            -2.2783                ENSTATITE-PR
-2.6837
 DIOPSIDE                 -.1012                HEDENBERGITE
-3.8634
 FERROSILITE             -4.5005                WOLLASTONITE
-3.5958
 PSEUDOWOLLASTONITE      -4.0819                TREMOLITE
-5.6388
 ANTIGORITE               -.5335                TALC
-7.0068
 CLINOCHLORE             -3.1129                CHAMOSITE
-7.2947
 GROSSULAR               -9.3692                QUARTZ-ALPHA
-5.6851
 QUARTZ-BETA             -5.9221                COESITE
-6.2814
 IRON-ALPHA              -8.6597                IRON-GAMMA
-7.8030
 HALITE                  -9.7500                CRISTOBALITE-ALPHA
-6.9710
 CRISTOBALITE-BETA       -7.6844
```

```
                         --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -25.1370
     ALBITE                     -25.13701     .9987581     1.00000
     ANORTHITE                  -25.13701     .0012419     1.00000

 ORTHOPYROXENE(SS)         -2.0008
     ENSTATITE-OR                -2.00078     .8243812     1.00000
     FERROSILITE                 -2.00078     .1756188     1.00000

 GARNET(SS)                -9.1196
     PYROPE                      -9.11963     .0821294     1.00000
     ALMANDINE                   -9.11963     .0773123     1.00000
     GROSSULAR                   -9.11963     .8405583     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .9320069     1.00000
     HEDENBERGITE                  .00000     .0679926     1.00000
     JADEITE                       .00000     .0000005     1.00000

 CPX_SUBCALCIC(SS)           .0000
     DIOPSIDE                      .00000     .9320073     1.00000
     HEDENBERGITE                  .00000     .0679927     1.00000

 CHLORITE(SS)              -3.0367
     CLINOCHLORE                 -3.03669     .9483341     1.00000
     CHAMOSITE                   -3.03669     .0516659     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
              .0000    1.0000     .0000   -6.3212     .0000   -6.3212


           --- summary of gas species ---
```

```
          gas                  log fugacity         fugacity
partial pressure

   O2(G)                         -26.80001       1.58487E-27
   H2(G)                           2.27783       1.89596E+02
   H2O(G)                          3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  3.9811E-08, delzi=  1.4692E-08, nord= 2
               ncycle=  0
 steps completed =     5, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =    -10.7764
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  3.98107170553496E-08
                     log of reaction progress =      -7.4000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        1.00000E+02    6.66949E-08    2.68618E+04
1.79154E-05
   CLINOPYROXENE(SS)      1.00000E+02    8.03858E-08    2.22861E+04
1.79148E-05
   MAGNETITE              1.00000E+02    8.59911E-09    2.31539E+04
1.99103E-06
   TREMOLITE              1.00000E+02    7.29332E-09    8.12370E+04
5.92488E-06
```

```
                current total mass =  1.53539E+05 grams
                delta total mass   =  4.37462E-05 grams
                delta total volume =       .00001 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           27.9527    1.67530E+00
   CLINOPYROXENE(SS)           .1345    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.6387    1.83200E-01

          affinity of the overall irreversible reaction=    47.862
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element          mg/kg soln.         molal conc.          moles

      O          8.434542E+05       5.775244E+01       5.775261E+01
      NA         1.205627E+04       5.745010E-01       5.745027E-01
      CA         3.534817E+01       9.661661E-04       9.661690E-04
      MG         2.393610E+04       1.078873E+00       1.078876E+00
      AL         2.692865E-02       1.093353E-06       1.093356E-06
      SI         6.668266E+01       2.601017E-03       2.601025E-03
      H          1.042623E+05       1.133241E+02       1.133244E+02
      CL         1.618114E+04       4.999985E-01       5.000000E-01
      FE         7.970848E+00       1.563569E-04       1.563574E-04

      co3--                         0.000000E+00       0.000000E+00
      so4--                         0.000000E+00       0.000000E+00
      s--                           0.000000E+00       0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                            ph            eh            pe
```

```
     internal ph scale              6.5998        .4548
3.1695E+00
     modified nbs ph scale          6.3533        .4901
3.4160E+00
     rational ph scale              6.3533        .4901
3.4160E+00

   phcl =      7.1857



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001



                             activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                    ionic strength =  5.170393E-01 molal
                 sum of molalities =    2.2049456249060
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999985E-01
molal

                         mass of solution =   1.095504 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095501 kg
                         conc of solutes  =   8.717509 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15714E-01   1.18561E+01   5.15712E-01     -.
28759    -.24649    -.53408
   CA++                 9.74304E-05   3.90501E-03   9.74301E-05
-4.01131    -.98596   -4.99727
   MG++                 7.45847E-07   1.81278E-05   7.45845E-07
-6.12735    -.98596   -7.11331
   AL+++                6.92187E-25   1.86763E-23   6.92185E-25
-24.15978   -2.21841   -26.37819
   H4SIO4(AQ)           1.44972E-03   1.39339E-01   1.44971E-03
-2.83872     .00000   -2.83872
   H+                   4.43271E-07   4.46773E-07   4.43270E-07
-6.35333    -.24649   -6.59982
   CL-                  4.57685E-01   1.62263E+01   4.57683E-01     -.
```

```
33944     -.24649     -.58593
   FE++                    3.02059E-09   1.68691E-07   3.02059E-09
-8.51991     -.98596    -9.50587
   O2(AQ)                  1.33381E-31   4.26805E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)                  3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                   1.31479E-22   7.34271E-21   1.31479E-22
-21.88114    -2.21841   -24.09956
   OH-                     5.86192E-02   9.96954E-01   5.86190E-02
-1.23196     -.24649    -1.47845
   H8SI3O10(AQ)            1.55022E-11   3.91143E-09   1.55022E-11
-10.80961      .00000   -10.80961
   H6SI2O7(AQ)             5.68511E-06   9.90427E-04   5.68509E-06
-5.24526      .00000    -5.24526
   AL(OH)3(AQ)             4.49235E-09   3.50419E-07   4.49234E-09
-8.34753      .00000    -8.34753
   AL(OH)4-                8.63317E-07   8.20244E-05   8.63315E-07
-6.06383     -.24649    -6.31032
   AL(OH)SI(OH)-           2.25546E-07   3.90444E-05   2.25546E-07
-6.64677     -.24649    -6.89326
   CACL+                   2.05778E-04   1.55430E-02   2.05777E-04
-3.68660     -.24649    -3.93309
   CACL2(AQ)               3.75845E-06   4.17135E-04   3.75843E-06
-5.42499      .00000    -5.42499
   CA(OH)+                 3.01072E-04   1.71874E-02   3.01071E-04
-3.52133     -.24649    -3.76782
   CA(H3SIO4)+             3.58131E-04   4.84145E-02   3.58130E-04
-3.44596     -.24649    -3.69245
   FE(OH)+                 8.46445E-08   6.16672E-06   8.46443E-08
-7.07240     -.24649    -7.31889
   FE(OH)2                 5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-                5.95082E-06   6.35957E-04   5.95080E-06
-5.22542     -.24649    -5.47191
   FECL+                   3.34890E-09   3.05755E-07   3.34889E-09
-8.47510     -.24649    -8.72159
   FECL2(AQ)               7.84123E-08   9.93900E-06   7.84121E-08
-7.10562      .00000    -7.10562
   FE(H3SIO4)+             1.49651E-04   2.25904E-02   1.49650E-04
-3.82492     -.24649    -4.07141
   MGCL+                   7.44154E-07   4.44691E-05   7.44151E-07
-6.12834     -.24649    -6.37483
   MG(OH)+                 1.63773E-05   6.76583E-04   1.63772E-05
-4.78576     -.24649    -5.03225
   MG(OH)2(AQ)             1.07886E+00   6.29186E+01   1.07886E+00      .
03296      .00000      .03296
   MG(H3SIO4)+             8.17804E-09   9.76554E-07   8.17801E-09
-8.08735     -.24649    -8.33384
   NACL(AQ)                4.21007E-02   2.46048E+00   4.21006E-02
```

```
-1.37571      .00000    -1.37571
   NAOH(AQ)             1.66880E-02   6.67471E-01   1.66880E-02
-1.77760      .00000    -1.77760
   H3SIO4-              6.31922E-04   6.01001E-02   6.31921E-04
-3.19934     -.24649    -3.44583
   HCL(AQ)              5.61023E-07   2.04554E-05   5.61021E-07
-6.25102      .00000    -6.25102

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657394
           log (CA++  /h+**0)            8.2023765
           log (MG++  /h+**0)            6.0863317
           log (AL+++ /h+**0)           -6.5787230
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE               -6.4906968    3.23075E-07    7.48043E-05
1.43833E-05

   CLINOPYROXENE(SS)       -4.4691264    3.39526E-05    7.42534E-03
2.24766E-03
   DIOPSIDE                -4.4997073    3.16441E-05    6.85260E-03
2.09484E-03
   HEDENBERGITE            -5.6366645    2.30853E-06    5.72733E-04
1.52825E-04
   JADEITE                -10.7763994    1.67340E-11    3.38260E-09
1.00973E-09


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)          2.0000000    1.00000E+02
```

```
   ALBITE                        1.7781513    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                     1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)             2.0000001    1.00000E+02

   DIOPSIDE                      1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE                  1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                     -10.7763994    1.67340E-11    3.38260E-09
1.00973E-09



                           mass, grams        volume, cc

           created         7.500146E-03       2.262048E-03
           destroyed       4.374617E-05       1.441583E-05
           net             7.456400E-03       2.247632E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3501
 PERICLASE              -4.8210                BRUCITE
-1.0847
 FORSTERITE              -.3962                FAYALITE
-1.7306
 CHRYSOTILE              -.6893                ENSTATITE-CL
-2.2002
 ENSTATITE-OR           -2.2783                ENSTATITE-PR
-2.6837
 DIOPSIDE                -.1012                HEDENBERGITE
-3.8634
 FERROSILITE            -4.5005                WOLLASTONITE
-3.5958
 PSEUDOWOLLASTONITE     -4.0819                TREMOLITE
```

```
-5.6387
 ANTIGORITE              -.5333                TALC
-7.0068
 CLINOCHLORE            -3.0945                CHAMOSITE
-7.2763
 GROSSULAR              -9.3386                QUARTZ-ALPHA
-5.6851
 QUARTZ-BETA            -5.9220                COESITE
-6.2814
 IRON-ALPHA             -8.6597                IRON-GAMMA
-7.8030
 HALITE                 -9.7500                CRISTOBALITE-ALPHA
-6.9710
 CRISTOBALITE-BETA      -7.6844


                     --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -25.0909
     ALBITE                     -25.09090     .9987177     1.00000
     ANORTHITE                  -25.09090     .0012823     1.00000

 ORTHOPYROXENE(SS)         -2.0008
     ENSTATITE-OR                -2.00077     .8243812     1.00000
     FERROSILITE                 -2.00077     .1756188     1.00000

 GARNET(SS)                -9.0890
     PYROPE                      -9.08899     .0821307     1.00000
     ALMANDINE                   -9.08899     .0773136     1.00000
     GROSSULAR                   -9.08899     .8405557     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .9320069     1.00000
     HEDENBERGITE                  .00000     .0679926     1.00000
     JADEITE                       .00000     .0000005     1.00000

 CPX_SUBCALCIC(SS)           .0000
     DIOPSIDE                      .00000     .9320073     1.00000
     HEDENBERGITE                  .00000     .0679927     1.00000

 CHLORITE(SS)              -3.0183
     CLINOCHLORE                 -3.01828     .9483341     1.00000
     CHAMOSITE                   -3.01828     .0516659     1.00000


 solid solution product phases
```

```
            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
              .0000    1.0000     .0000   -6.3073     .0000   -6.3073


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.80001       1.58487E-27
   H2(G)                          2.27783       1.89596E+02
   H2O(G)                         3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  6.3096E-08, delzi=  2.3285E-08, nord= 2
               ncycle=  0
 steps completed =     6, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =    -10.7540
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  6.30957344480192E-08
                     log of reaction progress =      -7.2000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---
```

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	1.00000E+02	1.05704E-07	2.68618E+04	2.83940E-05
CLINOPYROXENE(SS)	1.00000E+02	1.27403E-07	2.22861E+04	2.83931E-05
MAGNETITE	1.00000E+02	1.36287E-08	2.31539E+04	3.15557E-06
TREMOLITE	1.00000E+02	1.15591E-08	8.12370E+04	9.39030E-06

current total mass = 1.53539E+05 grams
delta total mass   = 6.93330E-05 grams
delta total volume =   .00002 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	27.8546	1.67530E+00
CLINOPYROXENE(SS)	.1345	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.6386	1.83200E-01

affinity of the overall irreversible reaction=   47.698 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434542E+05	5.775244E+01	5.775261E+01
NA	1.205627E+04	5.745010E-01	5.745028E-01
CA	3.534732E+01	9.661428E-04	9.661457E-04
MG	2.393610E+04	1.078873E+00	1.078876E+00
AL	2.827371E-02	1.147965E-06	1.147968E-06
SI	6.668370E+01	2.601058E-03	2.601066E-03
H	1.042623E+05	1.133241E+02	1.133244E+02
CL	1.618114E+04	4.999985E-01	5.000000E-01
FE	7.970973E+00	1.563594E-04	1.563599E-04

co3--		0.000000E+00	0.000000E+00

```
      so4--                              0.000000E+00        0.000000E+00
      s--                                0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                           ph            eh            pe


     internal ph scale                   6.5998         .4548
3.1695E+00
     modified nbs ph scale               6.3533         .4901
3.4160E+00
     rational ph scale                   6.3533         .4901
3.4160E+00

   phcl =      7.1857



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001



                           activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  5.170393E-01 molal
                 sum of molalities =    2.2049456371363
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999985E-01
molal

                         mass of solution =   1.095504 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095501 kg
                         conc of solutes  =   8.717510 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act
```

```
   H2O                    5.55088E+01   1.00000E+03
   NA+                    5.15714E-01   1.18561E+01   5.15712E-01      -.
28759     -.24649     -.53408
   CA++                   9.74275E-05   3.90490E-03   9.74272E-05
-4.01132     -.98596    -4.99728
   MG++                   7.45848E-07   1.81278E-05   7.45846E-07
-6.12735     -.98596    -7.11331
   AL+++                  7.26762E-25   1.96092E-23   7.26760E-25
-24.13861    -2.21841   -26.35702
   H4SIO4(AQ)             1.44974E-03   1.39341E-01   1.44974E-03
-2.83871      .00000    -2.83871
   H+                     4.43272E-07   4.46774E-07   4.43270E-07
-6.35333     -.24649    -6.59982
   CL-                    4.57685E-01   1.62263E+01   4.57683E-01      -.
33944     -.24649     -.58593
   FE++                   3.02060E-09   1.68691E-07   3.02059E-09
-8.51991     -.98596    -9.50587
   O2(AQ)                 1.33381E-31   4.26805E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)                 3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                  1.31479E-22   7.34273E-21   1.31479E-22
-21.88114    -2.21841   -24.09955
   OH-                    5.86191E-02   9.96953E-01   5.86189E-02
-1.23196     -.24649    -1.47845
   H8SI3O10(AQ)           1.55030E-11   3.91161E-09   1.55029E-11
-10.80959      .00000   -10.80959
   H6SI2O7(AQ)            5.68529E-06   9.90457E-04   5.68527E-06
-5.24525      .00000    -5.24525
   AL(OH)3(AQ)            4.71673E-09   3.67921E-07   4.71672E-09
-8.32636      .00000    -8.32636
   AL(OH)4-               9.06436E-07   8.61212E-05   9.06434E-07
-6.04266     -.24649    -6.28915
   AL(OH)SI(OH)-          2.36815E-07   4.09951E-05   2.36814E-07
-6.62559     -.24649    -6.87208
   CACL+                  2.05772E-04   1.55426E-02   2.05771E-04
-3.68662     -.24649    -3.93311
   CACL2(AQ)              3.75834E-06   4.17123E-04   3.75833E-06
-5.42501      .00000    -5.42501
   CA(OH)+                3.01063E-04   1.71868E-02   3.01062E-04
-3.52134     -.24649    -3.76783
   CA(H3SIO4)+            3.58126E-04   4.84138E-02   3.58124E-04
-3.44597     -.24649    -3.69246
   FE(OH)+                8.46446E-08   6.16672E-06   8.46443E-08
-7.07240     -.24649    -7.31889
   FE(OH)2                5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-               5.95081E-06   6.35957E-04   5.95079E-06
-5.22543     -.24649    -5.47192
```

```
   FECL+                 3.34891E-09   3.05756E-07   3.34890E-09
-8.47510     -.24649    -8.72159
   FECL2(AQ)             7.84125E-08   9.93902E-06   7.84122E-08
-7.10562      .00000    -7.10562
   FE(H3SIO4)+           1.49653E-04   2.25907E-02   1.49653E-04
-3.82491     -.24649    -4.07140
   MGCL+                 7.44155E-07   4.44692E-05   7.44153E-07
-6.12834     -.24649    -6.37483
   MG(OH)+               1.63773E-05   6.76584E-04   1.63772E-05
-4.78576     -.24649    -5.03225
   MG(OH)2(AQ)           1.07886E+00   6.29186E+01   1.07886E+00      .
03296      .00000      .03296
   MG(H3SIO4)+           8.17817E-09   9.76570E-07   8.17815E-09
-8.08734     -.24649    -8.33384
   NACL(AQ)              4.21007E-02   2.46048E+00   4.21006E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)              1.66880E-02   6.67471E-01   1.66879E-02
-1.77760      .00000    -1.77760
   H3SIO4-               6.31932E-04   6.01010E-02   6.31930E-04
-3.19933     -.24649    -3.44582
   HCL(AQ)               5.61023E-07   2.04554E-05   5.61022E-07
-6.25102      .00000    -6.25102

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657390
           log (CA++  /h+**0)            8.2023629
           log (MG++  /h+**0)            6.0863317
           log (AL+++ /h+**0)           -6.5575557
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                       log moles        moles         grams
volume, cc

   MAGNETITE                -6.4837610    3.28276E-07    7.60085E-05
1.46148E-05

   CLINOPYROXENE(SS)        -4.4679199    3.40471E-05    7.44600E-03
2.25392E-03
   DIOPSIDE                 -4.4985008    3.17321E-05    6.87167E-03
2.10067E-03
   HEDENBERGITE             -5.6354580    2.31495E-06    5.74327E-04
1.53250E-04
   JADEITE                 -10.7540124    1.76193E-11    3.56153E-09
```

```
1.06315E-09


               --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                 2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)           2.0000000    1.00000E+02

   ALBITE                    1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                 1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)         2.0000001    1.00000E+02

   DIOPSIDE                  1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE              1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                 -10.7540124    1.76193E-11    3.56153E-09
1.06315E-09



                           mass, grams        volume, cc

           created         7.522008E-03       2.268533E-03
           destroyed       6.933300E-05       2.284755E-05
           net             7.452675E-03       2.245685E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state
```

```
 MAGNETITE                  .0000  satd          HEMATITE
-3.3501
 PERICLASE                -4.8210                BRUCITE
-1.0847
 FORSTERITE                -.3962                FAYALITE
-1.7306
 CHRYSOTILE                -.6893                ENSTATITE-CL
-2.2002
 ENSTATITE-OR             -2.2783                ENSTATITE-PR
-2.6836
 DIOPSIDE                  -.1012                HEDENBERGITE
-3.8634
 FERROSILITE              -4.5005                WOLLASTONITE
-3.5958
 PSEUDOWOLLASTONITE       -4.0819                TREMOLITE
-5.6386
 ANTIGORITE                -.5329                TALC
-7.0067
 CLINOCHLORE              -3.0665                CHAMOSITE
-7.2483
 GROSSULAR                -9.2920                QUARTZ-ALPHA
-5.6851
 QUARTZ-BETA              -5.9220                COESITE
-6.2814
 IRON-ALPHA               -8.6597                IRON-GAMMA
-7.8030
 HALITE                   -9.7500                CRISTOBALITE-ALPHA
-6.9710
 CRISTOBALITE-BETA        -7.6844


                      --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -25.0207
     ALBITE                      -25.02069     .9986538     1.00000
     ANORTHITE                   -25.02069     .0013462     1.00000

 ORTHOPYROXENE(SS)          -2.0007
     ENSTATITE-OR                 -2.00074     .8243812     1.00000
     FERROSILITE                  -2.00074     .1756188     1.00000

 GARNET(SS)                 -9.0424
     PYROPE                       -9.04236     .0821329     1.00000
     ALMANDINE                    -9.04236     .0773156     1.00000
     GROSSULAR                    -9.04236     .8405515     1.00000

 CLINOPYROXENE(SS)            .0000
saturated
```

```
    DIOPSIDE                         .00000     .9320068     1.00000
    HEDENBERGITE                     .00000     .0679926     1.00000
    JADEITE                          .00000     .0000005     1.00000

CPX_SUBCALCIC(SS)          .0000
    DIOPSIDE                         .00000     .9320073     1.00000
    HEDENBERGITE                     .00000     .0679927     1.00000

CHLORITE(SS)             -2.9902
    CLINOCHLORE                    -2.99025     .9483341     1.00000
    CHAMOSITE                      -2.99025     .0516659     1.00000


solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

  CLINOPYROXENE(SS)
ideal solution

    DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0000    1.0000     .0000   -6.2861     .0000   -6.2861


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

  O2(G)                        -26.80001       1.58487E-27
  H2(G)                          2.27783       1.89596E+02
  H2O(G)                         3.80603       6.39774E+03



- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



stepping to zi=  1.0000E-07, delzi=  3.6904E-08, nord= 2
              ncycle=  0
steps completed =     7, iter =  4, ncorr = 0
most rapidly changing is zvclg1(JADEITE           ) =    -10.7205
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
                    reaction progress        =  9.99999999999996E-08
                    log of reaction progress =      -7.0000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         1.00000E+02    1.67530E-07    2.68618E+04
4.50015E-05
   CLINOPYROXENE(SS)       1.00000E+02    2.01920E-07    2.22861E+04
4.50001E-05
   MAGNETITE               1.00000E+02    2.16000E-08    2.31539E+04
5.00123E-06
   TREMOLITE               1.00000E+02    1.83200E-08    8.12370E+04
1.48826E-05


                current total mass =  1.53539E+05 grams
                delta total mass   =  1.09885E-04 grams
                delta total volume =       .00004 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           27.7083    1.67530E+00
   CLINOPYROXENE(SS)           .1345    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.6385    1.83200E-01

          affinity of the overall irreversible reaction=    47.453
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included
```

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434542E+05	5.775244E+01	5.775261E+01
NA	1.205627E+04	5.745011E-01	5.745028E-01
CA	3.534597E+01	9.661059E-04	9.661088E-04
MG	2.393610E+04	1.078873E+00	1.078876E+00
AL	3.040549E-02	1.234519E-06	1.234523E-06
SI	6.668535E+01	2.601123E-03	2.601130E-03
H	1.042623E+05	1.133241E+02	1.133244E+02
CL	1.618114E+04	4.999985E-01	5.000000E-01
FE	7.971173E+00	1.563633E-04	1.563638E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.5998	.4548	3.1695E+00
modified nbs ph scale	6.3533	.4901	3.4160E+00
rational ph scale	6.3533	.4901	3.4160E+00

phcl = 7.1857

oxygen fugacity = 1.58487E-27
log oxygen fugacity = -26.80001

activity of water = .98384
log activity of water = -.00707
alkalinity = 0.000000E+00 equiv/kg solvent
(not def. for t.gt.50 c)

```
                     ionic strength =  5.170393E-01 molal
                  sum of molalities =    2.2049456565244
                osmotic coefficient =     .41003
                     equiv. stoich. ionic strength =  4.999985E-01
molal

                          mass of solution =   1.095504 kg
                          mass of solvent  =   1.000003 kg
                          mass of solutes  =    .095501 kg
                          conc of solutes  =   8.717511 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15714E-01   1.18561E+01   5.15713E-01     -.
28759     -.24649     -.53408
   CA++                 9.74230E-05   3.90471E-03   9.74227E-05
-4.01134     -.98596    -4.99730
   MG++                 7.45850E-07   1.81279E-05   7.45848E-07
-6.12735     -.98596    -7.11331
   AL+++                7.81559E-25   2.10877E-23   7.81557E-25
-24.10704    -2.21841   -26.32545
   H4SIO4(AQ)           1.44978E-03   1.39345E-01   1.44977E-03
-2.83870      .00000    -2.83870
   H+                   4.43272E-07   4.46774E-07   4.43271E-07
-6.35333     -.24649    -6.59982
   CL-                  4.57685E-01   1.62263E+01   4.57683E-01     -.
33944     -.24649     -.58593
   FE++                 3.02061E-09   1.68692E-07   3.02060E-09
-8.51991     -.98596    -9.50587
   O2(AQ)               1.33381E-31   4.26805E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)               3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                1.31480E-22   7.34276E-21   1.31480E-22
-21.88114    -2.21841   -24.09955
   OH-                  5.86190E-02   9.96952E-01   5.86189E-02
-1.23196     -.24649    -1.47845
   H8SI3O10(AQ)         1.55041E-11   3.91190E-09   1.55041E-11
-10.80955      .00000   -10.80955
   H6SI2O7(AQ)          5.68557E-06   9.90506E-04   5.68555E-06
-5.24523      .00000    -5.24523
   AL(OH)3(AQ)          5.07235E-09   3.95660E-07   5.07233E-09
-8.29479      .00000    -8.29479
   AL(OH)4-             9.74775E-07   9.26141E-05   9.74772E-07
-6.01110     -.24649    -6.25759
   AL(OH)SI(OH)-        2.54676E-07   4.40870E-05   2.54675E-07
```

```
-6.59401     -.24649    -6.84050
   CACL+                2.05762E-04   1.55418E-02   2.05762E-04
-3.68664     -.24649    -3.93313
   CACL2(AQ)            3.75816E-06   4.17103E-04   3.75815E-06
-5.42503      .00000    -5.42503
   CA(OH)+              3.01048E-04   1.71860E-02   3.01047E-04
-3.52137     -.24649    -3.76786
   CA(H3SIO4)+          3.58117E-04   4.84127E-02   3.58116E-04
-3.44598     -.24649    -3.69247
   FE(OH)+              8.46447E-08   6.16673E-06   8.46445E-08
-7.07240     -.24649    -7.31889
   FE(OH)2              5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.95080E-06   6.35956E-04   5.95078E-06
-5.22543     -.24649    -5.47192
   FECL+                3.34892E-09   3.05757E-07   3.34891E-09
-8.47510     -.24649    -8.72159
   FECL2(AQ)            7.84127E-08   9.93905E-06   7.84125E-08
-7.10561      .00000    -7.10561
   FE(H3SIO4)+          1.49657E-04   2.25913E-02   1.49657E-04
-3.82490     -.24649    -4.07139
   MGCL+                7.44157E-07   4.44693E-05   7.44155E-07
-6.12834     -.24649    -6.37483
   MG(OH)+              1.63773E-05   6.76585E-04   1.63773E-05
-4.78576     -.24649    -5.03225
   MG(OH)2(AQ)          1.07886E+00   6.29186E+01   1.07886E+00      .
03296      .00000      .03296
   MG(H3SIO4)+          8.17839E-09   9.76596E-07   8.17836E-09
-8.08733     -.24649    -8.33382
   NACL(AQ)             4.21007E-02   2.46048E+00   4.21006E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)             1.66880E-02   6.67470E-01   1.66879E-02
-1.77760      .00000    -1.77760
   H3SIO4-              6.31946E-04   6.01024E-02   6.31944E-04
-3.19932     -.24649    -3.44581
   HCL(AQ)              5.61024E-07   2.04554E-05   5.61022E-07
-6.25102      .00000    -6.25102

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657384
           log (CA++  /h+**0)            8.2023415
           log (MG++  /h+**0)            6.0863316
           log (AL+++ /h+**0)           -6.5259880
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---
```

```
  product                        log moles        moles        grams
volume, cc

   MAGNETITE                    -6.4729904    3.36519E-07    7.79171E-05
1.49818E-05

   CLINOPYROXENE(SS)            -4.4660145    3.41968E-05    7.47874E-03
2.26383E-03
   DIOPSIDE                     -4.4965954    3.18717E-05    6.90188E-03
2.10990E-03
   HEDENBERGITE                 -5.6335526    2.32513E-06    5.76852E-04
1.53924E-04
   JADEITE                     -10.7205185    1.90319E-11    3.84708E-09
1.14838E-09


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                     2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                     2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)               2.0000000    1.00000E+02

   ALBITE                        1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                     1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)             2.0000001    1.00000E+02

   DIOPSIDE                      1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE                  1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                     -10.7205185    1.90319E-11    3.84708E-09
1.14838E-09


                             mass, grams        volume, cc
```

```
           created          7.556657E-03       2.278810E-03
           destroyed        1.098854E-04       3.621092E-05
           net              7.446771E-03       2.242599E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                 .0000  satd          HEMATITE
-3.3501
 PERICLASE               -4.8210                HRUCITE
-1.0847
 FORSTERITE               -.3962                FAYALITE
-1.7305
 CHRYSOTILE               -.6892                ENSTATITE-CL
-2.2001
 ENSTATITE-OR            -2.2782                ENSTATITE-PR
-2.6836
 DIOPSIDE                 -.1012                HEDENBERGITE
-3.8634
 FERROSILITE             -4.5004                WOLLASTONITE
-3.5959
 PSEUDOWOLLASTONITE      -4.0820                TREMOLITE
-5.6385
 ANTIGORITE               -.5323                TALC
-7.0066
 CLINOCHLORE             -3.0247                CHAMOSITE
-7.2065
 GROSSULAR               -9.2224                QUARTZ-ALPHA
-5.6851
 QUARTZ-BETA             -5.9220                COESITE
-6.2814
 IRON-ALPHA              -8.6597                IRON-GAMMA
-7.8030
 HALITE                  -9.7500                CRISTOBALITE-ALPHA
-6.9709
 CRISTOBALITE-BETA       -7.6844


                      --- summary of solid solutions  ---

 mineral                   aff. kcal/mol  mole frac.    lambda      state
```

```
 PLAGIOCLASE(SS)         -24.9160
     ALBITE                    -24.91599     .9985526     1.00000
     ANORTHITE                 -24.91599     .0014474     1.00000

 ORTHOPYROXENE(SS)        -2.0007
     ENSTATITE-OR               -2.00071     .8243812     1.00000
     FERROSILITE                -2.00071     .1756188     1.00000

 GARNET(SS)               -8.9728
     PYROPE                     -8.97281     .0821363     1.00000
     ALMANDINE                  -8.97281     .0773188     1.00000
     GROSSULAR                  -8.97281     .8405449     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9320068     1.00000
     HEDENBERGITE                 .00000     .0679926     1.00000
     JADEITE                      .00000     .0000006     1.00000

 CPX_SUBCALCIC(SS)          .0000
     DIOPSIDE                     .00000     .9320073     1.00000
     HEDENBERGITE                 .00000     .0679927     1.00000

 CHLORITE(SS)             -2.9484
     CLINOCHLORE                -2.94844     .9483341     1.00000
     CHAMOSITE                  -2.94844     .0516659     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
              .0000    1.0000     .0000   -6.2545     .0000   -6.2545


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.80001       1.58487E-27
```

```
  H2(G)                             2.27783       1.89596E+02
  H2O(G)                            3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.5849E-07, delzi=  5.8489E-08, nord= 2
               ncycle=  0
 steps completed =     8, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =    -10.6717
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                     reaction progress        =  1.58489319246111E-07
                     log of reaction progress =      -6.8000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant             moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        1.00000E+02    2.65517E-07    2.68618E+04
7.13226E-05
   CLINOPYROXENE(SS)      1.00000E+02    3.20022E-07    2.22861E+04
7.13203E-05
   MAGNETITE              1.00000E+02    3.42337E-08    2.31539E+04
7.92642E-06
   TREMOLITE              1.00000E+02    2.90352E-08    8.12370E+04
2.35874E-05


                current total mass =  1.53539E+05 grams
                delta total mass   =  1.74157E-04 grams
                delta total volume =       .00006 cc
```

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	27.4962	1.67530E+00
CLINOPYROXENE(SS)	.1345	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.6383	1.83200E-01

affinity of the overall irreversible reaction= 47.097
kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434542E+05	5.775244E+01	5.775261E+01
NA	1.205627E+04	5.745011E-01	5.745029E-01
CA	3.534383E+01	9.660473E-04	9.660503E-04
MG	2.393610E+04	1.078873E+00	1.078876E+00
AL	3.378414E-02	1.371699E-06	1.371703E-06
SI	6.668797E+01	2.601225E-03	2.601233E-03
H	1.042623E+05	1.133241E+02	1.133244E+02
CL	1.618114E+04	4.999985E-01	5.000000E-01
FE	7.971488E+00	1.563695E-04	1.563700E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.5998	.4548	3.1695E+00
modified nbs ph scale	6.3533	.4901	3.4160E+00
rational ph scale	6.3533	.4901	

```
3.4160E+00

   phcl =      7.1857



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001




                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  5.170393E-01 molal
                 sum of molalities =    2.2049456872631
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999985E-01
molal

                         mass of solution =   1.095504 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095501 kg
                         conc of solutes  =   8.717512 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15714E-01   1.18562E+01   5.15713E-01     -.
28759    -.24649    -.53408
   CA++                 9.74159E-05   3.90443E-03   9.74156E-05
-4.01137     -.98596    -4.99733
   MG++                 7.45854E-07   1.81280E-05   7.45852E-07
-6.12735     -.98596    -7.11331
   AL+++                8.68407E-25   2.34310E-23   8.68404E-25
-24.06128    -2.21841   -26.27969
   H4SIO4(AQ)           1.44983E-03   1.39350E-01   1.44983E-03
-2.83868      .00000    -2.83868
   H+                   4.43273E-07   4.46775E-07   4.43272E-07
-6.35333     -.24649    -6.59982
   CL-                  4.57685E-01   1.62263E+01   4.57683E-01     -.
33944    -.24649    -.58593
   FE++                 3.02062E-09   1.68693E-07   3.02062E-09
-8.51990     -.98596    -9.50586
   O2(AQ)               1.33381E-31   4.26805E-30   1.33381E-31
-30.87491      .00000   -30.87491
```

```
   H2(AQ)                   3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                    1.31481E-22   7.34281E-21   1.31481E-22
-21.88114    -2.21841   -24.09955
   OH-                      5.86189E-02   9.96949E-01   5.86187E-02
-1.23196     -.24649    -1.47845
   H8SI3O10(AQ)             1.55059E-11   3.91236E-09   1.55059E-11
-10.80950     .00000    -10.80950
   H6SI2O7(AQ)              5.68601E-06   9.90584E-04   5.68599E-06
-5.24519      .00000    -5.24519
   AL(OH)3(AQ)              5.63595E-09   4.39624E-07   5.63593E-09
-8.24903      .00000    -8.24903
   AL(OH)4-                 1.08308E-06   1.02905E-04   1.08308E-06
-5.96534     -.24649    -6.21183
   AL(OH)SI(OH)-            2.82984E-07   4.89874E-05   2.82983E-07
-6.54824     -.24649    -6.79473
   CACL+                    2.05747E-04   1.55407E-02   2.05746E-04
-3.68667     -.24649    -3.93316
   CACL2(AQ)                3.75789E-06   4.17073E-04   3.75787E-06
-5.42506      .00000    -5.42506
   CA(OH)+                  3.01025E-04   1.71847E-02   3.01024E-04
-3.52140     -.24649    -3.76789
   CA(H3SIO4)+              3.58104E-04   4.84109E-02   3.58103E-04
-3.44599     -.24649    -3.69248
   FE(OH)+                  8.46449E-08   6.16675E-06   8.46447E-08
-7.07240     -.24649    -7.31889
   FE(OH)2                  5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-                 5.95079E-06   6.35954E-04   5.95077E-06
-5.22543     -.24649    -5.47192
   FECL+                    3.34894E-09   3.05758E-07   3.34893E-09
-8.47509     -.24649    -8.72158
   FECL2(AQ)                7.84131E-08   9.93910E-06   7.84129E-08
-7.10561      .00000    -7.10561
   FE(H3SIO4)+              1.49664E-04   2.25923E-02   1.49663E-04
-3.82489     -.24649    -4.07138
   MGCL+                    7.44161E-07   4.44696E-05   7.44158E-07
-6.12833     -.24649    -6.37482
   MG(OH)+                  1.63774E-05   6.76586E-04   1.63773E-05
-4.78576     -.24649    -5.03225
   MG(OH)2(AQ)              1.07886E+00   6.29186E+01   1.07886E+00       .
03296      .00000      .03296
   MG(H3SIO4)+              8.17873E-09   9.76636E-07   8.17870E-09
-8.08732     -.24649    -8.33381
   NACL(AQ)                 4.21007E-02   2.46048E+00   4.21006E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)                 1.66879E-02   6.67468E-01   1.66879E-02
-1.77760      .00000    -1.77760
   H3SIO4-                  6.31970E-04   6.01046E-02   6.31968E-04
-3.19931     -.24649    -3.44580
```

```
   HCL(AQ)              5.61025E-07   2.04555E-05   5.61024E-07
-6.25102      .00000    -6.25102

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657374
           log (CA++  /h+**0)            8.2023075
           log (MG++  /h+**0)            6.0863316
           log (AL+++ /h+**0)           -6.4802297
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                        log moles        moles        grams
volume, cc

   MAGNETITE                   -6.4564492    3.49583E-07    8.09420E-05
1.55635E-05

   CLINOPYROXENE(SS)           -4.4630116    3.44341E-05    7.53063E-03
2.27954E-03
   DIOPSIDE                    -4.4935926    3.20928E-05    6.94977E-03
2.12454E-03
   HEDENBERGITE                -5.6305497    2.34126E-06    5.80854E-04
1.54992E-04
   JADEITE                    -10.6717243    2.12949E-11    4.30452E-09
1.28493E-09


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                    2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                    2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)              2.0000000    1.00000E+02

   ALBITE                       1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                    1.6020600    4.00000E+01    1.11284E+04
4.03000E+03
```

```
   CLINOPYROXENE(SS)          2.0000001    1.00000E+02

   DIOPSIDE                   1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE               1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -10.6717243    2.12949E-11    4.30452E-09
1.28493E-09



                            mass, grams        volume, cc

           created          7.611571E-03       2.295099E-03
           destroyed        1.741566E-04       5.739044E-05
           net              7.437414E-03       2.237708E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd         HEMATITE
-3.3501
 PERICLASE              -4.8210               BRUCITE
-1.0847
 FORSTERITE              -.3961               FAYALITE
-1.7305
 CHRYSOTILE              -.6891               ENSTATITE-CL
-2.2001
 ENSTATITE-OR           -2.2782               ENSTATITE-PR
-2.6835
 DIOPSIDE                -.1012               HEDENBERGITE
-3.8634
 FERROSILITE            -4.5004               WOLLASTONITE
-3.5959
 PSEUDOWOLLASTONITE     -4.0820               TREMOLITE
-5.6383
 ANTIGORITE              -.5313               TALC
-7.0063
 CLINOCHLORE            -2.9641               CHAMOSITE
-7.1459
```

```
 GROSSULAR              -9.1217              QUARTZ-ALPHA
-5.6850
 QUARTZ-BETA            -5.9219              COESITE
-6.2813
 IRON-ALPHA             -8.6597              IRON-GAMMA
-7.8030
 HALITE                 -9.7500              CRISTOBALITE-ALPHA
-6.9709
 CRISTOBALITE-BETA      -7.6843


                    --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -24.7642
     ALBITE                    -24.76418     .9983922     1.00000
     ANORTHITE                 -24.76418     .0016078     1.00000

 ORTHOPYROXENE(SS)        -2.0007
     ENSTATITE-OR               -2.00065     .8243812     1.00000
     FERROSILITE                -2.00065     .1756188     1.00000

 GARNET(SS)               -8.8720
     PYROPE                     -8.87201     .0821417     1.00000
     ALMANDINE                  -8.87201     .0773239     1.00000
     GROSSULAR                  -8.87201     .8405344     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9320067     1.00000
     HEDENBERGITE                 .00000     .0679926     1.00000
     JADEITE                      .00000     .0000006     1.00000

 CPX_SUBCALCIC(SS)          .0000
     DIOPSIDE                     .00000     .9320073     1.00000
     HEDENBERGITE                 .00000     .0679927     1.00000

 CHLORITE(SS)             -2.8878
     CLINOCHLORE                -2.88784     .9483341     1.00000
     CHAMOSITE                  -2.88784     .0516659     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution
```

```
     DIOPSIDE
              .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
              .0000    1.0000     .0000   -6.2087     .0000   -6.2087


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                         -26.80001       1.58487E-27
   H2(G)                           2.27783       1.89596E+02
   H2O(G)                          3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  2.5119E-07, delzi=  9.2699E-08, nord= 2
               ncycle=  0
 steps completed =     9, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =    -10.6031
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  2.511886431509 57E-07
                     log of reaction progress =      -6.6000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams
```

```
   PLAGIOCLASE(SS)         1.00000E+02    4.20816E-07    2.68618E+04
1.13039E-04
   CLINOPYROXENE(SS)       1.00000E+02    5.07200E-07    2.22861E+04
1.13035E-04
   MAGNETITE               1.00000E+02    5.42567E-08    2.31539E+04
1.25625E-05
   TREMOLITE               1.00000E+02    4.60178E-08    8.12370E+04
3.73835E-05


                current total mass =  1.53539E+05 grams
                delta total mass   =  2.76020E-04 grams
                delta total volume =       .00009 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           27.2001    1.67530E+00
   CLINOPYROXENE(SS)           .1345    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.6379    1.83200E-01

          affinity of the overall irreversible reaction=    46.601
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element          mg/kg soln.         molal conc.          moles

      O          8.434542E+05        5.775244E+01        5.775261E+01
      NA         1.205627E+04        5.745012E-01        5.745029E-01
      CA         3.534043E+01        9.659546E-04        9.659575E-04
      MG         2.393610E+04        1.078873E+00        1.078876E+00
      AL         3.913894E-02        1.589113E-06        1.589118E-06
      SI         6.669212E+01        2.601387E-03        2.601394E-03
      H          1.042623E+05        1.133241E+02        1.133244E+02
      CL         1.618114E+04        4.999985E-01        5.000000E-01
      FE         7.971989E+00        1.563793E-04        1.563798E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
```

```
     and non-sulfate sulfur aqueous species


    single ion activities and activity coefficients are here defined
    with respect to the internal ph scale



                                           ph           eh           pe

      internal ph scale                  6.5998        .4548
3.1695E+00
      modified nbs ph scale              6.3533        .4901
3.4160E+00
      rational ph scale                  6.3533        .4901
3.4160E+00

    phcl =      7.1857



           oxygen fugacity =  1.58487E-27
           log oxygen fugacity = -26.80001




                               activity of water =    .98384
                log activity of water =   -.00707
                alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                     ionic strength =  5.170394E-01 molal
                  sum of molalities =    2.2049457360076
                osmotic coefficient =     .41003
                     equiv. stoich. ionic strength =  4.999985E-01
molal

                          mass of solution =   1.095504 kg
                          mass of solvent  =   1.000003 kg
                          mass of solutes  =    .095501 kg
                          conc of solutes  =   8.717514 per cent (w/w)


    species                moles        grams          conc        log
conc      log g      log act

    H2O                  5.55088E+01   1.00000E+03
    NA+                  5.15714E-01   1.18562E+01   5.15713E-01     -.
28759     -.24649     -.53408
    CA++                 9.74045E-05   3.90397E-03   9.74042E-05
```

```
-4.01142     -.98596    -4.99738
   MG++                 7.45860E-07   1.81281E-05   7.45857E-07
-6.12734     -.98596    -7.11330
   AL+++                1.00605E-24   2.71448E-23   1.00605E-24
-23.99738    -2.21841   -26.21579
   H4SIO4(AQ)           1.44992E-03   1.39359E-01   1.44992E-03
-2.83866      .00000    -2.83866
   H+                   4.43275E-07   4.46777E-07   4.43274E-07
-6.35333     -.24649    -6.59982
   CL-                  4.57685E-01   1.62263E+01   4.57683E-01     -.
33944     -.24649     -.58593
   FE++                 3.02065E-09   1.68694E-07   3.02064E-09
-8.51990     -.98596    -9.50586
   O2(AQ)               1.33381E-31   4.26805E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)               3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                1.31482E-22   7.34290E-21   1.31482E-22
-21.88113    -2.21841   -24.09954
   OH-                  5.86187E-02   9.96945E-01   5.86185E-02
-1.23197     -.24649    -1.47846
   H8SI3O10(AQ)         1.55088E-11   3.91308E-09   1.55088E-11
-10.80942      .00000   -10.80942
   H6SI2O7(AQ)          5.68672E-06   9.90707E-04   5.68670E-06
-5.24514      .00000    -5.24514
   AL(OH)3(AQ)          6.52919E-09   5.09299E-07   6.52917E-09
-8.18514      .00000    -8.18514
   AL(OH)4-             1.25474E-06   1.19213E-04   1.25473E-06
-5.90145     -.24649    -6.14794
   AL(OH)SI(OH)-        3.27853E-07   5.67547E-05   3.27852E-07
-6.48432     -.24649    -6.73081
   CACL+                2.05723E-04   1.55389E-02   2.05723E-04
-3.68672     -.24649    -3.93321
   CACL2(AQ)            3.75745E-06   4.17024E-04   3.75744E-06
-5.42511      .00000    -5.42511
   CA(OH)+              3.00989E-04   1.71827E-02   3.00988E-04
-3.52145     -.24649    -3.76794
   CA(H3SIO4)+          3.58083E-04   4.84081E-02   3.58082E-04
-3.44602     -.24649    -3.69251
   FE(OH)+              8.46452E-08   6.16677E-06   8.46450E-08
-7.07240     -.24649    -7.31889
   FE(OH)2              5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.95077E-06   6.35952E-04   5.95075E-06
-5.22543     -.24649    -5.47192
   FECL+                3.34896E-09   3.05760E-07   3.34895E-09
-8.47509     -.24649    -8.72158
   FECL2(AQ)            7.84137E-08   9.93917E-06   7.84135E-08
-7.10561      .00000    -7.10561
   FE(H3SIO4)+          1.49673E-04   2.25938E-02   1.49673E-04
```

```
-3.82486     -.24649    -4.07135
   MGCL+                7.44166E-07   4.44699E-05   7.44164E-07
-6.12833     -.24649    -6.37482
   MG(OH)+              1.63774E-05   6.76589E-04   1.63774E-05
-4.78576     -.24649    -5.03225
   MG(OH)2(AQ)          1.07886E+00   6.29186E+01   1.07885E+00      .
03296      .00000      .03296
   MG(H3SIO4)+          8.17926E-09   9.76701E-07   8.17924E-09
-8.08729     -.24649    -8.33378
   NACL(AQ)             4.21007E-02   2.46048E+00   4.21006E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)             1.66879E-02   6.67466E-01   1.66878E-02
-1.77760      .00000    -1.77760
   H3SIO4-              6.32006E-04   6.01081E-02   6.32004E-04
-3.19928     -.24649    -3.44577
   HCL(AQ)              5.61028E-07   2.04556E-05   5.61026E-07
-6.25102      .00000    -6.25102

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657359
           log (CA++  /h+**0)            8.2022537
           log (MG++  /h+**0)            6.0863316
           log (AL+++ /h+**0)           -6.4163375
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                 -6.4314592    3.70289E-07    8.57362E-05
1.64853E-05

   CLINOPYROXENE(SS)         -4.4582947    3.48101E-05    7.61287E-03
2.30443E-03
   DIOPSIDE                  -4.4888757    3.24432E-05    7.02566E-03
2.14774E-03
   HEDENBERGITE              -5.6258328    2.36683E-06    5.87197E-04
1.56684E-04
   JADEITE                  -10.6030628    2.49423E-11    5.04181E-09
1.50502E-09


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---
```

```
      phase/end-member        log moles        moles        grams
volume, cc

   MAGNETITE                  2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                  2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)            2.0000000    1.00000E+02

   ALBITE                     1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                  1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)          2.0000001    1.00000E+02

   DIOPSIDE                   1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE               1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -10.6030628    2.49423E-11    5.04181E-09
1.50502E-09



                        mass, grams        volume, cc

           created        7.698602E-03       2.320914E-03
           destroyed      2.760197E-04       9.095773E-05
           net            7.422582E-03       2.229956E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE               .0000  satd          HEMATITE
-3.3501
 PERICLASE             -4.8210                BRUCITE
-1.0847
 FORSTERITE             -.3961                FAYALITE
```

```
-1.7305
 CHRYSOTILE               -.6889                ENSTATITE-CL
-2.2000
 ENSTATITE-OR            -2.2781                ENSTATITE-PR
-2.6835
 DIOPSIDE                 -.1012                HEDENBERGITE
-3.8634
 FERROSILITE             -4.5003                WOLLASTONITE
-3.5960
 PSEUDOWOLLASTONITE      -4.0821                TREMOLITE
-5.6379
 ANTIGORITE               -.5298                TALC
-7.0060
 CLINOCHLORE             -2.8795                CHAMOSITE
-7.0612
 GROSSULAR               -8.9809                QUARTZ-ALPHA
-5.6849
 QUARTZ-BETA             -5.9218                COESITE
-6.2812
 IRON-ALPHA              -8.6597                IRON-GAMMA
-7.8030
 HALITE                  -9.7500                CRISTOBALITE-ALPHA
-6.9708
 CRISTOBALITE-BETA       -7.6842


                --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -24.5521
     ALBITE                     -24.55213     .9981382     1.00000
     ANORTHITE                  -24.55213     .0018618     1.00000

 ORTHOPYROXENE(SS)         -2.0006
     ENSTATITE-OR                -2.00056     .8243812     1.00000
     FERROSILITE                 -2.00056     .1756188     1.00000

 GARNET(SS)                -8.7313
     PYROPE                      -8.73126     .0821502     1.00000
     ALMANDINE                   -8.73126     .0773320     1.00000
     GROSSULAR                   -8.73126     .8405178     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .9320066     1.00000
     HEDENBERGITE                  .00000     .0679926     1.00000
     JADEITE                       .00000     .0000007     1.00000

 CPX_SUBCALCIC(SS)           .0000
```

```
    DIOPSIDE                     .00000     .9320073     1.00000
    HEDENBERGITE                 .00000     .0679927     1.00000

CHLORITE(SS)            -2.8032
    CLINOCHLORE                -2.80322     .9483341     1.00000
    CHAMOSITE                  -2.80322     .0516659     1.00000


solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

  CLINOPYROXENE(SS)
ideal solution

    DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0000    1.0000     .0000   -6.1448     .0000   -6.1448


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

  O2(G)                          -26.80001       1.58487E-27
  H2(G)                            2.27783       1.89596E+02
  H2O(G)                           3.80603       6.39774E+03



- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



stepping to zi=  3.9811E-07, delzi=  1.4692E-07, nord= 2
              ncycle=  0
steps completed =    10, iter =  4, ncorr = 0
most rapidly changing is zvclg1(JADEITE           ) =    -10.5104
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  3.98107170553495E-07
                    log of reaction progress =      -6.4000000
```

temperature   =   450.000 degrees c
total pressure =   500.000 bars

computing units remaining =   .000

step size is limited by the print requirement

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	1.00000E+02	6.66949E-07	2.68618E+04	1.79154E-04
CLINOPYROXENE(SS)	1.00000E+02	8.03858E-07	2.22861E+04	1.79148E-04
MAGNETITE	1.00000E+02	8.59911E-08	2.31539E+04	1.99103E-05
TREMOLITE	1.00000E+02	7.29332E-08	8.12370E+04	5.92488E-05

current total mass = 1.53539E+05 grams
delta total mass   = 4.37462E-04 grams
delta total volume =   .00014 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	26.8050	1.67530E+00
CLINOPYROXENE(SS)	.1345	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.6373	1.83200E-01

affinity of the overall irreversible reaction=   45.939 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434542E+05	5.775244E+01	5.775261E+01

```
NA        1.205627E+04      5.745014E-01      5.745031E-01
CA        3.533506E+01      9.658076E-04      9.658105E-04
MG        2.393609E+04      1.078873E+00      1.078876E+00
AL        4.762571E-02      1.933692E-06      1.933698E-06
SI        6.669870E+01      2.601643E-03      2.601651E-03
H         1.042623E+05      1.133241E+02      1.133244E+02
CL        1.618114E+04      4.999985E-01      5.000000E-01
FE        7.972782E+00      1.563949E-04      1.563954E-04

co3--                       0.000000E+00      0.000000E+00
so4--                       0.000000E+00      0.000000E+00
s--                         0.000000E+00      0.000000E+00

 warning-- co3--, so4--, and s-- totals require that routine comp1
 have the names of non-carbonate carbon, sulfide sulfur,
 and non-sulfate sulfur aqueous species


single ion activities and activity coefficients are here defined
with respect to the internal ph scale



                                     ph           eh           pe

  internal ph scale               6.5998        .4548
3.1695E+00
  modified nbs ph scale           6.3533        .4901
3.4160E+00
  rational ph scale               6.3533        .4901
3.4160E+00

phcl =      7.1857


      oxygen fugacity =  1.58487E-27
      log oxygen fugacity = -26.80001


                         activity of water =    .98384
           log activity of water =   -.00707
           alkalinity =  0.000000E+00 equiv/kg solvent
                                      (not def. for t.gt.50 c)

                ionic strength =  5.170394E-01 molal
             sum of molalities =    2.2049458133304
           osmotic coefficient =     .41003
                equiv. stoich. ionic strength =  4.999985E-01
```

molal

mass of solution = 1.095504 kg
mass of solvent = 1.000003 kg
mass of solutes = .095501 kg
conc of solutes = 8.717517 per cent (w/w)

species	moles	grams	conc	log conc	log g	log act
H2O	5.55088E+01	1.00000E+03				
NA+	5.15715E-01	1.18562E+01	5.15713E-01	-.28759	-.24649	-.53408
CA++	9.73866E-05	3.90325E-03	9.73863E-05	-4.01150	-.98596	-4.99746
MG++	7.45868E-07	1.81283E-05	7.45866E-07	-6.12734	-.98596	-7.11330
AL+++	1.22421E-24	3.30310E-23	1.22420E-24	-23.91215	-2.21841	-26.13056
H4SIO4(AQ)	1.45006E-03	1.39373E-01	1.45006E-03	-2.83861	.00000	-2.83861
H+	4.43278E-07	4.46780E-07	4.43276E-07	-6.35333	-.24649	-6.59982
CL-	4.57685E-01	1.62263E+01	4.57683E-01	-.33944	-.24649	-.58593
FE++	3.02068E-09	1.68696E-07	3.02067E-09	-8.51990	-.98596	-9.50586
O2(AQ)	1.33381E-31	4.26805E-30	1.33381E-31	-30.87491	.00000	-30.87491
H2(AQ)	3.20576E-02	6.46217E-02	3.20575E-02	-1.49407	.00000	-1.49407
FE+++	1.31485E-22	7.34303E-21	1.31484E-22	-21.88113	-2.21841	-24.09954
OH-	5.86183E-02	9.96939E-01	5.86182E-02	-1.23197	-.24649	-1.47846
H8SI3O10(AQ)	1.55134E-11	3.91424E-09	1.55133E-11	-10.80929	.00000	-10.80929
H6SI2O7(AQ)	5.68783E-06	9.90901E-04	5.68782E-06	-5.24505	.00000	-5.24505
AL(OH)3(AQ)	7.94485E-09	6.19726E-07	7.94483E-09	-8.09992	.00000	-8.09992
AL(OH)4-	1.52678E-06	1.45060E-04	1.52677E-06	-5.81623	-.24649	-6.06272
AL(OH)SI(OH)-	3.98975E-07	6.90666E-05	3.98974E-07	-6.39906	-.24649	-6.64555
CACL+	2.05685E-04	1.55360E-02	2.05685E-04	-3.68680	-.24649	-3.93329
CACL2(AQ)	3.75676E-06	4.16947E-04	3.75674E-06	-5.42519	.00000	-5.42519

```
   CA(OH)+                 3.00932E-04   1.71794E-02   3.00931E-04
-3.52153     -.24649    -3.76802
   CA(H3SIO4)+             3.58050E-04   4.84037E-02   3.58049E-04
-3.44606     -.24649    -3.69255
   FE(OH)+                 8.46457E-08   6.16681E-06   8.46455E-08
-7.07240     -.24649    -7.31889
   FE(OH)2                 5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-                5.95073E-06   6.35948E-04   5.95071E-06
-5.22543     -.24649    -5.47192
   FECL+                   3.34900E-09   3.05764E-07   3.34899E-09
-8.47509     -.24649    -8.72158
   FECL2(AQ)               7.84146E-08   9.93929E-06   7.84144E-08
-7.10560      .00000    -7.10560
   FE(H3SIO4)+             1.49689E-04   2.25961E-02   1.49689E-04
-3.82481     -.24649    -4.07130
   MGCL+                   7.44175E-07   4.44704E-05   7.44173E-07
-6.12833     -.24649    -6.37482
   MG(OH)+                 1.63775E-05   6.76593E-04   1.63775E-05
-4.78575     -.24649    -5.03224
   MG(OH)2(AQ)             1.07886E+00   6.29186E+01   1.07885E+00      .
03296      .00000      .03296
   MG(H3SIO4)+             8.18011E-09   9.76802E-07   8.18009E-09
-8.08724     -.24649    -8.33373
   NACL(AQ)                4.21008E-02   2.46049E+00   4.21006E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)                1.66878E-02   6.67462E-01   1.66877E-02
-1.77760      .00000    -1.77760
   H3SIO4-                 6.32065E-04   6.01137E-02   6.32063E-04
-3.19924     -.24649    -3.44573
   HCL(AQ)                 5.61031E-07   2.04557E-05   5.61029E-07
-6.25101      .00000    -6.25101

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657335
           log (CA++  /h+**0)            8.2021684
           log (MG++  /h+**0)            6.0863315
           log (AL+++ /h+**0)           -6.3311113
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc
```

```
   MAGNETITE                 -6.3945819    4.03105E-07    9.33344E-05
1.79462E-05

   CLINOPYROXENE(SS)         -4.4509224    3.54061E-05    7.74320E-03
2.34388E-03
   DIOPSIDE                  -4.4815035    3.29987E-05    7.14594E-03
2.18451E-03
   HEDENBERGITE              -5.6184605    2.40735E-06    5.97250E-04
1.59367E-04
   JADEITE                  -10.5103814    3.08758E-11    6.24120E-09
1.86305E-09


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                  2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)            2.0000000    1.00000E+02

   ALBITE                     1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                  1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)          2.0000002    1.00000E+02

   DIOPSIDE                   1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE               1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -10.5103814    3.08758E-11    6.24120E-09
1.86305E-09



                             mass, grams        volume, cc

           created          7.836534E-03       2.361827E-03
           destroyed        4.374617E-04       1.441583E-04
           net              7.399072E-03       2.217669E-03

          warning-- these volume totals may be incomplete because
```

```
          of missing partial molar volume data in the data base


          --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3501
 PERICLASE              -4.8210                BRUCITE
-1.0847
 FORSTERITE              -.3960                FAYALITE
-1.7304
 CHRYSOTILE              -.6886                ENSTATITE-CL
-2.1999
 ENSTATITE-OR           -2.2780                ENSTATITE-PR
-2.6833
 DIOPSIDE                -.1012                HEDENBERGITE
-3.8634
 FERROSILITE            -4.5001                WOLLASTONITE
-3.5961
 PSEUDOWOLLASTONITE     -4.0822                TREMOLITE
-5.6373
 ANTIGORITE              -.5274                TALC
-7.0054
 CLINOCHLORE            -2.7666                CHAMOSITE
-6.9484
 GROSSULAR              -8.7933                QUARTZ-ALPHA
-5.6848
 QUARTZ-BETA            -5.9217                COESITE
-6.2811
 IRON-ALPHA             -8.6597                IRON-GAMMA
-7.8030
 HALITE                 -9.7500                CRISTOBALITE-ALPHA
-6.9707
 CRISTOBALITE-BETA      -7.6841


                    --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -24.2691
     ALBITE                     -24.26912     .9977361     1.00000
     ANORTHITE                  -24.26912     .0022639     1.00000

 ORTHOPYROXENE(SS)         -2.0004
```

```
    ENSTATITE-OR                  -2.00042     .8243812     1.00000
    FERROSILITE                   -2.00042     .1756188     1.00000

 GARNET(SS)                -8.5435
    PYROPE                        -8.54354     .0821638     1.00000
    ALMANDINE                     -8.54354     .0773448     1.00000
    GROSSULAR                     -8.54354     .8404914     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
    DIOPSIDE                        .00000     .9320065     1.00000
    HEDENBERGITE                    .00000     .0679926     1.00000
    JADEITE                         .00000     .0000009     1.00000

 CPX_SUBCALCIC(SS)           .0000
    DIOPSIDE                        .00000     .9320073     1.00000
    HEDENBERGITE                    .00000     .0679927     1.00000

 CHLORITE(SS)              -2.6903
    CLINOCHLORE                   -2.69033     .9483341     1.00000
    CHAMOSITE                     -2.69033     .0516659     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0000    1.0000     .0000   -6.0595     .0000   -6.0595


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                          -26.80001       1.58487E-27
   H2(G)                            2.27783       1.89596E+02
   H2O(G)                           3.80603       6.39774E+03
```

```
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  6.3096E-07, delzi=  2.3285E-07, nord= 2
               ncycle=  0
 steps completed =    11, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =    -10.3908
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  6.30957344480189E-07
                     log of reaction progress =      -6.2000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         1.00000E+02    1.05704E-06    2.68618E+04
2.83940E-04
   CLINOPYROXENE(SS)       1.00000E+02    1.27403E-06    2.22861E+04
2.83931E-04
   MAGNETITE               1.00000E+02    1.36287E-07    2.31539E+04
3.15557E-05
   TREMOLITE               1.00000E+02    1.15591E-07    8.12370E+04
9.39030E-05


                current total mass =  1.53539E+05 grams
                delta total mass   =  6.93330E-04 grams
                delta total volume =       .00023 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           26.3042    1.67530E+00
   CLINOPYROXENE(SS)           .1345    0.00000E+00
```

```
   MAGNETITE                    .0000    0.00000E+00
   TREMOLITE                   5.6364    1.83200E-01

          affinity of the overall irreversible reaction=    45.100
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O          8.434542E+05        5.775244E+01        5.775262E+01
      NA         1.205628E+04        5.745016E-01        5.745033E-01
      CA         3.532653E+01        9.655747E-04        9.655775E-04
      MG         2.393609E+04        1.078872E+00        1.078876E+00
      AL         6.107633E-02        2.479812E-06        2.479819E-06
      SI         6.670913E+01        2.602050E-03        2.602058E-03
      H          1.042623E+05        1.133241E+02        1.133244E+02
      CL         1.618114E+04        4.999985E-01        5.000000E-01
      FE         7.974040E+00        1.564196E-04        1.564201E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                             ph            eh            pe

     internal ph scale                     6.5998         .4548
3.1695E+00
     modified nbs ph scale                 6.3533         .4901
3.4160E+00
     rational ph scale                     6.3533         .4901
3.4160E+00

   phcl =      7.1857
```

```
          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001



                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                    ionic strength =  5.170395E-01 molal
                 sum of molalities =    2.2049459360491
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999985E-01
molal

                         mass of solution =   1.095504 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095501 kg
                         conc of solutes  =   8.717522 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15715E-01   1.18562E+01   5.15713E-01     -.
28759     -.24649     -.53408
   CA++                 9.73581E-05   3.90211E-03   9.73578E-05
-4.01163     -.98596    -4.99759
   MG++                 7.45882E-07   1.81287E-05   7.45880E-07
-6.12733     -.98596    -7.11329
   AL+++                1.56996E-24   4.23599E-23   1.56995E-24
-23.80411    -2.21841   -26.02252
   H4SIO4(AQ)           1.45029E-03   1.39394E-01   1.45029E-03
-2.83855      .00000    -2.83855
   H+                   4.43282E-07   4.46784E-07   4.43281E-07
-6.35332     -.24649    -6.59981
   CL-                  4.57685E-01   1.62263E+01   4.57683E-01     -.
33943     -.24649     -.58593
   FE++                 3.02074E-09   1.68699E-07   3.02073E-09
-8.51989     -.98596    -9.50585
   O2(AQ)               1.33381E-31   4.26804E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)               3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                1.31489E-22   7.34324E-21   1.31488E-22
-21.88111    -2.21841   -24.09952
   OH-                  5.86178E-02   9.96930E-01   5.86176E-02
```

```
-1.23197     -.24649    -1.47846
   H8SI3O10(AQ)         1.55206E-11   3.91607E-09   1.55206E-11
-10.80909      .00000   -10.80909
   H6SI2O7(AQ)          5.68960E-06   9.91210E-04   5.68959E-06
-5.24492      .00000    -5.24492
   AL(OH)3(AQ)          1.01884E-08   7.94733E-07   1.01884E-08
-7.99189      .00000    -7.99189
   AL(OH)4-             1.95791E-06   1.86023E-04   1.95791E-06
-5.70821     -.24649    -5.95470
   AL(OH)SI(OH)-        5.11718E-07   8.85836E-05   5.11716E-07
-6.29097     -.24649    -6.53746
   CACL+                2.05625E-04   1.55315E-02   2.05624E-04
-3.68693     -.24649    -3.93342
   CACL2(AQ)            3.75566E-06   4.16825E-04   3.75565E-06
-5.42532      .00000    -5.42532
   CA(OH)+              3.00841E-04   1.71742E-02   3.00840E-04
-3.52166     -.24649    -3.76815
   CA(H3SIO4)+          3.57998E-04   4.83966E-02   3.57997E-04
-3.44612     -.24649    -3.69261
   FE(OH)+              8.46465E-08   6.16687E-06   8.46463E-08
-7.07239     -.24649    -7.31888
   FE(OH)2              5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.95067E-06   6.35942E-04   5.95066E-06
-5.22544     -.24649    -5.47193
   FECL+                3.34907E-09   3.05770E-07   3.34906E-09
-8.47508     -.24649    -8.72157
   FECL2(AQ)            7.84161E-08   9.93948E-06   7.84159E-08
-7.10560      .00000    -7.10560
   FE(H3SIO4)+          1.49714E-04   2.25999E-02   1.49713E-04
-3.82474     -.24649    -4.07123
   MGCL+                7.44189E-07   4.44712E-05   7.44187E-07
-6.12832     -.24649    -6.37481
   MG(OH)+              1.63777E-05   6.76599E-04   1.63776E-05
-4.78575     -.24649    -5.03224
   MG(OH)2(AQ)          1.07886E+00   6.29186E+01   1.07885E+00      .
03296      .00000      .03296
   MG(H3SIO4)+          8.18146E-09   9.76963E-07   8.18144E-09
-8.08717     -.24649    -8.33366
   NACL(AQ)             4.21008E-02   2.46049E+00   4.21007E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)             1.66876E-02   6.67456E-01   1.66876E-02
-1.77761      .00000    -1.77761
   H3SIO4-              6.32157E-04   6.01224E-02   6.32155E-04
-3.19918     -.24649    -3.44567
   HCL(AQ)              5.61036E-07   2.04559E-05   5.61035E-07
-6.25101      .00000    -6.25101

           --- activity ratios of cations ---
```

```
           log (NA+   /h+**0)            6.0657297
           log (CA++  /h+**0)            8.2020331
           log (MG++  /h+**0)            6.0863314
           log (AL+++ /h+**0)           -6.2230897
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                  -6.3418795    4.55114E-07    1.05377E-04
2.02617E-05

   CLINOPYROXENE(SS)          -4.4394891    3.63505E-05    7.94976E-03
2.40641E-03
   DIOPSIDE                   -4.4700703    3.38789E-05    7.33656E-03
2.24279E-03
   HEDENBERGITE               -5.6070272    2.47157E-06    6.13183E-04
1.63618E-04
   JADEITE                   -10.3907950    4.06635E-11    8.21967E-09
2.45364E-09


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member        log moles        moles        grams
volume, cc

   MAGNETITE                   2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                   2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)             2.0000000    1.00000E+02

   ALBITE                      1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                   1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)           2.0000002    1.00000E+02

   DIOPSIDE                    1.9030902    8.00000E+01    1.73242E+04
```

```
5.29600E+03
   HEDENBERGITE              1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                 -10.3907950    4.06635E-11    8.21967E-09
2.45364E-09


                           mass, grams        volume, cc

           created         8.055132E-03       2.426667E-03
           destroyed       6.933300E-04       2.284755E-04
           net             7.361802E-03       2.198192E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base


           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3501
 PERICLASE              -4.8210                BRUCITE
-1.0847
 FORSTERITE              -.3959                FAYALITE
-1.7303
 CHRYSOTILE              -.6882                ENSTATITE-CL
-2.1996
 ENSTATITE-OR           -2.2777                ENSTATITE-PR
-2.6831
 DIOPSIDE                -.1012                HEDENBERGITE
-3.8634
 FERROSILITE            -4.4999                WOLLASTONITE
-3.5964
 PSEUDOWOLLASTONITE     -4.0825                TREMOLITE
-5.6364
 ANTIGORITE              -.5236                TALC
-7.0045
 CLINOCHLORE            -2.6235                CHAMOSITE
-6.8052
 GROSSULAR              -8.5554                QUARTZ-ALPHA
-5.6846
 QUARTZ-BETA            -5.9215                COESITE
-6.2808
 IRON-ALPHA             -8.6597                IRON-GAMMA
```

```
-7.8030
 HALITE                 -9.7500                CRISTOBALITE-ALPHA
-6.9704
 CRISTOBALITE-BETA      -7.6839


                    --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -23.9101
     ALBITE                    -23.91010     .9971000     1.00000
     ANORTHITE                 -23.91010     .0029000     1.00000

 ORTHOPYROXENE(SS)        -2.0002
     ENSTATITE-OR               -2.00020     .8243811     1.00000
     FERROSILITE                -2.00020     .1756189     1.00000

 GARNET(SS)               -8.3056
     PYROPE                     -8.30563     .0821853     1.00000
     ALMANDINE                  -8.30563     .0773651     1.00000
     GROSSULAR                  -8.30563     .8404496     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9320062     1.00000
     HEDENBERGITE                 .00000     .0679926     1.00000
     JADEITE                      .00000     .0000011     1.00000

 CPX_SUBCALCIC(SS)          .0000
     DIOPSIDE                     .00000     .9320073     1.00000
     HEDENBERGITE                 .00000     .0679927     1.00000

 CHLORITE(SS)             -2.5472
     CLINOCHLORE                -2.54722     .9483340     1.00000
     CHAMOSITE                  -2.54722     .0516660     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
```

```
     JADEITE
              .0000    1.0000     .0000   -5.9513     .0000   -5.9513


           --- summary of gas species ---

           gas               log fugacity         fugacity
partial pressure

   O2(G)                          -26.80001       1.58487E-27
   H2(G)                            2.27783       1.89596E+02
   H2O(G)                           3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.0000E-06, delzi=  3.6904E-07, nord= 3
               ncycle=  0
 steps completed =    12, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =    -10.2431
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  9.99999999999993E-07
                     log of reaction progress =      -6.0000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         1.00000E+02    1.67530E-06    2.68618E+04
4.50015E-04
   CLINOPYROXENE(SS)       1.00000E+02    2.01920E-06    2.22861E+04
4.50001E-04
```

```
   MAGNETITE              1.00000E+02    2.16000E-07    2.31539E+04
5.00123E-05
   TREMOLITE              1.00000E+02    1.83200E-07    8.12370E+04
1.48826E-04


                current total mass =  1.53539E+05 grams
                delta total mass   =  1.09885E-03 grams
                delta total volume =       .00036 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           25.7013    1.67530E+00
   CLINOPYROXENE(SS)           .1345    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.6350    1.83200E-01

          affinity of the overall irreversible reaction=    44.090
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O          8.434541E+05        5.775245E+01        5.775262E+01
      NA         1.205629E+04        5.745020E-01        5.745037E-01
      CA         3.531303E+01        9.652056E-04        9.652084E-04
      MG         2.393607E+04        1.078872E+00        1.078875E+00
      AL         8.239409E-02        3.345353E-06        3.345363E-06
      SI         6.672566E+01        2.602695E-03        2.602703E-03
      H          1.042623E+05        1.133241E+02        1.133244E+02
      CL         1.618114E+04        4.999985E-01        5.000000E-01
      FE         7.976034E+00        1.564587E-04        1.564592E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale
```

```
                                         ph            eh            pe

     internal ph scale              6.5998        .4548
3.1695E+00
     modified nbs ph scale          6.3533        .4901
3.4160E+00
     rational ph scale              6.3533        .4901
3.4160E+00

   phcl =      7.1857



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001



                           activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                    ionic strength =  5.170397E-01 molal
                 sum of molalities =    2.2049461309733
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999985E-01
molal

                         mass of solution =   1.095504 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095501 kg
                         conc of solutes  =   8.717529 per cent (w/w)


   species               moles        grams          conc        log
conc      log g      log act

   H2O                 5.55088E+01   1.00000E+03
   NA+                 5.15715E-01   1.18562E+01   5.15714E-01     -.
28759     -.24649     -.53408
   CA++                9.73130E-05   3.90030E-03   9.73127E-05
-4.01183     -.98596    -4.99779
   MG++                7.45904E-07   1.81292E-05   7.45902E-07
-6.12732     -.98596    -7.11328
   AL+++               2.11795E-24   5.71455E-23   2.11794E-24
-23.67409    -2.21841   -25.89250
```

```
   H4SIO4(AQ)          1.45065E-03   1.39429E-01   1.45064E-03
-2.83844      .00000    -2.83844
   H+                  4.43289E-07   4.46791E-07   4.43287E-07
-6.35331     -.24649    -6.59980
   CL-                 4.57685E-01   1.62263E+01   4.57683E-01      -.
33943     -.24649     -.58593
   FE++                3.02083E-09   1.68704E-07   3.02082E-09
-8.51987     -.98596    -9.50584
   O2(AQ)              1.33381E-31   4.26804E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)              3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++               1.31494E-22   7.34357E-21   1.31494E-22
-21.88109    -2.21841   -24.09950
   OH-                 5.86169E-02   9.96915E-01   5.86167E-02
-1.23198     -.24649    -1.47847
   H8SI3O10(AQ)        1.55321E-11   3.91897E-09   1.55321E-11
-10.80877      .00000   -10.80877
   H6SI2O7(AQ)         5.69241E-06   9.91699E-04   5.69240E-06
-5.24470      .00000    -5.24470
   AL(OH)3(AQ)         1.37441E-08   1.07208E-06   1.37440E-08
-7.86189      .00000    -7.86189
   AL(OH)4-            2.64116E-06   2.50938E-04   2.64115E-06
-5.57821     -.24649    -5.82470
   AL(OH)SI(OH)-       6.90460E-07   1.19526E-04   6.90458E-07
-6.16086     -.24649    -6.40735
   CACL+               2.05530E-04   1.55243E-02   2.05529E-04
-3.68713     -.24649    -3.93362
   CACL2(AQ)           3.75392E-06   4.16632E-04   3.75391E-06
-5.42552      .00000    -5.42552
   CA(OH)+             3.00697E-04   1.71660E-02   3.00696E-04
-3.52187     -.24649    -3.76836
   CA(H3SIO4)+         3.57915E-04   4.83854E-02   3.57914E-04
-3.44622     -.24649    -3.69271
   FE(OH)+             8.46478E-08   6.16696E-06   8.46476E-08
-7.07239     -.24649    -7.31888
   FE(OH)2             5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-            5.95059E-06   6.35933E-04   5.95057E-06
-5.22544     -.24649    -5.47193
   FECL+               3.34917E-09   3.05779E-07   3.34916E-09
-8.47506     -.24649    -8.72155
   FECL2(AQ)           7.84185E-08   9.93978E-06   7.84183E-08
-7.10558      .00000    -7.10558
   FE(H3SIO4)+         1.49753E-04   2.26058E-02   1.49752E-04
-3.82463     -.24649    -4.07112
   MGCL+               7.44211E-07   4.44726E-05   7.44209E-07
-6.12831     -.24649    -6.37480
   MG(OH)+             1.63779E-05   6.76609E-04   1.63779E-05
-4.78574     -.24649    -5.03223
```

```
   MG(OH)2(AQ)          1.07886E+00   6.29185E+01   1.07885E+00      .
03296      .00000      .03296
   MG(H3SIO4)+          8.18360E-09   9.77219E-07   8.18358E-09
-8.08706    -.24649    -8.33355
   NACL(AQ)             4.21008E-02   2.46049E+00   4.21007E-02
-1.37571      .00000   -1.37571
   NAOH(AQ)             1.66874E-02   6.67447E-01   1.66873E-02
-1.77761      .00000   -1.77761
   H3SIO4-              6.32304E-04   6.01364E-02   6.32302E-04
-3.19908    -.24649    -3.44557
   HCL(AQ)              5.61045E-07   2.04562E-05   5.61043E-07
-6.25100      .00000   -6.25100

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657237
           log (CA++  /h+**0)            8.2018187
           log (MG++  /h+**0)            6.0863312
           log (AL+++ /h+**0)           -6.0930821
           log (FE++  /h+**0)            3.6937745
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE               -6.2695870    5.37543E-07    1.24462E-04
2.39314E-05

   CLINOPYROXENE(SS)       -4.4219645    3.78473E-05    8.27710E-03
2.50549E-03
   DIOPSIDE                -4.4525459    3.52739E-05    7.63866E-03
2.33514E-03
   HEDENBERGITE            -5.5895026    2.57334E-06    6.38432E-04
1.70355E-04
   JADEITE                -10.2430546    5.71407E-11    1.15503E-08
3.44787E-09


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                2.0000000    1.00000E+02    2.31539E+04
```

```
4.45200E+03
   TREMOLITE                  2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)            2.0000000    1.00000E+02

   ALBITE                     1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                  1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)          2.0000002    1.00000E+02

   DIOPSIDE                   1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE               1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -10.2430546    5.71407E-11    1.15503E-08
3.44787E-09



                            mass, grams        volume, cc

           created          8.401563E-03       2.529425E-03
           destroyed        1.098854E-03       3.621092E-04
           net              7.302709E-03       2.167316E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3501
 PERICLASE              -4.8210                BRUCITE
-1.0847
 FORSTERITE              -.3957                FAYALITE
-1.7301
 CHRYSOTILE              -.6875                ENSTATITE-CL
-2.1993
 ENSTATITE-OR           -2.2774                ENSTATITE-PR
-2.6827
```

```
 DIOPSIDE                  -.1012                HEDENBERGITE
-3.8634
 FERROSILITE              -4.4996                WOLLASTONITE
-3.5967
 PSEUDOWOLLASTONITE       -4.0828                TREMOLITE
-5.6350
 ANTIGORITE                -.5176                TALC
-7.0031
 CLINOCHLORE              -2.4512                CHAMOSITE
-6.6330
 GROSSULAR                -8.2693                QUARTZ-ALPHA
-5.6842
 QUARTZ-BETA              -5.9211                COESITE
-6.2805
 IRON-ALPHA               -8.6597                IRON-GAMMA
-7.8030
 HALITE                   -9.7500                CRISTOBALITE-ALPHA
-6.9701
 CRISTOBALITE-BETA        -7.6835


                     --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -23.4774
     ALBITE                      -23.47741     .9960947     1.00000
     ANORTHITE                   -23.47741     .0039053     1.00000

 ORTHOPYROXENE(SS)          -1.9998
     ENSTATITE-OR                 -1.99984     .8243811     1.00000
     FERROSILITE                  -1.99984     .1756189     1.00000

 GARNET(SS)                 -8.0194
     PYROPE                       -8.01936     .0822194     1.00000
     ALMANDINE                    -8.01936     .0773972     1.00000
     GROSSULAR                    -8.01936     .8403834     1.00000

 CLINOPYROXENE(SS)            .0000
saturated
     DIOPSIDE                       .00000     .9320058     1.00000
     HEDENBERGITE                   .00000     .0679926     1.00000
     JADEITE                        .00000     .0000015     1.00000

 CPX_SUBCALCIC(SS)            .0000
     DIOPSIDE                       .00000     .9320072     1.00000
     HEDENBERGITE                   .00000     .0679928     1.00000

 CHLORITE(SS)               -2.3749
     CLINOCHLORE                  -2.37493     .9483340     1.00000
```

```
    CHAMOSITE                  -2.37493     .0516660     1.00000


  solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
 activity

   CLINOPYROXENE(SS)
  ideal solution

     DIOPSIDE
              .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
              .0000    1.0000     .0000   -5.8211     .0000   -5.8211


           --- summary of gas species ---

           gas                log fugacity         fugacity
 partial pressure

   O2(G)                        -26.80001       1.58487E-27
   H2(G)                          2.27783       1.89596E+02
   H2O(G)                         3.80603       6.39774E+03



  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



  stepping to zi=  1.5849E-06, delzi=  5.8489E-07, nord= 3
                ncycle=  0
  steps completed =    13, iter =  5, ncorr = 0
  most rapidly changing is zvclg1(JADEITE          ) =    -10.0671
  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  1.58489319246110E-06
                    log of reaction progress =      -5.8000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000
```

step size is limited by the print requirement

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	1.00000E+02	2.65517E-06	2.68618E+04	7.13226E-04
CLINOPYROXENE(SS)	1.00000E+02	3.20022E-06	2.22861E+04	7.13203E-04
MAGNETITE	1.00000E+02	3.42337E-07	2.31539E+04	7.92642E-05
TREMOLITE	1.00000E+02	2.90352E-07	8.12370E+04	2.35874E-04

current total mass = 1.53539E+05 grams
delta total mass = 1.74157E-03 grams
delta total volume = .00057 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	25.0091	1.67530E+00
CLINOPYROXENE(SS)	.1345	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.6328	1.83200E-01

affinity of the overall irreversible reaction= 42.930 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434541E+05	5.775245E+01	5.775262E+01
NA	1.205630E+04	5.745026E-01	5.745043E-01
CA	3.529163E+01	9.646209E-04	9.646237E-04
MG	2.393606E+04	1.078871E+00	1.078874E+00
AL	1.161804E-01	4.717141E-06	4.717155E-06
SI	6.675188E+01	2.603718E-03	2.603726E-03

```
    H          1.042622E+05       1.133241E+02       1.133244E+02
    CL         1.618114E+04       4.999986E-01       5.000000E-01
    FE         7.979195E+00       1.565207E-04       1.565212E-04

    co3--                         0.000000E+00       0.000000E+00
    so4--                         0.000000E+00       0.000000E+00
    s--                           0.000000E+00       0.000000E+00

  warning-- co3--, so4--, and s-- totals require that routine comp1
  have the names of non-carbonate carbon, sulfide sulfur,
  and non-sulfate sulfur aqueous species


 single ion activities and activity coefficients are here defined
 with respect to the internal ph scale



                                         ph           eh            pe

     internal ph scale                6.5998        .4548
3.1695E+00
     modified nbs ph scale            6.3533        .4901
3.4160E+00
     rational ph scale                6.3533        .4901
3.4160E+00

   phcl =      7.1857



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001



                     activity of water =    .98384
          log activity of water =   -.00707
          alkalinity =  0.000000E+00 equiv/kg solvent
                                  (not def. for t.gt.50 c)

               ionic strength =  5.170399E-01 molal
            sum of molalities =    2.2049464409827
          osmotic coefficient =     .41003
               equiv. stoich. ionic strength =  4.999986E-01
molal

                    mass of solution =   1.095504 kg
                    mass of solvent  =   1.000003 kg
                    mass of solutes  =    .095501 kg
```

conc of solutes = 8.717541 per cent (w/w)

species	moles	grams	conc	log conc	log g	log act
H2O	5.55088E+01	1.00000E+03				
NA+	5.15716E-01	1.18562E+01	5.15715E-01	-.28759	-.24649	-.53408
CA++	9.72415E-05	3.89744E-03	9.72412E-05	-4.01215	-.98596	-4.99811
MG++	7.45940E-07	1.81301E-05	7.45937E-07	-6.12730	-.98596	-7.11326
AL+++	2.98647E-24	8.05797E-23	2.98647E-24	-23.52484	-2.21841	-25.74325
H4SIO4(AQ)	1.45122E-03	1.39483E-01	1.45121E-03	-2.83827	.00000	-2.83827
H+	4.43299E-07	4.46801E-07	4.43298E-07	-6.35330	-.24649	-6.59979
CL-	4.57685E-01	1.62263E+01	4.57683E-01	-.33943	-.24649	-.58592
FE++	3.02098E-09	1.68712E-07	3.02097E-09	-8.51985	-.98596	-9.50581
O2(AQ)	1.33381E-31	4.26804E-30	1.33381E-31	-30.87491	.00000	-30.87491
H2(AQ)	3.20576E-02	6.46217E-02	3.20575E-02	-1.49407	.00000	-1.49407
FE+++	1.31504E-22	7.34410E-21	1.31504E-22	-21.88106	-2.21841	-24.09947
OH-	5.86155E-02	9.96892E-01	5.86153E-02	-1.23199	-.24649	-1.47848
H8SI3O10(AQ)	1.55504E-11	3.92357E-09	1.55503E-11	-10.80826	.00000	-10.80826
H6SI2O7(AQ)	5.69687E-06	9.92475E-04	5.69685E-06	-5.24437	.00000	-5.24437
AL(OH)3(AQ)	1.93788E-08	1.51161E-06	1.93787E-08	-7.71267	.00000	-7.71267
AL(OH)4-	3.72388E-06	3.53809E-04	3.72387E-06	-5.42901	-.24649	-5.67550
AL(OH)SI(OH)-	9.73891E-07	1.68591E-04	9.73888E-07	-6.01149	-.24649	-6.25798
CACL+	2.05379E-04	1.55129E-02	2.05378E-04	-3.68745	-.24649	-3.93394
CACL2(AQ)	3.75116E-06	4.16326E-04	3.75115E-06	-5.42584	.00000	-5.42584
CA(OH)+	3.00469E-04	1.71530E-02	3.00468E-04	-3.52220	-.24649	-3.76869
CA(H3SIO4)+	3.57783E-04	4.83676E-02	3.57782E-04	-3.44638	-.24649	-3.69287
FE(OH)+	8.46498E-08	6.16710E-06	8.46496E-08			

```
-7.07238     -.24649    -7.31887
   FE(OH)2                5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-               5.95045E-06   6.35918E-04   5.95043E-06
-5.22545     -.24649    -5.47194
   FECL+                  3.34933E-09   3.05794E-07   3.34932E-09
-8.47504     -.24649    -8.72153
   FECL2(AQ)              7.84222E-08   9.94025E-06   7.84220E-08
-7.10556      .00000    -7.10556
   FE(H3SIO4)+            1.49815E-04   2.26152E-02   1.49815E-04
-3.82445     -.24649    -4.07094
   MGCL+                  7.44246E-07   4.44747E-05   7.44244E-07
-6.12828     -.24649    -6.37477
   MG(OH)+                1.63783E-05   6.76625E-04   1.63782E-05
-4.78573     -.24649    -5.03222
   MG(OH)2(AQ)            1.07886E+00   6.29185E+01   1.07885E+00      .
03296      .00000      .03296
   MG(H3SIO4)+            8.18699E-09   9.77624E-07   8.18697E-09
-8.08688     -.24649    -8.33337
   NACL(AQ)               4.21009E-02   2.46049E+00   4.21008E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)               1.66870E-02   6.67432E-01   1.66870E-02
-1.77762      .00000    -1.77762
   H3SIO4-                6.32536E-04   6.01585E-02   6.32534E-04
-3.19892     -.24649    -3.44541
   HCL(AQ)                5.61058E-07   2.04567E-05   5.61056E-07
-6.25099      .00000    -6.25099

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0657141
           log (CA++  /h+**0)            8.2014790
           log (MG++  /h+**0)            6.0863310
           log (AL+++ /h+**0)           -5.9438701
           log (FE++  /h+**0)            3.6937746
           log (FE+++ /h+**0)           -4.3000902


           --- summary of solid product phases---


  product                     log moles        moles         grams
volume, cc

   MAGNETITE                 -6.1751063    6.68180E-07    1.54710E-04
2.97474E-05

   CLINOPYROXENE(SS)         -4.3955648    4.02194E-05    8.79585E-03
2.66252E-03
```

```
   DIOPSIDE                  -4.4261465    3.74847E-05    8.11739E-03
2.48148E-03
   HEDENBERGITE              -5.5631029    2.73462E-06    6.78444E-04
1.81032E-04
   JADEITE                  -10.0671126    8.56816E-11    1.73196E-08
5.17003E-09


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                  2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)            2.0000000    1.00000E+02

   ALBITE                     1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                  1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)          2.0000002    1.00000E+02

   DIOPSIDE                   1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE               1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -10.0671126    8.56816E-11    1.73196E-08
5.17003E-09



                          mass, grams        volume, cc

           created        8.950563E-03       2.692269E-03
           destroyed      1.741566E-03       5.739044E-04
           net            7.208997E-03       2.118364E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---
```

mineral	affinity, kcal	state	mineral	affinity, kcal	state
MAGNETITE	.0000	satd	HEMATITE	-3.3501	
PERICLASE	-4.8210		BRUCITE	-1.0847	
FORSTERITE	-.3954		FAYALITE	-1.7298	
CHRYSOTILE	-.6864		ENSTATITE-CL	-2.1987	
ENSTATITE-OR	-2.2768		ENSTATITE-PR	-2.6822	
DIOPSIDE	-.1012		HEDENBERGITE	-3.8634	
FERROSILITE	-4.4990		WOLLASTONITE	-3.5973	
PSEUDOWOLLASTONITE	-4.0834		TREMOLITE	-5.6328	
ANTIGORITE	-.5081		TALC	-7.0009	
CLINOCHLORE	-2.2533		CHAMOSITE	-6.4351	
GROSSULAR	-7.9410		QUARTZ-ALPHA	-5.6836	
QUARTZ-BETA	-5.9206		COESITE	-6.2799	
IRON-ALPHA	-8.6597		IRON-GAMMA	-7.8030	
HALITE	-9.7500		CRISTOBALITE-ALPHA	-6.9695	
CRISTOBALITE-BETA	-7.6829				

--- summary of solid solutions ---

mineral	aff. kcal/mol		mole frac.	lambda	state
PLAGIOCLASE(SS)	-22.9797				
ALBITE		-22.97972	.9945087	1.00000	
ANORTHITE		-22.97972	.0054913	1.00000	
ORTHOPYROXENE(SS)	-1.9993				
ENSTATITE-OR		-1.99928	.8243810	1.00000	
FERROSILITE		-1.99928	.1756190	1.00000	
GARNET(SS)	-7.6909				
PYROPE		-7.69091	.0822735	1.00000	

```
    ALMANDINE                    -7.69091     .0774482     1.00000
    GROSSULAR                    -7.69091     .8402783     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
    DIOPSIDE                       .00000     .9320052     1.00000
    HEDENBERGITE                   .00000     .0679926     1.00000
    JADEITE                        .00000     .0000021     1.00000

 CPX_SUBCALCIC(SS)          .0000
    DIOPSIDE                       .00000     .9320072     1.00000
    HEDENBERGITE                   .00000     .0679928     1.00000

 CHLORITE(SS)             -2.1771
    CLINOCHLORE                  -2.17709     .9483340     1.00000
    CHAMOSITE                    -2.17709     .0516660     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0000    1.0000     .0000   -5.6715     .0000   -5.6715


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                         -26.80001       1.58487E-27
   H2(G)                           2.27783       1.89596E+02
   H2O(G)                          3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  2.5119E-06, delzi=  9.2699E-07, nord= 3
```

```
                 ncycle=  0
 steps completed =    14, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =    -9.8632
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                       reaction progress        =  2.51188643150956E-06
                       log of reaction progress =      -5.6000000

                       temperature    =    450.000 degrees c
                       total pressure =    500.000 bars

                       computing units remaining =       .000


 step size is limited by the print requirement


                                 --- reactant summary ---



          reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         1.00000E+02    4.20816E-06    2.68618E+04
1.13039E-03
   CLINOPYROXENE(SS)       1.00000E+02    5.07200E-06    2.22861E+04
1.13035E-03
   MAGNETITE               1.00000E+02    5.42567E-07    2.31539E+04
1.25625E-04
   TREMOLITE               1.00000E+02    4.60178E-07    8.12370E+04
3.73835E-04


                  current total mass =  1.53539E+05 grams
                  delta total mass   =  2.76020E-03 grams
                  delta total volume =       .00091 cc


          reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           24.2450    1.67530E+00
   CLINOPYROXENE(SS)           .1345    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.6292    1.83200E-01

           affinity of the overall irreversible reaction=    41.649
kcal
```

```
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

    element         mg/kg soln.         molal conc.          moles

       O          8.434541E+05        5.775246E+01        5.775263E+01
       NA         1.205632E+04        5.745036E-01        5.745052E-01
       CA         3.525774E+01        9.636949E-04        9.636977E-04
       MG         2.393603E+04        1.078870E+00        1.078873E+00
       AL         1.697280E-01        6.891272E-06        6.891292E-06
       SI         6.679347E+01        2.605341E-03        2.605348E-03
       H          1.042622E+05        1.133241E+02        1.133244E+02
       CL         1.618114E+04        4.999986E-01        5.000000E-01
       FE         7.984208E+00        1.566191E-04        1.566196E-04

       co3--                          0.000000E+00        0.000000E+00
       so4--                          0.000000E+00        0.000000E+00
       s--                            0.000000E+00        0.000000E+00

     warning-- co3--, so4--, and s-- totals require that routine comp1
     have the names of non-carbonate carbon, sulfide sulfur,
     and non-sulfate sulfur aqueous species


    single ion activities and activity coefficients are here defined
    with respect to the internal ph scale



                                        ph           eh            pe

      internal ph scale               6.5998        .4548
  3.1696E+00
      modified nbs ph scale           6.3533        .4901
  3.4160E+00
      rational ph scale               6.3533        .4901
  3.4160E+00

    phcl =      7.1857



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001
```

```
                        activity of water =    .98384
              log activity of water =   -.00707
              alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                   ionic strength =  5.170403E-01 molal
                sum of molalities =    2.2049469350158
              osmotic coefficient =     .41003
                   equiv. stoich. ionic strength =  4.999986E-01
molal

                        mass of solution =   1.095504 kg
                        mass of solvent  =   1.000003 kg
                        mass of solutes  =    .095501 kg
                        conc of solutes  =   8.717560 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15718E-01   1.18562E+01   5.15716E-01     -.
28759     -.24649     -.53408
   CA++                 9.71283E-05   3.89290E-03   9.71280E-05
-4.01266     -.98596    -4.99862
   MG++                 7.45995E-07   1.81314E-05   7.45993E-07
-6.12727     -.98596    -7.11323
   AL+++                4.36304E-24   1.17722E-22   4.36303E-24
-23.36021    -2.21841   -25.57862
   H4SIO4(AQ)           1.45212E-03   1.39570E-01   1.45211E-03
-2.83800      .00000    -2.83800
   H+                   4.43316E-07   4.46818E-07   4.43314E-07
-6.35329     -.24649    -6.59978
   CL-                  4.57685E-01   1.62263E+01   4.57684E-01     -.
33943     -.24649     -.58592
   FE++                 3.02120E-09   1.68725E-07   3.02120E-09
-8.51982     -.98596    -9.50578
   O2(AQ)               1.33381E-31   4.26804E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)               3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                1.31519E-22   7.34493E-21   1.31518E-22
-21.88101    -2.21841   -24.09943
   OH-                  5.86133E-02   9.96854E-01   5.86131E-02
-1.23201     -.24649    -1.47850
   H8SI3O10(AQ)         1.55793E-11   3.93087E-09   1.55793E-11
-10.80745      .00000   -10.80745
   H6SI2O7(AQ)          5.70394E-06   9.93707E-04   5.70392E-06
-5.24383      .00000    -5.24383
```

```
   AL(OH)3(AQ)           2.83079E-08   2.20812E-06   2.83078E-08
-7.54809      .00000    -7.54809
   AL(OH)4-              5.43953E-06   5.16813E-04   5.43951E-06
-5.26444     -.24649    -5.51093
   AL(OH)SI(OH)-         1.42346E-06   2.46415E-04   1.42345E-06
-5.84666     -.24649    -6.09315
   CACL+                 2.05140E-04   1.54948E-02   2.05139E-04
-3.68795     -.24649    -3.93444
   CACL2(AQ)             3.74679E-06   4.15842E-04   3.74678E-06
-5.42634      .00000    -5.42634
   CA(OH)+               3.00108E-04   1.71323E-02   3.00107E-04
-3.52272     -.24649    -3.76921
   CA(H3SIO4)+           3.57575E-04   4.83394E-02   3.57574E-04
-3.44663     -.24649    -3.69312
   FE(OH)+               8.46530E-08   6.16734E-06   8.46528E-08
-7.07236     -.24649    -7.31885
   FE(OH)2               5.86244E-07   5.26808E-05   5.86242E-07
-6.23192      .00000    -6.23192
   FE(OH)3-              5.95022E-06   6.35894E-04   5.95021E-06
-5.22547     -.24649    -5.47196
   FECL+                 3.34958E-09   3.05817E-07   3.34957E-09
-8.47501     -.24649    -8.72150
   FECL2(AQ)             7.84282E-08   9.94101E-06   7.84279E-08
-7.10553      .00000    -7.10553
   FE(H3SIO4)+           1.49914E-04   2.26300E-02   1.49913E-04
-3.82416     -.24649    -4.07065
   MGCL+                 7.44301E-07   4.44780E-05   7.44299E-07
-6.12825     -.24649    -6.37474
   MG(OH)+               1.63789E-05   6.76649E-04   1.63788E-05
-4.78572     -.24649    -5.03221
   MG(OH)2(AQ)           1.07886E+00   6.29184E+01   1.07885E+00      .
03296      .00000      .03296
   MG(H3SIO4)+           8.19237E-09   9.78266E-07   8.19235E-09
-8.08659     -.24649    -8.33308
   NACL(AQ)              4.21010E-02   2.46050E+00   4.21009E-02
-1.37571      .00000    -1.37571
   NAOH(AQ)              1.66864E-02   6.67409E-01   1.66864E-02
-1.77764      .00000    -1.77764
   H3SIO4-               6.32905E-04   6.01935E-02   6.32903E-04
-3.19866     -.24649    -3.44515
   HCL(AQ)               5.61079E-07   2.04575E-05   5.61078E-07
-6.25098      .00000    -6.25098

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0656989
           log (CA++  /h+**0)            8.2009404
           log (MG++  /h+**0)            6.0863305
           log (AL+++ /h+**0)           -5.7792889
```

```
           log (FE++  /h+**0)            3.6937746
           log (FE+++ /h+**0)           -4.3000903


           --- summary of solid product phases---


  product                       log moles        moles        grams
volume, cc

   MAGNETITE                   -6.0578823    8.75221E-07    2.02647E-04
3.89648E-05

   CLINOPYROXENE(SS)           -4.3567635    4.39781E-05    9.61788E-03
2.91135E-03
   DIOPSIDE                    -4.3873456    4.09878E-05    8.87600E-03
2.71339E-03
   HEDENBERGITE                -5.5243016    2.99019E-06    7.41849E-04
1.97950E-04
   JADEITE                     -9.8632067    1.37023E-10    2.76976E-08
8.26796E-09


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member          log moles        moles        grams
volume, cc

   MAGNETITE                    2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                    2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)              2.0000000    1.00000E+02

   ALBITE                       1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                    1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)            2.0000002    1.00000E+02

   DIOPSIDE                     1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE                 1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                     -9.8632067    1.37023E-10    2.76976E-08
8.26796E-09
```

	mass, grams	volume, cc
created	9.820526E-03	2.950315E-03
destroyed	2.760197E-03	9.095773E-04
net	7.060329E-03	2.040737E-03

warning-- these volume totals may be incomplete because
of missing partial molar volume data in the data base

--- mineral saturation state summary ---

mineral	affinity, kcal	state	mineral	affinity, kcal	state
MAGNETITE	.0000	satd	HEMATITE	-3.3501	
PERICLASE	-4.8210		BRUCITE	-1.0847	
FORSTERITE	-.3950		FAYALITE	-1.7294	
CHRYSOTILE	-.6846		ENSTATITE-CL	-2.1978	
ENSTATITE-OR	-2.2759		ENSTATITE-PR	-2.6813	
DIOPSIDE	-.1012		HEDENBERGITE	-3.8634	
FERROSILITE	-4.4981		WOLLASTONITE	-3.5982	
PSEUDOWOLLASTONITE	-4.0843		TREMOLITE	-5.6292	
ANTIGORITE	-.4930		TALC	-6.9973	
CLINOCHLORE	-2.0350		CHAMOSITE	-6.2167	
GROSSULAR	-7.5792		QUARTZ-ALPHA	-5.6827	
QUARTZ-BETA	-5.9197		COESITE	-6.2790	
IRON-ALPHA	-8.6597		IRON-GAMMA	-7.8030	
HALITE	-9.7500		CRISTOBALITE-ALPHA	-6.9686	
CRISTOBALITE-BETA	-7.6821				

```
                     --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -22.4289
     ALBITE                    -22.42888     .9920131     1.00000
     ANORTHITE                 -22.42888     .0079869     1.00000

 ORTHOPYROXENE(SS)        -1.9984
     ENSTATITE-OR               -1.99839     .8243808     1.00000
     FERROSILITE                -1.99839     .1756192     1.00000

 GARNET(SS)               -7.3288
     PYROPE                     -7.32881     .0823593     1.00000
     ALMANDINE                  -7.32881     .0775290     1.00000
     GROSSULAR                  -7.32881     .8401117     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9320042     1.00000
     HEDENBERGITE                 .00000     .0679927     1.00000
     JADEITE                      .00000     .0000031     1.00000

 CPX_SUBCALCIC(SS)          .0000
     DIOPSIDE                     .00000     .9320071     1.00000
     HEDENBERGITE                 .00000     .0679929     1.00000

 CHLORITE(SS)             -1.9587
     CLINOCHLORE                -1.95872     .9483339     1.00000
     CHAMOSITE                  -1.95872     .0516661     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
              .0000    1.0000     .0000   -5.5064     .0000   -5.5064


          --- summary of gas species ---
```

```
          gas                  log fugacity         fugacity
partial pressure

   O2(G)                          -26.80001       1.58487E-27
   H2(G)                            2.27783       1.89596E+02
   H2O(G)                           3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  3.9811E-06, delzi=  1.4692E-06, nord= 3
               ncycle=  0
 steps completed =    15, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -9.6312
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  3.98107170553494E-06
                     log of reaction progress =      -5.4000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         1.00000E+02    6.66949E-06    2.68618E+04
1.79154E-03
   CLINOPYROXENE(SS)       1.00000E+02    8.03858E-06    2.22861E+04
1.79148E-03
   MAGNETITE               1.00000E+02    8.59911E-07    2.31539E+04
1.99103E-04
   TREMOLITE               1.00000E+02    7.29332E-07    8.12370E+04
5.92488E-04
```

```
                 current total mass =  1.53539E+05 grams
                 delta total mass   =  4.37462E-03 grams
                 delta total volume =       .00144 cc


          reactant           affinity     rel. rate

      PLAGIOCLASE(SS)         23.4271    1.67530E+00
      CLINOPYROXENE(SS)         .1345    0.00000E+00
      MAGNETITE                 .0000    0.00000E+00
      TREMOLITE                5.6236    1.83200E-01

           affinity of the overall irreversible reaction=    40.278
 kcal
           contributions from irreversible reactions
           with no thermodynamic data are not included



        --- element totals for the aqueous phase ---

      element         mg/kg soln.         molal conc.          moles

         O          8.434540E+05        5.775248E+01        5.775263E+01
         NA         1.205634E+04        5.745051E-01        5.745067E-01
         CA         3.520410E+01        9.622290E-04        9.622316E-04
         MG         2.393598E+04        1.078868E+00        1.078871E+00
         AL         2.545947E-01        1.033702E-05        1.033705E-05
         SI         6.685946E+01        2.607916E-03        2.607923E-03
         H          1.042622E+05        1.133241E+02        1.133244E+02
         CL         1.618113E+04        4.999986E-01        5.000000E-01
         FE         7.992161E+00        1.567752E-04        1.567756E-04

         co3--                          0.000000E+00        0.000000E+00
         so4--                          0.000000E+00        0.000000E+00
         s--                            0.000000E+00        0.000000E+00

       warning-- co3--, so4--, and s-- totals require that routine comp1
       have the names of non-carbonate carbon, sulfide sulfur,
       and non-sulfate sulfur aqueous species


      single ion activities and activity coefficients are here defined
      with respect to the internal ph scale



                                              ph            eh             pe
```

```
     internal ph scale              6.5998        .4548
3.1696E+00
     modified nbs ph scale          6.3533        .4901
3.4161E+00
     rational ph scale              6.3533        .4901
3.4161E+00

   phcl =      7.1857



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001



                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                    ionic strength =  5.170409E-01 molal
                 sum of molalities =    2.2049477247920
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999986E-01
molal

                         mass of solution =   1.095504 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095502 kg
                         conc of solutes  =   8.717591 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15720E-01   1.18563E+01   5.15719E-01     -.
28759     -.24649     -.53408
   CA++                 9.69492E-05   3.88572E-03   9.69489E-05
-4.01346     -.98596    -4.99942
   MG++                 7.46083E-07   1.81336E-05   7.46081E-07
-6.12721     -.98596    -7.11318
   AL+++                6.54487E-24   1.76591E-22   6.54485E-24
-23.18410    -2.21841   -25.40251
   H4SIO4(AQ)           1.45354E-03   1.39707E-01   1.45354E-03
-2.83757      .00000    -2.83757
   H+                   4.43342E-07   4.46845E-07   4.43341E-07
-6.35326     -.24649    -6.59975
   CL-                  4.57685E-01   1.62263E+01   4.57684E-01     -.
```

```
33943     -.24649     -.58592
   FE++                   3.02157E-09   1.68745E-07   3.02156E-09
-8.51977     -.98596    -9.50573
   O2(AQ)                 1.33381E-31   4.26803E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)                 3.20576E-02   6.46217E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                  1.31543E-22   7.34626E-21   1.31542E-22
-21.88094    -2.21841   -24.09935
   OH-                    5.86098E-02   9.96795E-01   5.86097E-02
-1.23203     -.24649    -1.47852
   H8SI3O10(AQ)           1.56253E-11   3.94248E-09   1.56253E-11
-10.80617      .00000   -10.80617
   H6SI2O7(AQ)            5.71516E-06   9.95662E-04   5.71514E-06
-5.24297      .00000    -5.24297
   AL(OH)3(AQ)            4.24562E-08   3.31173E-06   4.24561E-08
-7.37206      .00000    -7.37206
   AL(OH)4-               8.15772E-06   7.75071E-04   8.15770E-06
-5.08843     -.24649    -5.33492
   AL(OH)SI(OH)-          2.13687E-06   3.69915E-04   2.13687E-06
-5.67022     -.24649    -5.91671
   CACL+                  2.04761E-04   1.54662E-02   2.04761E-04
-3.68875     -.24649    -3.93524
   CACL2(AQ)              3.73988E-06   4.15075E-04   3.73987E-06
-5.42714      .00000    -5.42714
   CA(OH)+                2.99536E-04   1.70997E-02   2.99535E-04
-3.52355     -.24649    -3.77004
   CA(H3SIO4)+            3.57245E-04   4.82948E-02   3.57244E-04
-3.44704     -.24649    -3.69353
   FE(OH)+                8.46581E-08   6.16771E-06   8.46579E-08
-7.07233     -.24649    -7.31882
   FE(OH)2                5.86244E-07   5.26808E-05   5.86243E-07
-6.23192      .00000    -6.23192
   FE(OH)3-               5.94987E-06   6.35856E-04   5.94985E-06
-5.22549     -.24649    -5.47198
   FECL+                  3.34998E-09   3.05853E-07   3.34997E-09
-8.47496     -.24649    -8.72145
   FECL2(AQ)              7.84376E-08   9.94220E-06   7.84374E-08
-7.10548      .00000    -7.10548
   FE(H3SIO4)+            1.50070E-04   2.26536E-02   1.50070E-04
-3.82371     -.24649    -4.07020
   MGCL+                  7.44389E-07   4.44832E-05   7.44387E-07
-6.12820     -.24649    -6.37469
   MG(OH)+                1.63798E-05   6.76689E-04   1.63798E-05
-4.78569     -.24649    -5.03218
   MG(OH)2(AQ)            1.07885E+00   6.29183E+01   1.07885E+00      .
03296      .00000      .03296
   MG(H3SIO4)+            8.20090E-09   9.79285E-07   8.20088E-09
-8.08614     -.24649    -8.33263
   NACL(AQ)               4.21012E-02   2.46051E+00   4.21011E-02
```

```
-1.37571      .00000    -1.37571
   NAOH(AQ)             1.66855E-02   6.67372E-01   1.66855E-02
-1.77766      .00000    -1.77766
   H3SIO4-              6.33489E-04   6.02491E-02   6.33488E-04
-3.19826     -.24649    -3.44475
   HCL(AQ)              5.61113E-07   2.04587E-05   5.61111E-07
-6.25095      .00000    -6.25095

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0656749
           log (CA++  /h+**0)            8.2000866
           log (MG++  /h+**0)            6.0863298
           log (AL+++ /h+**0)           -5.6032553
           log (FE++  /h+**0)            3.6937747
           log (FE+++ /h+**0)           -4.3000903


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE                -5.9196109    1.20334E-06    2.78620E-04
5.35728E-05

   CLINOPYROXENE(SS)        -4.3016065    4.99337E-05    1.09203E-02
3.30561E-03
   DIOPSIDE                 -4.3321894    4.65383E-05    1.00780E-02
3.08084E-03
   HEDENBERGITE             -5.4691446    3.39512E-06    8.42311E-04
2.24757E-04
   JADEITE                  -9.6311865    2.33783E-10    4.72567E-08
1.41065E-08


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                 2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)           2.0000000    1.00000E+02
```

```
   ALBITE                     1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                  1.6020600    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)          2.0000002    1.00000E+02

   DIOPSIDE                   1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE               1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                   -9.6311865    2.33783E-10    4.72567E-08
1.41065E-08



                          mass, grams        volume, cc

           created        1.119896E-02       3.359180E-03
           destroyed      4.374617E-03       1.441583E-03
           net            6.824345E-03       1.917598E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                 .0000  satd          HEMATITE
-3.3501
 PERICLASE               -4.8210                BRUCITE
-1.0848
 FORSTERITE               -.3943                FAYALITE
-1.7287
 CHRYSOTILE               -.6818                ENSTATITE-CL
-2.1964
 ENSTATITE-OR            -2.2745                ENSTATITE-PR
-2.6799
 DIOPSIDE                 -.1012                HEDENBERGITE
-3.8634
 FERROSILITE             -4.4967                WOLLASTONITE
-3.5996
 PSEUDOWOLLASTONITE      -4.0857                TREMOLITE
```

```
-5.6236
 ANTIGORITE               -.4690                TALC
-6.9916
 CLINOCHLORE             -1.8011                CHAMOSITE
-5.9829
 GROSSULAR               -7.1927                QUARTZ-ALPHA
-5.6813
 QUARTZ-BETA             -5.9183                COESITE
-6.2776
 IRON-ALPHA              -8.6597                IRON-GAMMA
-7.8030
 HALITE                  -9.7500                CRISTOBALITE-ALPHA
-6.9672
 CRISTOBALITE-BETA       -7.6806


                     --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -21.8366
     ALBITE                     -21.83655     .9881030     1.00000
     ANORTHITE                  -21.83655     .0118970     1.00000

 ORTHOPYROXENE(SS)         -1.9970
     ENSTATITE-OR                -1.99698     .8243806     1.00000
     FERROSILITE                 -1.99698     .1756194     1.00000

 GARNET(SS)                -6.9418
     PYROPE                      -6.94183     .0824954     1.00000
     ALMANDINE                   -6.94183     .0776573     1.00000
     GROSSULAR                   -6.94183     .8398473     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .9320027     1.00000
     HEDENBERGITE                  .00000     .0679927     1.00000
     JADEITE                       .00000     .0000047     1.00000

 CPX_SUBCALCIC(SS)           .0000
     DIOPSIDE                     -.00001     .9320070     1.00000
     HEDENBERGITE                 -.00001     .0679930     1.00000

 CHLORITE(SS)              -1.7249
     CLINOCHLORE                 -1.72488     .9483339     1.00000
     CHAMOSITE                   -1.72488     .0516661     1.00000


 solid solution product phases
```

```
           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
             .0000    1.0000     .0000   -5.3296     .0000   -5.3296


          --- summary of gas species ---

          gas               log fugacity         fugacity
partial pressure

   O2(G)                       -26.80001       1.58487E-27
   H2(G)                         2.27783       1.89596E+02
   H2O(G)                        3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  6.3096E-06, delzi=  2.3285E-06, nord= 3
               ncycle=  0
 steps completed =    16, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -9.3706
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  6.30957344480188E-06
                    log of reaction progress =      -5.2000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---
```

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	1.00000E+02	1.05704E-05	2.68617E+04	2.83940E-03
CLINOPYROXENE(SS)	1.00000E+02	1.27403E-05	2.22861E+04	2.83931E-03
MAGNETITE	1.00000E+02	1.36287E-06	2.31539E+04	3.15557E-04
TREMOLITE	1.00000E+02	1.15591E-06	8.12370E+04	9.39030E-04

current total mass = 1.53539E+05 grams
delta total mass = 6.93330E-03 grams
delta total volume = .00228 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	22.5702	1.67530E+00
CLINOPYROXENE(SS)	.1345	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.6146	1.83200E-01

affinity of the overall irreversible reaction= 38.840 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434539E+05	5.775250E+01	5.775265E+01
NA	1.205639E+04	5.745076E-01	5.745090E-01
CA	3.511923E+01	9.599098E-04	9.599122E-04
MG	2.393591E+04	1.078866E+00	1.078869E+00
AL	3.890984E-01	1.579813E-05	1.579817E-05
SI	6.696426E+01	2.612005E-03	2.612012E-03
H	1.042622E+05	1.133241E+02	1.133244E+02
CL	1.618113E+04	4.999987E-01	5.000000E-01
FE	8.004787E+00	1.570229E-04	1.570233E-04
co3--		0.000000E+00	0.000000E+00

```
      so4--                          0.000000E+00       0.000000E+00
      s--                            0.000000E+00       0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                       ph           eh            pe

     internal ph scale               6.5997        .4548
3.1696E+00
     modified nbs ph scale           6.3532        .4901
3.4161E+00
     rational ph scale               6.3532        .4901
3.4161E+00

   phcl =      7.1856



          oxygen fugacity =  1.58487E-27
          log oxygen fugacity = -26.80001



                         activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                    ionic strength =  5.170419E-01 molal
                 sum of molalities =    2.2049489935532
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999987E-01
molal

                         mass of solution =   1.095505 kg
                         mass of solvent  =   1.000003 kg
                         mass of solutes  =    .095502 kg
                         conc of solutes  =   8.717639 per cent (w/w)


   species                moles        grams         conc        log
conc      log g      log act
```

```
   H2O                   5.55088E+01   1.00000E+03
   NA+                   5.15723E-01   1.18564E+01   5.15722E-01      -.
28758     -.24649     -.53407
   CA++                  9.66658E-05   3.87436E-03   9.66655E-05
-4.01473     -.98596    -5.00069
   MG++                  7.46223E-07   1.81369E-05   7.46221E-07
-6.12713     -.98596    -7.11309
   AL+++                 1.00031E-23   2.69900E-22   1.00031E-23
-22.99987    -2.21841   -25.21828
   H4SIO4(AQ)            1.45581E-03   1.39925E-01   1.45581E-03
-2.83690      .00000    -2.83690
   H+                    4.43384E-07   4.46887E-07   4.43383E-07
-6.35322     -.24649    -6.59971
   CL-                   4.57685E-01   1.62263E+01   4.57684E-01      -.
33943     -.24649     -.58592
   FE++                  3.02214E-09   1.68777E-07   3.02213E-09
-8.51969     -.98596    -9.50565
   O2(AQ)                1.33381E-31   4.26803E-30   1.33381E-31
-30.87491      .00000   -30.87491
   H2(AQ)                3.20576E-02   6.46218E-02   3.20575E-02
-1.49407      .00000    -1.49407
   FE+++                 1.31580E-22   7.34835E-21   1.31580E-22
-21.88081    -2.21841   -24.09922
   OH-                   5.86043E-02   9.96701E-01   5.86041E-02
-1.23207     -.24649    -1.47856
   H8SI3O10(AQ)          1.56985E-11   3.96095E-09   1.56985E-11
-10.80414      .00000   -10.80414
   H6SI2O7(AQ)           5.73300E-06   9.98770E-04   5.73298E-06
-5.24162      .00000    -5.24162
   AL(OH)3(AQ)           6.48713E-08   5.06018E-06   6.48711E-08
-7.18795      .00000    -7.18795
   AL(OH)4-              1.24635E-05   1.18416E-03   1.24634E-05
-4.90436     -.24649    -5.15085
   AL(OH)SI(OH)-         3.26984E-06   5.66042E-04   3.26983E-06
-5.48548     -.24649    -5.73197
   CACL+                 2.04163E-04   1.54210E-02   2.04162E-04
-3.69002     -.24649    -3.93651
   CACL2(AQ)             3.72895E-06   4.13862E-04   3.72894E-06
-5.42841      .00000    -5.42841
   CA(OH)+               2.98632E-04   1.70481E-02   2.98632E-04
-3.52486     -.24649    -3.77135
   CA(H3SIO4)+           3.56722E-04   4.82241E-02   3.56721E-04
-3.44767     -.24649    -3.69416
   FE(OH)+               8.46661E-08   6.16829E-06   8.46659E-08
-7.07229     -.24649    -7.31878
   FE(OH)2               5.86244E-07   5.26808E-05   5.86243E-07
-6.23192      .00000    -6.23192
   FE(OH)3-              5.94931E-06   6.35796E-04   5.94930E-06
-5.22553     -.24649    -5.47202
```

```
   FECL+                 3.35062E-09   3.05911E-07   3.35061E-09
-8.47488     -.24649    -8.72137
   FECL2(AQ)             7.84525E-08   9.94409E-06   7.84523E-08
-7.10539      .00000    -7.10539
   FE(H3SIO4)+           1.50318E-04   2.26911E-02   1.50318E-04
-3.82299     -.24649    -4.06948
   MGCL+                 7.44528E-07   4.44915E-05   7.44526E-07
-6.12812     -.24649    -6.37461
   MG(OH)+               1.63813E-05   6.76751E-04   1.63813E-05
-4.78565     -.24649    -5.03214
   MG(OH)2(AQ)           1.07885E+00   6.29181E+01   1.07885E+00      .
03296      .00000      .03296
   MG(H3SIO4)+           8.21445E-09   9.80902E-07   8.21443E-09
-8.08542     -.24649    -8.33191
   NACL(AQ)              4.21015E-02   2.46053E+00   4.21014E-02
-1.37570      .00000    -1.37570
   NAOH(AQ)              1.66841E-02   6.67313E-01   1.66840E-02
-1.77770      .00000    -1.77770
   H3SIO4-               6.34417E-04   6.03374E-02   6.34416E-04
-3.19763     -.24649    -3.44412
   HCL(AQ)               5.61166E-07   2.04606E-05   5.61165E-07
-6.25091      .00000    -6.25091

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0656369
           log (CA++  /h+**0)            8.1987330
           log (MG++  /h+**0)            6.0863288
           log (AL+++ /h+**0)           -5.4191443
           log (FE++  /h+**0)            3.6937748
           log (FE+++ /h+**0)           -4.3000903


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                  -5.7636291    1.72334E-06    3.99020E-04
7.67231E-05

   CLINOPYROXENE(SS)          -4.2264439    5.93685E-05    1.29837E-02
3.93019E-03
   DIOPSIDE                   -4.2570279    5.53315E-05    1.19822E-02
3.66294E-03
   HEDENBERGITE               -5.3939820    4.03662E-06    1.00146E-03
2.67224E-04
   JADEITE                    -9.3705975    4.25993E-10    8.61097E-08
```

```
2.57044E-08


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                 2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)           2.0000000    1.00000E+02

   ALBITE                    1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                 1.6020599    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)         2.0000002    1.00000E+02

   DIOPSIDE                  1.9030902    8.00000E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE              1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -9.3705975    4.25993E-10    8.61097E-08
2.57044E-08



                       mass, grams        volume, cc

           created        1.338273E-02       4.006915E-03
           destroyed      6.933300E-03       2.284755E-03
           net            6.449427E-03       1.722160E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state
```

```
 MAGNETITE                  .0000  satd          HEMATITE
-3.3501
 PERICLASE                -4.8211                BRUCITE
-1.0848
 FORSTERITE                -.3932                FAYALITE
-1.7275
 CHRYSOTILE                -.6773                ENSTATITE-CL
-2.1942
 ENSTATITE-OR             -2.2723                ENSTATITE-PR
-2.6776
 DIOPSIDE                  -.1012                HEDENBERGITE
-3.8634
 FERROSILITE              -4.4945                WOLLASTONITE
-3.6018
 PSEUDOWOLLASTONITE       -4.0879                TREMOLITE
-5.6146
 ANTIGORITE                -.4310                TALC
-6.9827
 CLINOCHLORE              -1.5561                CHAMOSITE
-5.7379
 GROSSULAR                -6.7892                QUARTZ-ALPHA
-5.6791
 QUARTZ-BETA              -5.9160                COESITE
-6.2754
 IRON-ALPHA               -8.6597                IRON-GAMMA
-7.8030
 HALITE                   -9.7500                CRISTOBALITE-ALPHA
-6.9650
 CRISTOBALITE-BETA        -7.6784


                    --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -21.2119
     ALBITE                      -21.21185     .9820166     1.00000
     ANORTHITE                   -21.21185     .0179834     1.00000

 ORTHOPYROXENE(SS)          -1.9947
     ENSTATITE-OR                 -1.99475     .8243802     1.00000
     FERROSILITE                  -1.99475     .1756198     1.00000

 GARNET(SS)                 -6.5376
     PYROPE                       -6.53761     .0827116     1.00000
     ALMANDINE                    -6.53761     .0778610     1.00000
     GROSSULAR                    -6.53761     .8394274     1.00000

 CLINOPYROXENE(SS)            .0000
saturated
```

```
    DIOPSIDE                      .00000     .9320002     1.00000
    HEDENBERGITE                  .00000     .0679927     1.00000
    JADEITE                       .00000     .0000072     1.00000

CPX_SUBCALCIC(SS)          .0000
    DIOPSIDE                     -.00001     .9320069     1.00000
    HEDENBERGITE                 -.00001     .0679931     1.00000

CHLORITE(SS)             -1.4798
    CLINOCHLORE                 -1.47985     .9483337     1.00000
    CHAMOSITE                   -1.47985     .0516663     1.00000


solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

  CLINOPYROXENE(SS)
ideal solution

    DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0000    1.0000     .0000   -5.1442     .0000   -5.1442


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

  O2(G)                         -26.80001       1.58487E-27
  H2(G)                           2.27783       1.89596E+02
  H2O(G)                          3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.0000E-05, delzi=  3.6904E-06, nord= 4
               ncycle=  0
 steps completed =    17, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -9.0814
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
                    reaction progress        =  9.99999999999991E-06
                    log of reaction progress =      -5.0000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         1.00000E+02    1.67530E-05    2.68617E+04
4.50015E-03
   CLINOPYROXENE(SS)       1.00000E+02    2.01920E-05    2.22861E+04
4.50001E-03
   MAGNETITE               1.00000E+02    2.16000E-06    2.31539E+04
5.00123E-04
   TREMOLITE               1.00000E+02    1.83200E-06    8.12370E+04
1.48826E-03


                current total mass =  1.53539E+05 grams
                delta total mass   =  1.09885E-02 grams
                delta total volume =       .00362 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           21.6857    1.67530E+00
   CLINOPYROXENE(SS)           .1345    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.6005    1.83200E-01

          affinity of the overall irreversible reaction=    37.356
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included
```

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434538E+05	5.775254E+01	5.775267E+01
NA	1.205646E+04	5.745115E-01	5.745127E-01
CA	3.498510E+01	9.562445E-04	9.562467E-04
MG	2.393579E+04	1.078862E+00	1.078864E+00
AL	6.022697E-01	2.445332E-05	2.445337E-05
SI	6.713090E+01	2.618507E-03	2.618513E-03
H	1.042621E+05	1.133242E+02	1.133244E+02
CL	1.618112E+04	4.999989E-01	5.000000E-01
FE	8.024848E+00	1.574166E-04	1.574169E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.5996	.4548	3.1697E+00
modified nbs ph scale	6.3532	.4902	3.4162E+00
rational ph scale	6.3532	.4902	3.4162E+00

phcl = 7.1856

oxygen fugacity = 1.58486E-27
log oxygen fugacity = -26.80001

activity of water = .98384
log activity of water = -.00707
alkalinity = 0.000000E+00 equiv/kg solvent
(not def. for t.gt.50 c)

```
                    ionic strength =  5.170435E-01 molal
                 sum of molalities =    2.2049510472453
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999989E-01
molal

                         mass of solution =   1.095505 kg
                         mass of solvent  =   1.000002 kg
                         mass of solutes  =    .095503 kg
                         conc of solutes  =   8.717716 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15729E-01   1.18565E+01   5.15728E-01     -.
28758     -.24649     -.53407
   CA++                 9.62181E-05   3.85642E-03   9.62179E-05
-4.01674     -.98596    -5.00271
   MG++                 7.46444E-07   1.81423E-05   7.46442E-07
-6.12700     -.98596    -7.11297
   AL+++                1.54848E-23   4.17804E-22   1.54848E-23
-22.81009    -2.21842   -25.02851
   H4SIO4(AQ)           1.45941E-03   1.40271E-01   1.45941E-03
-2.83582      .00000    -2.83582
   H+                   4.43450E-07   4.46954E-07   4.43449E-07
-6.35316     -.24649    -6.59965
   CL-                  4.57686E-01   1.62263E+01   4.57685E-01     -.
33943     -.24649     -.58592
   FE++                 3.02305E-09   1.68828E-07   3.02304E-09
-8.51956     -.98596    -9.50552
   O2(AQ)               1.33381E-31   4.26802E-30   1.33380E-31
-30.87491      .00000   -30.87491
   H2(AQ)               3.20577E-02   6.46218E-02   3.20576E-02
-1.49407      .00000    -1.49407
   FE+++                1.31639E-22   7.35167E-21   1.31639E-22
-21.88061    -2.21842   -24.09903
   OH-                  5.85956E-02   9.96552E-01   5.85954E-02
-1.23214     -.24649    -1.47863
   H8SI3O10(AQ)         1.58153E-11   3.99042E-09   1.58153E-11
-10.80092      .00000   -10.80092
   H6SI2O7(AQ)          5.76140E-06   1.00372E-03   5.76138E-06
-5.23947      .00000    -5.23947
   AL(OH)3(AQ)          1.00375E-07   7.82961E-06   1.00375E-07
-6.99837      .00000    -6.99837
   AL(OH)4-             1.92818E-05   1.83198E-03   1.92818E-05
-4.71485     -.24649    -4.96134
   AL(OH)SI(OH)-        5.07117E-06   8.77872E-04   5.07116E-06
```

```
-5.29489     -.24649    -5.54138
   CACL+                2.03217E-04   1.53496E-02   2.03217E-04
-3.69204     -.24649    -3.93853
   CACL2(AQ)            3.71168E-06   4.11945E-04   3.71168E-06
-5.43043      .00000    -5.43043
   CA(OH)+              2.97205E-04   1.69666E-02   2.97204E-04
-3.52695     -.24649    -3.77344
   CA(H3SIO4)+          3.55895E-04   4.81123E-02   3.55894E-04
-3.44868     -.24649    -3.69517
   FE(OH)+              8.46788E-08   6.16921E-06   8.46786E-08
-7.07223     -.24649    -7.31872
   FE(OH)2              5.86244E-07   5.26808E-05   5.86243E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.94842E-06   6.35702E-04   5.94841E-06
-5.22560     -.24649    -5.47209
   FECL+                3.35162E-09   3.06003E-07   3.35161E-09
-8.47475     -.24649    -8.72124
   FECL2(AQ)            7.84761E-08   9.94708E-06   7.84759E-08
-7.10526      .00000    -7.10526
   FE(H3SIO4)+          1.50713E-04   2.27507E-02   1.50712E-04
-3.82185     -.24649    -4.06834
   MGCL+                7.44749E-07   4.45047E-05   7.44747E-07
-6.12799     -.24649    -6.37448
   MG(OH)+              1.63837E-05   6.76849E-04   1.63837E-05
-4.78559     -.24649    -5.03208
   MG(OH)2(AQ)          1.07885E+00   6.29179E+01   1.07884E+00      .
03296      .00000      .03296
   MG(H3SIO4)+          8.23597E-09   9.83472E-07   8.23595E-09
-8.08429     -.24649    -8.33078
   NACL(AQ)             4.21020E-02   2.46056E+00   4.21019E-02
-1.37570      .00000    -1.37570
   NAOH(AQ)             1.66817E-02   6.67221E-01   1.66817E-02
-1.77776      .00000    -1.77776
   H3SIO4-              6.35892E-04   6.04777E-02   6.35891E-04
-3.19662     -.24649    -3.44311
   HCL(AQ)              5.61250E-07   2.04637E-05   5.61249E-07
-6.25084      .00000    -6.25084

           --- activity ratios of cations ---


           log (NA+   /h+**0)           6.0655766
           log (CA++  /h+**0)           8.1965867
           log (MG++  /h+**0)           6.0863270
           log (AL+++ /h+**0)          -5.2295703
           log (FE++  /h+**0)           3.6937750
           log (FE+++ /h+**0)          -4.3000904


           --- summary of solid product phases---
```

```
  product                          log moles        moles        grams
volume, cc

   MAGNETITE                      -5.5939061    2.54738E-06    5.89817E-04
1.13409E-04

   CLINOPYROXENE(SS)              -4.1289448    7.43114E-05    1.62517E-02
4.91941E-03
   DIOPSIDE                       -4.1595306    6.92579E-05    1.49980E-02
4.58487E-03
   HEDENBERGITE                   -5.2964828    5.05263E-06    1.25353E-03
3.34484E-04
   JADEITE                        -9.0814383    8.29014E-10    1.67576E-07
5.00227E-08


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member            log moles        moles        grams
volume, cc

   MAGNETITE                       2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                       2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)                 1.9999999    1.00000E+02

   ALBITE                          1.7781512    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                       1.6020599    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)               2.0000002    1.00000E+02

   DIOPSIDE                        1.9030903    8.00001E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE                    1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                        -9.0814383    8.29014E-10    1.67576E-07
5.00227E-08


                                 mass, grams        volume, cc
```

```
              created          1.684148E-02       5.032817E-03
              destroyed        1.098854E-02       3.621092E-03
              net              5.852939E-03       1.411725E-03

             warning-- these volume totals may be incomplete because
             of missing partial molar volume data in the data base



              --- mineral saturation state summary ---


     mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                  .0000  satd          HEMATITE
-3.3501
 PERICLASE               -4.8211                 BRUCITE
-1.0848
 DIASPORE                -9.9632                 FORSTERITE
-.3914
 FAYALITE                -1.7258                 CHRYSOTILE
-.6702
 ENSTATITE-CL            -2.1906                 ENSTATITE-OR
-2.2687
 ENSTATITE-PR            -2.6741                 DIOPSIDE
-.1012
 HEDENBERGITE            -3.8634                 FERROSILITE
-4.4909
 WOLLASTONITE            -3.6054                 PSEUDOWOLLASTONITE
-4.0915
 TREMOLITE               -5.6005                 ANTIGORITE
-.3708
 TALC                    -6.9685                 CLINOCHLORE
-1.3030
 CHAMOSITE               -5.4848                 PYROPE
-9.6981
 ALMANDINE               -9.7849                 GROSSULAR
-6.3749
 QUARTZ-ALPHA            -5.6755                 QUARTZ-BETA
-5.9125
 COESITE                 -6.2718                 IRON-ALPHA
-8.6597
 IRON-GAMMA              -7.8030                 HALITE
-9.7500
 CRISTOBALITE-ALPHA      -6.9614                 CRISTOBALITE-BETA
-7.6749

                        --- summary of solid solutions  ---
```

```
 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -20.5603
     ALBITE                    -20.56031     .9726397     1.00000
     ANORTHITE                 -20.56031     .0273603     1.00000

 ORTHOPYROXENE(SS)        -1.9912
     ENSTATITE-OR               -1.99120     .8243795     1.00000
     FERROSILITE                -1.99120     .1756205     1.00000

 GARNET(SS)               -6.1222
     PYROPE                     -6.12225     .0830553     1.00000
     ALMANDINE                  -6.12225     .0781849     1.00000
     GROSSULAR                  -6.12225     .8387597     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9319962     1.00000
     HEDENBERGITE                 .00000     .0679927     1.00000
     JADEITE                      .00000     .0000112     1.00000

 CPX_SUBCALCIC(SS)          .0000
     DIOPSIDE                    -.00002     .9320066     1.00000
     HEDENBERGITE                -.00002     .0679934     1.00000

 CHLORITE(SS)             -1.2268
     CLINOCHLORE                -1.22680     .9483335     1.00000
     CHAMOSITE                  -1.22680     .0516665     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
             .0000    1.0000     .0000   -4.9525     .0000   -4.9525


           --- summary of gas species ---

           gas                log fugacity         fugacity
```

```
partial pressure

   O2(G)                            -26.80001       1.58486E-27
   H2(G)                              2.27783       1.89597E+02
   H2O(G)                             3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.5849E-05, delzi=  5.8489E-06, nord= 4
               ncycle=  0
 steps completed =    18, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -8.7650
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  1.58489319246110E-05
                     log of reaction progress =      -4.8000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         1.00000E+02    2.65517E-05    2.68617E+04
7.13226E-03
   CLINOPYROXENE(SS)       1.00000E+02    3.20022E-05    2.22861E+04
7.13203E-03
   MAGNETITE               1.00000E+02    3.42337E-06    2.31539E+04
7.92642E-04
   TREMOLITE               1.00000E+02    2.90352E-06    8.12370E+04
2.35874E-03


                current total mass =  1.53539E+05 grams
```

delta total mass = 1.74157E-02 grams
delta total volume = .00574 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	20.7810	1.67530E+00
CLINOPYROXENE(SS)	.1345	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.5780	1.83200E-01

affinity of the overall irreversible reaction= 35.836
kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434535E+05	5.775260E+01	5.775270E+01
NA	1.205657E+04	5.745176E-01	5.745186E-01
CA	3.477349E+01	9.504617E-04	9.504634E-04
MG	2.393561E+04	1.078855E+00	1.078857E+00
AL	9.401168E-01	3.817062E-05	3.817068E-05
SI	6.739632E+01	2.628864E-03	2.628869E-03
H	1.042620E+05	1.133242E+02	1.133244E+02
CL	1.618110E+04	4.999991E-01	5.000000E-01
FE	8.056771E+00	1.580430E-04	1.580433E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.5995	.4548	3.1698E+00

```
     modified nbs ph scale           6.3531         .4902
3.4163E+00
     rational ph scale               6.3531         .4902
3.4163E+00

   phcl =      7.1855



          oxygen fugacity =  1.58486E-27
          log oxygen fugacity = -26.80001



                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                    ionic strength =  5.170460E-01 molal
                 sum of molalities =    2.2049544097865
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999991E-01
molal

                         mass of solution =   1.095506 kg
                         mass of solvent  =   1.000002 kg
                         mass of solutes  =    .095504 kg
                         conc of solutes  =   8.717838 per cent (w/w)


   species                moles        grams         conc        log
conc      log g      log act

   H2O                  5.55088E+01   1.00000E+03
   NA+                  5.15738E-01   1.18567E+01   5.15737E-01     -.
28757     -.24649     -.53406
   CA++                 9.55122E-05   3.82813E-03   9.55120E-05
-4.01994     -.98596    -5.00591
   MG++                 7.46794E-07   1.81508E-05   7.46792E-07
-6.12680     -.98596    -7.11276
   AL+++                2.41744E-23   6.52264E-22   2.41744E-23
-22.61664    -2.21842   -24.83506
   H4SIO4(AQ)           1.46514E-03   1.40822E-01   1.46514E-03
-2.83412      .00000    -2.83412
   H+                   4.43555E-07   4.47059E-07   4.43554E-07
-6.35305     -.24649    -6.59954
   CL-                  4.57687E-01   1.62264E+01   4.57686E-01     -.
33943     -.24649     -.58592
   FE++                 3.02449E-09   1.68908E-07   3.02448E-09
```

```
-8.51935     -.98596    -9.50531
   O2(AQ)               1.33380E-31   4.26800E-30   1.33380E-31
-30.87491      .00000   -30.87491
   H2(AQ)               3.20577E-02   6.46219E-02   3.20576E-02
-1.49407      .00000    -1.49407
   FE+++                1.31734E-22   7.35692E-21   1.31733E-22
-21.88030    -2.21842   -24.09872
   OH-                  5.85817E-02   9.96317E-01   5.85816E-02
-1.23224     -.24649    -1.47873
   H8SI3O10(AQ)         1.60023E-11   4.03761E-09   1.60023E-11
-10.79582      .00000   -10.79582
   H6SI2O7(AQ)          5.80673E-06   1.01161E-03   5.80672E-06
-5.23607      .00000    -5.23607
   AL(OH)3(AQ)          1.56591E-07   1.22146E-05   1.56590E-07
-6.80523      .00000    -6.80523
   AL(OH)4-             3.00736E-05   2.85731E-03   3.00735E-05
-4.52182     -.24649    -4.76831
   AL(OH)SI(OH)-        7.94049E-06   1.37458E-03   7.94048E-06
-5.10015     -.24649    -5.34664
   CACL+                2.01726E-04   1.52370E-02   2.01726E-04
-3.69524     -.24649    -3.94173
   CACL2(AQ)            3.68445E-06   4.08923E-04   3.68445E-06
-5.43363      .00000    -5.43363
   CA(OH)+              2.94954E-04   1.68381E-02   2.94953E-04
-3.53025     -.24649    -3.77674
   CA(H3SIO4)+          3.54587E-04   4.79354E-02   3.54586E-04
-3.45028     -.24649    -3.69677
   FE(OH)+              8.46989E-08   6.17068E-06   8.46987E-08
-7.07212     -.24649    -7.31861
   FE(OH)2              5.86244E-07   5.26809E-05   5.86243E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.94702E-06   6.35552E-04   5.94701E-06
-5.22570     -.24649    -5.47219
   FECL+                3.35321E-09   3.06148E-07   3.35321E-09
-8.47454     -.24649    -8.72103
   FECL2(AQ)            7.85134E-08   9.95181E-06   7.85133E-08
-7.10506      .00000    -7.10506
   FE(H3SIO4)+          1.51340E-04   2.28454E-02   1.51340E-04
-3.82005     -.24649    -4.06654
   MGCL+                7.45097E-07   4.45255E-05   7.45096E-07
-6.12779     -.24649    -6.37428
   MG(OH)+              1.63875E-05   6.77005E-04   1.63875E-05
-4.78549     -.24649    -5.03198
   MG(OH)2(AQ)          1.07884E+00   6.29174E+01   1.07884E+00       .
03296      .00000      .03296
   MG(H3SIO4)+          8.27021E-09   9.87561E-07   8.27020E-09
-8.08248     -.24649    -8.32898
   NACL(AQ)             4.21028E-02   2.46060E+00   4.21027E-02
-1.37569      .00000    -1.37569
   NAOH(AQ)             1.66781E-02   6.67074E-01   1.66780E-02
```

```
-1.77786      .00000    -1.77786
   H3SIO4-              6.38238E-04   6.07008E-02   6.38237E-04
-3.19502     -.24649    -3.44151
   HCL(AQ)              5.61383E-07   2.04685E-05   5.61382E-07
-6.25074      .00000    -6.25074

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0654813
           log (CA++  /h+**0)            8.1931825
           log (MG++  /h+**0)            6.0863243
           log (AL+++ /h+**0)           -5.0364304
           log (FE++  /h+**0)            3.6937752
           log (FE+++ /h+**0)           -4.3000905


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE                -5.4141841    3.85315E-06    8.92153E-04
1.71542E-04

   CLINOPYROXENE(SS)        -4.0089147    9.79682E-05    2.14253E-02
6.48549E-03
   DIOPSIDE                 -4.0395035    9.13054E-05    1.97724E-02
6.04442E-03
   HEDENBERGITE             -5.1764527    6.66112E-06    1.65259E-03
4.40966E-04
   JADEITE                  -8.7649597    1.71807E-09    3.47288E-07
1.03668E-07


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

       phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                 2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)           1.9999999    1.00000E+02

   ALBITE                    1.7781511    6.00000E+01    1.57334E+04
```

```
6.04980E+03
   ANORTHITE                 1.6020599    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)         2.0000003    1.00000E+02

   DIOPSIDE                  1.9030903    8.00001E+01    1.73242E+04
5.29600E+03
   HEDENBERGITE              1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -8.7649597    1.71807E-09    3.47288E-07
1.03668E-07



                           mass, grams        volume, cc

           created         2.231749E-02       6.657030E-03
           destroyed       1.741566E-02       5.739044E-03
           net             4.901829E-03       9.179856E-04

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state         mineral
affinity, kcal    state

 MAGNETITE                .0000  satd           HEMATITE
-3.3501
 PERICLASE              -4.8211                 BRUCITE
-1.0848
 DIASPORE               -9.3241                 FORSTERITE
-.3886
 FAYALITE               -1.7230                 CHRYSOTILE
-.6590
 ENSTATITE-CL           -2.1850                 ENSTATITE-OR
-2.2631
 ENSTATITE-PR           -2.6685                 DIOPSIDE
-.1012
 HEDENBERGITE           -3.8634                 FERROSILITE
-4.4853
 WOLLASTONITE           -3.6110                 PSEUDOWOLLASTONITE
-4.0971
 TREMOLITE              -5.5780                 ANTIGORITE
```

```
-.2753
 TALC                   -6.9460                CLINOCHLORE
-1.0440
 CHAMOSITE              -5.2258                PYROPE
-9.2668
 ALMANDINE              -9.3536                GROSSULAR
-5.9549
 QUARTZ-ALPHA           -5.6699                QUARTZ-BETA
-5.9068
 COESITE                -6.2662                IRON-ALPHA
-8.6597
 IRON-GAMMA             -7.8030                HALITE
-9.7500
 CRISTOBALITE-ALPHA     -6.9558                CRISTOBALITE-BETA
-7.6692


                              --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -19.8835
     ALBITE                      -19.88346     .9584228     1.00000
     ANORTHITE                   -19.88346     .0415772     1.00000

 ORTHOPYROXENE(SS)          -1.9856
     ENSTATITE-OR                 -1.98558     .8243785     1.00000
     FERROSILITE                  -1.98558     .1756215     1.00000

 GARNET(SS)                 -5.7004
     PYROPE                       -5.70042     .0836029     1.00000
     ALMANDINE                    -5.70042     .0787009     1.00000
     GROSSULAR                    -5.70042     .8376962     1.00000

 CLINOPYROXENE(SS)            .0000
saturated
     DIOPSIDE                       .00000     .9319898     1.00000
     HEDENBERGITE                   .00000     .0679927     1.00000
     JADEITE                        .00000     .0000175     1.00000

 CPX_SUBCALCIC(SS)            .0000
     DIOPSIDE                      -.00003     .9320061     1.00000
     HEDENBERGITE                  -.00003     .0679939     1.00000

 CHLORITE(SS)                -.9678
     CLINOCHLORE                   -.96779     .9483332     1.00000
     CHAMOSITE                     -.96779     .0516668     1.00000


 solid solution product phases
```

```
            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
              .0000    1.0000     .0000   -4.7560     .0000   -4.7560


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.80001       1.58486E-27
   H2(G)                          2.27783       1.89597E+02
   H2O(G)                         3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  2.5119E-05, delzi=  9.2699E-06, nord= 4
               ncycle=  0
 steps completed =    19, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -8.4238
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  2.511886431509 55E-05
                    log of reaction progress =      -4.6000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement
```

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	1.00000E+02	4.20816E-05	2.68617E+04	1.13039E-02
CLINOPYROXENE(SS)	9.99999E+01	5.07200E-05	2.22861E+04	1.13035E-02
MAGNETITE	1.00000E+02	5.42567E-06	2.31539E+04	1.25625E-03
TREMOLITE	1.00000E+02	4.60178E-06	8.12370E+04	3.73835E-03

current total mass = 1.53539E+05 grams
delta total mass = 2.76020E-02 grams
delta total volume = .00910 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	19.8601	1.67530E+00
CLINOPYROXENE(SS)	.1345	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.5423	1.83200E-01

affinity of the overall irreversible reaction= 34.287 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434531E+05	5.775270E+01	5.775275E+01
NA	1.205675E+04	5.745274E-01	5.745279E-01
CA	3.444051E+01	9.413625E-04	9.413634E-04
MG	2.393533E+04	1.078844E+00	1.078845E+00
AL	1.475551E+00	5.991046E-05	5.991052E-05
SI	6.782033E+01	2.645409E-03	2.645411E-03
H	1.042619E+05	1.133243E+02	1.133244E+02
CL	1.618108E+04	4.999995E-01	5.000000E-01
FE	8.107686E+00	1.590421E-04	1.590422E-04

```
     co3--                              0.000000E+00        0.000000E+00
     so4--                              0.000000E+00        0.000000E+00
     s--                                0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                          ph            eh            pe


     internal ph scale                  6.5994        .4548
3.1700E+00
     modified nbs ph scale              6.3529        .4902
3.4164E+00
     rational ph scale                  6.3529        .4902
3.4164E+00

   phcl =      7.1853



          oxygen fugacity =  1.58485E-27
          log oxygen fugacity = -26.80001



                           activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                    ionic strength =  5.170500E-01 molal
                 sum of molalities =    2.2049600096388
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999995E-01
molal

                        mass of solution =   1.095508 kg
                        mass of solvent  =   1.000001 kg
                        mass of solutes  =    .095507 kg
                        conc of solutes  =   8.718034 per cent (w/w)


   species                     moles         grams           conc         log
```

```
conc      log g      log act

   H2O                  5.55087E+01   1.00000E+03
   NA+                  5.15752E-01   1.18570E+01   5.15751E-01     -.
28756     -.24649     -.53405
   CA++                 9.44025E-05   3.78365E-03   9.44024E-05
-4.02502     -.98597    -5.01098
   MG++                 7.47348E-07   1.81643E-05   7.47347E-07
-6.12648     -.98597    -7.11244
   AL+++                3.79506E-23   1.02397E-21   3.79506E-23
-22.42078    -2.21842   -24.63920
   H4SIO4(AQ)           1.47428E-03   1.41700E-01   1.47428E-03
-2.83142      .00000    -2.83142
   H+                   4.43721E-07   4.47227E-07   4.43721E-07
-6.35289     -.24649    -6.59938
   CL-                  4.57688E-01   1.62264E+01   4.57687E-01     -.
33943     -.24649     -.58592
   FE++                 3.02676E-09   1.69036E-07   3.02676E-09
-8.51902     -.98597    -9.50499
   O2(AQ)               1.33379E-31   4.26797E-30   1.33379E-31
-30.87491      .00000   -30.87491
   H2(AQ)               3.20578E-02   6.46220E-02   3.20577E-02
-1.49407      .00000    -1.49407
   FE+++                1.31882E-22   7.36524E-21   1.31882E-22
-21.87981    -2.21842   -24.09824
   OH-                  5.85599E-02   9.95945E-01   5.85598E-02
-1.23240     -.24649    -1.47889
   H8SI3O10(AQ)         1.63037E-11   4.11363E-09   1.63036E-11
-10.78772      .00000   -10.78772
   H6SI2O7(AQ)          5.87939E-06   1.02427E-03   5.87938E-06
-5.23067      .00000    -5.23067
   AL(OH)3(AQ)          2.45548E-07   1.91536E-05   2.45548E-07
-6.60986      .00000    -6.60986
   AL(OH)4-             4.71406E-05   4.47886E-03   4.71405E-05
-4.32661     -.24649    -4.57310
   AL(OH)SI(OH)-        1.25244E-05   2.16810E-03   1.25244E-05
-4.90224     -.24649    -5.14873
   CACL+                1.99382E-04   1.50599E-02   1.99382E-04
-3.70031     -.24649    -3.94681
   CACL2(AQ)            3.64165E-06   4.04172E-04   3.64164E-06
-5.43870      .00000    -5.43870
   CA(OH)+              2.91417E-04   1.66362E-02   2.91417E-04
-3.53549     -.24649    -3.78198
   CA(H3SIO4)+          3.52520E-04   4.76561E-02   3.52520E-04
-3.45282     -.24649    -3.69931
   FE(OH)+              8.47306E-08   6.17299E-06   8.47305E-08
-7.07196     -.24649    -7.31845
   FE(OH)2              5.86244E-07   5.26809E-05   5.86244E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.94481E-06   6.35315E-04   5.94480E-06
```

```
-5.22586     -.24649    -5.47235
   FECL+                3.35573E-09   3.06378E-07   3.35573E-09
-8.47421     -.24649    -8.72070
   FECL2(AQ)            7.85725E-08   9.95930E-06   7.85724E-08
-7.10473      .00000    -7.10473
   FE(H3SIO4)+          1.52342E-04   2.29965E-02   1.52341E-04
-3.81718     -.24649    -4.06367
   MGCL+                7.45649E-07   4.45585E-05   7.45648E-07
-6.12747     -.24649    -6.37396
   MG(OH)+              1.63935E-05   6.77252E-04   1.63934E-05
-4.78533     -.24649    -5.03182
   MG(OH)2(AQ)          1.07883E+00   6.29168E+01   1.07883E+00      .
03295      .00000      .03295
   MG(H3SIO4)+          8.32483E-09   9.94083E-07   8.32482E-09
-8.07963     -.24649    -8.32612
   NACL(AQ)             4.21039E-02   2.46067E+00   4.21039E-02
-1.37568      .00000    -1.37568
   NAOH(AQ)             1.66723E-02   6.66842E-01   1.66723E-02
-1.77801      .00000    -1.77801
   H3SIO4-              6.41980E-04   6.10566E-02   6.41979E-04
-3.19248     -.24649    -3.43897
   HCL(AQ)              5.61594E-07   2.04762E-05   5.61594E-07
-6.25058      .00000    -6.25058

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0653306
           log (CA++  /h+**0)            8.1877810
           log (MG++  /h+**0)            6.0863201
           log (AL+++ /h+**0)           -4.8410590
           log (FE++  /h+**0)            3.6937756
           log (FE+++ /h+**0)           -4.3000907


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE               -5.2275290    5.92204E-06    1.37118E-03
2.63649E-04

   CLINOPYROXENE(SS)       -3.8683923    1.35397E-04    2.96108E-02
8.96323E-03
   DIOPSIDE                -3.8989859    1.26187E-04    2.73261E-02
8.35357E-03
   HEDENBERGITE            -5.0359304    9.20597E-06    2.28395E-03
6.09435E-04
```

```
   JADEITE                 -8.4238156    3.76864E-09    7.61788E-07
2.27400E-07


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                2.0000000    1.00000E+02    8.12370E+04
2.72680E+04

   PLAGIOCLASE(SS)          1.9999998    1.00000E+02

   ALBITE                   1.7781511    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                1.6020598    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)        2.0000004    1.00000E+02

   DIOPSIDE                 1.9030905    8.00001E+01    1.73242E+04
5.29601E+03
   HEDENBERGITE             1.3010300    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                 -8.4238156    3.76864E-09    7.61788E-07
2.27400E-07



                           mass, grams        volume, cc

           created        3.098195E-02       9.226880E-03
           destroyed      2.760197E-02       9.095773E-03
           net            3.379988E-03       1.311077E-04

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state
```

```
 MAGNETITE                  .0000  satd           HEMATITE
-3.3501
 PERICLASE                -4.8211                 BRUCITE
-1.0848
 DIASPORE                 -8.6776                 FORSTERITE
-.3841
 FAYALITE                 -1.7185                 CHRYSOTILE
-.6411
 ENSTATITE-CL             -2.1761                 ENSTATITE-OR
-2.2542
 ENSTATITE-PR             -2.6595                 DIOPSIDE
-.1012
 HEDENBERGITE             -3.8634                 FERROSILITE
-4.4763
 WOLLASTONITE             -3.6200                 PSEUDOWOLLASTONITE
-4.1060
 TREMOLITE                -5.5423                 ANTIGORITE
-.1237
 TALC                     -6.9103                 CLINOCHLORE
-.7801
 CHAMOSITE                -4.9618                 PYROPE
-8.8273
 ALMANDINE                -8.9141                 GROSSULAR
-5.5333
 QUARTZ-ALPHA             -5.6610                 QUARTZ-BETA
-5.8979
 COESITE                  -6.2573                 IRON-ALPHA
-8.6597
 IRON-GAMMA               -7.8030                 HALITE
-9.7499
 CRISTOBALITE-ALPHA       -6.9469                 CRISTOBALITE-BETA
-7.6603


                     --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -19.1788
     ALBITE                     -19.17878     .9373907     1.00000
     ANORTHITE                  -19.17878     .0626093     1.00000

 ORTHOPYROXENE(SS)         -1.9767
     ENSTATITE-OR                -1.97665     .8243770     1.00000
     FERROSILITE                 -1.97665     .1756230     1.00000

 GARNET(SS)                -5.2759
     PYROPE                      -5.27590     .0844777     1.00000
     ALMANDINE                   -5.27590     .0795253     1.00000
```

```
    GROSSULAR                  -5.27590     .8359969     1.00000

 CLINOPYROXENE(SS)         .0000
saturated
    DIOPSIDE                     .00000     .9319795     1.00000
    HEDENBERGITE                 .00000     .0679926     1.00000
    JADEITE                      .00000     .0000278     1.00000

 CPX_SUBCALCIC(SS)         .0000
    DIOPSIDE                    -.00004     .9320055     1.00000
    HEDENBERGITE                -.00004     .0679945     1.00000

 CHLORITE(SS)             -.7038
    CLINOCHLORE                 -.70384     .9483326     1.00000
    CHAMOSITE                   -.70384     .0516674     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0000    1.0000     .0000   -4.5554     .0000   -4.5554


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                       -26.80001       1.58485E-27
   H2(G)                         2.27783       1.89598E+02
   H2O(G)                        3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  3.3128E-05, delzi=  8.0092E-06, nord= 4
              ncycle=  0
```

```
 iter =    5
       1 supersaturated pure minerals
       0 supersaturated solid solutions

                         the most supersaturated phases     affinity,
kcal

                           1      39   ANTIGORITE              .
00743984


   attempted species assemblage no.   2

              1      1  H2O
              2      2  NA+
              3      4  CA++
              4      5  MG++
              5      6  AL+++
              6      7  H4SIO4(AQ)
              7     13  H+
              8     16  CL-
              9     21  FE++
             10     32  O2(G)
             11      1  MAGNETITE
             12     39  ANTIGORITE
             13      1  CLINOPYRDIOPSIDE
             14      2  CLINOPYRHEDENBERGITE
             15      3  CLINOPYRJADEITE

 steps completed =    20, iter = 11, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  3.31280282222572E-05
                    log of reaction progress =      -4.4798044

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 change in the product phase assemblage

                              --- reactant summary ---
```

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.99999E+01	5.54994E-05	2.68617E+04	1.49081E-02
CLINOPYROXENE(SS)	9.99999E+01	6.68921E-05	2.22861E+04	1.49076E-02
MAGNETITE	1.00000E+02	7.15565E-06	2.31539E+04	1.65681E-03
TREMOLITE	1.00000E+02	6.06905E-06	8.12370E+04	4.93032E-03

current total mass = 1.53539E+05 grams
delta total mass = 3.64029E-02 grams
delta total volume = .01200 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	19.3001	1.67530E+00
CLINOPYROXENE(SS)	.1346	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.5132	1.83200E-01

affinity of the overall irreversible reaction= 33.343 kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434528E+05	5.775277E+01	5.775280E+01
NA	1.205691E+04	5.745358E-01	5.745360E-01
CA	3.417158E+01	9.340136E-04	9.340139E-04
MG	2.393504E+04	1.078833E+00	1.078834E+00
AL	1.938147E+00	7.869294E-05	7.869297E-05
SI	6.817481E+01	2.659240E-03	2.659241E-03
H	1.042618E+05	1.133244E+02	1.133244E+02
CL	1.618106E+04	4.999998E-01	5.000000E-01
FE	8.149560E+00	1.598638E-04	1.598638E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

```
    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                          ph           eh           pe

     internal ph scale              6.5992        .4548
3.1701E+00
     modified nbs ph scale          6.3528        .4902
3.4166E+00
     rational ph scale              6.3528        .4902
3.4166E+00

   phcl =      7.1852



          oxygen fugacity =  1.58484E-27
          log oxygen fugacity = -26.80002



                          activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                           (not def. for t.gt.50 c)

                    ionic strength =  5.170540E-01 molal
                 sum of molalities =    2.2049636876641
               osmotic coefficient =     .41003
                    equiv. stoich. ionic strength =  4.999998E-01
molal

                         mass of solution =   1.095509 kg
                         mass of solvent  =   1.000000 kg
                         mass of solutes  =    .095509 kg
                         conc of solutes  =   8.718194 per cent (w/w)


   species                moles        grams         conc        log
conc      log g      log act

   H2O                  5.55087E+01   1.00000E+03
   NA+                  5.15764E-01   1.18573E+01   5.15763E-01     -.
```

```
28755     -.24649     -.53404
   CA++                   9.35075E-05   3.74778E-03   9.35075E-05
-4.02915     -.98597    -5.01512
   MG++                   7.47809E-07   1.81755E-05   7.47809E-07
-6.12621     -.98597    -7.11218
   AL+++                  4.98580E-23   1.34524E-21   4.98580E-23
-22.30227    -2.21843   -24.52069
   H4SIO4(AQ)             1.48178E-03   1.42421E-01   1.48178E-03
-2.82922      .00000    -2.82922
   H+                     4.43860E-07   4.47366E-07   4.43860E-07
-6.35275     -.24649    -6.59925
   CL-                    4.57689E-01   1.62264E+01   4.57689E-01     -.
33943     -.24649     -.58592
   FE++                   3.02866E-09   1.69142E-07   3.02866E-09
-8.51875     -.98597    -9.50472
   O2(AQ)                 1.33378E-31   4.26794E-30   1.33378E-31
-30.87492      .00000   -30.87492
   H2(AQ)                 3.20578E-02   6.46222E-02   3.20578E-02
-1.49407      .00000    -1.49407
   FE+++                  1.32007E-22   7.37220E-21   1.32007E-22
-21.87940    -2.21843   -24.09783
   OH-                    5.85416E-02   9.95635E-01   5.85416E-02
-1.23254     -.24649    -1.47903
   H8SI3O10(AQ)           1.65539E-11   4.17676E-09   1.65538E-11
-10.78110      .00000   -10.78110
   H6SI2O7(AQ)            5.93939E-06   1.03473E-03   5.93938E-06
-5.22626      .00000    -5.22626
   AL(OH)3(AQ)            3.22287E-07   2.51395E-05   3.22287E-07
-6.49176      .00000    -6.49176
   AL(OH)4-               6.18536E-05   5.87676E-03   6.18536E-05
-4.20863     -.24649    -4.45513
   AL(OH)SI(OH)-          1.65171E-05   2.85927E-03   1.65170E-05
-4.78207     -.24649    -5.02856
   CACL+                  1.97492E-04   1.49171E-02   1.97492E-04
-3.70445     -.24649    -3.95094
   CACL2(AQ)              3.60712E-06   4.00339E-04   3.60712E-06
-5.44284      .00000    -5.44284
   CA(OH)+                2.88563E-04   1.64733E-02   2.88563E-04
-3.53976     -.24649    -3.78625
   CA(H3SIO4)+            3.50844E-04   4.74295E-02   3.50844E-04
-3.45489     -.24649    -3.70138
   FE(OH)+                8.47572E-08   6.17493E-06   8.47572E-08
-7.07182     -.24649    -7.31832
   FE(OH)2                5.86245E-07   5.26809E-05   5.86244E-07
-6.23192      .00000    -6.23192
   FE(OH)3-               5.94297E-06   6.35118E-04   5.94296E-06
-5.22600     -.24649    -5.47249
   FECL+                  3.35784E-09   3.06571E-07   3.35784E-09
-8.47394     -.24649    -8.72043
   FECL2(AQ)              7.86218E-08   9.96555E-06   7.86218E-08
```

```
-7.10446      .00000    -7.10446
   FE(H3SIO4)+           1.53165E-04   2.31208E-02   1.53165E-04
-3.81484     -.24649    -4.06133
   MGCL+                 7.46108E-07   4.45859E-05   7.46108E-07
-6.12720     -.24649    -6.37369
   MG(OH)+               1.63984E-05   6.77456E-04   1.63984E-05
-4.78520     -.24649    -5.03169
   MG(OH)2(AQ)           1.07882E+00   6.29161E+01   1.07882E+00      .
03295      .00000      .03295
   MG(H3SIO4)+           8.36973E-09   9.99444E-07   8.36972E-09
-8.07729     -.24649    -8.32378
   NACL(AQ)              4.21049E-02   2.46073E+00   4.21049E-02
-1.37567      .00000    -1.37567
   NAOH(AQ)              1.66674E-02   6.66649E-01   1.66674E-02
-1.77813      .00000    -1.77813
   H3SIO4-               6.45046E-04   6.13483E-02   6.45046E-04
-3.19041     -.24649    -3.43690
   HCL(AQ)               5.61770E-07   2.04826E-05   5.61770E-07
-6.25044      .00000    -6.25044

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0652050
           log (CA++  /h+**0)            8.1833714
           log (MG++  /h+**0)            6.0863157
           log (AL+++ /h+**0)           -4.7229533
           log (FE++  /h+**0)            3.6937761
           log (FE+++ /h+**0)           -4.3000910


           --- summary of solid product phases---


  product                     log moles        moles        grams
volume, cc

   MAGNETITE                -5.1115406    7.73498E-06    1.79095E-03
3.44361E-04
   ANTIGORITE               -7.0579966    8.74991E-08    1.98446E-04
7.62318E-05

   CLINOPYROXENE(SS)        -3.7767059    1.67222E-04    3.65709E-02
1.10701E-02
   DIOPSIDE                 -3.8073038    1.55846E-04    3.37489E-02
1.03170E-02
   HEDENBERGITE             -4.9442435    1.13699E-05    2.82081E-03
7.52687E-04
   JADEITE                  -8.2097395    6.16965E-09    1.24713E-06
3.72277E-07
```

--- grand summary of solid phases (e.s.+p.r.s. +reactants) ---

phase/end-member	log moles	moles	grams	volume, cc
MAGNETITE	2.0000000	1.00000E+02	2.31539E+04	4.45200E+03
TREMOLITE	2.0000000	1.00000E+02	8.12370E+04	2.72680E+04
ANTIGORITE	-7.0579966	8.74991E-08	1.98446E-04	7.62318E-05
PLAGIOCLASE(SS)	1.9999998	9.99999E+01		
ALBITE	1.7781510	6.00000E+01	1.57334E+04	6.04980E+03
ANORTHITE	1.6020598	4.00000E+01	1.11284E+04	4.03000E+03
CLINOPYROXENE(SS)	2.0000004	1.00000E+02		
DIOPSIDE	1.9030905	8.00001E+01	1.73242E+04	5.29601E+03
HEDENBERGITE	1.3010300	2.00000E+01	4.96189E+03	1.32400E+03
JADEITE	-8.2097395	6.16965E-09	1.24713E-06	3.72277E-07

	mass, grams	volume, cc
created	3.856031E-02	1.149067E-02
destroyed	3.640287E-02	1.199596E-02
net	2.157446E-03	-5.052943E-04

warning-- these volume totals may be incomplete because of missing partial molar volume data in the data base

--- mineral saturation state summary ---

mineral affinity, kcal state mineral affinity, kcal state

```
 MAGNETITE                   .0000  satd          HEMATITE
-3.3501
 PERICLASE                 -4.8211                BRUCITE
-1.0848
 DIASPORE                  -8.2868                FORSTERITE
-.3805
 FAYALITE                  -1.7148                CHRYSOTILE
-.6266
 ENSTATITE-CL              -2.1688                ENSTATITE-OR
-2.2469
 ENSTATITE-PR              -2.6523                DIOPSIDE
-.1012
 HEDENBERGITE              -3.8634                FERROSILITE
-4.4690
 WOLLASTONITE              -3.6272                PSEUDOWOLLASTONITE
-4.1133
 TREMOLITE                 -5.5132
ANTIGORITE                  .0000  satd
 TALC                      -6.8812                CLINOCHLORE
-.6194
 CHAMOSITE                 -4.8011                PYROPE
-8.5598
 ALMANDINE                 -8.6466                GROSSULAR
-5.2804
 QUARTZ-ALPHA              -5.6537                QUARTZ-BETA
-5.8906
 COESITE                   -6.2500                IRON-ALPHA
-8.6597
 IRON-GAMMA                -7.8030                HALITE
-9.7499
 CRISTOBALITE-ALPHA        -6.9396                CRISTOBALITE-BETA
-7.6530


                    --- summary of solid solutions  ---

 mineral                  aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)            -18.7404
     ALBITE                       -18.74037     .9205014     1.00000
     ANORTHITE                    -18.74037     .0794986     1.00000

 ORTHOPYROXENE(SS)           -1.9694
     ENSTATITE-OR                  -1.96937     .8243754     1.00000
     FERROSILITE                   -1.96937     .1756246     1.00000

 GARNET(SS)                  -5.0205
     PYROPE                        -5.02052     .0851972     1.00000
     ALMANDINE                     -5.02052     .0802035     1.00000
```

```
     GROSSULAR                      -5.02052     .8345993     1.00000

 CLINOPYROXENE(SS)         .0000
saturated
     DIOPSIDE                         .00000     .9319704     1.00000
     HEDENBERGITE                     .00000     .0679927     1.00000
     JADEITE                          .00000     .0000369     1.00000

 CPX_SUBCALCIC(SS)        -.0001
     DIOPSIDE                        -.00005     .9320048     1.00000
     HEDENBERGITE                    -.00005     .0679952     1.00000

 CHLORITE(SS)             -.5432
     CLINOCHLORE                     -.54315     .9483321     1.00000
     CHAMOSITE                       -.54315     .0516679     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9320    1.0000     .9320    -.0306     .0000    -.0306
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1675     .0000   -1.1675
     JADEITE
              .0000    1.0000     .0000   -4.4330     .0000   -4.4330


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.80002       1.58484E-27
   H2(G)                          2.27783       1.89598E+02
   H2O(G)                         3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  3.3138E-05, delzi=  1.0000E-08, nord= 0
               ncycle=  0
```

```
steps completed =    21, iter =  5, ncorr = 0
most rapidly changing is zvclg1(ANTIGORITE       ) =    -7.0485

stepping to zi=  3.3148E-05, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =    22, iter =  5, ncorr = 0
most rapidly changing is zvclg1(ANTIGORITE       ) =    -7.0393

stepping to zi=  3.3158E-05, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =    23, iter =  5, ncorr = 0
most rapidly changing is zvclg1(ANTIGORITE       ) =    -7.0302

stepping to zi=  3.3168E-05, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =    24, iter =  5, ncorr = 0
most rapidly changing is zvclg1(ANTIGORITE       ) =    -7.0213

stepping to zi=  3.3268E-05, delzi=  1.0000E-07, nord= 2
              ncycle=  0
steps completed =    25, iter =  5, ncorr = 0
most rapidly changing is zvclg1(ANTIGORITE       ) =    -6.9413

stepping to zi=  3.4268E-05, delzi=  1.0000E-06, nord= 2
              ncycle=  0
steps completed =    26, iter =  7, ncorr = 0
most rapidly changing is zvclg1(ANTIGORITE       ) =    -6.5127

stepping to zi=  3.9811E-05, delzi=  5.5427E-06, nord= 3
              ncycle=  0
steps completed =    27, iter =  6, ncorr = 0
most rapidly changing is zvclg1(ANTIGORITE       ) =    -5.8617
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  3.98107170553493E-05
                    log of reaction progress =      -4.4000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


step size is limited by the print requirement


                              --- reactant summary ---
```

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.99999E+01	6.66949E-05	2.68617E+04	1.79154E-02
CLINOPYROXENE(SS)	9.99999E+01	8.03858E-05	2.22861E+04	1.79148E-02
MAGNETITE	1.00000E+02	8.59911E-06	2.31539E+04	1.99103E-03
TREMOLITE	1.00000E+02	7.29332E-06	8.12370E+04	5.92488E-03

current total mass = 1.53539E+05 grams
delta total mass = 4.37462E-02 grams
delta total volume = .01442 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	18.9345	1.67530E+00
CLINOPYROXENE(SS)	.1346	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.5131	1.83200E-01

affinity of the overall irreversible reaction= 32.731 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434529E+05	5.775277E+01	5.775278E+01
NA	1.205705E+04	5.745427E-01	5.745427E-01
CA	3.417538E+01	9.341172E-04	9.341173E-04
MG	2.393432E+04	1.078801E+00	1.078801E+00
AL	2.324127E+00	9.436455E-05	9.436455E-05
SI	6.826114E+01	2.662607E-03	2.662607E-03
H	1.042618E+05	1.133244E+02	1.133244E+02
CL	1.618107E+04	5.000000E-01	5.000000E-01
FE	8.150850E+00	1.598891E-04	1.598891E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00

```
      s--                                0.000000E+00       0.000000E+00

     warning-- co3--, so4--, and s-- totals require that routine comp1
     have the names of non-carbonate carbon, sulfide sulfur,
     and non-sulfate sulfur aqueous species


    single ion activities and activity coefficients are here defined
    with respect to the internal ph scale



                                        ph            eh            pe

      internal ph scale               6.5992        .4549
3.1701E+00
      modified nbs ph scale           6.3527        .4902
3.4166E+00
      rational ph scale               6.3527        .4902
3.4166E+00

    phcl =      7.1851



           oxygen fugacity =  1.58479E-27
           log oxygen fugacity = -26.80003



                         activity of water =    .98384
                log activity of water =   -.00707
                alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                     ionic strength =  5.170623E-01 molal
                  sum of molalities =    2.2049470417070
                osmotic coefficient =    .41003
                     equiv. stoich. ionic strength =  5.000000E-01
molal

                          mass of solution =   1.095509 kg
                          mass of solvent  =   1.000000 kg
                          mass of solutes  =    .095508 kg
                          conc of solutes  =   8.718184 per cent (w/w)


    species                 moles        grams          conc        log
conc      log g      log act
```

```
   H2O                  5.55087E+01   1.00000E+03
   NA+                  5.15772E-01   1.18575E+01   5.15772E-01     -.
28754     -.24649     -.53404
   CA++                 9.35247E-05   3.74847E-03   9.35246E-05
-4.02907     -.98597    -5.01505
   MG++                 7.47972E-07   1.81795E-05   7.47972E-07
-6.12611     -.98597    -7.11209
   AL+++                5.98163E-23   1.61394E-21   5.98163E-23
-22.22318    -2.21844   -24.44162
   H4SIO4(AQ)           1.48184E-03   1.42427E-01   1.48184E-03
-2.82920      .00000    -2.82920
   H+                   4.43914E-07   4.47421E-07   4.43914E-07
-6.35270     -.24649    -6.59919
   CL-                  4.57688E-01   1.62264E+01   4.57688E-01     -.
33943     -.24649     -.58592
   FE++                 3.02943E-09   1.69185E-07   3.02943E-09
-8.51864     -.98597    -9.50461
   O2(AQ)               1.33374E-31   4.26782E-30   1.33374E-31
-30.87493      .00000   -30.87493
   H2(AQ)               3.20583E-02   6.46231E-02   3.20583E-02
-1.49406      .00000    -1.49406
   FE+++                1.32057E-22   7.37498E-21   1.32057E-22
-21.87924    -2.21844   -24.09768
   OH-                  5.85347E-02   9.95518E-01   5.85347E-02
-1.23259     -.24649    -1.47908
   H8SI3O10(AQ)         1.65560E-11   4.17730E-09   1.65560E-11
-10.78105      .00000   -10.78105
   H6SI2O7(AQ)          5.93989E-06   1.03481E-03   5.93989E-06
-5.22622      .00000    -5.22622
   AL(OH)3(AQ)          3.86511E-07   3.01492E-05   3.86511E-07
-6.41284      .00000    -6.41284
   AL(OH)4-             7.41710E-05   7.04704E-03   7.41710E-05
-4.12977     -.24649    -4.37626
   AL(OH)SI(OH)-        1.98071E-05   3.42880E-03   1.98071E-05
-4.70318     -.24649    -4.94967
   CACL+                1.97526E-04   1.49197E-02   1.97526E-04
-3.70438     -.24649    -3.95087
   CACL2(AQ)            3.60772E-06   4.00407E-04   3.60772E-06
-5.44277      .00000    -5.44277
   CA(OH)+              2.88580E-04   1.64742E-02   2.88580E-04
-3.53973     -.24649    -3.78623
   CA(H3SIO4)+          3.50879E-04   4.74343E-02   3.50879E-04
-3.45484     -.24649    -3.70134
   FE(OH)+              8.47679E-08   6.17571E-06   8.47679E-08
-7.07177     -.24649    -7.31826
   FE(OH)2              5.86247E-07   5.26811E-05   5.86247E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.94229E-06   6.35046E-04   5.94229E-06
-5.22605     -.24649    -5.47254
   FECL+                3.35865E-09   3.06645E-07   3.35865E-09
```

```
-8.47383     -.24649    -8.72033
   FECL2(AQ)            7.86405E-08   9.96792E-06   7.86405E-08
-7.10435      .00000    -7.10435
   FE(H3SIO4)+          1.53191E-04   2.31247E-02   1.53191E-04
-3.81477     -.24649    -4.06126
   MGCL+                7.46264E-07   4.45952E-05   7.46263E-07
-6.12711     -.24649    -6.37360
   MG(OH)+              1.63999E-05   6.77518E-04   1.63999E-05
-4.78516     -.24649    -5.03165
   MG(OH)2(AQ)          1.07878E+00   6.29142E+01   1.07878E+00      .
03293      .00000      .03293
   MG(H3SIO4)+          8.37085E-09   9.99578E-07   8.37085E-09
-8.07723     -.24649    -8.32372
   NACL(AQ)             4.21054E-02   2.46075E+00   4.21054E-02
-1.37566      .00000    -1.37566
   NAOH(AQ)             1.66657E-02   6.66578E-01   1.66657E-02
-1.77818      .00000    -1.77818
   H3SIO4-              6.44998E-04   6.13437E-02   6.44998E-04
-3.19044     -.24649    -3.43693
   HCL(AQ)              5.61835E-07   2.04850E-05   5.61835E-07
-6.25039      .00000    -6.25039

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0651589
           log (CA++  /h+**0)            8.1833433
           log (MG++  /h+**0)            6.0863026
           log (AL+++ /h+**0)           -4.6440334
           log (FE++  /h+**0)            3.6937781
           log (FE+++ /h+**0)           -4.3000920


           --- summary of solid product phases---


  product                    log moles       moles        grams
volume, cc

   MAGNETITE                -5.0173225    9.60899E-06    2.22485E-03
4.27792E-04
   ANTIGORITE               -5.8617382    1.37487E-06    3.11817E-03
1.19783E-03

   CLINOPYROXENE(SS)        -3.7269028    1.87541E-04    4.10146E-02
1.24152E-02
   DIOPSIDE                 -3.7575049    1.74781E-04    3.78493E-02
1.15705E-02
   HEDENBERGITE             -4.8944295    1.27518E-05    3.16364E-03
8.44167E-04
```

```
   JADEITE                    -8.0810254    8.29802E-09    1.67735E-06
5.00703E-07


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                  2.0000000    1.00000E+02    8.12370E+04
2.72680E+04
   ANTIGORITE                -5.8617382    1.37487E-06    3.11817E-03
1.19783E-03

   PLAGIOCLASE(SS)            1.9999997    9.99999E+01

   ALBITE                     1.7781510    6.00000E+01    1.57334E+04
6.04980E+03
   ANORTHITE                  1.6020597    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)          2.0000005    1.00000E+02

   DIOPSIDE                   1.9030906    8.00001E+01    1.73242E+04
5.29601E+03
   HEDENBERGITE               1.3010299    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                   -8.0810254    8.29802E-09    1.67735E-06
5.00703E-07


                          mass, grams        volume, cc

           created        4.635766E-02       1.404081E-02
           destroyed      4.374617E-02       1.441583E-02
           net            2.611497E-03      -3.750136E-04

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---
```

```
   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3501
 PERICLASE              -4.8211                HRUCITE
-1.0848
 DIASPORE               -8.0256                FORSTERITE
-.3805
 FAYALITE               -1.7148                CHRYSOTILE
-.6266
 ENSTATITE-CL           -2.1688                ENSTATITE-OR
-2.2469
 ENSTATITE-PR           -2.6522                DIOPSIDE
-.1013
 HEDENBERGITE           -3.8634                FERROSILITE
-4.4690
 WOLLASTONITE           -3.6273                PSEUDOWOLLASTONITE
-4.1134
 TREMOLITE              -5.5131
ANTIGORITE               .0000  satd
 TALC                   -6.8811                CLINOCHLORE
-.5149
 CHAMOSITE              -4.6966                PYROPE
-8.3858
 ALMANDINE              -8.4726                GROSSULAR
-5.1065
 QUARTZ-ALPHA           -5.6536                QUARTZ-BETA
-5.8905
 COESITE                -6.2499                IRON-ALPHA
-8.6596
 IRON-GAMMA             -7.8029                HALITE
-9.7499
 CRISTOBALITE-ALPHA     -6.9395                CRISTOBALITE-BETA
-7.6529


                    --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -18.4566
     ALBITE                    -18.45660     .9061461     1.00000
     ANORTHITE                 -18.45660     .0938539     1.00000

 ORTHOPYROXENE(SS)        -1.9693
     ENSTATITE-OR               -1.96934     .8243703     1.00000
     FERROSILITE                -1.96934     .1756297     1.00000

 GARNET(SS)               -4.8466
```

```
    PYROPE                        -4.84662     .0851994     1.00000
    ALMANDINE                     -4.84662     .0802084     1.00000
    GROSSULAR                     -4.84662     .8345922     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
    DIOPSIDE                        .00000     .9319613     1.00000
    HEDENBERGITE                    .00000     .0679944     1.00000
    JADEITE                         .00000     .0000442     1.00000

 CPX_SUBCALCIC(SS)         -.0001
    DIOPSIDE                       -.00006     .9320026     1.00000
    HEDENBERGITE                   -.00006     .0679974     1.00000

 CHLORITE(SS)              -.4387
    CLINOCHLORE                    -.43870     .9483304     1.00000
    CHAMOSITE                      -.43870     .0516696     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
             .9320    1.0000     .9320    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0000    1.0000     .0000   -4.3541     .0000   -4.3541


          --- summary of gas species ---

          gas                log fugacity        fugacity
partial pressure

   O2(G)                          -26.80003      1.58479E-27
   H2(G)                            2.27784      1.89601E+02
   H2O(G)                           3.80603      6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
 stepping to zi=  6.3096E-05, delzi=  2.3285E-05, nord= 3
              ncycle=  0
 steps completed =    28, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -5.2321
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  6.30957344480186E-05
                    log of reaction progress =      -4.2000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.99999E+01    1.05704E-04    2.68617E+04
2.83940E-02
   CLINOPYROXENE(SS)      9.99999E+01    1.27403E-04    2.22861E+04
2.83931E-02
   MAGNETITE              1.00000E+02    1.36287E-05    2.31539E+04
3.15557E-03
   TREMOLITE              1.00000E+02    1.15591E-05    8.12370E+04
9.39030E-03


               current total mass =  1.53539E+05 grams
               delta total mass   =  6.93330E-02 grams
               delta total volume =       .02285 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)          18.0150    1.67530E+00
   CLINOPYROXENE(SS)          .1346    0.00000E+00
   MAGNETITE                  .0000    0.00000E+00
   TREMOLITE                 5.5128    1.83200E-01

          affinity of the overall irreversible reaction=    31.191
```

```
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.         moles

      O          8.434531E+05        5.775277E+01        5.775271E+01
      NA         1.205756E+04        5.745667E-01        5.745661E-01
      CA         3.418862E+01        9.344786E-04        9.344777E-04
      MG         2.393181E+04        1.078687E+00        1.078686E+00
      AL         3.668972E+00        1.489681E-04        1.489679E-04
      SI         6.856197E+01        2.674340E-03        2.674338E-03
      H          1.042618E+05        1.133244E+02        1.133243E+02
      CL         1.618109E+04        5.000005E-01        5.000000E-01
      FE         8.155347E+00        1.599772E-04        1.599771E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                                  ph            eh            pe

     internal ph scale                          6.5990        .4549
3.1703E+00
     modified nbs ph scale                      6.3525        .4902
3.4168E+00
     rational ph scale                          6.3525        .4902
3.4168E+00

   phcl =      7.1849



          oxygen fugacity =  1.58464E-27
          log oxygen fugacity = -26.80007
```

```
                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                           (not def. for t.gt.50 c)

                    ionic strength =  5.170915E-01 molal
                 sum of molalities =    2.2048890456704
               osmotic coefficient =     .41004
                    equiv. stoich. ionic strength =  5.000005E-01
molal

                         mass of solution =   1.095507 kg
                         mass of solvent  =    .999999 kg
                         mass of solutes  =    .095508 kg
                         conc of solutes  =   8.718147 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55086E+01   9.99999E+02
   NA+                  5.15800E-01   1.18581E+01   5.15800E-01     -.
28752     -.24650     -.53401
   CA++                 9.35845E-05   3.75087E-03   9.35846E-05
-4.02880     -.98599    -5.01478
   MG++                 7.48541E-07   1.81933E-05   7.48542E-07
-6.12578     -.98599    -7.11177
   AL+++                9.45893E-23   2.55216E-21   9.45894E-23
-22.02416    -2.21847   -24.24263
   H4SIO4(AQ)           1.48206E-03   1.42448E-01   1.48206E-03
-2.82913      .00000    -2.82913
   H+                   4.44102E-07   4.47610E-07   4.44102E-07
-6.35252     -.24650    -6.59901
   CL-                  4.57687E-01   1.62264E+01   4.57687E-01     -.
33943     -.24650     -.58593
   FE++                 3.03210E-09   1.69334E-07   3.03210E-09
-8.51826     -.98599    -9.50424
   O2(AQ)               1.33362E-31   4.26741E-30   1.33362E-31
-30.87497      .00000   -30.87497
   H2(AQ)               3.20598E-02   6.46261E-02   3.20598E-02
-1.49404      .00000    -1.49404
   FE+++                1.32231E-22   7.38469E-21   1.32231E-22
-21.87867    -2.21847   -24.09714
   OH-                  5.85107E-02   9.95110E-01   5.85108E-02
-1.23276     -.24650    -1.47926
   H8SI3O10(AQ)         1.65633E-11   4.17915E-09   1.65633E-11
-10.78085      .00000   -10.78085
   H6SI2O7(AQ)          5.94165E-06   1.03512E-03   5.94166E-06
```

```
-5.22609      .00000    -5.22609
   AL(OH)3(AQ)             6.10393E-07   4.76128E-05   6.10394E-07
-6.21439      .00000    -6.21439
   AL(OH)4-                1.17086E-04   1.11244E-02   1.17086E-04
-3.93150     -.24650    -4.17799
   AL(OH)SI(OH)-           3.12719E-05   5.41349E-03   3.12719E-05
-4.50485     -.24650    -4.75134
   CACL+                   1.97645E-04   1.49287E-02   1.97646E-04
-3.70411     -.24650    -3.95061
   CACL2(AQ)               3.60984E-06   4.00642E-04   3.60984E-06
-5.44251      .00000    -5.44251
   CA(OH)+                 2.88637E-04   1.64775E-02   2.88637E-04
-3.53965     -.24650    -3.78614
   CA(H3SIO4)+             3.51001E-04   4.74507E-02   3.51002E-04
-3.45469     -.24650    -3.70119
   FE(OH)+                 8.48052E-08   6.17842E-06   8.48053E-08
-7.07158     -.24650    -7.31807
   FE(OH)2                 5.86256E-07   5.26819E-05   5.86256E-07
-6.23191      .00000    -6.23191
   FE(OH)3-                5.93995E-06   6.34796E-04   5.93996E-06
-5.22622     -.24650    -5.47271
   FECL+                   3.36150E-09   3.06905E-07   3.36150E-09
-8.47347     -.24650    -8.71996
   FECL2(AQ)               7.87056E-08   9.97617E-06   7.87057E-08
-7.10399      .00000    -7.10399
   FE(H3SIO4)+             1.53281E-04   2.31383E-02   1.53281E-04
-3.81451     -.24650    -4.06101
   MGCL+                   7.46805E-07   4.46276E-05   7.46806E-07
-6.12679     -.24650    -6.37329
   MG(OH)+                 1.64052E-05   6.77735E-04   1.64052E-05
-4.78502     -.24650    -5.03152
   MG(OH)2(AQ)             1.07867E+00   6.29075E+01   1.07867E+00      .
03289      .00000      .03289
   MG(H3SIO4)+             8.37476E-09   1.00005E-06   8.37477E-09
-8.07703     -.24650    -8.32352
   NACL(AQ)                4.21069E-02   2.46084E+00   4.21069E-02
-1.37565      .00000    -1.37565
   NAOH(AQ)                1.66595E-02   6.66331E-01   1.66595E-02
-1.77834      .00000    -1.77834
   H3SIO4-                 6.44829E-04   6.13277E-02   6.44830E-04
-3.19055     -.24650    -3.43705
   HCL(AQ)                 5.62063E-07   2.04933E-05   5.62063E-07
-6.25021      .00000    -6.25021

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0649984
           log (CA++  /h+**0)            8.1832452
           log (MG++  /h+**0)            6.0862569
```

```
           log (AL+++ /h+**0)           -4.4455856
           log (FE++  /h+**0)            3.6937850
           log (FE+++ /h+**0)           -4.3000954


           --- summary of solid product phases---


  product                        log moles        moles        grams
volume, cc

   MAGNETITE                   -4.7921375    1.61385E-05    3.73668E-03
7.18485E-04
   ANTIGORITE                  -5.2320850    5.86023E-06    1.32909E-02
5.10561E-03

   CLINOPYROXENE(SS)           -3.5878029    2.58343E-04    5.64987E-02
1.71022E-02
   DIOPSIDE                    -3.6184197    2.40758E-04    5.21367E-02
1.59382E-02
   HEDENBERGITE                -4.7552917    1.75674E-05    4.35838E-03
1.16296E-03
   JADEITE                     -7.7435093    1.80506E-08    3.64872E-06
1.08917E-06


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                    2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                    1.9999999    1.00000E+02    8.12370E+04
2.72680E+04
   ANTIGORITE                  -5.2320850    5.86023E-06    1.32909E-02
5.10561E-03

   PLAGIOCLASE(SS)              1.9999995    9.99999E+01

   ALBITE                       1.7781508    5.99999E+01    1.57334E+04
6.04979E+03
   ANORTHITE                    1.6020595    4.00000E+01    1.11284E+04
4.03000E+03


   CLINOPYROXENE(SS)            2.0000006    1.00000E+02

   DIOPSIDE                     1.9030907    8.00001E+01    1.73242E+04
```

```
5.29601E+03
   HEDENBERGITE              1.3010298    2.00000E+01    4.96189E+03
1.32400E+03
   JADEITE                  -7.7435093    1.80506E-08    3.64872E-06
1.08917E-06


                           mass, grams        volume, cc

           created         7.352624E-02       2.292631E-02
           destroyed       6.933300E-02       2.284755E-02
           net             4.193235E-03       7.876517E-05

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE               .0000  satd          HEMATITE
-3.3501
 PERICLASE             -4.8213                BRUCITE
-1.0850
 DIASPORE              -7.3690                FORSTERITE
-.3806
 FAYALITE              -1.7147                CHRYSOTILE
-.6266
 ENSTATITE-CL          -2.1687                ENSTATITE-OR
-2.2468
 ENSTATITE-PR          -2.6522                DIOPSIDE
-.1013
 HEDENBERGITE          -3.8632                FERROSILITE
-4.4687
 WOLLASTONITE          -3.6274                PSEUDOWOLLASTONITE
-4.1135
 TREMOLITE             -5.5128
ANTIGORITE              .0000  satd
 TALC                  -6.8807                CLINOCHLORE
-.2523
 CHAMOSITE             -4.4338                PYROPE
-7.9484
 ALMANDINE             -8.0350                GROSSULAR
-4.6692
 QUARTZ-ALPHA          -5.6534                QUARTZ-BETA
```

```
-5.8903
 COESITE               -6.2497              IRON-ALPHA
-8.6595
 IRON-GAMMA            -7.8028              HALITE
-9.7498
 CRISTOBALITE-ALPHA    -6.9393              CRISTOBALITE-BETA
-7.6527


                    --- summary of solid solutions  ---

 mineral              aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)        -17.7237
     ALBITE                   -17.72375     .8594250     1.00000
     ANORTHITE                -17.72375     .1405750     1.00000

 ORTHOPYROXENE(SS)       -1.9692
     ENSTATITE-OR              -1.96925     .8243528     1.00000
     FERROSILITE               -1.96925     .1756472     1.00000

 GARNET(SS)              -4.4093
     PYROPE                    -4.40935     .0852072     1.00000
     ALMANDINE                 -4.40935     .0802254     1.00000
     GROSSULAR                 -4.40935     .8345674     1.00000

 CLINOPYROXENE(SS)         .0000
saturated
     DIOPSIDE                    .00000     .9319298     1.00000
     HEDENBERGITE                .00000     .0680004     1.00000
     JADEITE                     .00000     .0000699     1.00000

 CPX_SUBCALCIC(SS)        -.0001
     DIOPSIDE                   -.00010     .9319949     1.00000
     HEDENBERGITE               -.00010     .0680051     1.00000

 CHLORITE(SS)             -.1760
     CLINOCHLORE                -.17605     .9483245     1.00000
     CHAMOSITE                  -.17605     .0516755     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
```

```
             .9319    1.0000     .9319    -.0306     .0000    -.0306
    HEDENBERGITE
             .0680    1.0000     .0680   -1.1675     .0000   -1.1675
    JADEITE
             .0001    1.0000     .0001   -4.1557     .0000   -4.1557


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                          -26.80007       1.58464E-27
   H2(G)                            2.27786       1.89610E+02
   H2O(G)                           3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  8.7225E-05, delzi=  2.4129E-05, nord= 4
              ncycle=  0
 iter =    5
       0 supersaturated pure minerals
       1 supersaturated solid solutions

                          the most supersaturated phases     affinity,
kcal

                            1   51100   CHLORITE(SS)             .
00922456


   attempted species assemblage no.   2

             1      1  H2O
             2      2  NA+
             3      4  CA++
             4      5  MG++
             5      6  AL+++
             6      7  H4SIO4(AQ)
             7     13  H+
             8     16  CL-
             9     21  FE++
            10     32  O2(G)
            11      1  MAGNETITE
            12     39  ANTIGORITE
            13      1  CLINOPYRDIOPSIDE
```

```
            14      2  CLINOPYRHEDENBERGITE
            15      3  CLINOPYRJADEITE
            16      1  CHLORITECLINOCHLORE
            17      2  CHLORITECHAMOSITE

 steps completed =    29, iter =  8, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  8.72245078424350E-05
                    log of reaction progress =      -4.0593615

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 change in the product phase assemblage


                              --- reactant summary ---



        reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.99999E+01    1.46127E-04    2.68617E+04
3.92523E-02
   CLINOPYROXENE(SS)      9.99998E+01    1.76124E-04    2.22860E+04
3.92511E-02
   MAGNETITE              1.00000E+02    1.88405E-05    2.31539E+04
4.36230E-03
   TREMOLITE              1.00000E+02    1.59795E-05    8.12370E+04
1.29813E-02


                 current total mass =  1.53539E+05 grams
                 delta total mass   =  9.58470E-02 grams
                 delta total volume =       .03158 cc


        reactant           affinity     rel. rate

   PLAGIOCLASE(SS)          17.3987    1.67530E+00
   CLINOPYROXENE(SS)          .1346    0.00000E+00
   MAGNETITE                  .0000    0.00000E+00
   TREMOLITE                 5.5125    1.83200E-01
```

affinity of the overall irreversible reaction=   30.158
kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434535E+05	5.775275E+01	5.775264E+01
NA	1.205809E+04	5.745915E-01	5.745903E-01
CA	3.420044E+01	9.348010E-04	9.347991E-04
MG	2.392918E+04	1.078568E+00	1.078566E+00
AL	4.982084E+00	2.022831E-04	2.022827E-04
SI	6.885650E+01	2.685827E-03	2.685821E-03
H	1.042619E+05	1.133244E+02	1.133241E+02
CL	1.618112E+04	5.000010E-01	5.000000E-01
FE	8.159701E+00	1.600625E-04	1.600622E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.5988	.4549	3.1705E+00
modified nbs ph scale	6.3523	.4903	3.4170E+00
rational ph scale	6.3523	.4903	3.4170E+00

phcl =   7.1848

oxygen fugacity = 1.58450E-27

```
          log oxygen fugacity = -26.80011



                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                           (not def. for t.gt.50 c)

                    ionic strength =  5.171210E-01 molal
                 sum of molalities =    2.2048261589121
               osmotic coefficient =     .41005
                    equiv. stoich. ionic strength =  5.000010E-01
molal

                         mass of solution =   1.095505 kg
                         mass of solvent  =    .999998 kg
                         mass of solutes  =    .095507 kg
                         conc of solutes  =   8.718075 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55086E+01   9.99998E+02
   NA+                  5.15828E-01   1.18588E+01   5.15829E-01     -.
28749     -.24650     -.53399
   CA++                 9.36385E-05   3.75303E-03   9.36387E-05
-4.02854     -.98600    -5.01454
   MG++                 7.49067E-07   1.82061E-05   7.49068E-07
-6.12548     -.98600    -7.11148
   AL+++                1.28647E-22   3.47109E-21   1.28647E-22
-21.89060    -2.21850   -24.10910
   H4SIO4(AQ)           1.48229E-03   1.42470E-01   1.48230E-03
-2.82907      .00000    -2.82907
   H+                   4.44279E-07   4.47788E-07   4.44279E-07
-6.35234     -.24650    -6.59884
   CL-                  4.57685E-01   1.62263E+01   4.57686E-01     -.
33943     -.24650     -.58593
   FE++                 3.03461E-09   1.69474E-07   3.03462E-09
-8.51790     -.98600    -9.50390
   O2(AQ)               1.33349E-31   4.26702E-30   1.33350E-31
-30.87501      .00000   -30.87501
   H2(AQ)               3.20612E-02   6.46289E-02   3.20613E-02
-1.49402      .00000    -1.49402
   FE+++                1.32394E-22   7.39382E-21   1.32394E-22
-21.87813    -2.21850   -24.09663
   OH-                  5.84883E-02   9.94729E-01   5.84885E-02
-1.23293     -.24650    -1.47943
   H8SI3O10(AQ)         1.65711E-11   4.18111E-09   1.65711E-11
```

```
-10.78065      .00000   -10.78065
   H6SI2O7(AQ)          5.94350E-06   1.03544E-03   5.94351E-06
-5.22596      .00000    -5.22596
   AL(OH)3(AQ)          8.29137E-07   6.46755E-05   8.29139E-07
-6.08137      .00000    -6.08137
   AL(OH)4-             1.58984E-04   1.51052E-02   1.58985E-04
-3.79864     -.24650    -4.04514
   AL(OH)SI(OH)-        4.24691E-05   7.35183E-03   4.24692E-05
-4.37193     -.24650    -4.61843
   CACL+                1.97752E-04   1.49368E-02   1.97753E-04
-3.70388     -.24650    -3.95038
   CACL2(AQ)            3.61172E-06   4.00851E-04   3.61173E-06
-5.44228      .00000    -5.44228
   CA(OH)+              2.88684E-04   1.64802E-02   2.88684E-04
-3.53958     -.24650    -3.78608
   CA(H3SIO4)+          3.51113E-04   4.74658E-02   3.51114E-04
-3.45455     -.24650    -3.70105
   FE(OH)+              8.48402E-08   6.18097E-06   8.48404E-08
-7.07140     -.24650    -7.31790
   FE(OH)2              5.86264E-07   5.26826E-05   5.86265E-07
-6.23191      .00000    -6.23191
   FE(OH)3-             5.93777E-06   6.34563E-04   5.93778E-06
-5.22638     -.24650    -5.47288
   FECL+                3.36416E-09   3.07148E-07   3.36417E-09
-8.47312     -.24650    -8.71962
   FECL2(AQ)            7.87665E-08   9.98388E-06   7.87666E-08
-7.10366      .00000    -7.10366
   FE(H3SIO4)+          1.53368E-04   2.31515E-02   1.53368E-04
-3.81426     -.24650    -4.06076
   MGCL+                7.47303E-07   4.46573E-05   7.47304E-07
-6.12650     -.24650    -6.37300
   MG(OH)+              1.64099E-05   6.77929E-04   1.64099E-05
-4.78489     -.24650    -5.03139
   MG(OH)2(AQ)          1.07855E+00   6.29005E+01   1.07855E+00      .
03284      .00000      .03284
   MG(H3SIO4)+          8.37848E-09   1.00049E-06   8.37849E-09
-8.07683     -.24650    -8.32333
   NACL(AQ)             4.21084E-02   2.46093E+00   4.21085E-02
-1.37563      .00000    -1.37563
   NAOH(AQ)             1.66538E-02   6.66102E-01   1.66538E-02
-1.77849      .00000    -1.77849
   H3SIO4-              6.44683E-04   6.13137E-02   6.44684E-04
-3.19065     -.24650    -3.43715
   HCL(AQ)              5.62276E-07   2.05011E-05   5.62277E-07
-6.25005      .00000    -6.25005

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0648497
```

```
           log (CA++  /h+**0)            8.1831429
           log (MG++  /h+**0)            6.0862088
           log (AL+++ /h+**0)           -4.3125684
           log (FE++  /h+**0)            3.6937916
           log (FE+++ /h+**0)           -4.3000987


           --- summary of solid product phases---


  product                        log moles        moles        grams
volume, cc

   MAGNETITE                   -4.6427430    2.27644E-05    5.27085E-03
1.01347E-03
   ANTIGORITE                  -4.9891440    1.02531E-05    2.32538E-02
8.93283E-03

   CLINOPYROXENE(SS)           -3.4791681    3.31766E-04    7.25559E-02
2.19627E-02
   DIOPSIDE                    -3.5097995    3.09172E-04    6.69520E-02
2.04672E-02
   HEDENBERGITE                -4.6466168    2.25623E-05    5.59758E-03
1.49362E-03
   JADEITE                     -7.5018701    3.14869E-08    6.36472E-06
1.89992E-06

   CHLORITE(SS)                -5.0883145    8.15991E-06    9.20353E-04
3.45247E-04
   CLINOCHLORE                 -5.1113604    7.73819E-06    8.60173E-04
3.27248E-04
   CHAMOSITE                   -6.3749777    4.21718E-07    6.01798E-05
1.79989E-05


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                    2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                    1.9999999    1.00000E+02    8.12370E+04
2.72680E+04
   ANTIGORITE                  -4.9891440    1.02531E-05    2.32538E-02
8.93283E-03

   PLAGIOCLASE(SS)              1.9999994    9.99999E+01
```

```
   ALBITE                     1.7781506    5.99999E+01    1.57334E+04
6.04979E+03
   ANORTHITE                  1.6020594    3.99999E+01    1.11284E+04
4.02999E+03


   CLINOPYROXENE(SS)          2.0000007    1.00000E+02

   DIOPSIDE                   1.9030909    8.00002E+01    1.73242E+04
5.29601E+03
   HEDENBERGITE               1.3010297    2.00000E+01    4.96188E+03
1.32400E+03
   JADEITE                   -7.5018701    3.14869E-08    6.36472E-06
1.89992E-06


   CHLORITE(SS)              -5.0883145    8.15991E-06

   CLINOCHLORE               -5.1113604    7.73819E-06    8.60173E-04
3.27248E-04
   CHAMOSITE                 -6.3749777    4.21718E-07    6.01798E-05
1.79989E-05



                           mass, grams        volume, cc

           created         1.020009E-01       3.225427E-02
           destroyed       9.584700E-02       3.158480E-02
           net             6.153944E-03       6.694733E-04

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                 .0000  satd         HEMATITE
-3.3501
 PERICLASE               -4.8214               BRUCITE
-1.0852
 DIASPORE                -6.9288               FORSTERITE
-.3806
 FAYALITE                -1.7145               CHRYSOTILE
-.6267
```

```
 ENSTATITE-CL           -2.1687               ENSTATITE-OR
-2.2468
 ENSTATITE-PR           -2.6521               DIOPSIDE
-.1014
 HEDENBERGITE           -3.8631               FERROSILITE
-4.4685
 WOLLASTONITE           -3.6275               PSEUDOWOLLASTONITE
-4.1136
 TREMOLITE              -5.5125
ANTIGORITE               .0000  satd
 TALC                   -6.8802               CLINOCHLORE
-.0763
 CHAMOSITE              -4.2576               PYROPE
-7.6552
 ALMANDINE              -7.7416               GROSSULAR
-4.3762
 QUARTZ-ALPHA           -5.6532               QUARTZ-BETA
-5.8901
 COESITE                -6.2495               IRON-ALPHA
-8.6595
 IRON-GAMMA             -7.8028               HALITE
-9.7498
 CRISTOBALITE-ALPHA     -6.9391               CRISTOBALITE-BETA
-7.6525


                --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -17.2128
     ALBITE                    -17.21279     .8182132     1.00000
     ANORTHITE                 -17.21279     .1817868     1.00000

 ORTHOPYROXENE(SS)        -1.9691
     ENSTATITE-OR               -1.96915     .8243346     1.00000
     FERROSILITE                -1.96915     .1756654     1.00000

 GARNET(SS)               -4.1163
     PYROPE                     -4.11628     .0852152     1.00000
     ALMANDINE                  -4.11628     .0802430     1.00000
     GROSSULAR                  -4.11628     .8345418     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9318985     1.00000
     HEDENBERGITE                 .00000     .0680066     1.00000
     JADEITE                      .00000     .0000949     1.00000

 CPX_SUBCALCIC(SS)         -.0001
```

```
     DIOPSIDE                        -.00014     .9319869     1.00000
     HEDENBERGITE                    -.00014     .0680131     1.00000

 CHLORITE(SS)              .0000
saturated
     CLINOCHLORE                      .00000     .9483183     1.00000
     CHAMOSITE                        .00000     .0516817     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .9319    1.0000     .9319    -.0306     .0000    -.0306
     HEDENBERGITE
             .0680    1.0000     .0680   -1.1674     .0000   -1.1674
     JADEITE
             .0001    1.0000     .0001   -4.0227     .0000   -4.0227

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
             .9483    1.0000     .9483    -.0230     .0000    -.0230
     CHAMOSITE
             .0517    1.0000     .0517   -1.2867     .0000   -1.2867


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.80011       1.58450E-27
   H2(G)                          2.27788       1.89618E+02
   H2O(G)                         3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  8.7235E-05, delzi=  1.0000E-08, nord= 0
              ncycle=  0
```

```
steps completed =    30, iter =  4, ncorr = 0
most rapidly changing is zvclg1(CHAMOSITE        ) =     -6.3719

stepping to zi=  8.7245E-05, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =    31, iter =  4, ncorr = 0
most rapidly changing is zvclg1(CHAMOSITE        ) =     -6.3688

stepping to zi=  8.7255E-05, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =    32, iter =  4, ncorr = 0
most rapidly changing is zvclg1(CHAMOSITE        ) =     -6.3657

stepping to zi=  8.7265E-05, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =    33, iter =  4, ncorr = 0
most rapidly changing is zvclg1(CHAMOSITE        ) =     -6.3627

stepping to zi=  8.7365E-05, delzi=  1.0000E-07, nord= 2
              ncycle=  0
steps completed =    34, iter =  5, ncorr = 0
most rapidly changing is zvclg1(CHAMOSITE        ) =     -6.3334

stepping to zi=  8.8365E-05, delzi=  1.0000E-06, nord= 2
              ncycle=  0
steps completed =    35, iter =  7, ncorr = 0
most rapidly changing is zvclg1(CHAMOSITE        ) =     -6.1154

stepping to zi=  9.8365E-05, delzi=  1.0000E-05, nord= 2
              ncycle=  0
steps completed =    36, iter =  7, ncorr = 0
most rapidly changing is zvclg1(CHAMOSITE        ) =     -5.4210

stepping to zi=  1.0000E-04, delzi=  1.6355E-06, nord= 3
              ncycle=  0
steps completed =    37, iter =  4, ncorr = 0
most rapidly changing is zvclg1(CHAMOSITE        ) =     -5.3678
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  9.99999999999989E-05
                    log of reaction progress =      -4.0000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000
```

step size is limited by the print requirement

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.99998E+01	1.67530E-04	2.68617E+04	4.50015E-02
CLINOPYROXENE(SS)	9.99998E+01	2.01920E-04	2.22860E+04	4.50001E-02
MAGNETITE	1.00000E+02	2.16000E-05	2.31539E+04	5.00123E-03
TREMOLITE	1.00000E+02	1.83200E-05	8.12370E+04	1.48826E-02

current total mass = 1.53539E+05 grams
delta total mass = 1.09885E-01 grams
delta total volume = .03621 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	17.3982	1.67530E+00
CLINOPYROXENE(SS)	.1346	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.5122	1.83200E-01

affinity of the overall irreversible reaction= 30.157 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434546E+05	5.775261E+01	5.775251E+01
NA	1.205840E+04	5.746042E-01	5.746032E-01
CA	3.419022E+01	9.345182E-04	9.345166E-04
MG	2.392753E+04	1.078489E+00	1.078487E+00
AL	4.983095E+00	2.023234E-04	2.023230E-04
SI	6.886344E+01	2.686088E-03	2.686083E-03
H	1.042621E+05	1.133242E+02	1.133240E+02

```
    CL         1.618118E+04       5.000009E-01       5.000000E-01
    FE         8.159337E+00       1.600548E-04       1.600545E-04

    co3--                         0.000000E+00       0.000000E+00
    so4--                         0.000000E+00       0.000000E+00
    s--                           0.000000E+00       0.000000E+00

   warning-- co3--, so4--, and s-- totals require that routine comp1
   have the names of non-carbonate carbon, sulfide sulfur,
   and non-sulfate sulfur aqueous species


  single ion activities and activity coefficients are here defined
  with respect to the internal ph scale



                                           ph           eh            pe

     internal ph scale               6.5989        .4549
3.1704E+00
     modified nbs ph scale           6.3524        .4903
3.4169E+00
     rational ph scale               6.3524        .4903
3.4169E+00

  phcl =      7.1848



         oxygen fugacity =  1.58454E-27
         log oxygen fugacity = -26.80010



                   activity of water =    .98384
              log activity of water =   -.00707
              alkalinity =  0.000000E+00 equiv/kg solvent
                                       (not def. for t.gt.50 c)

                   ionic strength =  5.171300E-01 molal
                sum of molalities =    2.2047687061221
              osmotic coefficient =     .41006
                   equiv. stoich. ionic strength =  5.000009E-01
molal

                        mass of solution =   1.095501 kg
                        mass of solvent  =    .999998 kg
                        mass of solutes  =    .095503 kg
                        conc of solutes  =   8.717736 per cent (w/w)
```

```
   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55086E+01   9.99998E+02
   NA+                  5.15838E-01   1.18590E+01   5.15839E-01     -.
28749     -.24650     -.53399
   CA++                 9.35973E-05   3.75138E-03   9.35974E-05
-4.02874     -.98600    -5.01474
   MG++                 7.48785E-07   1.81992E-05   7.48786E-07
-6.12564     -.98600    -7.11165
   AL+++                1.28592E-22   3.46960E-21   1.28592E-22
-21.89079    -2.21851   -24.10930
   H4SIO4(AQ)           1.48245E-03   1.42485E-01   1.48245E-03
-2.82902      .00000    -2.82902
   H+                   4.44210E-07   4.47719E-07   4.44211E-07
-6.35241     -.24650    -6.59891
   CL-                  4.57685E-01   1.62263E+01   4.57686E-01     -.
33943     -.24650     -.58593
   FE++                 3.03368E-09   1.69422E-07   3.03368E-09
-8.51803     -.98600    -9.50403
   O2(AQ)               1.33353E-31   4.26715E-30   1.33354E-31
-30.87500      .00000   -30.87500
   H2(AQ)               3.20607E-02   6.46280E-02   3.20608E-02
-1.49403      .00000    -1.49403
   FE+++                1.32335E-22   7.39053E-21   1.32336E-22
-21.87832    -2.21851   -24.09683
   OH-                  5.84977E-02   9.94887E-01   5.84978E-02
-1.23286     -.24650    -1.47936
   H8SI3O10(AQ)         1.65762E-11   4.18240E-09   1.65762E-11
-10.78051      .00000   -10.78051
   H6SI2O7(AQ)          5.94473E-06   1.03566E-03   5.94474E-06
-5.22587      .00000    -5.22587
   AL(OH)3(AQ)          8.29153E-07   6.46768E-05   8.29155E-07
-6.08136      .00000    -6.08136
   AL(OH)4-             1.59013E-04   1.51079E-02   1.59013E-04
-3.79857     -.24650    -4.04507
   AL(OH)SI(OH)-        4.24810E-05   7.35390E-03   4.24811E-05
-4.37180     -.24650    -4.61831
   CACL+                1.97663E-04   1.49301E-02   1.97663E-04
-3.70407     -.24650    -3.95057
   CACL2(AQ)            3.61007E-06   4.00667E-04   3.61008E-06
-5.44248      .00000    -5.44248
   CA(OH)+              2.88599E-04   1.64754E-02   2.88600E-04
-3.53970     -.24650    -3.78620
   CA(H3SIO4)+          3.51047E-04   4.74569E-02   3.51047E-04
-3.45463     -.24650    -3.70114
   FE(OH)+              8.48267E-08   6.17999E-06   8.48269E-08
-7.07147     -.24650    -7.31797
```

```
   FE(OH)2               5.86261E-07   5.26824E-05   5.86262E-07
-6.23191      .00000    -6.23191
   FE(OH)3-              5.93869E-06   6.34661E-04   5.93870E-06
-5.22631     -.24650    -5.47281
   FECL+                 3.36309E-09   3.07050E-07   3.36309E-09
-8.47326     -.24650    -8.71976
   FECL2(AQ)             7.87408E-08   9.98064E-06   7.87410E-08
-7.10380      .00000    -7.10380
   FE(H3SIO4)+           1.53360E-04   2.31502E-02   1.53360E-04
-3.81429     -.24650    -4.06079
   MGCL+                 7.47013E-07   4.46400E-05   7.47015E-07
-6.12667     -.24650    -6.37317
   MG(OH)+               1.64061E-05   6.77775E-04   1.64062E-05
-4.78499     -.24650    -5.03149
   MG(OH)2(AQ)           1.07847E+00   6.28959E+01   1.07847E+00      .
03281      .00000      .03281
   MG(H3SIO4)+           8.37744E-09   1.00036E-06   8.37745E-09
-8.07689     -.24650    -8.32339
   NACL(AQ)              4.21089E-02   2.46096E+00   4.21090E-02
-1.37563      .00000    -1.37563
   NAOH(AQ)              1.66566E-02   6.66217E-01   1.66567E-02
-1.77841      .00000    -1.77841
   H3SIO4-               6.44852E-04   6.13298E-02   6.44853E-04
-3.19054     -.24650    -3.43704
   HCL(AQ)               5.62186E-07   2.04978E-05   5.62187E-07
-6.25012      .00000    -6.25012

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0649245
           log (CA++  /h+**0)            8.1830832
           log (MG++  /h+**0)            6.0861772
           log (AL+++ /h+**0)           -4.3125601
           log (FE++  /h+**0)            3.6937895
           log (FE+++ /h+**0)           -4.3000976


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                  -4.6009217    2.50656E-05    5.80366E-03
1.11592E-03
   ANTIGORITE                 -4.9837630    1.03809E-05    2.35437E-02
9.04419E-03

   CLINOPYROXENE(SS)          -3.4305200    3.71091E-04    8.11561E-02
```

```
2.45660E-02
   DIOPSIDE                  -3.4611534    3.45817E-04    7.48875E-02
2.28931E-02
   HEDENBERGITE              -4.5979412    2.52382E-05    6.26146E-03
1.67077E-03
   JADEITE                   -7.4530496    3.52331E-08    7.12197E-06
2.12596E-06

   CHLORITE(SS)              -4.0811343    8.29594E-05    9.35696E-03
3.51003E-03
   CLINOCHLORE               -4.1041817    7.86717E-05    8.74509E-03
3.32702E-03
   CHAMOSITE                 -5.3677695    4.28776E-06    6.11869E-04
1.83002E-04


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member        log moles        moles         grams
volume, cc

   MAGNETITE                  2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                  1.9999999    1.00000E+02    8.12370E+04
2.72680E+04
   ANTIGORITE                -4.9837630    1.03809E-05    2.35437E-02
9.04419E-03

   PLAGIOCLASE(SS)            1.9999993    9.99998E+01

   ALBITE                     1.7781505    5.99999E+01    1.57334E+04
6.04979E+03
   ANORTHITE                  1.6020593    3.99999E+01    1.11284E+04
4.02999E+03


   CLINOPYROXENE(SS)          2.0000007    1.00000E+02

   DIOPSIDE                   1.9030910    8.00002E+01    1.73242E+04
5.29601E+03
   HEDENBERGITE               1.3010297    2.00000E+01    4.96188E+03
1.32400E+03
   JADEITE                   -7.4530496    3.52331E-08    7.12197E-06
2.12596E-06


   CHLORITE(SS)              -4.0811343    8.29594E-05

   CLINOCHLORE               -4.1041817    7.86717E-05    8.74509E-03
```

```
3.32702E-03
   CHAMOSITE                -5.3677695    4.28776E-06    6.11869E-04
1.83002E-04



                          mass, grams        volume, cc

           created        1.198605E-01       3.823614E-02
           destroyed      1.098854E-01       3.621092E-02
           net            9.975072E-03       2.025215E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3501
 PERICLASE              -4.8216                BRUCITE
-1.0853
 DIASPORE               -6.9288                FORSTERITE
-.3806
 FAYALITE               -1.7145                CHRYSOTILE
-.6267
 ENSTATITE-CL           -2.1686                ENSTATITE-OR
-2.2467
 ENSTATITE-PR           -2.6521                DIOPSIDE
-.1014
 HEDENBERGITE           -3.8630                FERROSILITE
-4.4684
 WOLLASTONITE           -3.6276                PSEUDOWOLLASTONITE
-4.1136
 TREMOLITE              -5.5122
ANTIGORITE               .0000  satd
 TALC                   -6.8800                CLINOCHLORE
-.0763
 CHAMOSITE              -4.2575                PYROPE
-7.6551
 ALMANDINE              -7.7414                GROSSULAR
-4.3762
 QUARTZ-ALPHA           -5.6530                QUARTZ-BETA
-5.8900
 COESITE                -6.2493                IRON-ALPHA
```

```
-8.6595
 IRON-GAMMA              -7.8028                HALITE
-9.7498
 CRISTOBALITE-ALPHA      -6.9389                CRISTOBALITE-BETA
-7.6523


                     --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -17.2122
     ALBITE                    -17.21218     .8182718     1.00000
     ANORTHITE                 -17.21218     .1817282     1.00000

 ORTHOPYROXENE(SS)        -1.9691
     ENSTATITE-OR               -1.96909     .8243247     1.00000
     FERROSILITE                -1.96909     .1756753     1.00000

 GARNET(SS)               -4.1163
     PYROPE                     -4.11628     .0852193     1.00000
     ALMANDINE                  -4.11628     .0802524     1.00000
     GROSSULAR                  -4.11628     .8345283     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9318941     1.00000
     HEDENBERGITE                 .00000     .0680109     1.00000
     JADEITE                      .00000     .0000949     1.00000

 CPX_SUBCALCIC(SS)         -.0001
     DIOPSIDE                    -.00014     .9319826     1.00000
     HEDENBERGITE                -.00014     .0680174     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9483150     1.00000
     CHAMOSITE                    .00000     .0516850     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .9319    1.0000     .9319    -.0306     .0000    -.0306
```

```
     HEDENBERGITE
              .0680    1.0000     .0680   -1.1674     .0000   -1.1674
     JADEITE
              .0001    1.0000     .0001   -4.0225     .0000   -4.0225

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9483    1.0000     .9483    -.0230     .0000    -.0230
     CHAMOSITE
              .0517    1.0000     .0517   -1.2866     .0000   -1.2866


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.80010       1.58454E-27
   H2(G)                          2.27787       1.89616E+02
   H2O(G)                         3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.1635E-04, delzi=  1.6355E-05, nord= 2
              ncycle=  0
 steps completed =    38, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(CHAMOSITE         ) =     -5.0344

 stepping to zi=  1.5849E-04, delzi=  4.2134E-05, nord= 3
              ncycle=  0
 steps completed =    39, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(CHAMOSITE         ) =     -4.6577
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                     reaction progress        =  1.58489319246109E-04
                     log of reaction progress =      -3.8000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000
```

step size is limited by the print requirement

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.99997E+01	2.65517E-04	2.68617E+04	7.13226E-02
CLINOPYROXENE(SS)	9.99997E+01	3.20022E-04	2.22860E+04	7.13203E-02
MAGNETITE	1.00000E+02	3.42337E-05	2.31539E+04	7.92642E-03
TREMOLITE	1.00000E+02	2.90352E-05	8.12370E+04	2.35874E-02

current total mass = 1.53539E+05 grams
delta total mass = 1.74157E-01 grams
delta total volume = .05739 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	17.3959	1.67530E+00
CLINOPYROXENE(SS)	.1345	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.5110	1.83200E-01

affinity of the overall irreversible reaction= 30.153 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434593E+05	5.775195E+01	5.775191E+01
NA	1.205983E+04	5.746624E-01	5.746619E-01
CA	3.414349E+01	9.332250E-04	9.332244E-04
MG	2.391996E+04	1.078130E+00	1.078129E+00
AL	4.987725E+00	2.025079E-04	2.025078E-04
SI	6.889526E+01	2.687283E-03	2.687281E-03

```
    H          1.042633E+05       1.133236E+02       1.133235E+02
    CL         1.618144E+04       5.000004E-01       5.000000E-01
    FE         8.157670E+00       1.600193E-04       1.600192E-04

    co3--                         0.000000E+00       0.000000E+00
    so4--                         0.000000E+00       0.000000E+00
    s--                           0.000000E+00       0.000000E+00

  warning-- co3--, so4--, and s-- totals require that routine comp1
  have the names of non-carbonate carbon, sulfide sulfur,
  and non-sulfate sulfur aqueous species


 single ion activities and activity coefficients are here defined
 with respect to the internal ph scale



                                           ph           eh            pe

     internal ph scale                  6.5992        .4549
3.1701E+00
     modified nbs ph scale              6.3527        .4902
3.4166E+00
     rational ph scale                  6.3527        .4902
3.4166E+00

   phcl =      7.1852



          oxygen fugacity =  1.58476E-27
          log oxygen fugacity = -26.80004



                         activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                    ionic strength =  5.171710E-01 molal
                 sum of molalities =    2.2045056827591
               osmotic coefficient =     .41011
                    equiv. stoich. ionic strength =  5.000004E-01
molal

                         mass of solution =   1.095484 kg
                         mass of solvent  =    .999999 kg
                         mass of solutes  =    .095484 kg
```

```
                     conc of solutes  =   8.716183 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55086E+01   9.99999E+02
   NA+                  5.15881E-01   1.18600E+01   5.15881E-01     -.
28745     -.24651     -.53396
   CA++                 9.34087E-05   3.74382E-03   9.34087E-05
-4.02961     -.98602    -5.01564
   MG++                 7.47497E-07   1.81679E-05   7.47498E-07
-6.12639     -.98602    -7.11241
   AL+++                1.28340E-22   3.46281E-21   1.28340E-22
-21.89164    -2.21855   -24.11019
   H4SIO4(AQ)           1.48315E-03   1.42552E-01   1.48315E-03
-2.82882      .00000    -2.82882
   H+                   4.43897E-07   4.47404E-07   4.43898E-07
-6.35272     -.24651    -6.59922
   CL-                  4.57683E-01   1.62262E+01   4.57683E-01     -.
33944     -.24651     -.58594
   FE++                 3.02940E-09   1.69183E-07   3.02941E-09
-8.51864     -.98602    -9.50467
   O2(AQ)               1.33371E-31   4.26772E-30   1.33371E-31
-30.87494      .00000   -30.87494
   H2(AQ)               3.20586E-02   6.46238E-02   3.20587E-02
-1.49405      .00000    -1.49405
   FE+++                1.32066E-22   7.37550E-21   1.32066E-22
-21.87921    -2.21855   -24.09776
   OH-                  5.85404E-02   9.95613E-01   5.85404E-02
-1.23254     -.24651    -1.47905
   H8SI3O10(AQ)         1.65996E-11   4.18832E-09   1.65997E-11
-10.77990      .00000   -10.77990
   H6SI2O7(AQ)          5.95033E-06   1.03663E-03   5.95034E-06
-5.22546      .00000    -5.22546
   AL(OH)3(AQ)          8.29226E-07   6.46825E-05   8.29227E-07
-6.08133      .00000    -6.08133
   AL(OH)4-             1.59143E-04   1.51203E-02   1.59143E-04
-3.79821     -.24651    -4.04472
   AL(OH)SI(OH)-        4.25358E-05   7.36338E-03   4.25358E-05
-4.37125     -.24651    -4.61775
   CACL+                1.97255E-04   1.48992E-02   1.97255E-04
-3.70497     -.24651    -3.95148
   CACL2(AQ)            3.60251E-06   3.99828E-04   3.60251E-06
-5.44339      .00000    -5.44339
   CA(OH)+              2.88215E-04   1.64534E-02   2.88215E-04
-3.54028     -.24651    -3.78679
   CA(H3SIO4)+          3.50744E-04   4.74159E-02   3.50744E-04
-3.45501     -.24651    -3.70152
   FE(OH)+              8.47651E-08   6.17550E-06   8.47651E-08
```

```
-7.07178     -.24651    -7.31829
   FE(OH)2              5.86249E-07   5.26813E-05   5.86249E-07
-6.23192      .00000    -6.23192
   FE(OH)3-             5.94289E-06   6.35110E-04   5.94289E-06
-5.22600     -.24651    -5.47251
   FECL+                3.35818E-09   3.06602E-07   3.35818E-09
-8.47390     -.24651    -8.72040
   FECL2(AQ)            7.86237E-08   9.96579E-06   7.86238E-08
-7.10445      .00000    -7.10445
   FE(H3SIO4)+          1.53320E-04   2.31443E-02   1.53320E-04
-3.81440     -.24651    -4.06091
   MGCL+                7.45691E-07   4.45610E-05   7.45691E-07
-6.12744     -.24651    -6.37395
   MG(OH)+              1.63891E-05   6.77072E-04   1.63891E-05
-4.78544     -.24651    -5.03195
   MG(OH)2(AQ)          1.07811E+00   6.28750E+01   1.07811E+00      .
03266      .00000      .03266
   MG(H3SIO4)+          8.37269E-09   9.99798E-07   8.37269E-09
-8.07713     -.24651    -8.32364
   NACL(AQ)             4.21113E-02   2.46110E+00   4.21113E-02
-1.37560      .00000    -1.37560
   NAOH(AQ)             1.66698E-02   6.66743E-01   1.66698E-02
-1.77807      .00000    -1.77807
   H3SIO4-              6.45627E-04   6.14035E-02   6.45627E-04
-3.19002     -.24651    -3.43652
   HCL(AQ)              5.61774E-07   2.04828E-05   5.61774E-07
-6.25044      .00000    -6.25044

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0652670
           log (CA++  /h+**0)            8.1828098
           log (MG++  /h+**0)            6.0860324
           log (AL+++ /h+**0)           -4.3125222
           log (FE++  /h+**0)            3.6937798
           log (FE+++ /h+**0)           -4.3000928


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE               -4.4485820    3.55974E-05    8.24217E-03
1.58480E-03
   ANTIGORITE              -4.9599400    1.09663E-05    2.48713E-02
9.55417E-03
```

```
   CLINOPYROXENE(SS)          -3.2587483    5.51127E-04    1.20530E-01
3.64843E-02
   DIOPSIDE                   -3.2893910    5.13581E-04    1.11217E-01
3.39991E-02
   HEDENBERGITE               -4.4260436    3.74935E-05    9.30194E-03
2.48207E-03
   JADEITE                    -7.2804886    5.24217E-08    1.05965E-05
3.16313E-06

   CHLORITE(SS)               -3.3711927    4.25410E-04    4.79820E-02
1.79991E-02
   CLINOCHLORE                -3.3942471    4.03416E-04    4.48435E-02
1.70605E-02
   CHAMOSITE                  -4.6576997    2.19938E-05    3.13855E-03
9.38695E-04


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member         log moles        moles        grams
volume, cc

   MAGNETITE                   2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                   1.9999999    1.00000E+02    8.12370E+04
2.72680E+04
   ANTIGORITE                 -4.9599400    1.09663E-05    2.48713E-02
9.55417E-03

   PLAGIOCLASE(SS)             1.9999988    9.99997E+01

   ALBITE                      1.7781501    5.99998E+01    1.57333E+04
6.04978E+03
   ANORTHITE                   1.6020588    3.99999E+01    1.11283E+04
4.02999E+03


   CLINOPYROXENE(SS)           2.0000010    1.00000E+02

   DIOPSIDE                    1.9030914    8.00003E+01    1.73242E+04
5.29602E+03
   HEDENBERGITE                1.3010294    2.00000E+01    4.96188E+03
1.32400E+03
   JADEITE                    -7.2804886    5.24217E-08    1.05965E-05
3.16313E-06


   CHLORITE(SS)               -3.3711927    4.25410E-04
```

```
   CLINOCHLORE              -3.3942471    4.03416E-04    4.48435E-02
1.70605E-02
   CHAMOSITE                -4.6576997    2.19938E-05    3.13855E-03
9.38695E-04



                           mass, grams        volume, cc

           created         2.016252E-01       6.562241E-02
           destroyed       1.741566E-01       5.739044E-02
           net             2.746857E-02       8.231969E-03

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE               .0000  satd          HEMATITE
-3.3501
 PERICLASE             -4.8220                BRUCITE
-1.0857
 DIASPORE              -6.9286                FORSTERITE
-.3808
 FAYALITE              -1.7142                CHRYSOTILE
-.6268
 ENSTATITE-CL          -2.1684                ENSTATITE-OR
-2.2465
 ENSTATITE-PR          -2.6519                DIOPSIDE
-.1014
 HEDENBERGITE          -3.8626                FERROSILITE
-4.4677
 WOLLASTONITE          -3.6278                PSEUDOWOLLASTONITE
-4.1139
 TREMOLITE             -5.5110
ANTIGORITE              .0000  satd
 TALC                  -6.8787                CLINOCHLORE
-.0763
 CHAMOSITE             -4.2571                PYROPE
-7.6549
 ALMANDINE             -7.7407                GROSSULAR
-4.3764
 QUARTZ-ALPHA          -5.6524                QUARTZ-BETA
-5.8893
```

```
 COESITE                  -6.2486              IRON-ALPHA
-8.6596
 IRON-GAMMA               -7.8029              HALITE
-9.7497
 CRISTOBALITE-ALPHA       -6.9382              CRISTOBALITE-BETA
-7.6517


                      --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -17.2094
     ALBITE                     -17.20936     .8185395     1.00000
     ANORTHITE                  -17.20936     .1814605     1.00000

 ORTHOPYROXENE(SS)         -1.9688
     ENSTATITE-OR                -1.96881     .8242797     1.00000
     FERROSILITE                 -1.96881     .1757203     1.00000

 GARNET(SS)                -4.1163
     PYROPE                      -4.11632     .0852383     1.00000
     ALMANDINE                   -4.11632     .0802952     1.00000
     GROSSULAR                   -4.11632     .8344665     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .9318742     1.00000
     HEDENBERGITE                  .00000     .0680307     1.00000
     JADEITE                       .00000     .0000951     1.00000

 CPX_SUBCALCIC(SS)          -.0001
     DIOPSIDE                     -.00014     .9319629     1.00000
     HEDENBERGITE                 -.00014     .0680371     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9482997     1.00000
     CHAMOSITE                     .00000     .0517003     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
```

```
             .9319    1.0000     .9319    -.0306     .0000    -.0306
     HEDENBERGITE
             .0680    1.0000     .0680   -1.1673     .0000   -1.1673
     JADEITE
             .0001    1.0000     .0001   -4.0217     .0000   -4.0217

   CHLORITE(SS)
  ideal solution

     CLINOCHLORE
             .9483    1.0000     .9483    -.0231     .0000    -.0231
     CHAMOSITE
             .0517    1.0000     .0517   -1.2865     .0000   -1.2865


           --- summary of gas species ---

           gas                log fugacity         fugacity
 partial pressure

   O2(G)                        -26.80004      1.58476E-27
   H2(G)                          2.27785      1.89603E+02
   H2O(G)                         3.80603      6.39774E+03



  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



  stepping to zi=  2.5119E-04, delzi=  9.2699E-05, nord= 3
                ncycle=  0
  steps completed =    40, iter =  5, ncorr = 0
  most rapidly changing is zvclg1(CHAMOSITE         ) =     -4.3004
  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                      reaction progress        =  2.511886431509555E-04
                      log of reaction progress =      -3.6000000

                      temperature    =    450.000 degrees c
                      total pressure =    500.000 bars

                      computing units remaining =       .000


  step size is limited by the print requirement
```

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.99996E+01	4.20816E-04	2.68616E+04	1.13039E-01
CLINOPYROXENE(SS)	9.99995E+01	5.07200E-04	2.22860E+04	1.13035E-01
MAGNETITE	9.99999E+01	5.42567E-05	2.31538E+04	1.25625E-02
TREMOLITE	1.00000E+02	4.60178E-05	8.12370E+04	3.73835E-02

current total mass = 1.53538E+05 grams
delta total mass = 2.76020E-01 grams
delta total volume = .09096 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	17.3923	1.67530E+00
CLINOPYROXENE(SS)	.1344	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.5091	1.83200E-01

affinity of the overall irreversible reaction= 30.147 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434668E+05	5.775091E+01	5.775096E+01
NA	1.206209E+04	5.747546E-01	5.747551E-01
CA	3.406961E+01	9.311806E-04	9.311815E-04
MG	2.390796E+04	1.077560E+00	1.077561E+00
AL	4.995068E+00	2.028006E-04	2.028008E-04
SI	6.894578E+01	2.689181E-03	2.689184E-03
H	1.042651E+05	1.133225E+02	1.133226E+02
CL	1.618185E+04	4.999995E-01	5.000000E-01
FE	8.155038E+00	1.599634E-04	1.599636E-04

```
      co3--                              0.000000E+00       0.000000E+00
      so4--                              0.000000E+00       0.000000E+00
      s--                                0.000000E+00       0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                           ph            eh            pe


     internal ph scale                   6.5997        .4548
3.1696E+00
     modified nbs ph scale               6.3532        .4902
3.4161E+00
     rational ph scale                   6.3532        .4902
3.4161E+00

   phcl =      7.1857



          oxygen fugacity =  1.58509E-27
          log oxygen fugacity = -26.79995




                             activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                           (not def. for t.gt.50 c)

                    ionic strength =  5.172359E-01 molal
                 sum of molalities =    2.2040888508566
               osmotic coefficient =     .41019
                    equiv. stoich. ionic strength =  4.999995E-01
molal

                         mass of solution =   1.095456 kg
                         mass of solvent  =   1.000001 kg
                         mass of solutes  =    .095455 kg
                         conc of solutes  =   8.713721 per cent (w/w)


   species                      moles        grams          conc        log
```

```
conc       log g       log act

   H2O                  5.55087E+01   1.00000E+03
   NA+                  5.15949E-01   1.18616E+01   5.15949E-01     -.
28739     -.24651     -.53391
   CA++                 9.31107E-05   3.73188E-03   9.31106E-05
-4.03100     -.98606    -5.01706
   MG++                 7.45463E-07   1.81185E-05   7.45462E-07
-6.12757     -.98606    -7.11363
   AL+++                1.27942E-22   3.45208E-21   1.27942E-22
-21.89299    -2.21862   -24.11161
   H4SIO4(AQ)           1.48426E-03   1.42659E-01   1.48425E-03
-2.82849      .00000    -2.82849
   H+                   4.43402E-07   4.46905E-07   4.43402E-07
-6.35320     -.24651    -6.59972
   CL-                  4.57680E-01   1.62261E+01   4.57679E-01     -.
33944     -.24651     -.58595
   FE++                 3.02265E-09   1.68806E-07   3.02265E-09
-8.51961     -.98606    -9.50567
   O2(AQ)               1.33400E-31   4.26863E-30   1.33400E-31
-30.87485      .00000   -30.87485
   H2(AQ)               3.20553E-02   6.46170E-02   3.20553E-02
-1.49410      .00000    -1.49410
   FE+++                1.31641E-22   7.35175E-21   1.31641E-22
-21.88061    -2.21862   -24.09923
   OH-                  5.86080E-02   9.96764E-01   5.86080E-02
-1.23204     -.24651    -1.47856
   H8SI3O10(AQ)         1.66369E-11   4.19772E-09   1.66369E-11
-10.77893      .00000   -10.77893
   H6SI2O7(AQ)          5.95923E-06   1.03818E-03   5.95923E-06
-5.22481      .00000    -5.22481
   AL(OH)3(AQ)          8.29342E-07   6.46916E-05   8.29342E-07
-6.08127      .00000    -6.08127
   AL(OH)4-             1.59349E-04   1.51398E-02   1.59349E-04
-3.79765     -.24651    -4.04417
   AL(OH)SI(OH)-        4.26226E-05   7.37842E-03   4.26226E-05
-4.37036     -.24651    -4.61687
   CACL+                1.96610E-04   1.48505E-02   1.96609E-04
-3.70640     -.24651    -3.95291
   CACL2(AQ)            3.59057E-06   3.98503E-04   3.59057E-06
-5.44484      .00000    -5.44484
   CA(OH)+              2.87606E-04   1.64187E-02   2.87606E-04
-3.54120     -.24651    -3.78772
   CA(H3SIO4)+          3.50264E-04   4.73511E-02   3.50264E-04
-3.45560     -.24651    -3.70212
   FE(OH)+              8.46676E-08   6.16840E-06   8.46675E-08
-7.07228     -.24651    -7.31880
   FE(OH)2              5.86229E-07   5.26795E-05   5.86229E-07
-6.23193      .00000    -6.23193
   FE(OH)3-             5.94955E-06   6.35822E-04   5.94954E-06
```

```
-5.22552     -.24651    -5.47203
   FECL+                3.35042E-09   3.05893E-07   3.35042E-09
-8.47490     -.24651    -8.72142
   FECL2(AQ)            7.84386E-08   9.94232E-06   7.84385E-08
-7.10547      .00000    -7.10547
   FE(H3SIO4)+          1.53258E-04   2.31349E-02   1.53258E-04
-3.81458     -.24651    -4.06109
   MGCL+                7.43601E-07   4.44361E-05   7.43600E-07
-6.12866     -.24651    -6.37517
   MG(OH)+              1.63622E-05   6.75959E-04   1.63622E-05
-4.78616     -.24651    -5.03267
   MG(OH)2(AQ)          1.07754E+00   6.28419E+01   1.07754E+00      .
03243      .00000      .03243
   MG(H3SIO4)+          8.36517E-09   9.98900E-07   8.36516E-09
-8.07753     -.24651    -8.32404
   NACL(AQ)             4.21150E-02   2.46132E+00   4.21149E-02
-1.37556      .00000    -1.37556
   NAOH(AQ)             1.66907E-02   6.67577E-01   1.66906E-02
-1.77753      .00000    -1.77753
   H3SIO4-              6.46856E-04   6.15204E-02   6.46855E-04
-3.18919     -.24651    -3.43571
   HCL(AQ)              5.61122E-07   2.04590E-05   5.61122E-07
-6.25094      .00000    -6.25094

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0658093
           log (CA++  /h+**0)            8.1823764
           log (MG++  /h+**0)            6.0858027
           log (AL+++ /h+**0)           -4.3124621
           log (FE++  /h+**0)            3.6937645
           log (FE+++ /h+**0)           -4.3000851


           --- summary of solid product phases---


  product                     log moles        moles        grams
volume, cc

   MAGNETITE                -4.2816879    5.22772E-05    1.21042E-02
2.32738E-03
   ANTIGORITE               -4.9246572    1.18944E-05    2.69762E-02
1.03628E-02

   CLINOPYROXENE(SS)        -3.0775546    8.36460E-04    1.82932E-01
5.53732E-02
   DIOPSIDE                 -3.1082120    7.79450E-04    1.68792E-01
5.15996E-02
```

```
   HEDENBERGITE              -4.2446503    5.69311E-05    1.41243E-02
3.76884E-03
   JADEITE                   -7.0980441    7.97914E-08    1.61289E-05
4.81461E-06

   CHLORITE(SS)              -3.0140548    9.68156E-04    1.09199E-01
4.09628E-02
   CLINOCHLORE               -3.0371202    9.18078E-04    1.02053E-01
3.88255E-02
   CHAMOSITE                 -4.3003585    5.00774E-05    7.14611E-03
2.13730E-03


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                  1.9999998    1.00000E+02    8.12370E+04
2.72680E+04
   ANTIGORITE                -4.9246572    1.18944E-05    2.69762E-02
1.03628E-02

   PLAGIOCLASE(SS)            1.9999982    9.99996E+01

   ALBITE                     1.7781494    5.99997E+01    1.57333E+04
6.04977E+03
   ANORTHITE                  1.6020582    3.99998E+01    1.11283E+04
4.02998E+03


   CLINOPYROXENE(SS)          2.0000014    1.00000E+02

   DIOPSIDE                   1.9030920    8.00004E+01    1.73243E+04
5.29602E+03
   HEDENBERGITE               1.3010290    2.00000E+01    4.96188E+03
1.32400E+03
   JADEITE                   -7.0980441    7.97914E-08    1.61289E-05
4.81461E-06


   CHLORITE(SS)              -3.0140548    9.68156E-04

   CLINOCHLORE               -3.0371202    9.18078E-04    1.02053E-01
3.88255E-02
   CHAMOSITE                 -4.3003585    5.00774E-05    7.14611E-03
2.13730E-03
```

```
                     mass, grams        volume, cc

       created         3.312116E-01       1.090262E-01
       destroyed       2.760197E-01       9.095773E-02
       net             5.519197E-02       1.806847E-02

      warning-- these volume totals may be incomplete because
      of missing partial molar volume data in the data base



       --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                 .0000  satd          HEMATITE
-3.3500
 PERICLASE               -4.8228                HRUCITE
-1.0865
 DIASPORE                -6.9284                FORSTERITE
-.3810
 FAYALITE                -1.7137                CHRYSOTILE
-.6269
 ENSTATITE-CL            -2.1681                ENSTATITE-OR
-2.2462
 ENSTATITE-PR            -2.6516                DIOPSIDE
-.1014
 HEDENBERGITE            -3.8619                FERROSILITE
-4.4667
 WOLLASTONITE            -3.6281                PSEUDOWOLLASTONITE
-4.1142
 TREMOLITE               -5.5091
ANTIGORITE                .0000  satd
 TALC                    -6.8767                CLINOCHLORE
-.0763
 CHAMOSITE               -4.2564                PYROPE
-7.6544
 ALMANDINE               -7.7396                GROSSULAR
-4.3766
 QUARTZ-ALPHA            -5.6513                QUARTZ-BETA
-5.8882
 COESITE                 -6.2476                IRON-ALPHA
-8.6598
 IRON-GAMMA              -7.8031                HALITE
-9.7495
```

```
 CRISTOBALITE-ALPHA     -6.9372              CRISTOBALITE-BETA
-7.6506


                    --- summary of solid solutions  ---

 mineral              aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)        -17.2049
     ALBITE                   -17.20489     .8189632     1.00000
     ANORTHITE                -17.20489     .1810368     1.00000

 ORTHOPYROXENE(SS)       -1.9684
     ENSTATITE-OR              -1.96838     .8242082     1.00000
     FERROSILITE               -1.96838     .1757918     1.00000

 GARNET(SS)              -4.1164
     PYROPE                    -4.11638     .0852683     1.00000
     ALMANDINE                 -4.11638     .0803632     1.00000
     GROSSULAR                 -4.11638     .8343685     1.00000

 CLINOPYROXENE(SS)         .0000
saturated
     DIOPSIDE                    .00000     .9318427     1.00000
     HEDENBERGITE                .00000     .0680619     1.00000
     JADEITE                     .00000     .0000954     1.00000

 CPX_SUBCALCIC(SS)        -.0001
     DIOPSIDE                   -.00014     .9319316     1.00000
     HEDENBERGITE               -.00014     .0680684     1.00000

 CHLORITE(SS)              .0000
saturated
     CLINOCHLORE                 .00000     .9482755     1.00000
     CHAMOSITE                   .00000     .0517245     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9318    1.0000     .9318    -.0307     .0000    -.0307
     HEDENBERGITE
              .0681    1.0000     .0681   -1.1671     .0000   -1.1671
     JADEITE
```

```
             .0001    1.0000     .0001   -4.0205     .0000   -4.0205

   CHLORITE(SS)
  ideal solution

     CLINOCHLORE
             .9483    1.0000     .9483    -.0231     .0000    -.0231
     CHAMOSITE
             .0517    1.0000     .0517   -1.2863     .0000   -1.2863


           --- summary of gas species ---

           gas                log fugacity         fugacity
 partial pressure

   O2(G)                        -26.79995       1.58509E-27
   H2(G)                          2.27780       1.89583E+02
   H2O(G)                         3.80603       6.39774E+03



  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



  stepping to zi=  3.9811E-04, delzi=  1.4692E-04, nord= 3
                ncycle=  0
  steps completed =    41, iter =  5, ncorr = 0
  most rapidly changing is zvclg1(CHAMOSITE         ) =     -4.0239
  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                      reaction progress        =  3.98107170553492E-04
                      log of reaction progress =      -3.4000000

                      temperature    =    450.000 degrees c
                      total pressure =    500.000 bars

                      computing units remaining =       .000


  step size is limited by the print requirement


                               --- reactant summary ---
```

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.99993E+01	6.66949E-04	2.68616E+04	1.79154E-01
CLINOPYROXENE(SS)	9.99992E+01	8.03858E-04	2.22859E+04	1.79148E-01
MAGNETITE	9.99999E+01	8.59911E-05	2.31538E+04	1.99103E-02
TREMOLITE	9.99999E+01	7.29332E-05	8.12370E+04	5.92488E-02

current total mass = 1.53538E+05 grams
delta total mass = 4.37462E-01 grams
delta total volume = .14416 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	17.3867	1.67530E+00
CLINOPYROXENE(SS)	.1343	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.5061	1.83200E-01

affinity of the overall irreversible reaction= 30.137 kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.434787E+05	5.774925E+01	5.774946E+01
NA	1.206567E+04	5.749007E-01	5.749027E-01
CA	3.395298E+01	9.279533E-04	9.279567E-04
MG	2.388894E+04	1.076657E+00	1.076660E+00
AL	5.006718E+00	2.032649E-04	2.032656E-04
SI	6.902610E+01	2.692199E-03	2.692208E-03
H	1.042681E+05	1.133208E+02	1.133212E+02
CL	1.618250E+04	4.999982E-01	5.000000E-01
FE	8.150892E+00	1.598753E-04	1.598758E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

```
     warning-- co3--, so4--, and s-- totals require that routine comp1
     have the names of non-carbonate carbon, sulfide sulfur,
     and non-sulfate sulfur aqueous species


    single ion activities and activity coefficients are here defined
    with respect to the internal ph scale



                                             ph            eh            pe

      internal ph scale                    6.6005        .4547
3.1689E+00
      modified nbs ph scale                6.3540        .4900
3.4154E+00
      rational ph scale                    6.3540        .4900
3.4154E+00

    phcl =      7.1865



           oxygen fugacity =  1.58563E-27
           log oxygen fugacity = -26.79980



                              activity of water =    .98384
                   log activity of water =   -.00707
                   alkalinity =  0.000000E+00 equiv/kg solvent
                                            (not def. for t.gt.50 c)

                        ionic strength =  5.173390E-01 molal
                     sum of molalities =    2.2034282973412
                   osmotic coefficient =     .41031
                        equiv. stoich. ionic strength =  4.999982E-01
molal

                             mass of solution =   1.095412 kg
                             mass of solvent  =   1.000004 kg
                             mass of solutes  =    .095408 kg
                             conc of solutes  =   8.709820 per cent (w/w)


    species                moles        grams          conc        log
conc      log g      log act

    H2O                  5.55089E+01   1.00000E+03
    NA+                  5.16058E-01   1.18641E+01   5.16056E-01     -.
```

```
28730     -.24653     -.53383
   CA++                   9.26408E-05   3.71304E-03   9.26404E-05
-4.03320     -.98611    -5.01930
   MG++                   7.42253E-07   1.80404E-05   7.42250E-07
-6.12945     -.98611    -7.11556
   AL+++                  1.27315E-22   3.43517E-21   1.27315E-22
-21.89512    -2.21874   -24.11386
   H4SIO4(AQ)             1.48602E-03   1.42828E-01   1.48601E-03
-2.82798      .00000    -2.82798
   H+                     4.42620E-07   4.46117E-07   4.42618E-07
-6.35397     -.24653    -6.60050
   CL-                    4.57675E-01   1.62259E+01   4.57673E-01     -.
33944     -.24653     -.58597
   FE++                   3.01199E-09   1.68210E-07   3.01198E-09
-8.52115     -.98611    -9.50725
   O2(AQ)                 1.33445E-31   4.27008E-30   1.33445E-31
-30.87470     .00000    -30.87470
   H2(AQ)                 3.20500E-02   6.46063E-02   3.20498E-02
-1.49417      .00000    -1.49417
   FE+++                  1.30971E-22   7.31434E-21   1.30971E-22
-21.88283    -2.21874   -24.10156
   OH-                    5.87153E-02   9.98589E-01   5.87151E-02
-1.23125     -.24653    -1.47778
   H8SI3O10(AQ)           1.66961E-11   4.21266E-09   1.66961E-11
-10.77739     .00000    -10.77739
   H6SI2O7(AQ)            5.97338E-06   1.04065E-03   5.97335E-06
-5.22378      .00000    -5.22378
   AL(OH)3(AQ)            8.29527E-07   6.47059E-05   8.29524E-07
-6.08117      .00000    -6.08117
   AL(OH)4-               1.59675E-04   1.51709E-02   1.59675E-04
-3.79676     -.24653    -4.04329
   AL(OH)SI(OH)-          4.27606E-05   7.40230E-03   4.27605E-05
-4.36896     -.24653    -4.61548
   CACL+                  1.95592E-04   1.47737E-02   1.95592E-04
-3.70865     -.24653    -3.95518
   CACL2(AQ)              3.57174E-06   3.96413E-04   3.57173E-06
-5.44712      .00000    -5.44712
   CA(OH)+                2.86645E-04   1.63638E-02   2.86644E-04
-3.54266     -.24653    -3.78918
   CA(H3SIO4)+            3.49507E-04   4.72487E-02   3.49506E-04
-3.45655     -.24653    -3.70307
   FE(OH)+                8.45134E-08   6.15717E-06   8.45131E-08
-7.07308     -.24653    -7.31960
   FE(OH)2                5.86198E-07   5.26767E-05   5.86196E-07
-6.23196      .00000    -6.23196
   FE(OH)3-               5.96010E-06   6.36949E-04   5.96008E-06
-5.22475     -.24653    -5.47127
   FECL+                  3.33818E-09   3.04775E-07   3.33816E-09
-8.47649     -.24653    -8.72302
   FECL2(AQ)              7.81464E-08   9.90529E-06   7.81461E-08
```

```
-7.10709      .00000    -7.10709
   FE(H3SIO4)+          1.53161E-04   2.31202E-02   1.53160E-04
-3.81485     -.24653    -4.06138
   MGCL+                7.40304E-07   4.42391E-05   7.40302E-07
-6.13059     -.24653    -6.37712
   MG(OH)+              1.63196E-05   6.74201E-04   1.63196E-05
-4.78729     -.24653    -5.03382
   MG(OH)2(AQ)          1.07664E+00   6.27894E+01   1.07664E+00      .
03207      .00000      .03207
   MG(H3SIO4)+          8.35330E-09   9.97482E-07   8.35327E-09
-8.07814     -.24653    -8.32467
   NACL(AQ)             4.21209E-02   2.46166E+00   4.21207E-02
-1.37550      .00000    -1.37550
   NAOH(AQ)             1.67237E-02   6.68900E-01   1.67237E-02
-1.77667      .00000    -1.77667
   H3SIO4-              6.48807E-04   6.17060E-02   6.48805E-04
-3.18789     -.24653    -3.43441
   HCL(AQ)              5.60093E-07   2.04215E-05   5.60091E-07
-6.25174      .00000    -6.25174

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0666676
           log (CA++  /h+**0)            8.1816890
           log (MG++  /h+**0)            6.0854385
           log (AL+++ /h+**0)           -4.3123669
           log (FE++  /h+**0)            3.6937400
           log (FE+++ /h+**0)           -4.3000730


           --- summary of solid product phases---


  product                     log moles        moles         grams
volume, cc

   MAGNETITE                -4.1041199    7.86829E-05    1.82181E-02
3.50296E-03
   ANTIGORITE               -4.8739870    1.33664E-05    3.03146E-02
1.16452E-02

   CLINOPYROXENE(SS)        -2.8898580    1.28867E-03    2.81832E-01
8.53093E-02
   DIOPSIDE                 -2.9205387    1.20077E-03    2.60030E-01
7.94912E-02
   HEDENBERGITE             -4.0566373    8.77734E-05    2.17761E-02
5.81060E-03
   JADEITE                  -6.9083656    1.23491E-07    2.49623E-05
7.45143E-06
```

```
   CHLORITE(SS)              -2.7379410    1.82835E-03    2.06223E-01
7.73578E-02
   CLINOCHLORE               -2.7610240    1.73371E-03    1.92718E-01
7.33185E-02
   CHAMOSITE                 -4.0239226    9.46406E-05    1.35053E-02
4.03926E-03


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member        log moles        moles        grams
volume, cc

   MAGNETITE                  2.0000000    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                  1.9999997    9.99999E+01    8.12370E+04
2.72680E+04
   ANTIGORITE                -4.8739870    1.33664E-05    3.03146E-02
1.16452E-02

   PLAGIOCLASE(SS)            1.9999971    9.99993E+01

   ALBITE                     1.7781484    5.99996E+01    1.57333E+04
6.04976E+03
   ANORTHITE                  1.6020571    3.99997E+01    1.11283E+04
4.02997E+03


   CLINOPYROXENE(SS)          2.0000021    1.00000E+02

   DIOPSIDE                   1.9030930    8.00006E+01    1.73243E+04
5.29604E+03
   HEDENBERGITE               1.3010284    1.99999E+01    4.96187E+03
1.32400E+03
   JADEITE                   -6.9083656    1.23491E-07    2.49623E-05
7.45143E-06


   CHLORITE(SS)              -2.7379410    1.82835E-03

   CLINOCHLORE               -2.7610240    1.73371E-03    1.92718E-01
7.33185E-02
   CHAMOSITE                 -4.0239226    9.46406E-05    1.35053E-02
4.03926E-03


                           mass, grams        volume, cc
```

```
              created          5.365875E-01       1.778152E-01
              destroyed        4.374617E-01       1.441583E-01
              net              9.912582E-02       3.365691E-02

             warning-- these volume totals may be incomplete because
             of missing partial molar volume data in the data base



              --- mineral saturation state summary ---


       mineral        affinity, kcal    state        mineral
    affinity, kcal    state

     MAGNETITE                 .0000  satd          HEMATITE
    -3.3499
     PERICLASE               -4.8240                BRUCITE
    -1.0877
     DIASPORE                -6.9281                FORSTERITE
    -.3814
     FAYALITE                -1.7129                CHRYSOTILE
    -.6271
     ENSTATITE-CL            -2.1676                ENSTATITE-OR
    -2.2457
     ENSTATITE-PR            -2.6511                DIOPSIDE
    -.1015
     HEDENBERGITE            -3.8609                FERROSILITE
    -4.4651
     WOLLASTONITE            -3.6287                PSEUDOWOLLASTONITE
    -4.1148
     TREMOLITE               -5.5061
    ANTIGORITE                 .0000  satd
     TALC                    -6.8735                CLINOCHLORE
    -.0764
     CHAMOSITE               -4.2553                PYROPE
    -7.6537
     ALMANDINE               -7.7377                GROSSULAR
    -4.3770
     QUARTZ-ALPHA            -5.6496                QUARTZ-BETA
    -5.8865
     COESITE                 -6.2459                IRON-ALPHA
    -8.6601
     IRON-GAMMA              -7.8034                HALITE
    -9.7494
     CRISTOBALITE-ALPHA      -6.9355                CRISTOBALITE-BETA
    -7.6489
```

```
                        --- summary of solid solutions  ---

 mineral              aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)        -17.1978
     ALBITE                  -17.19780     .8196329     1.00000
     ANORTHITE               -17.19780     .1803671     1.00000

 ORTHOPYROXENE(SS)       -1.9677
     ENSTATITE-OR             -1.96768     .8240948     1.00000
     FERROSILITE              -1.96768     .1759052     1.00000

 GARNET(SS)              -4.1165
     PYROPE                   -4.11648     .0853159     1.00000
     ALMANDINE                -4.11648     .0804711     1.00000
     GROSSULAR                -4.11648     .8342129     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                   .00000     .9317926     1.00000
     HEDENBERGITE               .00000     .0681115     1.00000
     JADEITE                    .00000     .0000958     1.00000

 CPX_SUBCALCIC(SS)         -.0001
     DIOPSIDE                  -.00014     .9318819     1.00000
     HEDENBERGITE              -.00014     .0681181     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                .00000     .9482371     1.00000
     CHAMOSITE                  .00000     .0517629     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9318    1.0000     .9318    -.0307     .0000    -.0307
     HEDENBERGITE
              .0681    1.0000     .0681   -1.1668     .0000   -1.1668
     JADEITE
              .0001    1.0000     .0001   -4.0185     .0000   -4.0185

   CHLORITE(SS)
 ideal solution
```

```
     CLINOCHLORE
              .9482    1.0000     .9482    -.0231     .0000    -.0231
     CHAMOSITE
              .0518    1.0000     .0518   -1.2860     .0000   -1.2860


           --- summary of gas species ---

           gas                 log fugacity         fugacity
partial pressure

   O2(G)                          -26.79980       1.58563E-27
   H2(G)                            2.27773       1.89551E+02
   H2O(G)                           3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  6.3096E-04, delzi=  2.3285E-04, nord= 4
               ncycle=  0
 steps completed =    42, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(CHAMOSITE         ) =     -3.7815
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  6.30957344480185E-04
                     log of reaction progress =      -3.2000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.99989E+01    1.05704E-03    2.68615E+04
```

```
2.83940E-01
   CLINOPYROXENE(SS)       9.99987E+01    1.27403E-03    2.22858E+04
2.83931E-01
   MAGNETITE               9.99999E+01    1.36287E-04    2.31538E+04
3.15557E-02
   TREMOLITE               9.99999E+01    1.15591E-04    8.12369E+04
9.39030E-02


                current total mass =  1.53538E+05 grams
                delta total mass   =  6.93330E-01 grams
                delta total volume =       .22848 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           17.3777    1.67530E+00
   CLINOPYROXENE(SS)           .1340    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.5013    1.83200E-01

          affinity of the overall irreversible reaction=    30.121
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O          8.434975E+05        5.774663E+01        5.774708E+01
      NA         1.207135E+04        5.751323E-01        5.751367E-01
      CA         3.376929E+01        9.228705E-04        9.228777E-04
      MG         2.385880E+04        1.075225E+00        1.075234E+00
      AL         5.025209E+00        2.040018E-04        2.040034E-04
      SI         6.915400E+01        2.697004E-03        2.697025E-03
      H          1.042727E+05        1.133182E+02        1.133191E+02
      CL         1.618352E+04        4.999961E-01        5.000000E-01
      FE         8.144386E+00        1.597368E-04        1.597380E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species
```

```
   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                               ph            eh            pe


     internal ph scale                       6.6017        .4545
3.1677E+00
     modified nbs ph scale                   6.3552        .4899
3.4143E+00
     rational ph scale                       6.3552        .4899
3.4143E+00

   phcl =      7.1877



          oxygen fugacity =  1.58648E-27
          log oxygen fugacity = -26.79956



                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  5.175023E-01 molal
                 sum of molalities =    2.2023815930990
               osmotic coefficient =     .41050
                    equiv. stoich. ionic strength =  4.999961E-01
molal

                         mass of solution =   1.095342 kg
                         mass of solvent  =   1.000008 kg
                         mass of solutes  =    .095335 kg
                         conc of solutes  =   8.703639 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55091E+01   1.00001E+03
   NA+                  5.16230E-01   1.18680E+01   5.16226E-01     -.
28716     -.24655     -.53371
   CA++                 9.19018E-05   3.68343E-03   9.19011E-05
-4.03668     -.98618    -5.02286
   MG++                 7.37202E-07   1.79177E-05   7.37196E-07
```

```
-6.13242     -.98618    -7.11860
   AL+++                1.26331E-22   3.40860E-21   1.26330E-22
-21.89849    -2.21891   -24.11741
   H4SIO4(AQ)           1.48882E-03   1.43097E-01   1.48881E-03
-2.82716      .00000    -2.82716
   H+                   4.41386E-07   4.44873E-07   4.41383E-07
-6.35518     -.24655    -6.60173
   CL-                  4.57667E-01   1.62257E+01   4.57664E-01     -.
33945     -.24655     -.58600
   FE++                 2.99521E-09   1.67273E-07   2.99518E-09
-8.52358     -.98618    -9.50976
   O2(AQ)               1.33518E-31   4.27241E-30   1.33517E-31
-30.87446      .00000   -30.87446
   H2(AQ)               3.20414E-02   6.45891E-02   3.20412E-02
-1.49429      .00000    -1.49429
   FE+++                1.29919E-22   7.25557E-21   1.29918E-22
-21.88633    -2.21891   -24.10525
   OH-                  5.88853E-02   1.00148E+00   5.88848E-02
-1.23000     -.24655    -1.47654
   H8SI3O10(AQ)         1.67905E-11   4.23648E-09   1.67904E-11
-10.77494      .00000   -10.77494
   H6SI2O7(AQ)          5.99588E-06   1.04457E-03   5.99583E-06
-5.22215      .00000    -5.22215
   AL(OH)3(AQ)          8.29819E-07   6.47287E-05   8.29813E-07
-6.08102      .00000    -6.08102
   AL(OH)4-             1.60194E-04   1.52201E-02   1.60192E-04
-3.79536     -.24655    -4.04190
   AL(OH)SI(OH)-        4.29800E-05   7.44028E-03   4.29797E-05
-4.36674     -.24655    -4.61328
   CACL+                1.93993E-04   1.46529E-02   1.93991E-04
-3.71222     -.24655    -3.95876
   CACL2(AQ)            3.54214E-06   3.93128E-04   3.54211E-06
-5.45074      .00000    -5.45074
   CA(OH)+              2.85129E-04   1.62772E-02   2.85126E-04
-3.54496     -.24655    -3.79151
   CA(H3SIO4)+          3.48312E-04   4.70872E-02   3.48309E-04
-3.45803     -.24655    -3.70458
   FE(OH)+              8.42702E-08   6.13945E-06   8.42696E-08
-7.07433     -.24655    -7.32088
   FE(OH)2              5.86148E-07   5.26722E-05   5.86143E-07
-6.23200      .00000    -6.23200
   FE(OH)3-             5.97682E-06   6.38736E-04   5.97677E-06
-5.22353     -.24655    -5.47008
   FECL+                3.31890E-09   3.03016E-07   3.31888E-09
-8.47901     -.24655    -8.72555
   FECL2(AQ)            7.76865E-08   9.84700E-06   7.76859E-08
-7.10966      .00000    -7.10966
   FE(H3SIO4)+          1.53007E-04   2.30970E-02   1.53006E-04
-3.81529     -.24655    -4.06184
   MGCL+                7.35118E-07   4.39292E-05   7.35112E-07
```

```
-6.13365     -.24655    -6.38019
   MG(OH)+              1.62525E-05   6.71428E-04   1.62524E-05
-4.78908     -.24655    -5.03563
   MG(OH)2(AQ)          1.07522E+00   6.27062E+01   1.07521E+00      .
03149      .00000      .03149
   MG(H3SIO4)+          8.33457E-09   9.95246E-07   8.33451E-09
-8.07912     -.24655    -8.32567
   NACL(AQ)             4.21302E-02   2.46221E+00   4.21299E-02
-1.37541      .00000    -1.37541
   NAOH(AQ)             1.67761E-02   6.70997E-01   1.67760E-02
-1.77531      .00000    -1.77531
   H3SIO4-              6.51909E-04   6.20010E-02   6.51904E-04
-3.18582     -.24655    -3.43236
   HCL(AQ)              5.58469E-07   2.03623E-05   5.58465E-07
-6.25300      .00000    -6.25300

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0680251
           log (CA++  /h+**0)            8.1805985
           log (MG++  /h+**0)            6.0848607
           log (AL+++ /h+**0)           -4.3122158
           log (FE++  /h+**0)            3.6937009
           log (FE+++ /h+**0)           -4.3000534


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE                -3.9191659    1.20458E-04    2.78906E-02
5.36277E-03
   ANTIGORITE               -4.8040532    1.57017E-05    3.56111E-02
1.36798E-02

   CLINOPYROXENE(SS)        -2.6978109    2.00534E-03    4.38573E-01
1.32753E-01
   DIOPSIDE                 -2.7285287    1.86841E-03    4.04608E-01
1.23688E-01
   HEDENBERGITE             -3.8640886    1.36745E-04    3.39257E-02
9.05252E-03
   JADEITE                  -6.7131788    1.93563E-07    3.91265E-05
1.16796E-05

   CHLORITE(SS)             -2.4959837    3.19166E-03    3.60000E-01
1.35040E-01
   CLINOCHLORE              -2.5190946    3.02625E-03    3.36397E-01
```

```
1.27980E-01
   CHAMOSITE                -3.7814546    1.65404E-04    2.36033E-02
7.05943E-03


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 1.9999999    1.00000E+02    2.31539E+04
4.45200E+03
   TREMOLITE                 1.9999995    9.99999E+01    8.12369E+04
2.72680E+04
   ANTIGORITE               -4.8040532    1.57017E-05    3.56111E-02
1.36798E-02

   PLAGIOCLASE(SS)           1.9999954    9.99989E+01

   ALBITE                    1.7781467    5.99994E+01    1.57332E+04
6.04974E+03
   ANORTHITE                 1.6020554    3.99996E+01    1.11283E+04
4.02996E+03


   CLINOPYROXENE(SS)         2.0000032    1.00001E+02

   DIOPSIDE                  1.9030946    8.00008E+01    1.73244E+04
5.29606E+03
   HEDENBERGITE              1.3010274    1.99999E+01    4.96186E+03
1.32399E+03
   JADEITE                  -6.7131788    1.93563E-07    3.91265E-05
1.16796E-05


   CHLORITE(SS)             -2.4959837    3.19166E-03

   CLINOCHLORE              -2.5190946    3.02625E-03    3.36397E-01
1.27980E-01
   CHAMOSITE                -3.7814546    1.65404E-04    2.36033E-02
7.05943E-03



                           mass, grams        volume, cc

           created         8.620742E-01       2.868350E-01
           destroyed       6.933300E-01       2.284755E-01
           net             1.687442E-01       5.835950E-02
```

warning-- these volume totals may be incomplete because
of missing partial molar volume data in the data base

--- mineral saturation state summary ---

mineral	affinity, kcal	state	mineral	affinity, kcal	state
MAGNETITE	.0000	satd	HEMATITE	-3.3498	
PERICLASE	-4.8259		BRUCITE	-1.0896	
DIASPORE	-6.9276		FORSTERITE	-.3819	
FAYALITE	-1.7117		CHRYSOTILE	-.6274	
ENSTATITE-CL	-2.1668		ENSTATITE-OR	-2.2449	
ENSTATITE-PR	-2.6503		DIOPSIDE	-.1016	
HEDENBERGITE	-3.8592		FERROSILITE	-4.4625	
WOLLASTONITE	-3.6296		PSEUDOWOLLASTONITE	-4.1157	
TREMOLITE	-5.5013		ANTIGORITE	.0000	satd
TALC	-6.8684		CLINOCHLORE	-.0765	
CHAMOSITE	-4.2536		PYROPE	-7.6526	
ALMANDINE	-7.7348		GROSSULAR	-4.3776	
QUARTZ-ALPHA	-5.6469		QUARTZ-BETA	-5.8838	
COESITE	-6.2432		IRON-ALPHA	-8.6607	
IRON-GAMMA	-7.8040		HALITE	-9.7490	
CRISTOBALITE-ALPHA	-6.9328		CRISTOBALITE-BETA	-7.6462	

--- summary of solid solutions ---

mineral	aff. kcal/mol	mole frac.	lambda	state

```
 PLAGIOCLASE(SS)          -17.1866
     ALBITE                     -17.18657     .8206899     1.00000
     ANORTHITE                  -17.18657     .1793101     1.00000

 ORTHOPYROXENE(SS)         -1.9666
     ENSTATITE-OR                -1.96658     .8239149     1.00000
     FERROSILITE                 -1.96658     .1760851     1.00000

 GARNET(SS)                -4.1166
     PYROPE                      -4.11664     .0853915     1.00000
     ALMANDINE                   -4.11664     .0806425     1.00000
     GROSSULAR                   -4.11664     .8339660     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .9317132     1.00000
     HEDENBERGITE                  .00000     .0681903     1.00000
     JADEITE                       .00000     .0000965     1.00000

 CPX_SUBCALCIC(SS)          -.0001
     DIOPSIDE                     -.00014     .9318032     1.00000
     HEDENBERGITE                 -.00014     .0681968     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9481762     1.00000
     CHAMOSITE                     .00000     .0518238     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9317    1.0000     .9317    -.0307     .0000    -.0307
     HEDENBERGITE
              .0682    1.0000     .0682   -1.1663     .0000   -1.1663
     JADEITE
              .0001    1.0000     .0001   -4.0154     .0000   -4.0154

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9482    1.0000     .9482    -.0231     .0000    -.0231
     CHAMOSITE
```

```
              .0518    1.0000     .0518   -1.2855     .0000   -1.2855


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                         -26.79956       1.58648E-27
   H2(G)                           2.27761       1.89500E+02
   H2O(G)                          3.80603       6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.0000E-03, delzi=  3.6904E-04, nord= 4
               ncycle=  0
 steps completed =    43, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(CHAMOSITE         ) =     -3.5561
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  9.99999999999987E-04
                     log of reaction progress =      -3.0000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.99983E+01    1.67530E-03    2.68613E+04
4.50015E-01
   CLINOPYROXENE(SS)       9.99980E+01    2.01920E-03    2.22856E+04
4.50001E-01
   MAGNETITE               9.99998E+01    2.16000E-04    2.31538E+04
```

```
5.00123E-02
   TREMOLITE                9.99998E+01    1.83200E-04    8.12369E+04
1.48826E-01


                current total mass =  1.53538E+05 grams
                delta total mass   =  1.09885E+00 grams
                delta total volume =       .36211 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           17.3635    1.67530E+00
   CLINOPYROXENE(SS)           .1337    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.4936    1.83200E-01

          affinity of the overall irreversible reaction=    30.096
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O         8.435274E+05       5.774248E+01        5.774331E+01
      NA        1.208035E+04       5.754993E-01        5.755076E-01
      CA        3.348103E+01       9.148945E-04        9.149076E-04
      MG        2.381103E+04       1.072957E+00        1.072973E+00
      AL        5.054590E+00       2.051725E-04        2.051754E-04
      SI        6.935825E+01       2.704680E-03        2.704719E-03
      H         1.042800E+05       1.133140E+02        1.133156E+02
      CL        1.618515E+04       4.999929E-01        5.000000E-01
      FE        8.134232E+00       1.595206E-04        1.595228E-04

      co3--                        0.000000E+00        0.000000E+00
      so4--                        0.000000E+00        0.000000E+00
      s--                          0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale
```

```
                                      ph            eh            pe

     internal ph scale              6.6037        .4542
3.1659E+00
     modified nbs ph scale          6.3571        .4896
3.4124E+00
     rational ph scale              6.3571        .4896
3.4124E+00

   phcl =      7.1897



          oxygen fugacity =  1.58786E-27
          log oxygen fugacity = -26.79919




                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                    ionic strength =  5.177611E-01 molal
                 sum of molalities =    2.2007231883866
               osmotic coefficient =     .41081
                    equiv. stoich. ionic strength =  4.999929E-01
molal

                         mass of solution =   1.095232 kg
                         mass of solvent  =   1.000014 kg
                         mass of solutes  =    .095218 kg
                         conc of solutes  =   8.693844 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55095E+01   1.00001E+03
   NA+                  5.16503E-01   1.18743E+01   5.16496E-01     -.
28693     -.24658     -.53351
   CA++                 9.07452E-05   3.63707E-03   9.07439E-05
-4.04218     -.98631    -5.02849
   MG++                 7.29289E-07   1.77254E-05   7.29278E-07
-6.13711     -.98631    -7.12342
   AL+++                1.24792E-22   3.36708E-21   1.24790E-22
-21.90382    -2.21920   -24.12302
   H4SIO4(AQ)           1.49327E-03   1.43525E-01   1.49325E-03
```

```
-2.82587      .00000    -2.82587
   H+                   4.39444E-07   4.42916E-07   4.39438E-07
-6.35710     -.24658    -6.60368
   CL-                  4.57655E-01   1.62252E+01   4.57649E-01     -.
33947     -.24658     -.58605
   FE++                 2.96889E-09   1.65804E-07   2.96885E-09
-8.52741     -.98631    -9.51372
   O2(AQ)               1.33635E-31   4.27615E-30   1.33633E-31
-30.87409      .00000   -30.87409
   H2(AQ)               3.20277E-02   6.45615E-02   3.20273E-02
-1.49448      .00000    -1.49448
   FE+++                1.28275E-22   7.16375E-21   1.28273E-22
-21.89187    -2.21920   -24.11106
   OH-                  5.91548E-02   1.00606E+00   5.91539E-02
-1.22802     -.24658    -1.47459
   H8SI3O10(AQ)         1.69415E-11   4.27456E-09   1.69412E-11
-10.77106      .00000   -10.77106
   H6SI2O7(AQ)          6.03177E-06   1.05082E-03   6.03169E-06
-5.21956      .00000    -5.21956
   AL(OH)3(AQ)          8.30283E-07   6.47649E-05   8.30271E-07
-6.08078      .00000    -6.08078
   AL(OH)4-             1.61016E-04   1.52982E-02   1.61013E-04
-3.79314     -.24658    -4.03972
   AL(OH)SI(OH)-        4.33295E-05   7.50079E-03   4.33289E-05
-4.36322     -.24658    -4.60980
   CACL+                1.91490E-04   1.44638E-02   1.91487E-04
-3.71786     -.24658    -3.96444
   CACL2(AQ)            3.49581E-06   3.87986E-04   3.49576E-06
-5.45646      .00000    -5.45646
   CA(OH)+              2.82745E-04   1.61412E-02   2.82741E-04
-3.54861     -.24658    -3.79519
   CA(H3SIO4)+          3.46432E-04   4.68330E-02   3.46427E-04
-3.46039     -.24658    -3.70697
   FE(OH)+              8.38874E-08   6.11155E-06   8.38862E-08
-7.07631     -.24658    -7.32289
   FE(OH)2              5.86067E-07   5.26649E-05   5.86058E-07
-6.23206      .00000    -6.23206
   FE(OH)3-             6.00331E-06   6.41567E-04   6.00322E-06
-5.22162     -.24658    -5.46819
   FECL+                3.28869E-09   3.00257E-07   3.28864E-09
-8.48298     -.24658    -8.72956
   FECL2(AQ)            7.69656E-08   9.75562E-06   7.69645E-08
-7.11371      .00000    -7.11371
   FE(H3SIO4)+          1.52766E-04   2.30607E-02   1.52764E-04
-3.81598     -.24658    -4.06256
   MGCL+                7.26994E-07   4.34437E-05   7.26983E-07
-6.13848     -.24658    -6.38505
   MG(OH)+              1.61469E-05   6.67064E-04   1.61466E-05
-4.79192     -.24658    -5.03850
   MG(OH)2(AQ)          1.07296E+00   6.25743E+01   1.07294E+00      .
```

```
03058      .00000      .03058
   MG(H3SIO4)+          8.30512E-09   9.91730E-07   8.30500E-09
-8.08066     -.24658    -8.32724
   NACL(AQ)             4.21450E-02   2.46307E+00   4.21444E-02
-1.37526      .00000    -1.37526
   NAOH(AQ)             1.68593E-02   6.74322E-01   1.68590E-02
-1.77317      .00000    -1.77317
   H3SIO4-              6.56848E-04   6.24707E-02   6.56838E-04
-3.18254     -.24658    -3.42912
   HCL(AQ)              5.55914E-07   2.02691E-05   5.55906E-07
-6.25500      .00000    -6.25500

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0701694
           log (CA++  /h+**0)            8.1788676
           log (MG++  /h+**0)            6.0839437
           log (AL+++ /h+**0)           -4.3119760
           log (FE++  /h+**0)            3.6936380
           log (FE+++ /h+**0)           -4.3000221


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                  -3.7293773    1.86476E-04    4.31764E-02
8.30191E-03
   ANTIGORITE                 -4.7119953    1.94091E-05    4.40193E-02
1.69098E-02

   CLINOPYROXENE(SS)          -2.5029156    3.14112E-03    6.86981E-01
2.07940E-01
   DIOPSIDE                   -2.5336921    2.92623E-03    6.33681E-01
1.93716E-01
   HEDENBERGITE               -3.6683979    2.14586E-04    5.32377E-02
1.42056E-02
   JADEITE                    -6.5133103    3.06683E-07    6.19925E-05
1.85053E-05

   CHLORITE(SS)               -2.2714559    5.35234E-03    6.03729E-01
2.26459E-01
   CLINOCHLORE                -2.2946112    5.07445E-03    5.64073E-01
2.14598E-01
   CHAMOSITE                  -3.5561170    2.77896E-04    3.96562E-02
1.18606E-02
```

--- grand summary of solid phases (e.s.+p.r.s. +reactants) ---

phase/end-member	log moles	moles	grams	volume, cc
MAGNETITE	1.9999999	1.00000E+02	2.31539E+04	4.45200E+03
TREMOLITE	1.9999992	9.99998E+01	8.12369E+04	2.72680E+04
ANTIGORITE	-4.7119953	1.94091E-05	4.40193E-02	1.69098E-02
PLAGIOCLASE(SS)	1.9999927	9.99983E+01		
ALBITE	1.7781440	5.99990E+01	1.57331E+04	6.04970E+03
ANORTHITE	1.6020527	3.99993E+01	1.11282E+04	4.02993E+03
CLINOPYROXENE(SS)	2.0000049	1.00001E+02		
DIOPSIDE	1.9030971	8.00013E+01	1.73245E+04	5.29609E+03
HEDENBERGITE	1.3010259	1.99998E+01	4.96184E+03	1.32399E+03
JADEITE	-6.5133103	3.06683E-07	6.19925E-05	1.85053E-05
CHLORITE(SS)	-2.2714559	5.35234E-03		
CLINOCHLORE	-2.2946112	5.07445E-03	5.64073E-01	2.14598E-01
CHAMOSITE	-3.5561170	2.77896E-04	3.96562E-02	1.18606E-02

	mass, grams	volume, cc
created	1.377905E+00	4.596110E-01
destroyed	1.098854E+00	3.621092E-01
net	2.790513E-01	9.750177E-02

warning-- these volume totals may be incomplete because of missing partial molar volume data in the data base

```
          --- mineral saturation state summary ---

   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                  .0000  satd          HEMATITE
-3.3496
 PERICLASE                -4.8289                BRUCITE
-1.0926
 DIASPORE                 -6.9268                FORSTERITE
-.3828
 FAYALITE                 -1.7098                CHRYSOTILE
-.6280
 ENSTATITE-CL             -2.1656                ENSTATITE-OR
-2.2437
 ENSTATITE-PR             -2.6490                DIOPSIDE
-.1018
 HEDENBERGITE             -3.8566                FERROSILITE
-4.4584
 WOLLASTONITE             -3.6311                PSEUDOWOLLASTONITE
-4.1172
 TREMOLITE                -5.4936
ANTIGORITE                 .0000  satd
 TALC                     -6.8604                CLINOCHLORE
-.0766
 CHAMOSITE                -4.2510                PYROPE
-7.6508
 ALMANDINE                -7.7302                GROSSULAR
-4.3785
 QUARTZ-ALPHA             -5.6426                QUARTZ-BETA
-5.8795
 COESITE                  -6.2389                IRON-ALPHA
-8.6615
 IRON-GAMMA               -7.8048                HALITE
-9.7485
 CRISTOBALITE-ALPHA       -6.9285                CRISTOBALITE-BETA
-7.6419


                    --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -17.1687
     ALBITE                     -17.16874     .8223543     1.00000
     ANORTHITE                  -17.16874     .1776457     1.00000
```

```
 ORTHOPYROXENE(SS)        -1.9648
     ENSTATITE-OR               -1.96483     .8236294     1.00000
     FERROSILITE                -1.96483     .1763706     1.00000

 GARNET(SS)               -4.1169
     PYROPE                     -4.11688     .0855116     1.00000
     ALMANDINE                  -4.11688     .0809150     1.00000
     GROSSULAR                  -4.11688     .8335734     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9315871     1.00000
     HEDENBERGITE                 .00000     .0683153     1.00000
     JADEITE                      .00000     .0000976     1.00000

 CPX_SUBCALCIC(SS)         -.0001
     DIOPSIDE                    -.00014     .9316781     1.00000
     HEDENBERGITE                -.00014     .0683219     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9480795     1.00000
     CHAMOSITE                    .00000     .0519205     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .9316    1.0000     .9316    -.0308     .0000    -.0308
     HEDENBERGITE
             .0683    1.0000     .0683   -1.1655     .0000   -1.1655
     JADEITE
             .0001    1.0000     .0001   -4.0104     .0000   -4.0104

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
             .9481    1.0000     .9481    -.0232     .0000    -.0232
     CHAMOSITE
             .0519    1.0000     .0519   -1.2847     .0000   -1.2847


           --- summary of gas species ---
```

```
          gas                  log fugacity         fugacity
partial pressure

   O2(G)                         -26.79919      1.58786E-27
   H2(G)                           2.27742      1.89417E+02
   H2O(G)                          3.80603      6.39774E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.5849E-03, delzi=  5.8489E-04, nord= 4
               ncycle=  0
 steps completed =    44, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(CHAMOSITE         ) =     -3.3400
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  1.58489319246109E-03
                     log of reaction progress =      -2.8000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.99973E+01    2.65517E-03    2.68610E+04
7.13226E-01
   CLINOPYROXENE(SS)       9.99968E+01    3.20022E-03    2.22854E+04
7.13203E-01
   MAGNETITE               9.99997E+01    3.42337E-04    2.31538E+04
7.92642E-02
   TREMOLITE               9.99997E+01    2.90352E-04    8.12368E+04
2.35874E-01
```

```
                  current total mass =  1.53537E+05 grams
                  delta total mass   =  1.74157E+00 grams
                  delta total volume =       .57390 cc


           reactant           affinity     rel. rate

     PLAGIOCLASE(SS)           17.3410    1.67530E+00
     CLINOPYROXENE(SS)           .1331    0.00000E+00
     MAGNETITE                   .0000    0.00000E+00
     TREMOLITE                  5.4815    1.83200E-01

            affinity of the overall irreversible reaction=    30.056
 kcal
            contributions from irreversible reactions
            with no thermodynamic data are not included



        --- element totals for the aqueous phase ---

     element         mg/kg soln.         molal conc.          moles

        O          8.435747E+05       5.773591E+01       5.773733E+01
        NA         1.209462E+04       5.760811E-01       5.760953E-01
        CA         3.303124E+01       9.024502E-04       9.024725E-04
        MG         2.373533E+04       1.069364E+00       1.069391E+00
        AL         5.101337E+00       2.070348E-04       2.070399E-04
        SI         6.968585E+01       2.716993E-03       2.717060E-03
        H          1.042917E+05       1.133074E+02       1.133102E+02
        CL         1.618774E+04       4.999877E-01       5.000000E-01
        FE         8.118535E+00       1.591857E-04       1.591896E-04

        co3--                         0.000000E+00       0.000000E+00
        so4--                         0.000000E+00       0.000000E+00
        s--                           0.000000E+00       0.000000E+00

      warning-- co3--, so4--, and s-- totals require that routine comp1
      have the names of non-carbonate carbon, sulfide sulfur,
      and non-sulfate sulfur aqueous species


     single ion activities and activity coefficients are here defined
     with respect to the internal ph scale



                                             ph            eh            pe
```

```
     internal ph scale              6.6068        .4538
3.1629E+00
     modified nbs ph scale          6.3601        .4892
3.4096E+00
     rational ph scale              6.3601        .4892
3.4096E+00

   phcl =      7.1929



          oxygen fugacity =  1.59010E-27
          log oxygen fugacity = -26.79858



                              activity of water =    .98384
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                    ionic strength =  5.181716E-01 molal
                 sum of molalities =    2.1980960783759
               osmotic coefficient =     .41130
                    equiv. stoich. ionic strength =  4.999877E-01
molal

                         mass of solution =   1.095057 kg
                         mass of solvent  =   1.000025 kg
                         mass of solutes  =    .095033 kg
                         conc of solutes  =   8.678324 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55101E+01   1.00002E+03
   NA+                  5.16936E-01   1.18842E+01   5.16923E-01     -.
28657     -.24663     -.53320
   CA++                 8.89476E-05   3.56502E-03   8.89454E-05
-4.05088     -.98651    -5.03738
   MG++                 7.16974E-07   1.74260E-05   7.16956E-07
-6.14451     -.98651    -7.13102
   AL+++                1.22407E-22   3.30272E-21   1.22403E-22
-21.91221    -2.21964   -24.13185
   H4SIO4(AQ)           1.50038E-03   1.44208E-01   1.50034E-03
-2.82381      .00000    -2.82381
   H+                   4.36402E-07   4.39849E-07   4.36391E-07
-6.36012     -.24663    -6.60675
   CL-                  4.57636E-01   1.62246E+01   4.57624E-01     -.
```

```
33949     -.24663     -.58612
   FE++                    2.92787E-09   1.63513E-07   2.92780E-09
-8.53346     -.98651    -9.51997
   O2(AQ)                  1.33824E-31   4.28221E-30   1.33821E-31
-30.87348      .00000   -30.87348
   H2(AQ)                  3.20056E-02   6.45168E-02   3.20048E-02
-1.49479      .00000    -1.49479
   FE+++                   1.25727E-22   7.02148E-21   1.25724E-22
-21.90058    -2.21964   -24.12022
   OH-                     5.95820E-02   1.01333E+00   5.95806E-02
-1.22490     -.24663    -1.47152
   H8SI3O10(AQ)            1.71840E-11   4.33577E-09   1.71836E-11
-10.76489      .00000   -10.76489
   H6SI2O7(AQ)             6.08923E-06   1.06083E-03   6.08908E-06
-5.21545      .00000    -5.21545
   AL(OH)3(AQ)             8.31020E-07   6.48224E-05   8.31000E-07
-6.08040      .00000    -6.08040
   AL(OH)4-                1.62321E-04   1.54222E-02   1.62317E-04
-3.78964     -.24663    -4.03626
   AL(OH)SI(OH)-           4.38881E-05   7.59748E-03   4.38870E-05
-4.35766     -.24663    -4.60429
   CACL+                   1.87601E-04   1.41701E-02   1.87596E-04
-3.72678     -.24663    -3.97340
   CACL2(AQ)               3.42386E-06   3.80000E-04   3.42377E-06
-5.46550      .00000    -5.46550
   CA(OH)+                 2.79016E-04   1.59282E-02   2.79009E-04
-3.55438     -.24663    -3.80101
   CA(H3SIO4)+             3.43485E-04   4.64346E-02   3.43476E-04
-3.46410     -.24663    -3.71073
   FE(OH)+                 8.32871E-08   6.06782E-06   8.32850E-08
-7.07943     -.24663    -7.32606
   FE(OH)2                 5.85935E-07   5.26531E-05   5.85921E-07
-6.23216      .00000    -6.23216
   FE(OH)3-                6.04525E-06   6.46049E-04   6.04510E-06
-5.21860     -.24663    -5.46522
   FECL+                   3.24160E-09   2.95958E-07   3.24152E-09
-8.48925     -.24663    -8.73588
   FECL2(AQ)               7.58424E-08   9.61325E-06   7.58405E-08
-7.12010      .00000    -7.12010
   FE(H3SIO4)+             1.52393E-04   2.30043E-02   1.52389E-04
-3.81705     -.24663    -4.06367
   MGCL+                   7.14353E-07   4.26883E-05   7.14336E-07
-6.14610     -.24663    -6.39272
   MG(OH)+                 1.59814E-05   6.60228E-04   1.59810E-05
-4.79640     -.24663    -5.04302
   MG(OH)2(AQ)             1.06937E+00   6.23654E+01   1.06935E+00      .
02912      .00000      .02912
   MG(H3SIO4)+             8.25902E-09   9.86225E-07   8.25882E-09
-8.08308     -.24663    -8.32971
   NACL(AQ)                4.21684E-02   2.46444E+00   4.21674E-02
```

```
-1.37502      .00000    -1.37502
   NAOH(AQ)             1.69912E-02   6.79599E-01   1.69908E-02
-1.76979      .00000    -1.76979
   H3SIO4-              6.64732E-04   6.32205E-02   6.64716E-04
-3.17736     -.24663    -3.42399
   HCL(AQ)              5.51910E-07   2.01231E-05   5.51896E-07
-6.25814      .00000    -6.25814

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0735499
           log (CA++  /h+**0)            8.1761178
           log (MG++  /h+**0)            6.0824869
           log (AL+++ /h+**0)           -4.3115953
           log (FE++  /h+**0)            3.6935360
           log (FE+++ /h+**0)           -4.2999713


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                  -3.5366618    2.90628E-04    6.72917E-02
1.29388E-02
   ANTIGORITE                 -4.5968842    2.52997E-05    5.73791E-02
2.20419E-02

   CLINOPYROXENE(SS)          -2.3061844    4.94101E-03    1.08066E+00
3.27092E-01
   DIOPSIDE                   -2.3370544    4.60199E-03    9.96572E-01
3.04652E-01
   HEDENBERGITE               -3.4704053    3.38528E-04    8.39869E-02
2.24106E-02
   JADEITE                    -6.3087047    4.91242E-07    9.92990E-05
2.96415E-05

   CHLORITE(SS)               -2.0566652    8.77677E-03    9.90037E-01
3.71348E-01
   CLINOCHLORE                -2.0798909    8.31973E-03    9.24816E-01
3.51841E-01
   CHAMOSITE                  -3.3400418    4.57044E-04    6.52209E-02
1.95066E-02


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---
```

```
      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 1.9999998    9.99999E+01    2.31538E+04
4.45200E+03
   TREMOLITE                 1.9999987    9.99997E+01    8.12368E+04
2.72679E+04
   ANTIGORITE               -4.5968842    2.52997E-05    5.73791E-02
2.20419E-02

   PLAGIOCLASE(SS)           1.9999885    9.99973E+01

   ALBITE                    1.7781397    5.99984E+01    1.57330E+04
6.04964E+03
   ANORTHITE                 1.6020485    3.99989E+01    1.11281E+04
4.02989E+03


   CLINOPYROXENE(SS)         2.0000076    1.00002E+02

   DIOPSIDE                  1.9031011    8.00020E+01    1.73246E+04
5.29614E+03
   HEDENBERGITE              1.3010234    1.99997E+01    4.96181E+03
1.32398E+03
   JADEITE                  -6.3087047    4.91242E-07    9.92990E-05
2.96415E-05


   CHLORITE(SS)             -2.0566652    8.77677E-03

   CLINOCHLORE              -2.0798909    8.31973E-03    9.24816E-01
3.51841E-01
   CHAMOSITE                -3.3400418    4.57044E-04    6.52209E-02
1.95066E-02


                           mass, grams        volume, cc

              created        2.195366E+00       7.334205E-01
              destroyed      1.741566E+00       5.739044E-01
              net            4.537994E-01       1.595161E-01

             warning-- these volume totals may be incomplete because
             of missing partial molar volume data in the data base


              --- mineral saturation state summary ---
```

```
   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE               .0000  satd          HEMATITE
-3.3493
 PERICLASE             -4.8338                BRUCITE
-1.0975
 DIASPORE              -6.9256                FORSTERITE
-.3842
 FAYALITE              -1.7067                CHRYSOTILE
-.6288
 ENSTATITE-CL          -2.1636                ENSTATITE-OR
-2.2417
 ENSTATITE-PR          -2.6470                DIOPSIDE
-.1021
 HEDENBERGITE          -3.8524                FERROSILITE
-4.4520
 WOLLASTONITE          -3.6334                PSEUDOWOLLASTONITE
-4.1195
 TREMOLITE             -5.4815
ANTIGORITE               .0000  satd
 TALC                  -6.8476                CLINOCHLORE
-.0769
 CHAMOSITE             -4.2467                PYROPE
-7.6480
 ALMANDINE             -7.7229                GROSSULAR
-4.3799
 QUARTZ-ALPHA          -5.6358                QUARTZ-BETA
-5.8727
 COESITE               -6.2321                IRON-ALPHA
-8.6628
 IRON-GAMMA            -7.8061                HALITE
-9.7478
 CRISTOBALITE-ALPHA    -6.9217                CRISTOBALITE-BETA
-7.6351


                     --- summary of solid solutions  ---

 mineral              aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)        -17.1404
     ALBITE                   -17.14043     .8249649     1.00000
     ANORTHITE                -17.14043     .1750351     1.00000

 ORTHOPYROXENE(SS)       -1.9621
     ENSTATITE-OR              -1.96206     .8231758     1.00000
     FERROSILITE               -1.96206     .1768242     1.00000
```

```
 GARNET(SS)                -4.1173
     PYROPE                       -4.11727     .0857025     1.00000
     ALMANDINE                    -4.11727     .0813493     1.00000
     GROSSULAR                    -4.11727     .8329482     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                       .00000     .9313866     1.00000
     HEDENBERGITE                   .00000     .0685140     1.00000
     JADEITE                        .00000     .0000994     1.00000

 CPX_SUBCALCIC(SS)          -.0001
     DIOPSIDE                      -.00014     .9314792     1.00000
     HEDENBERGITE                  -.00014     .0685208     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                    .00000     .9479257     1.00000
     CHAMOSITE                      .00000     .0520743     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9314    1.0000     .9314    -.0309     .0000    -.0309
     HEDENBERGITE
              .0685    1.0000     .0685   -1.1642     .0000   -1.1642
     JADEITE
              .0001    1.0000     .0001   -4.0025     .0000   -4.0025

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9479    1.0000     .9479    -.0232     .0000    -.0232
     CHAMOSITE
              .0521    1.0000     .0521   -1.2834     .0000   -1.2834


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure
```

```
  O2(G)                            -26.79858      1.59010E-27
  H2(G)                              2.27711      1.89284E+02
  H2O(G)                             3.80603      6.39774E+03


 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


 stepping to zi=  2.5119E-03, delzi=  9.2699E-04, nord= 5
              ncycle=  0
 steps completed =    45, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(CHAMOSITE        ) =     -3.1289
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                     reaction progress        =  2.51188643150955E-03
                     log of reaction progress =      -2.6000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.99958E+01    4.20816E-03    2.68606E+04
1.13039E+00
   CLINOPYROXENE(SS)       9.99949E+01    5.07200E-03    2.22849E+04
1.13035E+00
   MAGNETITE               9.99995E+01    5.42567E-04    2.31537E+04
1.25625E-01
   TREMOLITE               9.99995E+01    4.60178E-04    8.12367E+04
3.73835E-01


                 current total mass =  1.53536E+05 grams
                 delta total mass   =  2.76020E+00 grams
                 delta total volume =       .90958 cc
```

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	17.3053	1.67530E+00
CLINOPYROXENE(SS)	.1322	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.4622	1.83200E-01

affinity of the overall irreversible reaction= 29.992 kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.436497E+05	5.772550E+01	5.772787E+01
NA	1.211723E+04	5.770031E-01	5.770268E-01
CA	3.233566E+01	8.832084E-04	8.832447E-04
MG	2.361537E+04	1.063674E+00	1.063717E+00
AL	5.175889E+00	2.100039E-04	2.100126E-04
SI	7.021481E+01	2.736880E-03	2.736993E-03
H	1.043101E+05	1.132969E+02	1.133016E+02
CL	1.619183E+04	4.999795E-01	5.000000E-01
FE	8.094634E+00	1.586743E-04	1.586808E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.6116	.4532	3.1584E+00
modified nbs ph scale	6.3649	.4886	3.4051E+00

```
     rational ph scale              6.3649        .4886
3.4051E+00

   phcl =      7.1978



          oxygen fugacity =  1.59377E-27
          log oxygen fugacity = -26.79757



                        activity of water =    .98385
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                           (not def. for t.gt.50 c)

                    ionic strength =  5.188225E-01 molal
                 sum of molalities =    2.1939356318226
               osmotic coefficient =     .41207
                    equiv. stoich. ionic strength =  4.999795E-01
molal

                         mass of solution =   1.094781 kg
                         mass of solvent  =   1.000041 kg
                         mass of solutes  =    .094739 kg
                         conc of solutes  =   8.653739 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55110E+01   1.00004E+03
   NA+                  5.17621E-01   1.19000E+01   5.17599E-01     -.
28601     -.24671     -.53271
   CA++                 8.61853E-05   3.45431E-03   8.61817E-05
-4.06458     -.98682    -5.05141
   MG++                 6.98006E-07   1.69650E-05   6.97978E-07
-6.15616     -.98682    -7.14298
   AL+++                1.18755E-22   3.20419E-21   1.18750E-22
-21.92537    -2.22035   -24.14571
   H4SIO4(AQ)           1.51175E-03   1.45301E-01   1.51168E-03
-2.82054      .00000    -2.82054
   H+                   4.31667E-07   4.35077E-07   4.31649E-07
-6.36487     -.24671    -6.61157
   CL-                  4.57605E-01   1.62235E+01   4.57586E-01     -.
33953     -.24671     -.58623
   FE++                 2.86457E-09   1.59977E-07   2.86445E-09
-8.54296     -.98682    -9.52978
   O2(AQ)               1.34136E-31   4.29218E-30   1.34130E-31
```

```
-30.87247      .00000   -30.87247
   H2(AQ)               3.19692E-02   6.44435E-02   3.19679E-02
-1.49529      .00000    -1.49529
   FE+++                1.21830E-22   6.80384E-21   1.21825E-22
-21.91426    -2.22035   -24.13461
   OH-                  6.02594E-02   1.02485E+00   6.02569E-02
-1.21999     -.24671    -1.46670
   H8SI3O10(AQ)         1.75771E-11   4.43495E-09   1.75764E-11
-10.75507      .00000   -10.75507
   H6SI2O7(AQ)          6.18177E-06   1.07695E-03   6.18152E-06
-5.20890      .00000    -5.20890
   AL(OH)3(AQ)          8.32193E-07   6.49139E-05   8.32159E-07
-6.07979      .00000    -6.07979
   AL(OH)4-             1.64395E-04   1.56193E-02   1.64389E-04
-3.78413     -.24671    -4.03083
   AL(OH)SI(OH)-        4.47851E-05   7.75276E-03   4.47833E-05
-4.34888     -.24671    -4.59559
   CACL+                1.81628E-04   1.37189E-02   1.81621E-04
-3.74083     -.24671    -3.98754
   CACL2(AQ)            3.31337E-06   3.67738E-04   3.31324E-06
-5.47975      .00000    -5.47975
   CA(OH)+              2.73222E-04   1.55975E-02   2.73211E-04
-3.56350     -.24671    -3.81021
   CA(H3SIO4)+          3.38896E-04   4.58142E-02   3.38882E-04
-3.46995     -.24671    -3.71666
   FE(OH)+              8.23517E-08   5.99967E-06   8.23483E-08
-7.08435     -.24671    -7.33105
   FE(OH)2              5.85720E-07   5.26337E-05   5.85696E-07
-6.23233      .00000    -6.23233
   FE(OH)3-             6.11162E-06   6.53143E-04   6.11137E-06
-5.21386     -.24671    -5.46057
   FECL+                3.16895E-09   2.89325E-07   3.16882E-09
-8.49910     -.24671    -8.74581
   FECL2(AQ)            7.41096E-08   9.39361E-06   7.41065E-08
-7.13014      .00000    -7.13014
   FE(H3SIO4)+          1.51821E-04   2.29180E-02   1.51815E-04
-3.81869     -.24671    -4.06539
   MGCL+                6.94894E-07   4.15255E-05   6.94866E-07
-6.15810     -.24671    -6.40480
   MG(OH)+              1.57238E-05   6.49588E-04   1.57232E-05
-4.80346     -.24671    -5.05016
   MG(OH)2(AQ)          1.06370E+00   6.20346E+01   1.06366E+00      .
02680      .00000      .02680
   MG(H3SIO4)+          8.18738E-09   9.77670E-07   8.18704E-09
-8.08687     -.24671    -8.33358
   NACL(AQ)             4.22055E-02   2.46661E+00   4.22038E-02
-1.37465      .00000    -1.37465
   NAOH(AQ)             1.72007E-02   6.87976E-01   1.71999E-02
-1.76447      .00000    -1.76447
   H3SIO4-              6.77373E-04   6.44228E-02   6.77345E-04
```

```
-3.16919     -.24671    -3.41590
   HCL(AQ)              5.45678E-07   1.98959E-05   5.45656E-07
-6.26308      .00000    -6.26308

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.0788631
           log (CA++  /h+**0)            8.1717431
           log (MG++  /h+**0)            6.0801694
           log (AL+++ /h+**0)           -4.3109901
           log (FE++  /h+**0)            3.6933689
           log (FE+++ /h+**0)           -4.2998879


           --- summary of solid product phases---


  product                       log moles        moles        grams
volume, cc

   MAGNETITE                  -3.3424781    4.54487E-04    1.05231E-01
2.02338E-02
   ANTIGORITE                 -4.4600267    3.46716E-05    7.86342E-02
3.02069E-02

   CLINOPYROXENE(SS)          -2.1082856    7.79317E-03    1.70454E+00
5.15903E-01
   DIOPSIDE                   -2.1393046    7.25597E-03    1.57130E+00
4.80345E-01
   HEDENBERGITE               -3.2705051    5.36408E-04    1.33080E-01
3.55102E-02
   JADEITE                    -6.0983442    7.97362E-07    1.61178E-04
4.81129E-05

   CHLORITE(SS)               -1.8475879    1.42040E-02    1.60235E+00
6.00979E-01
   CLINOCHLORE                -1.8709258    1.34609E-02    1.49631E+00
5.69262E-01
   CHAMOSITE                  -3.1289264    7.43145E-04    1.06048E-01
3.17174E-02


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                   1.9999996    9.99999E+01    2.31538E+04
```

```
4.45200E+03
   TREMOLITE                 1.9999980    9.99995E+01    8.12367E+04
2.72679E+04
   ANTIGORITE               -4.4600267    3.46716E-05    7.86342E-02
3.02069E-02

   PLAGIOCLASE(SS)           1.9999817    9.99958E+01

   ALBITE                    1.7781330    5.99975E+01    1.57327E+04
6.04955E+03
   ANORTHITE                 1.6020417    3.99983E+01    1.11279E+04
4.02983E+03


   CLINOPYROXENE(SS)         2.0000118    1.00003E+02

   DIOPSIDE                  1.9031073    8.00032E+01    1.73249E+04
5.29621E+03
   HEDENBERGITE              1.3010196    1.99995E+01    4.96177E+03
1.32397E+03
   JADEITE                  -6.0983442    7.97362E-07    1.61178E-04
4.81129E-05


   CHLORITE(SS)             -1.8475879    1.42040E-02

   CLINOCHLORE              -1.8709258    1.34609E-02    1.49631E+00
5.69262E-01
   CHAMOSITE                -3.1289264    7.43145E-04    1.06048E-01
3.17174E-02



                           mass, grams        volume, cc

           created         3.490758E+00       1.167323E+00
           destroyed       2.760197E+00       9.095773E-01
           net             7.305610E-01       2.577459E-01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state
```

```
 MAGNETITE                  .0000  satd          HEMATITE
-3.3487
 PERICLASE                -4.8414                BRUCITE
-1.1051
 DIASPORE                 -6.9236                FORSTERITE
-.3865
 FAYALITE                 -1.7018                CHRYSOTILE
-.6302
 ENSTATITE-CL             -2.1604                ENSTATITE-OR
-2.2385
 ENSTATITE-PR             -2.6439                DIOPSIDE
-.1026
 HEDENBERGITE             -3.8458                FERROSILITE
-4.4417
 WOLLASTONITE             -3.6370                PSEUDOWOLLASTONITE
-4.1231
 TREMOLITE                -5.4622
ANTIGORITE                 .0000  satd
 TALC                     -6.8273                CLINOCHLORE
-.0772
 CHAMOSITE                -4.2400                PYROPE
-7.6435
 ALMANDINE                -7.7113                GROSSULAR
-4.3823
 QUARTZ-ALPHA             -5.6250                QUARTZ-BETA
-5.8619
 COESITE                  -6.2213                IRON-ALPHA
-8.6650
 IRON-GAMMA               -7.8083                HALITE
-9.7465
 CRISTOBALITE-ALPHA       -6.9109                CRISTOBALITE-BETA
-7.6243


                     --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -17.0954
     ALBITE                      -17.09544     .8290345     1.00000
     ANORTHITE                   -17.09544     .1709655     1.00000

 ORTHOPYROXENE(SS)          -1.9576
     ENSTATITE-OR                 -1.95764     .8224539     1.00000
     FERROSILITE                  -1.95764     .1775461     1.00000

 GARNET(SS)                 -4.1179
     PYROPE                       -4.11787     .0860066     1.00000
     ALMANDINE                    -4.11787     .0820436     1.00000
     GROSSULAR                    -4.11787     .8319498     1.00000
```

```
 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9310672     1.00000
     HEDENBERGITE                 .00000     .0688304     1.00000
     JADEITE                      .00000     .0001023     1.00000

 CPX_SUBCALCIC(SS)         -.0001
     DIOPSIDE                    -.00015     .9311625     1.00000
     HEDENBERGITE                -.00015     .0688375     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9476807     1.00000
     CHAMOSITE                    .00000     .0523193     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9311    1.0000     .9311    -.0310     .0000    -.0310
     HEDENBERGITE
              .0688    1.0000     .0688   -1.1622     .0000   -1.1622
     JADEITE
              .0001    1.0000     .0001   -3.9901     .0000   -3.9901

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9477    1.0000     .9477    -.0233     .0000    -.0233
     CHAMOSITE
              .0523    1.0000     .0523   -1.2813     .0000   -1.2813


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                         -26.79757       1.59377E-27
   H2(G)                           2.27661       1.89066E+02
   H2O(G)                          3.80603       6.39774E+03
```

```
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  3.9811E-03, delzi=  1.4692E-03, nord= 6
               ncycle=  0
 steps completed =    46, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =     -5.8800
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                     reaction progress        =  3.98107170553492E-03
                     log of reaction progress =      -2.4000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.99933E+01    6.66949E-03    2.68600E+04
1.79154E+00
   CLINOPYROXENE(SS)       9.99920E+01    8.03858E-03    2.22843E+04
1.79148E+00
   MAGNETITE               9.99991E+01    8.59911E-04    2.31537E+04
1.99103E-01
   TREMOLITE               9.99993E+01    7.29332E-04    8.12364E+04
5.92488E-01


                current total mass =  1.53534E+05 grams
                delta total mass   =  4.37462E+00 grams
                delta total volume =      1.44158 cc


         reactant           affinity     rel. rate
```

```
   PLAGIOCLASE(SS)           17.2487    1.67530E+00
   CLINOPYROXENE(SS)           .1307    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.4314    1.83200E-01

          affinity of the overall irreversible reaction=    29.892
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O          8.437683E+05        5.770902E+01        5.771288E+01
      NA         1.215310E+04        5.784643E-01        5.785031E-01
      CA         3.127485E+01        8.538699E-04        8.539271E-04
      MG         2.342531E+04        1.054663E+00        1.054734E+00
      AL         5.295220E+00        2.147541E-04        2.147684E-04
      SI         7.107778E+01        2.769337E-03        2.769523E-03
      H          1.043392E+05        1.132803E+02        1.132879E+02
      CL         1.619831E+04        4.999665E-01        5.000000E-01
      FE         8.059142E+00        1.579113E-04        1.579218E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                               ph           eh            pe

     internal ph scale               6.6191        .4521
3.1512E+00
     modified nbs ph scale           6.3723        .4876
3.3981E+00
     rational ph scale               6.3723        .4876
3.3981E+00

   phcl =      7.2055
```

```
          oxygen fugacity =  1.59993E-27
          log oxygen fugacity = -26.79590



                              activity of water =    .98385
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  5.198550E-01 molal
                 sum of molalities =    2.1873499784086
               osmotic coefficient =     .41330
                    equiv. stoich. ionic strength =  4.999665E-01
molal

                         mass of solution =   1.094342 kg
                         mass of solvent  =   1.000067 kg
                         mass of solutes  =    .094275 kg
                         conc of solutes  =   8.614806 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55124E+01   1.00007E+03
   NA+                  5.18705E-01   1.19249E+01   5.18671E-01     -.
28511     -.24683     -.53194
   CA++                 8.20147E-05   3.28715E-03   8.20092E-05
-4.08614     -.98732    -5.07346
   MG++                 6.69265E-07   1.62665E-05   6.69220E-07
-6.17443     -.98732    -7.16175
   AL+++                1.13275E-22   3.05633E-21   1.13267E-22
-21.94590    -2.22147   -24.16736
   H4SIO4(AQ)           1.53005E-03   1.47060E-01   1.52995E-03
-2.81532      .00000    -2.81532
   H+                   4.24372E-07   4.27724E-07   4.24343E-07
-6.37228     -.24683    -6.61911
   CL-                  4.57556E-01   1.62217E+01   4.57525E-01     -.
33959     -.24683     -.58641
   FE++                 2.76830E-09   1.54601E-07   2.76811E-09
-8.55782     -.98732    -9.54513
   O2(AQ)               1.34657E-31   4.30887E-30   1.34648E-31
-30.87080      .00000   -30.87080
   H2(AQ)               3.19085E-02   6.43211E-02   3.19063E-02
-1.49612      .00000    -1.49612
   FE+++                1.15988E-22   6.47756E-21   1.15980E-22
```

```
-21.93562    -2.22147   -24.15709
   OH-                  6.13336E-02   1.04312E+00   6.13294E-02
-1.21233     -.24683    -1.45916
   H8SI3O10(AQ)         1.82224E-11   4.59777E-09   1.82212E-11
-10.73942      .00000   -10.73942
   H6SI2O7(AQ)          6.33223E-06   1.10316E-03   6.33180E-06
-5.19847      .00000    -5.19847
   AL(OH)3(AQ)          8.34065E-07   6.50599E-05   8.34009E-07
-6.07883      .00000    -6.07883
   AL(OH)4-             1.67698E-04   1.59331E-02   1.67686E-04
-3.77550     -.24683    -4.02233
   AL(OH)SI(OH)-        4.62367E-05   8.00405E-03   4.62336E-05
-4.33504     -.24683    -4.58187
   CACL+                1.72618E-04   1.30384E-02   1.72607E-04
-3.76294     -.24683    -4.00977
   CACL2(AQ)            3.14678E-06   3.49249E-04   3.14657E-06
-5.50216      .00000    -5.50216
   CA(OH)+              2.64325E-04   1.50896E-02   2.64308E-04
-3.57789     -.24683    -3.82472
   CA(H3SIO4)+          3.31822E-04   4.48580E-02   3.31800E-04
-3.47912     -.24683    -3.72595
   FE(OH)+              8.09080E-08   5.89450E-06   8.09026E-08
-7.09204     -.24683    -7.33887
   FE(OH)2              5.85359E-07   5.26013E-05   5.85320E-07
-6.23261      .00000    -6.23261
   FE(OH)3-             6.21657E-06   6.64358E-04   6.21616E-06
-5.20648     -.24683    -5.45331
   FECL+                3.05854E-09   2.79245E-07   3.05834E-09
-8.51451     -.24683    -8.76134
   FECL2(AQ)            7.14771E-08   9.05993E-06   7.14723E-08
-7.14586      .00000    -7.14586
   FE(H3SIO4)+          1.50962E-04   2.27882E-02   1.50952E-04
-3.82116     -.24683    -4.06799
   MGCL+                6.65430E-07   3.97647E-05   6.65385E-07
-6.17693     -.24683    -6.42376
   MG(OH)+              1.53272E-05   6.33201E-04   1.53262E-05
-4.81457     -.24683    -5.06140
   MG(OH)2(AQ)          1.05472E+00   6.15107E+01   1.05465E+00      .
02311      .00000      .02311
   MG(H3SIO4)+          8.07726E-09   9.64521E-07   8.07672E-09
-8.09276     -.24683    -8.33959
   NACL(AQ)             4.22641E-02   2.47003E+00   4.22613E-02
-1.37406      .00000    -1.37406
   NAOH(AQ)             1.75335E-02   7.01287E-01   1.75323E-02
-1.75616      .00000    -1.75616
   H3SIO4-              6.97777E-04   6.63634E-02   6.97731E-04
-3.15631     -.24683    -3.40314
   HCL(AQ)              5.36078E-07   1.95459E-05   5.36042E-07
-6.27080      .00000    -6.27080
```

--- activity ratios of cations ---

```
log (NA+   /h+**0)            6.0871743
log (CA++  /h+**0)            8.1647680
log (MG++  /h+**0)            6.0764746
log (AL+++ /h+**0)           -4.3100263
log (FE++  /h+**0)            3.6930897
log (FE+++ /h+**0)           -4.2997487
```

--- summary of solid product phases---

```
  product                    log moles       moles        grams
volume, cc

   MAGNETITE                -3.1480616    7.11113E-04    1.64650E-01
3.16587E-02
   ANTIGORITE               -4.3044433    4.96086E-05    1.12511E-01
4.32205E-02

   CLINOPYROXENE(SS)        -1.9096562    1.23124E-02    2.69319E+00
8.15075E-01
   DIOPSIDE                 -1.9409132    1.14574E-02    2.48113E+00
7.58481E-01
   HEDENBERGITE             -3.0686981    8.53693E-04    2.11797E-01
5.65145E-02
   JADEITE                  -5.8800079    1.31823E-06    2.66466E-04
7.95422E-05

   CHLORITE(SS)             -1.6419605    2.28055E-02    2.57296E+00
9.64913E-01
   CLINOCHLORE              -1.6654778    2.16034E-02    2.40142E+00
9.13608E-01
   CHAMOSITE                -2.9200627    1.20209E-03    1.71540E-01
5.13052E-02
```

```
                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles       moles        grams
volume, cc

   MAGNETITE                 1.9999994    9.99999E+01    2.31538E+04
4.45199E+03
   TREMOLITE                 1.9999968    9.99993E+01    8.12364E+04
2.72678E+04
   ANTIGORITE               -4.3044433    4.96086E-05    1.12511E-01
```

```
4.32205E-02

   PLAGIOCLASE(SS)            1.9999710    9.99933E+01

   ALBITE                     1.7781223    5.99960E+01    1.57323E+04
6.04940E+03
   ANORTHITE                  1.6020310    3.99973E+01    1.11276E+04
4.02973E+03


   CLINOPYROXENE(SS)          2.0000186    1.00004E+02

   DIOPSIDE                   1.9031173    8.00050E+01    1.73253E+04
5.29633E+03
   HEDENBERGITE               1.3010136    1.99992E+01    4.96170E+03
1.32395E+03
   JADEITE                   -5.8800079    1.31823E-06    2.66466E-04
7.95422E-05


   CHLORITE(SS)              -1.6419605    2.28055E-02

   CLINOCHLORE               -1.6654778    2.16034E-02    2.40142E+00
9.13608E-01
   CHAMOSITE                 -2.9200627    1.20209E-03    1.71540E-01
5.13052E-02



                           mass, grams        volume, cc

           created         5.543317E+00       1.854868E+00
           destroyed       4.374617E+00       1.441583E+00
           net             1.168701E+00       4.132849E-01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3478
 PERICLASE              -4.8537                BRUCITE
-1.1174
```

```
 DIASPORE                -6.9204                FORSTERITE
-.3901
 FAYALITE                -1.6941                CHRYSOTILE
-.6323
 ENSTATITE-CL            -2.1554                ENSTATITE-OR
-2.2335
 ENSTATITE-PR            -2.6389                DIOPSIDE
-.1034
 HEDENBERGITE            -3.8353                FERROSILITE
-4.4253
 WOLLASTONITE            -3.6428                PSEUDOWOLLASTONITE
-4.1289
 TREMOLITE               -5.4314
ANTIGORITE                .0000  satd
 TALC                    -6.7950                CLINOCHLORE
-.0778
 CHAMOSITE               -4.2293                PYROPE
-7.6364
 ALMANDINE               -7.6929                GROSSULAR
-4.3860
 QUARTZ-ALPHA            -5.6077                QUARTZ-BETA
-5.8446
 COESITE                 -6.2040                IRON-ALPHA
-8.6687
 IRON-GAMMA              -7.8120                HALITE
-9.7446
 CRISTOBALITE-ALPHA      -6.8936                CRISTOBALITE-BETA
-7.6070


                    --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -17.0238
     ALBITE                     -17.02382     .8353168     1.00000
     ANORTHITE                  -17.02382     .1646832     1.00000

 ORTHOPYROXENE(SS)         -1.9506
     ENSTATITE-OR                -1.95059     .8213026     1.00000
     FERROSILITE                 -1.95059     .1786974     1.00000

 GARNET(SS)                -4.1188
     PYROPE                      -4.11882     .0864925     1.00000
     ALMANDINE                   -4.11882     .0831592     1.00000
     GROSSULAR                   -4.11882     .8303483     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .9305570     1.00000
```

```
    HEDENBERGITE                  .00000    .0693359    1.00000
    JADEITE                       .00000    .0001071    1.00000

 CPX_SUBCALCIC(SS)        -.0002
    DIOPSIDE                     -.00015    .9306567    1.00000
    HEDENBERGITE                 -.00015    .0693433    1.00000

 CHLORITE(SS)              .0000
saturated
    CLINOCHLORE                   .00000    .9472894    1.00000
    CHAMOSITE                     .00000    .0527106    1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
            .9306    1.0000     .9306    -.0313     .0000    -.0313
    HEDENBERGITE
            .0693    1.0000     .0693   -1.1590     .0000   -1.1590
    JADEITE
            .0001    1.0000     .0001   -3.9704     .0000   -3.9704

   CHLORITE(SS)
 ideal solution

    CLINOCHLORE
            .9473    1.0000     .9473    -.0235     .0000    -.0235
    CHAMOSITE
            .0527    1.0000     .0527   -1.2781     .0000   -1.2781


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.79590       1.59993E-27
   H2(G)                          2.27578       1.88702E+02
   H2O(G)                         3.80603       6.39775E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
 stepping to zi=  6.3096E-03, delzi=  2.3285E-03, nord= 6
              ncycle=  0
 steps completed =    47, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =     -5.6498
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  6.30957344480185E-03
                    log of reaction progress =      -2.2000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.99894E+01    1.05704E-02    2.68589E+04
2.83940E+00
   CLINOPYROXENE(SS)       9.99873E+01    1.27403E-02    2.22832E+04
2.83931E+00
   MAGNETITE               9.99986E+01    1.36287E-03    2.31535E+04
3.15557E-01
   TREMOLITE               9.99988E+01    1.15591E-03    8.12361E+04
9.39030E-01


               current total mass =  1.53532E+05 grams
               delta total mass   =  6.93330E+00 grams
               delta total volume =      2.28475 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           17.1589    1.67530E+00
   CLINOPYROXENE(SS)           .1283    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.3821    1.83200E-01
```

```
          affinity of the overall irreversible reaction=    29.732
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.        molal conc.          moles

      O          8.439562E+05       5.768297E+01       5.768917E+01
      NA         1.220998E+04       5.807803E-01       5.808427E-01
      CA         2.969137E+01       8.100913E-04       8.101784E-04
      MG         2.312423E+04       1.040407E+00       1.040518E+00
      AL         5.487347E+00       2.223961E-04       2.224200E-04
      SI         7.250785E+01       2.823152E-03       2.823456E-03
      H          1.043854E+05       1.132540E+02       1.132662E+02
      CL         1.620858E+04       4.999463E-01       5.000000E-01
      FE         8.008654E+00       1.568163E-04       1.568331E-04

      co3--                         0.000000E+00       0.000000E+00
      so4--                         0.000000E+00       0.000000E+00
      s--                           0.000000E+00       0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                                ph           eh            pe

     internal ph scale                        6.6308        .4506
3.1403E+00
     modified nbs ph scale                    6.3838        .4860
3.3873E+00
     rational ph scale                        6.3838        .4860
3.3873E+00

   phcl =      7.2175



          oxygen fugacity =  1.61055E-27
```

```
          log oxygen fugacity = -26.79303



                            activity of water =    .98385
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  5.214935E-01 molal
                 sum of molalities =    2.1769333168195
               osmotic coefficient =     .41526
                    equiv. stoich. ionic strength =  4.999463E-01
molal

                         mass of solution =   1.093649 kg
                         mass of solvent  =   1.000107 kg
                         mass of solutes  =    .093542 kg
                         conc of solutes  =   8.553181 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55146E+01   1.00011E+03
   NA+                  5.20423E-01   1.19644E+01   5.20367E-01     -.
28369     -.24703     -.53072
   CA++                 7.58872E-05   3.04156E-03   7.58790E-05
-4.11988     -.98811    -5.10798
   MG++                 6.26794E-07   1.52342E-05   6.26726E-07
-6.20292     -.98811    -7.19103
   AL+++                1.05296E-22   2.84105E-21   1.05285E-22
-21.97764    -2.22324   -24.20087
   H4SIO4(AQ)           1.55980E-03   1.49920E-01   1.55963E-03
-2.80698      .00000    -2.80698
   H+                   4.13311E-07   4.16577E-07   4.13267E-07
-6.38377     -.24703    -6.63080
   CL-                  4.57477E-01   1.62189E+01   4.57428E-01     -.
33968     -.24703     -.58670
   FE++                 2.62526E-09   1.46613E-07   2.62497E-09
-8.58087     -.98811    -9.56898
   O2(AQ)               1.35556E-31   4.33765E-30   1.35542E-31
-30.86793      .00000   -30.86793
   H2(AQ)               3.18044E-02   6.41113E-02   3.18010E-02
-1.49756      .00000    -1.49756
   FE+++                1.07495E-22   6.00328E-21   1.07484E-22
-21.96866    -2.22324   -24.19190
   OH-                  6.30371E-02   1.07209E+00   6.30304E-02
-1.20045     -.24703    -1.44748
   H8SI3O10(AQ)         1.93045E-11   4.87079E-09   1.93024E-11
```

```
-10.71439      .00000   -10.71439
   H6SI2O7(AQ)          6.58058E-06   1.14643E-03   6.57987E-06
-5.18178      .00000    -5.18178
   AL(OH)3(AQ)          8.37062E-07   6.52937E-05   8.36972E-07
-6.07729      .00000    -6.07729
   AL(OH)4-             1.72968E-04   1.64338E-02   1.72949E-04
-3.76208     -.24703    -4.00911
   AL(OH)SI(OH)-        4.86150E-05   8.41576E-03   4.86098E-05
-4.31328     -.24703    -4.56030
   CACL+                1.59398E-04   1.20398E-02   1.59381E-04
-3.79756     -.24703    -4.04459
   CACL2(AQ)            2.90254E-06   3.22141E-04   2.90223E-06
-5.53727      .00000    -5.53727
   CA(OH)+              2.50905E-04   1.43235E-02   2.50878E-04
-3.60054     -.24703    -3.84756
   CA(H3SIO4)+          3.21085E-04   4.34065E-02   3.21051E-04
-3.49343     -.24703    -3.74045
   FE(OH)+              7.87124E-08   5.73454E-06   7.87040E-08
-7.10400     -.24703    -7.35103
   FE(OH)2              5.84738E-07   5.25455E-05   5.84675E-07
-6.23309      .00000    -6.23309
   FE(OH)3-             6.38221E-06   6.82059E-04   6.38152E-06
-5.19508     -.24703    -5.44210
   FECL+                2.89463E-09   2.64280E-07   2.89432E-09
-8.53845     -.24703    -8.78548
   FECL2(AQ)            6.75709E-08   8.56481E-06   6.75636E-08
-7.17029      .00000    -7.17029
   FE(H3SIO4)+          1.49714E-04   2.26000E-02   1.49698E-04
-3.82478     -.24703    -4.07181
   MGCL+                6.21941E-07   3.71659E-05   6.21874E-07
-6.20630     -.24703    -6.45332
   MG(OH)+              1.47259E-05   6.08361E-04   1.47243E-05
-4.83196     -.24703    -5.07899
   MG(OH)2(AQ)          1.04050E+00   6.06817E+01   1.04039E+00      .
01720      .00000      .01720
   MG(H3SIO4)+          7.91096E-09   9.44662E-07   7.91011E-09
-8.10182     -.24703    -8.34884
   NACL(AQ)             4.23566E-02   2.47544E+00   4.23521E-02
-1.37313      .00000    -1.37313
   NAOH(AQ)             1.80630E-02   7.22468E-01   1.80611E-02
-1.74326      .00000    -1.74326
   H3SIO4-              7.31072E-04   6.95299E-02   7.30993E-04
-3.13609     -.24703    -3.38311
   HCL(AQ)              5.21522E-07   1.90152E-05   5.21466E-07
-6.28277      .00000    -6.28277

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.1000792
```

```
           log (CA++  /h+**0)            8.1536072
           log (MG++  /h+**0)            6.0705634
           log (AL+++ /h+**0)           -4.3084869
           log (FE++  /h+**0)            3.6926105
           log (FE+++ /h+**0)           -4.2995097


           --- summary of solid product phases---


  product                        log moles        moles        grams
volume, cc

   MAGNETITE                    -2.9546794    1.10999E-03    2.57006E-01
4.94169E-02
   ANTIGORITE                   -4.1338947    7.34692E-05    1.66626E-01
6.40086E-02

   CLINOPYROXENE(SS)            -1.7105816    1.94724E-02    4.25984E+00
1.28906E+00
   DIOPSIDE                     -1.7422209    1.81042E-02    3.92051E+00
1.19850E+00
   HEDENBERGITE                 -2.8645739    1.36592E-03    3.38878E-01
9.04241E-02
   JADEITE                      -5.6497996    2.23975E-06    4.52741E-04
1.35147E-04

   CHLORITE(SS)                 -1.4384532    3.64374E-02    4.11166E+00
1.54169E+00
   CLINOCHLORE                  -1.4622585    3.44938E-02    3.83431E+00
1.45874E+00
   CHAMOSITE                    -2.7114115    1.94352E-03    2.77343E-01
8.29493E-02


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                     1.9999989    9.99997E+01    2.31538E+04
4.45199E+03
   TREMOLITE                     1.9999950    9.99988E+01    8.12361E+04
2.72677E+04
   ANTIGORITE                   -4.1338947    7.34692E-05    1.66626E-01
6.40086E-02

   PLAGIOCLASE(SS)               1.9999541    9.99894E+01
```

```
   ALBITE                      1.7781053    5.99937E+01    1.57317E+04
6.04916E+03
   ANORTHITE                   1.6020141    3.99958E+01    1.11272E+04
4.02957E+03


   CLINOPYROXENE(SS)           2.0000292    1.00007E+02

   DIOPSIDE                    1.9031329    8.00079E+01    1.73259E+04
5.29652E+03
   HEDENBERGITE                1.3010043    1.99988E+01    4.96159E+03
1.32392E+03
   JADEITE                    -5.6497996    2.23975E-06    4.52741E-04
1.35147E-04


   CHLORITE(SS)               -1.4384532    3.64374E-02

   CLINOCHLORE                -1.4622585    3.44938E-02    3.83431E+00
1.45874E+00
   CHAMOSITE                  -2.7114115    1.94352E-03    2.77343E-01
8.29493E-02



                           mass, grams        volume, cc

           created         8.795125E+00       2.944176E+00
           destroyed       6.933300E+00       2.284755E+00
           net             1.861825E+00       6.594208E-01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3462
 PERICLASE              -4.8732                BRUCITE
-1.1369
 DIASPORE               -6.9153                FORSTERITE
-.3958
 FAYALITE               -1.6819                CHRYSOTILE
-.6358
```

```
 ENSTATITE-CL           -2.1474                ENSTATITE-OR
-2.2255
 ENSTATITE-PR           -2.6308                DIOPSIDE
-.1047
 HEDENBERGITE           -3.8186                FERROSILITE
-4.3993
 WOLLASTONITE           -3.6522                PSEUDOWOLLASTONITE
-4.1382
 TREMOLITE              -5.3821
ANTIGORITE               .0000  satd
 TALC                   -6.7432                CLINOCHLORE
-.0788
 CHAMOSITE              -4.2122                PYROPE
-7.6250
 ALMANDINE              -7.6634                GROSSULAR
-4.3920
 QUARTZ-ALPHA           -5.5801                QUARTZ-BETA
-5.8170
 COESITE                -6.1764                IRON-ALPHA
-8.6751
 IRON-GAMMA             -7.8184                HALITE
-9.7415
 CRISTOBALITE-ALPHA     -6.8660                CRISTOBALITE-BETA
-7.5794


                --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -16.9095
     ALBITE                    -16.90952     .8448634     1.00000
     ANORTHITE                 -16.90952     .1551366     1.00000

 ORTHOPYROXENE(SS)        -1.9393
     ENSTATITE-OR               -1.93931     .8194595     1.00000
     FERROSILITE                -1.93931     .1805405     1.00000

 GARNET(SS)               -4.1203
     PYROPE                     -4.12030     .0872726     1.00000
     ALMANDINE                  -4.12030     .0849664     1.00000
     GROSSULAR                  -4.12030     .8277610     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9297382     1.00000
     HEDENBERGITE                 .00000     .0701468     1.00000
     JADEITE                      .00000     .0001150     1.00000

 CPX_SUBCALCIC(SS)         -.0002
```

```
     DIOPSIDE                         -.00017     .9298452     1.00000
     HEDENBERGITE                     -.00017     .0701548     1.00000

 CHLORITE(SS)              .0000
saturated
     CLINOCHLORE                       .00000     .9466614     1.00000
     CHAMOSITE                         .00000     .0533386     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .9297    1.0000     .9297    -.0316     .0000    -.0316
     HEDENBERGITE
             .0701    1.0000     .0701   -1.1540     .0000   -1.1540
     JADEITE
             .0001    1.0000     .0001   -3.9392     .0000   -3.9392

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
             .9467    1.0000     .9467    -.0238     .0000    -.0238
     CHAMOSITE
             .0533    1.0000     .0533   -1.2730     .0000   -1.2730


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.79303       1.61055E-27
   H2(G)                          2.27434       1.88079E+02
   H2O(G)                         3.80603       6.39775E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.0000E-02, delzi=  3.6904E-03, nord= 6
              ncycle=  0
```

```
 steps completed =    48, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -5.4013
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  9.99999999999987E-03
                    log of reaction progress =      -2.0000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



        reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.99832E+01    1.67530E-02    2.68573E+04
4.50015E+00
   CLINOPYROXENE(SS)      9.99798E+01    2.01920E-02    2.22816E+04
4.50001E+00
   MAGNETITE              9.99978E+01    2.16000E-03    2.31534E+04
5.00123E-01
   TREMOLITE              9.99982E+01    1.83200E-03    8.12356E+04
1.48826E+00


                current total mass =  1.53528E+05 grams
                delta total mass   =  1.09885E+01 grams
                delta total volume =      3.62109 cc


        reactant           affinity     rel. rate

   PLAGIOCLASE(SS)          17.0164    1.67530E+00
   CLINOPYROXENE(SS)          .1247    0.00000E+00
   MAGNETITE                  .0000    0.00000E+00
   TREMOLITE                 5.3029    1.83200E-01

          affinity of the overall irreversible reaction=    29.479
kcal
          contributions from irreversible reactions
```

with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.442531E+05	5.764183E+01	5.765167E+01
NA	1.230024E+04	5.844508E-01	5.845505E-01
CA	2.740323E+01	7.468663E-04	7.469938E-04
MG	2.264751E+04	1.017873E+00	1.018047E+00
AL	5.799619E+00	2.348019E-04	2.348419E-04
SI	7.493358E+01	2.914494E-03	2.914991E-03
H	1.044583E+05	1.132124E+02	1.132318E+02
CL	1.622483E+04	4.999147E-01	5.000000E-01
FE	7.942242E+00	1.553503E-04	1.553768E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.6487	.4482	3.1237E+00
modified nbs ph scale	6.4013	.4837	3.3710E+00
rational ph scale	6.4013	.4837	3.3710E+00

phcl = 7.2358

oxygen fugacity = 1.62967E-27
log oxygen fugacity = -26.78790

```
                         activity of water =    .98385
              log activity of water =   -.00707
              alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                   ionic strength =  5.240949E-01 molal
                sum of molalities =    2.1604776605373
              osmotic coefficient =     .41840
                   equiv. stoich. ionic strength =  4.999147E-01
molal

                        mass of solution =   1.092554 kg
                        mass of solvent  =   1.000171 kg
                        mass of solutes  =    .092383 kg
                        conc of solutes  =   8.455727 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55182E+01   1.00017E+03
   NA+                  5.23141E-01   1.20269E+01   5.23052E-01     -.
28146     -.24734     -.52879
   CA++                 6.72520E-05   2.69546E-03   6.72406E-05
-4.17237     -.98935    -5.16172
   MG++                 5.66384E-07   1.37660E-05   5.66287E-07
-6.24696     -.98935    -7.23631
   AL+++                9.41990E-23   2.54163E-21   9.41829E-23
-22.02603    -2.22604   -24.25207
   H4SIO4(AQ)           1.60887E-03   1.54637E-01   1.60860E-03
-2.79355      .00000    -2.79355
   H+                   3.96943E-07   4.00079E-07   3.96875E-07
-6.40135     -.24734    -6.64868
   CL-                  4.57350E-01   1.62144E+01   4.57272E-01     -.
33983     -.24734     -.58716
   FE++                 2.41999E-09   1.35149E-07   2.41958E-09
-8.61626     -.98935    -9.60561
   O2(AQ)               1.37175E-31   4.38943E-30   1.37151E-31
-30.86280      .00000   -30.86280
   H2(AQ)               3.16193E-02   6.37381E-02   3.16139E-02
-1.50012      .00000    -1.50012
   FE+++                9.57150E-23   5.34539E-21   9.56986E-23
-22.01909    -2.22604   -24.24513
   OH-                  6.57391E-02   1.11804E+00   6.57278E-02
-1.18225     -.24734    -1.42959
   H8SI3O10(AQ)         2.11818E-11   5.34446E-09   2.11782E-11
-10.67411      .00000   -10.67411
   H6SI2O7(AQ)          7.00072E-06   1.21962E-03   6.99952E-06
-5.15493      .00000    -5.15493
   AL(OH)3(AQ)          8.41892E-07   6.56705E-05   8.41748E-07
```

```
-6.07482      .00000    -6.07482
   AL(OH)4-             1.81411E-04   1.72360E-02   1.81380E-04
-3.74141     -.24734    -3.98875
   AL(OH)SI(OH)-        5.25889E-05   9.10368E-03   5.25799E-05
-4.27918     -.24734    -4.52652
   CACL+                1.40808E-04   1.06357E-02   1.40784E-04
-3.85145     -.24734    -4.09878
   CACL2(AQ)            2.55949E-06   2.84067E-04   2.55905E-06
-5.59192      .00000    -5.59192
   CA(OH)+              2.31207E-04   1.31990E-02   2.31167E-04
-3.63607     -.24734    -3.88341
   CA(H3SIO4)+          3.05167E-04   4.12545E-02   3.05115E-04
-3.51554     -.24734    -3.76287
   FE(OH)+              7.54466E-08   5.49661E-06   7.54337E-08
-7.12243     -.24734    -7.36977
   FE(OH)2              5.83626E-07   5.24456E-05   5.83527E-07
-6.23394      .00000    -6.23394
   FE(OH)3-             6.64269E-06   7.09897E-04   6.64155E-06
-5.17773     -.24734    -5.42507
   FECL+                2.65976E-09   2.42836E-07   2.65931E-09
-8.57523     -.24734    -8.82257
   FECL2(AQ)            6.19782E-08   7.85592E-06   6.19676E-08
-7.20784      .00000    -7.20784
   FE(H3SIO4)+          1.48008E-04   2.23424E-02   1.47983E-04
-3.82979     -.24734    -4.07713
   MGCL+                5.60200E-07   3.34764E-05   5.60104E-07
-6.25173     -.24734    -6.49907
   MG(OH)+              1.38364E-05   5.71614E-04   1.38340E-05
-4.85905     -.24734    -5.10639
   MG(OH)2(AQ)          1.01803E+00   5.93712E+01   1.01786E+00      .
00769      .00000      .00769
   MG(H3SIO4)+          7.66647E-09   9.15467E-07   7.66516E-09
-8.11548     -.24734    -8.36282
   NACL(AQ)             4.25024E-02   2.48396E+00   4.24952E-02
-1.37166      .00000    -1.37166
   NAOH(AQ)             1.89073E-02   7.56237E-01   1.89041E-02
-1.72344      .00000    -1.72344
   H3SIO4-              7.86344E-04   7.47866E-02   7.86210E-04
-3.10446     -.24734    -3.35180
   HCL(AQ)              4.99981E-07   1.82298E-05   4.99896E-07
-6.30112      .00000    -6.30112

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.1198905
           log (CA++  /h+**0)            8.1356477
           log (MG++  /h+**0)            6.0610534
           log (AL+++ /h+**0)           -4.3060170
           log (FE++  /h+**0)            3.6917556
```

```
          log (FE+++ /h+**0)           -4.2990832


          --- summary of solid product phases---


  product                       log moles        moles        grams
volume, cc

   MAGNETITE                   -2.7639687    1.72199E-03    3.98708E-01
7.66631E-02
   ANTIGORITE                  -3.9520583    1.11671E-04    2.53268E-01
9.72914E-02

   CLINOPYROXENE(SS)           -1.5112495    3.08142E-02    6.74228E+00
2.03988E+00
   DIOPSIDE                    -1.5435076    2.86083E-02    6.19520E+00
1.89387E+00
   HEDENBERGITE                -2.6572054    2.20188E-03    5.46275E-01
1.45765E-01
   JADEITE                     -5.4013353    3.96885E-06    8.02258E-04
2.39480E-04

   CHLORITE(SS)                -1.2362653    5.80410E-02    6.55131E+00
2.45578E+00
   CLINOCHLORE                 -1.2605367    5.48862E-02    6.10112E+00
2.32114E+00
   CHAMOSITE                   -2.5010345    3.15475E-03    4.50188E-01
1.34645E-01


               --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member        log moles        moles        grams
volume, cc

   MAGNETITE                    1.9999981    9.99996E+01    2.31538E+04
4.45198E+03
   TREMOLITE                    1.9999920    9.99982E+01    8.12356E+04
2.72675E+04
   ANTIGORITE                  -3.9520583    1.11671E-04    2.53268E-01
9.72914E-02

   PLAGIOCLASE(SS)              1.9999272    9.99832E+01

   ALBITE                       1.7780785    5.99899E+01    1.57307E+04
6.04879E+03
   ANORTHITE                    1.6019872    3.99933E+01    1.11265E+04
4.02932E+03
```

```
   CLINOPYROXENE(SS)         2.0000461    1.00011E+02

   DIOPSIDE                  1.9031576    8.00125E+01    1.73269E+04
5.29682E+03
   HEDENBERGITE              1.3009901    1.99982E+01    4.96143E+03
1.32388E+03
   JADEITE                  -5.4013353    3.96885E-06    8.02258E-04
2.39480E-04


   CHLORITE(SS)             -1.2362653    5.80410E-02

   CLINOCHLORE              -1.2605367    5.48862E-02    6.10112E+00
2.32114E+00
   CHAMOSITE                -2.5010345    3.15475E-03    4.50188E-01
1.34645E-01



                           mass, grams        volume, cc

           created         1.394556E+01       4.669613E+00
           destroyed       1.098854E+01       3.621092E+00
           net             2.957020E+00       1.048521E+00

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3434
 PERICLASE              -4.9047                BRUCITE
-1.1684
 DIASPORE               -6.9071                FORSTERITE
-.4051
 FAYALITE               -1.6625                CHRYSOTILE
-.6413
 ENSTATITE-CL           -2.1344                ENSTATITE-OR
-2.2125
 ENSTATITE-PR           -2.6178                DIOPSIDE
-.1067
```

```
 HEDENBERGITE           -3.7920                FERROSILITE
-4.3577
 WOLLASTONITE           -3.6672                PSEUDOWOLLASTONITE
-4.1533
 TREMOLITE              -5.3029
ANTIGORITE               .0000  satd
 TALC                   -6.6599                CLINOCHLORE
-.0803
 CHAMOSITE              -4.1851                PYROPE
-7.6066
 ALMANDINE              -7.6164                GROSSULAR
-4.4016
 QUARTZ-ALPHA           -5.5357                QUARTZ-BETA
-5.7726
 COESITE                -6.1320                IRON-ALPHA
-8.6864
 IRON-GAMMA             -7.8297                HALITE
-9.7366
 CRISTOBALITE-ALPHA     -6.8216                CRISTOBALITE-BETA
-7.5350


                  --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -16.7264
     ALBITE                    -16.72638     .8590064     1.00000
     ANORTHITE                 -16.72638     .1409936     1.00000

 ORTHOPYROXENE(SS)        -1.9211
     ENSTATITE-OR               -1.92114     .8164923     1.00000
     FERROSILITE                -1.92114     .1835077     1.00000

 GARNET(SS)               -4.1226
     PYROPE                     -4.12256     .0885345     1.00000
     ALMANDINE                  -4.12256     .0879317     1.00000
     GROSSULAR                  -4.12256     .8235338     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9284143     1.00000
     HEDENBERGITE                 .00000     .0714569     1.00000
     JADEITE                      .00000     .0001288     1.00000

 CPX_SUBCALCIC(SS)         -.0002
     DIOPSIDE                    -.00019     .9285339     1.00000
     HEDENBERGITE                -.00019     .0714661     1.00000

 CHLORITE(SS)               .0000
```

```
saturated
     CLINOCHLORE                  .00000     .9456461     1.00000
     CHAMOSITE                    .00000     .0543539     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9284    1.0000     .9284    -.0323     .0000    -.0323
     HEDENBERGITE
              .0715    1.0000     .0715   -1.1460     .0000   -1.1460
     JADEITE
              .0001    1.0000     .0001   -3.8901     .0000   -3.8901

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9456    1.0000     .9456    -.0243     .0000    -.0243
     CHAMOSITE
              .0544    1.0000     .0544   -1.2648     .0000   -1.2648


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.78790       1.62967E-27
   H2(G)                          2.27178       1.86972E+02
   H2O(G)                         3.80603       6.39776E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.5849E-02, delzi=  5.8489E-03, nord= 6
               ncycle=  0
 steps completed =    49, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -5.1244
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
                    reaction progress        =  1.58489319246109E-02
                    log of reaction progress =      -1.8000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.99734E+01    2.65517E-02    2.68546E+04
7.13226E+00
   CLINOPYROXENE(SS)       9.99680E+01    3.20022E-02    2.22789E+04
7.13203E+00
   MAGNETITE               9.99966E+01    3.42337E-03    2.31531E+04
7.92642E-01
   TREMOLITE               9.99971E+01    2.90352E-03    8.12347E+04
2.35874E+00


               current total mass =  1.53521E+05 grams
               delta total mass   =  1.74157E+01 grams
               delta total volume =      5.73904 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           16.7896    1.67530E+00
   CLINOPYROXENE(SS)           .1189    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  5.1744    1.83200E-01

          affinity of the overall irreversible reaction=    29.076
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included
```

```
     --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.         moles

      O         8.447217E+05        5.757705E+01        5.759250E+01
      NA        1.244355E+04        5.902679E-01        5.904262E-01
      CA        2.425178E+01        6.598655E-04        6.600425E-04
      MG        2.189334E+04        9.823267E-01        9.825902E-01
      AL        6.315102E+00        2.552426E-04        2.553110E-04
      SI        7.919149E+01        3.074934E-03        3.075759E-03
      H         1.045732E+05        1.131469E+02        1.131772E+02
      CL        1.625051E+04        4.998659E-01        5.000000E-01
      FE        7.868133E+00        1.536425E-04        1.536837E-04

      co3--                         0.000000E+00        0.000000E+00
      so4--                         0.000000E+00        0.000000E+00
      s--                           0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                         ph            eh            pe

     internal ph scale                 6.6756        .4447
3.0992E+00
     modified nbs ph scale             6.4277        .4802
3.3470E+00
     rational ph scale                 6.4277        .4802
3.3470E+00

   phcl =      7.2635



          oxygen fugacity =  1.66627E-27
          log oxygen fugacity = -26.77825



                            activity of water =    .98385
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)
```

```
                    ionic strength =  5.282266E-01 molal
                 sum of molalities =    2.1345369209454
               osmotic coefficient =     .42344
                    equiv. stoich. ionic strength =  4.998659E-01
molal

                         mass of solution =   1.090827 kg
                         mass of solvent  =   1.000268 kg
                         mass of solutes  =    .090559 kg
                         conc of solutes  =   8.301861 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55236E+01   1.00027E+03
   NA+                  5.27438E-01   1.21257E+01   5.27296E-01     -.
27795     -.24783     -.52577
   CA++                 5.58192E-05   2.23724E-03   5.58043E-05
-4.25333     -.99132    -5.24465
   MG++                 4.85195E-07   1.17927E-05   4.85065E-07
-6.31420     -.99132    -7.30552
   AL+++                7.97732E-23   2.15240E-21   7.97519E-23
-22.09826    -2.23046   -24.32872
   H4SIO4(AQ)           1.69184E-03   1.62611E-01   1.69139E-03
-2.77176      .00000    -2.77176
   H+                   3.73577E-07   3.76528E-07   3.73477E-07
-6.42774     -.24783    -6.67557
   CL-                  4.57147E-01   1.62072E+01   4.57024E-01     -.
34006     -.24783     -.58789
   FE++                 2.14017E-09   1.19522E-07   2.13960E-09
-8.66967     -.99132    -9.66098
   O2(AQ)               1.40269E-31   4.48845E-30   1.40232E-31
-30.85315      .00000   -30.85315
   H2(AQ)               3.12732E-02   6.30404E-02   3.12648E-02
-1.50494      .00000    -1.50494
   FE+++                8.04638E-23   4.49366E-21   8.04422E-23
-22.09452    -2.23046   -24.32498
   OH-                  7.00228E-02   1.19090E+00   7.00040E-02
-1.15488     -.24783    -1.40271
   H8SI3O10(AQ)         2.46258E-11   6.21343E-09   2.46192E-11
-10.60873      .00000   -10.60873
   H6SI2O7(AQ)          7.74061E-06   1.34852E-03   7.73854E-06
-5.11134      .00000    -5.11134
   AL(OH)3(AQ)          8.49756E-07   6.62839E-05   8.49528E-07
-6.07082      .00000    -6.07082
   AL(OH)4-             1.95018E-04   1.85288E-02   1.94966E-04
-3.71004     -.24783    -3.95787
   AL(OH)SI(OH)-        5.94430E-05   1.02902E-02   5.94270E-05
```

```
-4.22602     -.24783    -4.47384
   CACL+                1.16280E-04   8.78301E-03   1.16249E-04
-3.93461     -.24783    -4.18244
   CACL2(AQ)            2.10772E-06   2.33928E-04   2.10716E-06
-5.67630      .00000    -5.67630
   CA(OH)+              2.03464E-04   1.16152E-02   2.03410E-04
-3.69163     -.24783    -3.93946
   CA(H3SIO4)+          2.82371E-04   3.81728E-02   2.82295E-04
-3.54930     -.24783    -3.79713
   FE(OH)+              7.07431E-08   5.15394E-06   7.07241E-08
-7.15043     -.24783    -7.39826
   FE(OH)2              5.81527E-07   5.22570E-05   5.81372E-07
-6.23555      .00000    -6.23555
   FE(OH)3-             7.04941E-06   7.53363E-04   7.04752E-06
-5.15196     -.24783    -5.39979
   FECL+                2.34033E-09   2.13672E-07   2.33971E-09
-8.63084     -.24783    -8.87867
   FECL2(AQ)            5.43821E-08   6.89309E-06   5.43675E-08
-7.26466      .00000    -7.26466
   FE(H3SIO4)+          1.45923E-04   2.20277E-02   1.45884E-04
-3.83599     -.24783    -4.08382
   MGCL+                4.77472E-07   2.85328E-05   4.77344E-07
-6.32117     -.24783    -6.56900
   MG(OH)+              1.25672E-05   5.19178E-04   1.25638E-05
-4.90088     -.24783    -5.14871
   MG(OH)2(AQ)          9.82577E-01   5.73035E+01   9.82313E-01     -.
00775      .00000     -.00775
   MG(H3SIO4)+          7.32157E-09   8.74282E-07   7.31961E-09
-8.13551     -.24783    -8.38334
   NACL(AQ)             4.27315E-02   2.49735E+00   4.27201E-02
-1.36937      .00000    -1.36937
   NAOH(AQ)             2.02569E-02   8.10217E-01   2.02515E-02
-1.69354      .00000    -1.69354
   H3SIO4-              8.80690E-04   8.37596E-02   8.80454E-04
-3.05529     -.24783    -3.30312
   HCL(AQ)              4.69232E-07   1.71086E-05   4.69106E-07
-6.32873      .00000    -6.32873

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.1497913
           log (CA++  /h+**0)            8.1064826
           log (MG++  /h+**0)            6.0456147
           log (AL+++ /h+**0)           -4.3020236
           log (FE++  /h+**0)            3.6901473
           log (FE+++ /h+**0)           -4.2982804


           --- summary of solid product phases---
```

product	log moles	moles	grams	volume, cc
MAGNETITE	-2.5785172	2.63926E-03	6.11091E-01	1.17500E-01
ANTIGORITE	-3.7622259	1.72892E-04	3.92114E-01	1.50628E-01
CLINOPYROXENE(SS)	-1.3117817	4.87774E-02	1.06760E+01	3.22902E+00
DIOPSIDE	-1.3450539	4.51800E-02	9.78383E+00	2.99092E+00
HEDENBERGITE	-2.4449214	3.58987E-03	8.90626E-01	2.37649E-01
JADEITE	-5.1243836	7.50959E-06	1.51798E-03	4.53129E-04
CHLORITE(SS)	-1.0349091	9.22765E-02	1.04204E+01	3.90439E+00
CLINOCHLORE	-1.0599436	8.71077E-02	9.68284E+00	3.68378E+00
CHAMOSITE	-2.2866111	5.16879E-03	7.37594E-01	2.20604E-01

--- grand summary of solid phases (e.s.+p.r.s. +reactants) ---

phase/end-member	log moles	moles	grams	volume, cc
MAGNETITE	1.9999966	9.99992E+01	2.31537E+04	4.45197E+03
TREMOLITE	1.9999874	9.99971E+01	8.12347E+04	2.72672E+04
ANTIGORITE	-3.7622259	1.72892E-04	3.92114E-01	1.50628E-01
PLAGIOCLASE(SS)	1.9998847	9.99734E+01		
ALBITE	1.7780359	5.99841E+01	1.57292E+04	6.04819E+03
ANORTHITE	1.6019447	3.99894E+01	1.11254E+04	4.02893E+03
CLINOPYROXENE(SS)	2.0000728	1.00017E+02		

```
   DIOPSIDE                    1.9031963    8.00196E+01    1.73284E+04
5.29730E+03
   HEDENBERGITE                1.3009690    1.99972E+01    4.96119E+03
1.32381E+03
   JADEITE                    -5.1243836    7.50959E-06    1.51798E-03
4.53129E-04


   CHLORITE(SS)               -1.0349091    9.22765E-02

   CLINOCHLORE                -1.0599436    8.71077E-02    9.68284E+00
3.68378E+00
   CHAMOSITE                  -2.2866111    5.16879E-03    7.37594E-01
2.20604E-01



                           mass, grams        volume, cc

           created         2.209961E+01       7.401533E+00
           destroyed       1.741566E+01       5.739044E+00
           net             4.683950E+00       1.662489E+00

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state         mineral
affinity, kcal    state

 MAGNETITE                .0000  satd           HEMATITE
-3.3381
 PERICLASE              -4.9558                 BRUCITE
-1.2195
 DIASPORE               -6.8939                 FORSTERITE
-.4201
 FAYALITE               -1.6318                 CHRYSOTILE
-.6504
 ENSTATITE-CL           -2.1134                 ENSTATITE-OR
-2.1915
 ENSTATITE-PR           -2.5968                 DIOPSIDE
-.1101
 HEDENBERGITE           -3.7496                 FERROSILITE
-4.2909
 WOLLASTONITE           -3.6915                 PSEUDOWOLLASTONITE
-4.1776
```

```
 TREMOLITE              -5.1744
ANTIGORITE               .0000  satd
 TALC                   -6.5247                CLINOCHLORE
-.0828
 CHAMOSITE              -4.1419                PYROPE
-7.5768
 ALMANDINE              -7.5408                GROSSULAR
-4.4173
 QUARTZ-ALPHA           -5.4636                QUARTZ-BETA
-5.7005
 COESITE                -6.0598                IRON-ALPHA
-8.7077
 IRON-GAMMA             -7.8510                HALITE
-9.7290
 CRISTOBALITE-ALPHA     -6.7494                CRISTOBALITE-BETA
-7.4629


                    --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -16.4311
     ALBITE                    -16.43111     .8791124     1.00000
     ANORTHITE                 -16.43111     .1208876     1.00000

 ORTHOPYROXENE(SS)        -1.8916
     ENSTATITE-OR               -1.89160     .8116726     1.00000
     FERROSILITE                -1.89160     .1883274     1.00000

 GARNET(SS)               -4.1259
     PYROPE                     -4.12592     .0906001     1.00000
     ALMANDINE                  -4.12592     .0928978     1.00000
     GROSSULAR                  -4.12592     .8165021     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9262490     1.00000
     HEDENBERGITE                 .00000     .0735970     1.00000
     JADEITE                      .00000     .0001540     1.00000

 CPX_SUBCALCIC(SS)         -.0002
     DIOPSIDE                    -.00022     .9263916     1.00000
     HEDENBERGITE                -.00022     .0736084     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9439858     1.00000
     CHAMOSITE                    .00000     .0560142     1.00000
```

```
 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9262    1.0000     .9262    -.0333     .0000    -.0333
     HEDENBERGITE
              .0736    1.0000     .0736   -1.1331     .0000   -1.1331
     JADEITE
              .0002    1.0000     .0002   -3.8126     .0000   -3.8126

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9440    1.0000     .9440    -.0250     .0000    -.0250
     CHAMOSITE
              .0560    1.0000     .0560   -1.2517     .0000   -1.2517


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.77825       1.66627E-27
   H2(G)                          2.26696       1.84908E+02
   H2O(G)                         3.80603       6.39777E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


 * note - a search for where a phase supersaturates
        indicates that the event being searched for
        does not take place in the interval being
        examined (search)
               the phase is CPX_SUBCALCIC(SS)
               delzi will not be decreased

 stepping to zi=  2.5119E-02, delzi=  9.2699E-03, nord= 6
               ncycle=  0
 steps completed =    50, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -4.8025
```

- -

reaction progress = 2.51188643150955E-02
log of reaction progress = -1.6000000

temperature = 450.000 degrees c
total pressure = 500.000 bars

computing units remaining = .000

step size is limited by the print requirement

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.99579E+01	4.20816E-02	2.68504E+04	1.13039E+01
CLINOPYROXENE(SS)	9.99493E+01	5.07200E-02	2.22748E+04	1.13035E+01
MAGNETITE	9.99946E+01	5.42567E-03	2.31526E+04	1.25625E+00
TREMOLITE	9.99954E+01	4.60178E-03	8.12333E+04	3.73835E+00

current total mass = 1.53511E+05 grams
delta total mass = 2.76020E+01 grams
delta total volume = 9.09577 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	16.4266	1.67530E+00
CLINOPYROXENE(SS)	.1098	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	4.9629	1.83200E-01

affinity of the overall irreversible reaction= 28.429 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.454590E+05	5.747551E+01	5.749940E+01
NA	1.267127E+04	5.994867E-01	5.997359E-01
CA	2.019846E+01	5.481311E-04	5.483590E-04
MG	2.070256E+04	9.264509E-01	9.268361E-01
AL	7.188788E+00	2.897897E-04	2.899102E-04
SI	8.705167E+01	3.371234E-03	3.372636E-03
H	1.047539E+05	1.130438E+02	1.130908E+02
CL	1.629103E+04	4.997922E-01	5.000000E-01
FE	7.819182E+00	1.522844E-04	1.523477E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.7149	.4397	3.0648E+00
modified nbs ph scale	6.4663	.4754	3.3134E+00
rational ph scale	6.4663	.4754	3.3134E+00

phcl = 7.3039

oxygen fugacity = 1.74271E-27
log oxygen fugacity = -26.75877

activity of water = .98385
log activity of water = -.00707

```
               alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                    ionic strength =  5.347893E-01 molal
                 sum of molalities =    2.0937967663332
               osmotic coefficient =     .43161
                    equiv. stoich. ionic strength =  4.997922E-01
molal

                         mass of solution =   1.088114 kg
                         mass of solvent  =   1.000416 kg
                         mass of solutes  =    .087699 kg
                         conc of solutes  =   8.059679 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55318E+01   1.00042E+03
   NA+                  5.34224E-01   1.22817E+01   5.34002E-01     -.
27246     -.24860     -.52106
   CA++                 4.19996E-05   1.68334E-03   4.19821E-05
-4.37694     -.99441    -5.37134
   MG++                 3.84605E-07   9.34783E-06   3.84445E-07
-6.41517     -.99441    -7.40957
   AL+++                6.27311E-23   1.69258E-21   6.27051E-23
-22.20270    -2.23741   -24.44011
   H4SIO4(AQ)           1.83794E-03   1.76653E-01   1.83718E-03
-2.73585      .00000    -2.73585
   H+                   3.41906E-07   3.44607E-07   3.41764E-07
-6.46627     -.24860    -6.71488
   CL-                  4.56819E-01   1.61956E+01   4.56629E-01     -.
34044     -.24860     -.58904
   FE++                 1.78540E-09   9.97092E-08   1.78466E-09
-8.74845     -.99441    -9.74285
   O2(AQ)               1.46726E-31   4.69504E-30   1.46665E-31
-30.83367      .00000   -30.83367
   H2(AQ)               3.05842E-02   6.16517E-02   3.05715E-02
-1.51468      .00000    -1.51468
   FE+++                6.25617E-23   3.49388E-21   6.25357E-23
-22.20387    -2.23741   -24.44128
   OH-                  7.68045E-02   1.30624E+00   7.67726E-02
-1.11479     -.24860    -1.36340
   H8SI3O10(AQ)         3.15629E-11   7.96375E-09   3.15498E-11
-10.50100      .00000   -10.50100
   H6SI2O7(AQ)          9.13386E-06   1.59125E-03   9.13007E-06
-5.03953      .00000    -5.03953
   AL(OH)3(AQ)          8.62782E-07   6.72999E-05   8.62423E-07
-6.06428      .00000    -6.06428
   AL(OH)4-             2.17153E-04   2.06318E-02   2.17062E-04
```

```
-3.66342     -.24860    -3.91202
   AL(OH)SI(OH)-        7.18948E-05   1.24457E-02   7.18649E-05
-4.14348     -.24860    -4.39208
   CACL+                8.67966E-05   6.55600E-03   8.67605E-05
-4.06168     -.24860    -4.31028
   CACL2(AQ)            1.56635E-06   1.73843E-04   1.56570E-06
-5.80529      .00000    -5.80529
   CA(OH)+              1.66703E-04   9.51662E-03   1.66634E-04
-3.77824     -.24860    -4.02684
   CA(H3SIO4)+          2.51294E-04   3.39716E-02   2.51189E-04
-3.60000     -.24860    -3.84860
   FE(OH)+              6.42635E-08   4.68187E-06   6.42367E-08
-7.19222     -.24860    -7.44082
   FE(OH)2              5.77283E-07   5.18756E-05   5.77043E-07
-6.23879      .00000    -6.23879
   FE(OH)3-             7.67458E-06   8.20174E-04   7.67139E-06
-5.11513     -.24860    -5.36373
   FECL+                1.93686E-09   1.76836E-07   1.93606E-09
-8.71308     -.24860    -8.96168
   FECL2(AQ)            4.48081E-08   5.67956E-06   4.47895E-08
-7.34882      .00000    -7.34882
   FE(H3SIO4)+          1.43983E-04   2.17348E-02   1.43923E-04
-3.84187     -.24860    -4.09047
   MGCL+                3.75475E-07   2.24377E-05   3.75319E-07
-6.42560     -.24860    -6.67420
   MG(OH)+              1.08475E-05   4.48135E-04   1.08430E-05
-4.96485     -.24860    -5.21345
   MG(OH)2(AQ)          9.26825E-01   5.40520E+01   9.26439E-01     -.
03318      .00000     -.03318
   MG(H3SIO4)+          6.86442E-09   8.19693E-07   6.86157E-09
-8.16358     -.24860    -8.41218
   NACL(AQ)             4.30903E-02   2.51832E+00   4.30724E-02
-1.36580      .00000    -1.36580
   NAOH(AQ)             2.24215E-02   8.96793E-01   2.24121E-02
-1.64952      .00000    -1.64952
   H3SIO4-              1.04925E-03   9.97905E-02   1.04881E-03
-2.97930     -.24860    -3.22790
   HCL(AQ)              4.27557E-07   1.55891E-05   4.27379E-07
-6.36919      .00000    -6.36919

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.1938168
           log (CA++  /h+**0)            8.0584096
           log (MG++  /h+**0)            6.0201796
           log (AL+++ /h+**0)           -4.2954842
           log (FE++  /h+**0)            3.6868997
           log (FE+++ /h+**0)           -4.2966587
```

--- summary of solid product phases---

product	log moles	moles	grams	volume, cc
MAGNETITE	-2.4031140	3.95263E-03	9.15186E-01	1.75971E-01
ANTIGORITE	-3.5676232	2.70631E-04	6.13783E-01	2.35781E-01
CLINOPYROXENE(SS)	-1.1122499	7.72236E-02	1.69107E+01	5.11211E+00
DIOPSIDE	-1.1472163	7.12498E-02	1.54293E+01	4.71674E+00
HEDENBERGITE	-2.2248962	5.95805E-03	1.47816E+00	3.94423E-01
JADEITE	-4.8024730	1.57589E-05	3.18549E-03	9.50895E-04
CHLORITE(SS)	-.8340911	1.46524E-01	1.65592E+01	6.19986E+00
CLINOCHLORE	-.8603989	1.37912E-01	1.53302E+01	5.83229E+00
CHAMOSITE	-2.0648788	8.61234E-03	1.22899E+00	3.67575E-01

--- grand summary of solid phases (e.s.+p.r.s. +reactants) ---

phase/end-member	log moles	moles	grams	volume, cc
MAGNETITE	1.9999936	9.99985E+01	2.31535E+04	4.45193E+03
TREMOLITE	1.9999800	9.99954E+01	8.12333E+04	2.72667E+04
ANTIGORITE	-3.5676232	2.70631E-04	6.13783E-01	2.35781E-01
PLAGIOCLASE(SS)	1.9998172	9.99579E+01		
ALBITE	1.7779685	5.99748E+01	1.57268E+04	6.04725E+03
ANORTHITE	1.6018772	3.99832E+01	1.11237E+04	4.02830E+03

```
   CLINOPYROXENE(SS)         2.0001151    1.00027E+02

   DIOPSIDE                  1.9032565    8.00307E+01    1.73308E+04
5.29803E+03
   HEDENBERGITE              1.3009391    1.99958E+01    4.96085E+03
1.32372E+03
   JADEITE                  -4.8024730    1.57589E-05    3.18549E-03
9.50895E-04


   CHLORITE(SS)              -.8340911    1.46524E-01

   CLINOCHLORE               -.8603989    1.37912E-01    1.53302E+01
5.83229E+00
   CHAMOSITE                -2.0648788    8.61234E-03    1.22899E+00
3.67575E-01



                        mass, grams        volume, cc

           created         3.499880E+01       1.172372E+01
           destroyed       2.760197E+01       9.095773E+00
           net             7.396839E+00       2.627952E+00

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE               .0000  satd          HEMATITE
-3.3273
 PERICLASE             -5.0399                BRUCITE
-1.3036
 DIASPORE              -6.8722                FORSTERITE
-.4449
 FAYALITE              -1.5831                CHRYSOTILE
-.6652
 ENSTATITE-CL          -2.0787                ENSTATITE-OR
-2.1568
 ENSTATITE-PR          -2.5622                DIOPSIDE
-.1157
 HEDENBERGITE          -3.6818                FERROSILITE
-4.1829
```

```
 WOLLASTONITE            -3.7318                PSEUDOWOLLASTONITE
-4.2179
 TREMOLITE               -4.9629
ANTIGORITE                .0000  satd
 TALC                    -6.3019                CLINOCHLORE
-.0871
 CHAMOSITE               -4.0727                PYROPE
-7.5278
 ALMANDINE               -7.4183                GROSSULAR
-4.4433
 QUARTZ-ALPHA            -5.3447                QUARTZ-BETA
-5.5817
 COESITE                 -5.9410                IRON-ALPHA
-8.7506
 IRON-GAMMA              -7.8939                HALITE
-9.7172
 CRISTOBALITE-ALPHA      -6.6306                CRISTOBALITE-BETA
-7.3441


                    --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -15.9504
     ALBITE                    -15.95037     .9058283     1.00000
     ANORTHITE                 -15.95037     .0941717     1.00000

 ORTHOPYROXENE(SS)        -1.8428
     ENSTATITE-OR               -1.84283     .8037386     1.00000
     FERROSILITE                -1.84283     .1962614     1.00000

 GARNET(SS)               -4.1306
     PYROPE                     -4.13058     .0940456     1.00000
     ALMANDINE                  -4.13058     .1014905     1.00000
     GROSSULAR                  -4.13058     .8044640     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9226428     1.00000
     HEDENBERGITE                 .00000     .0771532     1.00000
     JADEITE                      .00000     .0002041     1.00000

 CPX_SUBCALCIC(SS)         -.0003
     DIOPSIDE                    -.00029     .9228311     1.00000
     HEDENBERGITE                -.00029     .0771689     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9412223     1.00000
```

```
    CHAMOSITE                    .00000     .0587777     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
             .9226    1.0000     .9226    -.0350     .0000    -.0350
    HEDENBERGITE
             .0772    1.0000     .0772   -1.1126     .0000   -1.1126
    JADEITE
             .0002    1.0000     .0002   -3.6902     .0000   -3.6902

   CHLORITE(SS)
 ideal solution

    CLINOCHLORE
             .9412    1.0000     .9412    -.0263     .0000    -.0263
    CHAMOSITE
             .0588    1.0000     .0588   -1.2308     .0000   -1.2308


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                       -26.75877       1.74271E-27
   H2(G)                         2.25722       1.80808E+02
   H2O(G)                        3.80603       6.39778E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


 * note - a search for where a phase supersaturates
       indicates that the event being searched for
       does not take place in the interval being
       examined (search)
              the phase is CPX_SUBCALCIC(SS)
              delzi will not be decreased

 stepping to zi=  3.6285E-02, delzi=  1.1166E-02, nord= 6
              ncycle=  0
```

```
 steps completed =    51, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -4.4952

 stepping to zi=  3.9811E-02, delzi=  3.5257E-03, nord= 6
               ncycle=  0
 steps completed =    52, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -4.4080
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                     reaction progress        =  3.98107170553492E-02
                     log of reaction progress =      -1.4000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.99333E+01    6.66949E-02    2.68438E+04
1.79154E+01
   CLINOPYROXENE(SS)       9.99196E+01    8.03858E-02    2.22682E+04
1.79148E+01
   MAGNETITE               9.99914E+01    8.59911E-03    2.31519E+04
1.99103E+00
   TREMOLITE               9.99927E+01    7.29332E-03    8.12311E+04
5.92488E+00


                current total mass =  1.53495E+05 grams
                delta total mass   =  4.37462E+01 grams
                delta total volume =     14.41583 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           15.8374    1.67530E+00
   CLINOPYROXENE(SS)           .0958    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
```

```
   TREMOLITE                  4.6060    1.83200E-01

          affinity of the overall irreversible reaction=    27.376
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O          8.466111E+05        5.731773E+01        5.735388E+01
      NA         1.303348E+04        6.140933E-01        6.144805E-01
      CA         1.544832E+01        4.175057E-04        4.177690E-04
      MG         1.883051E+04        8.392188E-01        8.397480E-01
      AL         8.742066E+00        3.509588E-04        3.511801E-04
      SI         1.027247E+02        3.961880E-03        3.964379E-03
      H          1.050355E+05        1.128828E+02        1.129539E+02
      CL         1.635462E+04        4.996849E-01        5.000000E-01
      FE         7.885946E+00        1.529547E-04        1.530511E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                        ph           eh            pe

     internal ph scale                6.7702        .4334
3.0203E+00
     modified nbs ph scale            6.5204        .4692
3.2701E+00
     rational ph scale                6.5204        .4692
3.2701E+00

   phcl =      7.3610
```

```
          oxygen fugacity =  1.92498E-27
          log oxygen fugacity = -26.71557



                              activity of water =    .98385
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  5.452070E-01 molal
                 sum of molalities =    2.0302677137147
               osmotic coefficient =     .44502
                    equiv. stoich. ionic strength =  4.996849E-01
molal

                         mass of solution =   1.083883 kg
                         mass of solvent  =   1.000631 kg
                         mass of solutes  =    .083253 kg
                         conc of solutes  =   7.680969 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55437E+01   1.00063E+03
   NA+                  5.44925E-01   1.25277E+01   5.44582E-01     -.
26394     -.24981     -.51374
   CA++                 2.73093E-05   1.09456E-03   2.72921E-05
-4.56396     -.99923    -5.56320
   MG++                 2.73126E-07   6.63833E-06   2.72954E-07
-6.56391     -.99923    -7.56314
   AL+++                4.50256E-23   1.21486E-21   4.49973E-23
-22.34681    -2.24827   -24.59509
   H4SIO4(AQ)           2.11378E-03   2.03165E-01   2.11245E-03
-2.67521      .00000    -2.67521
   H+                   3.01922E-07   3.04307E-07   3.01732E-07
-6.52038     -.24981    -6.77019
   CL-                  4.56291E-01   1.61769E+01   4.56004E-01     -.
34103     -.24981     -.59084
   FE++                 1.37667E-09   7.68831E-08   1.37581E-09
-8.86144     -.99923    -9.86068
   O2(AQ)               1.62106E-31   5.18721E-30   1.62004E-31
-30.79047      .00000   -30.79047
   H2(AQ)               2.91066E-02   5.86731E-02   2.90883E-02
-1.53628      .00000    -1.53628
   FE+++                4.41496E-23   2.46562E-21   4.41217E-23
-22.35535    -2.24827   -24.60362
   OH-                  8.74984E-02   1.48811E+00   8.74432E-02
-1.05827     -.24981    -1.30808
```

```
   H8SI3O10(AQ)          4.79921E-11   1.21091E-08   4.79618E-11
-10.31910      .00000   -10.31910
   H6SI2O7(AQ)           1.20785E-05   2.10425E-03   1.20709E-05
-4.91826      .00000    -4.91826
   AL(OH)3(AQ)           8.85025E-07   6.90350E-05   8.84467E-07
-6.05332      .00000    -6.05332
   AL(OH)4-              2.53711E-04   2.41053E-02   2.53551E-04
-3.59593     -.24981    -3.84574
   AL(OH)SI(OH)-         9.65839E-05   1.67197E-02   9.65230E-05
-4.01537     -.24981    -4.26518
   CACL+                 5.57373E-05   4.21000E-03   5.57021E-05
-4.25413     -.24981    -4.50394
   CACL2(AQ)             9.98902E-07   1.10864E-04   9.98272E-07
-6.00075      .00000    -6.00075
   CA(OH)+               1.22096E-04   6.97013E-03   1.22019E-04
-3.91357     -.24981    -4.16338
   CA(H3SIO4)+           2.11628E-04   2.86093E-02   2.11494E-04
-3.67470     -.24981    -3.92451
   FE(OH)+               5.58152E-08   4.06638E-06   5.57800E-08
-7.25352     -.24981    -7.50333
   FE(OH)2               5.67915E-07   5.10338E-05   5.67557E-07
-6.24599      .00000    -6.24599
   FE(OH)3-              8.59942E-06   9.19011E-04   8.59400E-06
-5.06580     -.24981    -5.31561
   FECL+                 1.47493E-09   1.34661E-07   1.47400E-09
-8.83150     -.24981    -9.08131
   FECL2(AQ)             3.38861E-08   4.29516E-06   3.38647E-08
-7.47025      .00000    -7.47025
   FE(H3SIO4)+           1.43791E-04   2.17058E-02   1.43701E-04
-3.84254     -.24981    -4.09235
   MGCL+                 2.63334E-07   1.57363E-05   2.63168E-07
-6.57977     -.24981    -6.82958
   MG(OH)+               8.67701E-06   3.58467E-04   8.67154E-06
-5.06190     -.24981    -5.31171
   MG(OH)2(AQ)           8.39739E-01   4.89732E+01   8.39210E-01     -.
07613      .00000     -.07613
   MG(H3SIO4)+           6.31360E-09   7.53918E-07   6.30962E-09
-8.20000     -.24981    -8.44981
   NACL(AQ)              4.36501E-02   2.55103E+00   4.36226E-02
-1.36029      .00000    -1.36029
   NAOH(AQ)              2.59050E-02   1.03612E+00   2.58887E-02
-1.58689      .00000    -1.58689
   H3SIO4-               1.37443E-03   1.30718E-01   1.37357E-03
-2.86215     -.24981    -3.11196
   HCL(AQ)               3.74950E-07   1.36710E-05   3.74714E-07
-6.42630      .00000    -6.42630

           --- activity ratios of cations ---
```

```
           log (NA+   /h+**0)            6.2564420
           log (CA++  /h+**0)            7.9771777
           log (MG++  /h+**0)            5.9772300
           log (AL+++ /h+**0)           -4.2845276
           log (FE++  /h+**0)            3.6796980
           log (FE+++ /h+**0)           -4.2930609


           --- summary of solid product phases---


  product                     log moles        moles        grams
volume, cc

   MAGNETITE                 -2.2480701    5.64846E-03    1.30784E+00
2.51469E-01
   ANTIGORITE                -3.3724984    4.24133E-04    9.61922E-01
3.69517E-01

   CLINOPYROXENE(SS)          -.9126740    1.22272E-01    2.67986E+01
8.09416E+00
   DIOPSIDE                   -.9505565    1.12058E-01    2.42665E+01
7.41825E+00
   HEDENBERGITE              -1.9924885    1.01745E-02    2.52423E+00
6.73549E-01
   JADEITE                   -4.4080498    3.90796E-05    7.89950E-03
2.35806E-03

   CHLORITE(SS)               -.6336537    2.32459E-01    2.63056E+01
9.83645E+00
   CLINOCHLORE                -.6621460    2.17698E-01    2.41992E+01
9.20644E+00
   CHAMOSITE                 -1.8308781    1.47612E-02    2.10645E+00
6.30008E-01


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  1.9999872    9.99970E+01    2.31532E+04
4.45187E+03
   TREMOLITE                  1.9999683    9.99927E+01    8.12311E+04
2.72660E+04
   ANTIGORITE                -3.3724984    4.24133E-04    9.61922E-01
3.69517E-01

   PLAGIOCLASE(SS)            1.9997103    9.99333E+01
```

```
   ALBITE                     1.7778615    5.99600E+01    1.57229E+04
6.04577E+03
   ANORTHITE                  1.6017702    3.99733E+01    1.11209E+04
4.02731E+03


   CLINOPYROXENE(SS)          2.0001819    1.00042E+02

   DIOPSIDE                   1.9033491    8.00477E+01    1.73345E+04
5.29916E+03
   HEDENBERGITE               1.3009018    1.99941E+01    4.96042E+03
1.32361E+03
   JADEITE                   -4.4080498    3.90796E-05    7.89950E-03
2.35806E-03


   CHLORITE(SS)               -.6336537    2.32459E-01

   CLINOCHLORE                -.6621460    2.17698E-01    2.41992E+01
9.20644E+00
   CHAMOSITE                 -1.8308781    1.47612E-02    2.10645E+00
6.30008E-01



                          mass, grams         volume, cc

           created        5.537395E+01        1.855159E+01
           destroyed      4.374617E+01        1.441583E+01
           net            1.162778E+01        4.135764E+00

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-3.3035
 PERICLASE              -5.1820                BRUCITE
-1.4457
 DIASPORE               -6.8360                FORSTERITE
-.4867
 FAYALITE               -1.5066                CHRYSOTILE
```

```
-.6903
 ENSTATITE-CL           -2.0202               ENSTATITE-OR
-2.0983
 ENSTATITE-PR           -2.5037               DIOPSIDE
-.1254
 HEDENBERGITE           -3.5731               FERROSILITE
-4.0060
 WOLLASTONITE           -3.8000               PSEUDOWOLLASTONITE
-4.2861
 TREMOLITE              -4.6060
ANTIGORITE               .0000  satd
 TALC                   -5.9258               CLINOCHLORE
-.0943
 CHAMOSITE              -3.9616               PYROPE
-7.4453
 ALMANDINE              -7.2174               GROSSULAR
-4.4875
 QUARTZ-ALPHA           -5.1441               QUARTZ-BETA
-5.3810
 COESITE                -5.7404               IRON-ALPHA
-8.8459
 IRON-GAMMA             -7.9892               HALITE
-9.6990
 CRISTOBALITE-ALPHA     -6.4300               CRISTOBALITE-BETA
-7.1434


                     --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)         -15.1545
     ALBITE                    -15.15449     .9375759     1.00000
     ANORTHITE                 -15.15449     .0624241     1.00000

 ORTHOPYROXENE(SS)        -1.7603
     ENSTATITE-OR               -1.76032     .7904291     1.00000
     FERROSILITE                -1.76032     .2095709     1.00000

 GARNET(SS)               -4.1358
     PYROPE                     -4.13579     .0999661     1.00000
     ALMANDINE                  -4.13579     .1171448     1.00000
     GROSSULAR                  -4.13579     .7828891     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9164685     1.00000
     HEDENBERGITE                 .00000     .0832119     1.00000
     JADEITE                      .00000     .0003196     1.00000
```

```
 CPX_SUBCALCIC(SS)          -.0005
     DIOPSIDE                     -.00046     .9167615     1.00000
     HEDENBERGITE                 -.00046     .0832385     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9364997     1.00000
     CHAMOSITE                     .00000     .0635003     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9165    1.0000     .9165    -.0379     .0000    -.0379
     HEDENBERGITE
              .0832    1.0000     .0832   -1.0798     .0000   -1.0798
     JADEITE
              .0003    1.0000     .0003   -3.4954     .0000   -3.4954

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9365    1.0000     .9365    -.0285     .0000    -.0285
     CHAMOSITE
              .0635    1.0000     .0635   -1.1972     .0000   -1.1972


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.71557       1.92498E-27
   H2(G)                          2.23562       1.72035E+02
   H2O(G)                         3.80603       6.39780E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  4.6862E-02, delzi=  7.0514E-03, nord= 5
```

```
               ncycle=  0
 steps completed =    53, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =     -4.2426

 stepping to zi=  5.8898E-02, delzi=  1.2036E-02, nord= 6
               ncycle=  0
 steps completed =    54, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =     -3.9788

 stepping to zi=  6.3096E-02, delzi=  4.1974E-03, nord= 6
               ncycle=  0
 steps completed =    55, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =     -3.8903
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                     reaction progress        =  6.30957344480185E-02
                     log of reaction progress =      -1.2000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.98943E+01    1.05704E-01    2.68334E+04
2.83940E+01
   CLINOPYROXENE(SS)      9.98726E+01    1.27403E-01    2.22577E+04
2.83931E+01
   MAGNETITE              9.99864E+01    1.36287E-02    2.31507E+04
3.15557E+00
   TREMOLITE              9.99884E+01    1.15591E-02    8.12276E+04
9.39030E+00


                current total mass =  1.53469E+05 grams
                delta total mass   =  6.93330E+01 grams
                delta total volume =     22.84755 cc
```

```
      reactant           affinity     rel. rate

   PLAGIOCLASE(SS)          14.8496    1.67530E+00
   CLINOPYROXENE(SS)          .0751    0.00000E+00
   MAGNETITE                  .0000    0.00000E+00
   TREMOLITE                 3.9776    1.83200E-01

          affinity of the overall irreversible reaction=    25.606
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.           moles

      O          8.483835E+05        5.707722E+01        5.712949E+01
      NA         1.360959E+04        6.372129E-01        6.377965E-01
      CA         1.051086E+01        2.822832E-04        2.825417E-04
      MG         1.591820E+04        7.049730E-01        7.056186E-01
      AL         1.178224E+01        4.700405E-04        4.704710E-04
      SI         1.382990E+02        5.300431E-03        5.305285E-03
      H          1.054666E+05        1.126346E+02        1.127378E+02
      CL         1.645323E+04        4.995425E-01        5.000000E-01
      FE         8.288384E+00        1.597513E-04        1.598976E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                         ph            eh            pe

     internal ph scale                 6.8440         .4267
2.9738E+00
     modified nbs ph scale             6.5923         .4628
3.2255E+00
     rational ph scale                 6.5923         .4628
```

```
3.2255E+00

   phcl =      7.4376



          oxygen fugacity =  2.47646E-27
          log oxygen fugacity = -26.60617



                              activity of water =    .98386
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                   ionic strength =  5.617122E-01 molal
                 sum of molalities =    1.9326849690891
               osmotic coefficient =     .46736
                   equiv. stoich. ionic strength =  4.995425E-01
molal

                        mass of solution =   1.077387 kg
                        mass of solvent  =   1.000916 kg
                        mass of solutes  =    .076471 kg
                        conc of solutes  =   7.097857 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55595E+01   1.00092E+03
   NA+                  5.61760E-01   1.29147E+01   5.61246E-01     -.
25085     -.25167     -.50252
   CA++                 1.42220E-05   5.70017E-04   1.42090E-05
-4.84744    -1.00670    -5.85413
   MG++                 1.66183E-07   4.03909E-06   1.66031E-07
-6.77981    -1.00670    -7.78651
   AL+++                2.93847E-23   7.92845E-22   2.93578E-23
-22.53228    -2.26507   -24.79734
   H4SIO4(AQ)           2.70434E-03   2.59927E-01   2.70187E-03
-2.56834      .00000    -2.56834
   H+                   2.55892E-07   2.57914E-07   2.55658E-07
-6.59234     -.25167    -6.84401
   CL-                  4.55451E-01   1.61471E+01   4.55035E-01     -.
34196     -.25167     -.59363
   FE++                 9.56149E-10   5.33981E-08   9.55274E-10
-9.01987    -1.00670   -10.02657
   O2(AQ)               2.08607E-31   6.67516E-30   2.08416E-31
-30.68107      .00000   -30.68107
```

```
   H2(AQ)                   2.56694E-02   5.17443E-02   2.56459E-02
-1.59098      .00000    -1.59098
   FE+++                    2.81496E-23   1.57207E-21   2.81238E-23
-22.55093    -2.26507   -24.81599
   OH-                      1.04188E-01   1.77196E+00   1.04093E-01      -.
98258     -.25167    -1.23425
   H8SI3O10(AQ)             1.00444E-10   2.53434E-08   1.00352E-10
-9.99847      .00000    -9.99847
   H6SI2O7(AQ)              1.97648E-05   3.44332E-03   1.97468E-05
-4.70450      .00000    -4.70450
   AL(OH)3(AQ)              9.25370E-07   7.21821E-05   9.24524E-07
-6.03408      .00000    -6.03408
   AL(OH)4-                 3.15788E-04   3.00032E-02   3.15499E-04
-3.50100     -.25167    -3.75268
   AL(OH)SI(OH)-            1.53758E-04   2.66170E-02   1.53617E-04
-3.81356     -.25167    -4.06523
   CACL+                    2.84713E-05   2.15053E-03   2.84453E-05
-4.54599     -.25167    -4.79766
   CACL2(AQ)                5.04812E-07   5.60270E-05   5.04350E-07
-6.29727      .00000    -6.29727
   CA(OH)+                  7.44018E-05   4.24740E-03   7.43337E-05
-4.12881     -.25167    -4.38049
   CA(H3SIO4)+              1.64942E-04   2.22980E-02   1.64791E-04
-3.78307     -.25167    -4.03474
   FE(OH)+                  4.53607E-08   3.30472E-06   4.53192E-08
-7.34372     -.25167    -7.59539
   FE(OH)2                  5.44722E-07   4.89496E-05   5.44224E-07
-6.26422      .00000    -6.26422
   FE(OH)3-                 9.81876E-06   1.04932E-03   9.80978E-06
-5.00834     -.25167    -5.26001
   FECL+                    1.00480E-09   9.17383E-08   1.00388E-09
-8.99832     -.25167    -9.24999
   FECL2(AQ)                2.28388E-08   2.89489E-06   2.28179E-08
-7.64172      .00000    -7.64172
   FE(H3SIO4)+              1.49464E-04   2.25621E-02   1.49327E-04
-3.82586     -.25167    -4.07754
   MGCL+                    1.57161E-07   9.39162E-06   1.57017E-07
-6.80405     -.25167    -7.05573
   MG(OH)+                  6.17771E-06   2.55216E-04   6.17206E-06
-5.20957     -.25167    -5.46124
   MG(OH)2(AQ)              7.05612E-01   4.11510E+01   7.04966E-01      -.
15183      .00000     -.15183
   MG(H3SIO4)+              5.74925E-09   6.86528E-07   5.74399E-09
-8.24079     -.25167    -8.49246
   NACL(AQ)                 4.45187E-02   2.60180E+00   4.44780E-02
-1.35185      .00000    -1.35185
   NAOH(AQ)                 3.15182E-02   1.26064E+00   3.14894E-02
-1.50184      .00000    -1.50184
   H3SIO4-                  2.09324E-03   1.99082E-01   2.09133E-03
-2.67958     -.25167    -2.93125
```

```
   HCL(AQ)              3.14398E-07   1.14632E-05   3.14110E-07
-6.50292      .00000    -6.50292

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.3414938
           log (CA++  /h+**0)            7.8338961
           log (MG++  /h+**0)            5.9015239
           log (AL+++ /h+**0)           -4.2652973
           log (FE++  /h+**0)            3.6614619
           log (FE+++ /h+**0)           -4.2839470


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                  -2.1402139    7.24079E-03    1.67652E+00
3.22360E-01
   ANTIGORITE                 -3.1853824    6.52556E-04    1.47998E+00
5.68526E-01

   CLINOPYROXENE(SS)           -.7129846    1.93649E-01    4.25065E+01
1.28188E+01
   DIOPSIDE                    -.7561018    1.75347E-01    3.79718E+01
1.16080E+01
   HEDENBERGITE               -1.7405638    1.81734E-02    4.50872E+00
1.20308E+00
   JADEITE                    -3.8903254    1.28728E-04    2.60210E-02
7.76748E-03

   CHLORITE(SS)                -.4335985    3.68469E-01    4.17938E+01
1.55929E+01
   CLINOCHLORE                 -.4659752    3.41999E-01    3.80164E+01
1.44631E+01
   CHAMOSITE                  -1.5772373    2.64705E-02    3.77738E+00
1.12976E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                   1.9999723    9.99936E+01    2.31524E+04
4.45172E+03
```

```
   TREMOLITE                   1.9999498    9.99884E+01    8.12276E+04
2.72648E+04
   ANTIGORITE                 -3.1853824    6.52556E-04    1.47998E+00
5.68526E-01

   PLAGIOCLASE(SS)             1.9995407    9.98943E+01

   ALBITE                      1.7776919    5.99366E+01    1.57167E+04
6.04341E+03
   ANORTHITE                   1.6016007    3.99577E+01    1.11166E+04
4.02574E+03


   CLINOPYROXENE(SS)           2.0002876    1.00066E+02

   DIOPSIDE                    1.9034884    8.00734E+01    1.73401E+04
5.30086E+03
   HEDENBERGITE                1.3008713    1.99927E+01    4.96008E+03
1.32352E+03
   JADEITE                    -3.8903254    1.28728E-04    2.60210E-02
7.76748E-03


   CHLORITE(SS)                -.4335985    3.68469E-01

   CLINOCHLORE                 -.4659752    3.41999E-01    3.80164E+01
1.44631E+01
   CHAMOSITE                  -1.5772373    2.64705E-02    3.77738E+00
1.12976E+00


                           mass, grams         volume, cc

           created         8.745683E+01        2.930260E+01
           destroyed       6.933300E+01        2.284755E+01
           net             1.812382E+01        6.455052E+00

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral          affinity, kcal    state          mineral
affinity, kcal    state

 MAGNETITE                .0000  satd           HEMATITE
```

```
-3.2431
 PERICLASE              -5.4326                BRUCITE
-1.6962
 DIASPORE               -6.7723                FORSTERITE
-.5604
 FAYALITE               -1.3901                CHRYSOTILE
-.7345
 ENSTATITE-CL           -1.9171                ENSTATITE-OR
-1.9952
 ENSTATITE-PR           -2.4005                DIOPSIDE
-.1427
 HEDENBERGITE           -3.4003                FERROSILITE
-3.7127
 WOLLASTONITE           -3.9204                PSEUDOWOLLASTONITE
-4.4065
 TREMOLITE              -3.9776
ANTIGORITE               .0000  satd
 TALC                   -5.2627                CLINOCHLORE
-.1071
 CHAMOSITE              -3.7843                PYROPE
-7.3000
 ALMANDINE              -6.8818                GROSSULAR
-4.5661
 QUARTZ-ALPHA           -4.7905                QUARTZ-BETA
-5.0274
 COESITE                -5.3868                IRON-ALPHA
-9.0873
 IRON-GAMMA             -8.2306                HALITE
-9.6711
 CRISTOBALITE-ALPHA     -6.0764                CRISTOBALITE-BETA
-6.7898


                        --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -13.7956
     ALBITE                     -13.79559     .9688381     1.00000
     ANORTHITE                  -13.79559     .0311619     1.00000

 ORTHOPYROXENE(SS)         -1.6152
     ENSTATITE-OR                -1.61519     .7676670     1.00000
     FERROSILITE                 -1.61519     .2323330     1.00000

 GARNET(SS)                -4.1361
     PYROPE                      -4.13606     .1106216     1.00000
     ALMANDINE                   -4.13606     .1479919     1.00000
     GROSSULAR                   -4.13606     .7413864     1.00000
```

```
 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .9054882     1.00000
     HEDENBERGITE                 .00000     .0938471     1.00000
     JADEITE                      .00000     .0006648     1.00000

 CPX_SUBCALCIC(SS)         -.0010
     DIOPSIDE                    -.00096     .9060905     1.00000
     HEDENBERGITE                -.00096     .0939095     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9281608     1.00000
     CHAMOSITE                    .00000     .0718392     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .9055    1.0000     .9055    -.0431     .0000    -.0431
     HEDENBERGITE
              .0938    1.0000     .0938   -1.0276     .0000   -1.0276
     JADEITE
              .0007    1.0000     .0007   -3.1773     .0000   -3.1773

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9282    1.0000     .9282    -.0324     .0000    -.0324
     CHAMOSITE
              .0718    1.0000     .0718   -1.1436     .0000   -1.1436


           --- summary of gas species ---

           gas                 log fugacity         fugacity
partial pressure

   O2(G)                          -26.60617       2.47646E-27
   H2(G)                            2.18092       1.51676E+02
   H2O(G)                           3.80603       6.39783E+03
```

```
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  7.7265E-02, delzi=  1.4169E-02, nord= 6
               ncycle=  0
 steps completed =    56, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =     -3.5989

 stepping to zi=  8.8166E-02, delzi=  1.0901E-02, nord= 6
               ncycle=  0
 steps completed =    57, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =     -3.3775
 * note - a search for where a phase supersaturates
        indicates that the event being searched for
        does not take place in the interval being
        examined (search)
               the phase is CPX_SUBCALCIC(SS)
               delzi will not be decreased

 stepping to zi=  1.0000E-01, delzi=  1.1834E-02, nord= 6
               ncycle=  0
 steps completed =    58, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE          ) =     -3.1355
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  9.99999999999986E-02
                     log of reaction progress =      -1.0000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant             moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.98325E+01    1.67530E-01    2.68168E+04
4.50015E+01
```

```
   CLINOPYROXENE(SS)        9.97981E+01    2.01920E-01    2.22411E+04
4.50001E+01
   MAGNETITE                9.99784E+01    2.16000E-02    2.31489E+04
5.00123E+00
   TREMOLITE                9.99817E+01    1.83200E-02    8.12222E+04
1.48826E+01


                current total mass =  1.53429E+05 grams
                delta total mass   =  1.09885E+02 grams
                delta total volume =     36.21092 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           13.0634    1.67530E+00
   CLINOPYROXENE(SS)           .0496    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  2.7743    1.83200E-01

          affinity of the overall irreversible reaction=    22.393
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O          8.509970E+05        5.672811E+01        5.679584E+01
      NA         1.451738E+04        6.734847E-01        6.742888E-01
      CA         6.097913E+00        1.622660E-04        1.624597E-04
      MG         1.151301E+04        5.052048E-01        5.058080E-01
      AL         1.926436E+01        7.614857E-04        7.623949E-04
      SI         2.422134E+02        9.197927E-03        9.208909E-03
      H          1.060946E+05        1.122664E+02        1.124005E+02
      CL         1.660087E+04        4.994037E-01        5.000000E-01
      FE         9.535489E+00        1.821030E-04        1.823204E-04

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species
```

```
   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                            ph           eh           pe

     internal ph scale              6.9349        .4260
2.9693E+00
     modified nbs ph scale          6.6804        .4626
3.2238E+00
     rational ph scale              6.6804        .4626
3.2238E+00

   phcl =      7.5327



          oxygen fugacity =  5.48901E-27
          log oxygen fugacity = -26.26051



                           activity of water =    .98386
               log activity of water =   -.00706
               alkalinity =  0.000000E+00 equiv/kg solvent
                                      (not def. for t.gt.50 c)

                    ionic strength =  5.876771E-01 molal
                 sum of molalities =    1.7882979557710
               osmotic coefficient =     .50495
                    equiv. stoich. ionic strength =  4.994037E-01
molal

                         mass of solution =   1.067806 kg
                         mass of solvent  =   1.001194 kg
                         mass of solutes  =    .066612 kg
                         conc of solutes  =   6.238189 per cent (w/w)


   species                moles        grams         conc        log
conc      log g      log act

   H2O                  5.55750E+01   1.00119E+03
   NA+                  5.88031E-01   1.35187E+01   5.87330E-01     -.
23112     -.25450     -.48562
   CA++                 5.11797E-06   2.05128E-04   5.11186E-06
-5.29142    -1.01800    -6.30942
   MG++                 8.04642E-08   1.95568E-06   8.03682E-08
-7.09492    -1.01800    -8.11292
```

```
   AL+++                     1.81663E-23   4.90154E-22   1.81446E-23
-22.74125    -2.29050   -25.03176
   H4SIO4(AQ)                4.32988E-03   4.16165E-01   4.32472E-03
-2.36404       .00000    -2.36404
   H+                        2.09003E-07   2.10654E-07   2.08754E-07
-6.68037     -.25450    -6.93487
   CL-                       4.54137E-01   1.61005E+01   4.53595E-01      -.
34333     -.25450     -.59783
   FE++                      5.65765E-10   3.15963E-08   5.65091E-10
-9.24788    -1.01800   -10.26588
   O2(AQ)                    4.62501E-31   1.47995E-29   4.61949E-31
-30.33541       .00000   -30.33541
   H2(AQ)                    1.72467E-02   3.47659E-02   1.72261E-02
-1.76381       .00000    -1.76381
   FE+++                     1.70325E-23   9.51213E-22   1.70122E-23
-22.76924    -2.29050   -25.05974
   OH-                       1.29306E-01   2.19915E+00   1.29152E-01      -.
88890     -.25450    -1.14340
   H8SI3O10(AQ)              4.12023E-10   1.03959E-07   4.11532E-10
-9.38560       .00000    -9.38560
   H6SI2O7(AQ)               5.06522E-05   8.82434E-03   5.05918E-05
-4.29592       .00000    -4.29592
   AL(OH)3(AQ)               1.01061E-06   7.88309E-05   1.00940E-06
-5.99594       .00000    -5.99594
   AL(OH)4-                  4.27900E-04   4.06551E-02   4.27390E-04
-3.36918     -.25450    -3.62368
   AL(OH)SI(OH)-             3.33484E-04   5.77295E-02   3.33086E-04
-3.47744     -.25450    -3.73194
   CACL+                     9.95093E-06   7.51624E-04   9.93907E-06
-5.00265     -.25450    -5.25715
   CACL2(AQ)                 1.73603E-07   1.92675E-05   1.73396E-07
-6.76096       .00000    -6.76096
   CA(OH)+                   3.23664E-05   1.84771E-03   3.23279E-05
-4.49042     -.25450    -4.74492
   CA(H3SIO4)+               1.14851E-04   1.55263E-02   1.14714E-04
-3.94038     -.25450    -4.19488
   FE(OH)+                   3.24463E-08   2.36385E-06   3.24076E-08
-7.48935     -.25450    -7.74385
   FE(OH)2                   4.77186E-07   4.28807E-05   4.76616E-07
-6.32183       .00000    -6.32183
   FE(OH)3-                  1.06721E-05   1.14051E-03   1.06593E-05
-4.97227     -.25450    -5.22677
   FECL+                     5.77443E-10   5.27205E-08   5.76754E-10
-9.23901     -.25450    -9.49351
   FECL2(AQ)                 1.29144E-08   1.63694E-06   1.28990E-08
-7.88944       .00000    -7.88944
   FE(H3SIO4)+               1.71125E-04   2.58319E-02   1.70921E-04
-3.76721     -.25450    -4.02171
   MGCL+                     7.39057E-08   4.41646E-06   7.38176E-08
-7.13184     -.25450    -7.38634
```

```
   MG(OH)+              3.61590E-06   1.49381E-04   3.61159E-06
-5.44230     -.25450    -5.69680
   MG(OH)2(AQ)          5.05804E-01   2.94983E+01   5.05201E-01     -.
29654      .00000     -.29654
   MG(H3SIO4)+          5.38631E-09   6.43189E-07   5.37989E-09
-8.26923     -.25450    -8.52373
   NACL(AQ)             4.58526E-02   2.67975E+00   4.57979E-02
-1.33915      .00000    -1.33915
   NAOH(AQ)             4.04053E-02   1.61609E+00   4.03571E-02
-1.39408      .00000    -1.39408
   H3SIO4-              4.15826E-03   3.95479E-01   4.15330E-03
-2.38161     -.25450    -2.63611
   HCL(AQ)              2.52666E-07   9.21241E-06   2.52364E-07
-6.59797      .00000    -6.59797

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.4492480
           log (CA++  /h+**0)            7.5603105
           log (MG++  /h+**0)            5.7568157
           log (AL+++ /h+**0)           -4.2271569
           log (FE++  /h+**0)            3.6038493
           log (FE+++ /h+**0)           -4.2551447


           --- summary of solid product phases---


  product                        log moles        moles        grams
volume, cc

   MAGNETITE                    -2.1681658    6.78944E-03    1.57202E+00
3.02266E-01
   ANTIGORITE                   -3.0378349    9.16569E-04    2.07875E+00
7.98542E-01

   CLINOPYROXENE(SS)             -.5126615    3.07141E-01    6.75882E+01
2.03285E+01
   DIOPSIDE                      -.5654899    2.71963E-01    5.88943E+01
1.80040E+01
   HEDENBERGITE                 -1.4628563    3.44464E-02    8.54596E+00
2.28035E+00
   JADEITE                      -3.1355252    7.31939E-04    1.47953E-01
4.41652E-02

   CHLORITE(SS)                  -.2346134    5.82622E-01    6.63519E+01
2.46587E+01
   CLINOCHLORE                   -.2738638    5.32275E-01    5.91674E+01
2.25099E+01
```

```
   CHAMOSITE                 -1.2980302    5.03466E-02    7.18452E+00
2.14879E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  1.9999357    9.99852E+01    2.31504E+04
4.45134E+03
   TREMOLITE                  1.9999204    9.99817E+01    8.12222E+04
2.72630E+04
   ANTIGORITE                -3.0378349    9.16569E-04    2.07875E+00
7.98542E-01

   PLAGIOCLASE(SS)            1.9992718    9.98325E+01

   ALBITE                     1.7774231    5.98995E+01    1.57070E+04
6.03966E+03
   ANORTHITE                  1.6013318    3.99330E+01    1.11097E+04
4.02325E+03


   CLINOPYROXENE(SS)          2.0004567    1.00105E+02

   DIOPSIDE                   1.9036890    8.01104E+01    1.73481E+04
5.30331E+03
   HEDENBERGITE               1.3009010    1.99941E+01    4.96041E+03
1.32361E+03
   JADEITE                   -3.1355252    7.31939E-04    1.47953E-01
4.41652E-02


   CHLORITE(SS)               -.2346134    5.82622E-01

   CLINOCHLORE                -.2738638    5.32275E-01    5.91674E+01
2.25099E+01
   CHAMOSITE                 -1.2980302    5.03466E-02    7.18452E+00
2.14879E+00



                       mass, grams        volume, cc

           created        1.375909E+02       4.608799E+01
           destroyed      1.098854E+02       3.621092E+01
           net            2.770545E+01       9.877068E+00
```

warning-- these volume totals may be incomplete because
of missing partial molar volume data in the data base

--- mineral saturation state summary ---

mineral	affinity, kcal	state	mineral	affinity, kcal	state
MAGNETITE	.0000	satd	HEMATITE	-3.0525	
PERICLASE	-5.9114		BRUCITE	-2.1751	
DIASPORE	-6.6461		FORSTERITE	-.7012	
FAYALITE	-1.2428		CHRYSOTILE	-.8190	
ENSTATITE-CL	-1.7199		ENSTATITE-OR	-1.7980	
ENSTATITE-PR	-2.2033		DIOPSIDE	-.1748	
HEDENBERGITE	-3.1442		JADEITE	-8.6791	
FERROSILITE	-3.2274		WOLLASTONITE	-4.1497	
PSEUDOWOLLASTONITE	-4.6358		TREMOLITE	-2.7743	
ANTIGORITE	.0000	satd	TALC	-3.9952	
CLINOCHLORE	-.1299		CHAMOSITE	-3.5189	
PYROPE	-7.0193		ALMANDINE	-6.3125	
GROSSULAR	-4.7122		QUARTZ-ALPHA	-4.1145	
QUARTZ-BETA	-4.3514		COESITE	-4.7108	
IRON-ALPHA	-9.8498		IRON-GAMMA	-8.9931	
HALITE	-9.6291		CRISTOBALITE-ALPHA	-5.4004	
CRISTOBALITE-BETA	-6.1138				

--- summary of solid solutions ---

mineral	aff. kcal/mol	mole frac.	lambda	state

```
 PLAGIOCLASE(SS)         -11.3173
     ALBITE                    -11.31728     .9909646     1.00000
     ANORTHITE                 -11.31728     .0090354     1.00000

 ORTHOPYROXENE(SS)        -1.3457
     ENSTATITE-OR               -1.34573     .7300033     1.00000
     FERROSILITE                -1.34573     .2699967     1.00000

 GARNET(SS)               -4.1018
     PYROPE                     -4.10183     .1313218     1.00000
     ALMANDINE                  -4.10183     .2147423     1.00000
     GROSSULAR                  -4.10183     .6539359     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .8854654     1.00000
     HEDENBERGITE                 .00000     .1121515     1.00000
     JADEITE                      .00000     .0023831     1.00000

 CPX_SUBCALCIC(SS)         -.0034
     DIOPSIDE                    -.00343     .8875806     1.00000
     HEDENBERGITE                -.00343     .1124194     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9135862     1.00000
     CHAMOSITE                    .00000     .0864138     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .8855    1.0000     .8855    -.0528     .0000    -.0528
     HEDENBERGITE
              .1122    1.0000     .1122    -.9502     .0000    -.9502
     JADEITE
              .0024    1.0000     .0024   -2.6229     .0000   -2.6229

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9136    1.0000     .9136    -.0393     .0000    -.0393
     CHAMOSITE
```

```
              .0864    1.0000     .0864   -1.0634     .0000   -1.0634


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -26.26051       5.48901E-27
   H2(G)                          2.00809       1.01880E+02
   H2O(G)                         3.80604       6.39786E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.1190E-01, delzi=  1.1903E-02, nord= 6
               ncycle=  0
 steps completed =    59, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -2.8865

 stepping to zi=  1.2562E-01, delzi=  1.3716E-02, nord= 6
               ncycle=  0
 steps completed =    60, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(JADEITE           ) =     -2.5886
 * note - a search for where a phase supersaturates
        indicates that the event being searched for
        does not take place in the interval being
        examined (search)
               the phase is CPX_SUBCALCIC(SS)
               delzi will not be decreased

 stepping to zi=  1.3909E-01, delzi=  1.3471E-02, nord= 6
               ncycle=  0
 steps completed =    61, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(O2(G)             ) =    -25.4270

 stepping to zi=  1.5190E-01, delzi=  1.2811E-02, nord= 6
               ncycle=  0
 steps completed =    62, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(O2(G)             ) =    -25.0185

 stepping to zi=  1.5849E-01, delzi=  6.5890E-03, nord= 6
               ncycle=  0
 steps completed =    63, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(O2(G)             ) =    -24.8002
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
                    reaction progress        =  1.58489319246109E-01
                    log of reaction progress =       -.8000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.97345E+01    2.65517E-01    2.67904E+04
7.13226E+01
   CLINOPYROXENE(SS)      9.96800E+01    3.20022E-01    2.22148E+04
7.13203E+01
   MAGNETITE              9.99658E+01    3.42337E-02    2.31459E+04
7.92642E+00
   TREMOLITE              9.99710E+01    2.90352E-02    8.12135E+04
2.35874E+01


                current total mass =  1.53365E+05 grams
                delta total mass   =  1.74157E+02 grams
                delta total volume =     57.39044 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)            9.4162    1.67530E+00
   CLINOPYROXENE(SS)           .0696    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                   .1939    1.83200E-01

          affinity of the overall irreversible reaction=    15.810
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included
```

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.541967E+05	5.632641E+01	5.638867E+01
NA	1.566855E+04	7.190384E-01	7.198331E-01
CA	3.029912E+00	7.975543E-05	7.984358E-05
MG	5.712166E+03	2.479494E-01	2.482235E-01
AL	5.177941E+01	2.024642E-03	2.026880E-03
SI	7.396092E+02	2.778293E-02	2.781364E-02
H	1.068322E+05	1.118259E+02	1.119495E+02
CL	1.678361E+04	4.994480E-01	5.000000E-01
FE	1.241291E+01	2.344940E-04	2.347532E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	7.0083	.4679	3.2610E+00
modified nbs ph scale	6.7502	.5049	3.5190E+00
rational ph scale	6.7502	.5049	3.5190E+00

phcl = 7.6112

oxygen fugacity = 1.58429E-25
log oxygen fugacity = -24.80017

activity of water = .98386
log activity of water = -.00707
alkalinity = 0.000000E+00 equiv/kg solvent
(not def. for t.gt.50 c)

```
                   ionic strength =  6.216962E-01 molal
                sum of molalities =    1.6043879003053
              osmotic coefficient =     .56288
                   equiv. stoich. ionic strength =  4.994480E-01
molal

                        mass of solution =   1.056179 kg
                        mass of solvent  =   1.001105 kg
                        mass of solutes  =    .055074 kg
                        conc of solutes  =   5.214458 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55700E+01   1.00111E+03
   NA+                  6.22073E-01   1.43013E+01   6.21386E-01     -.
20664     -.25802     -.46466
   CA++                 9.85067E-07   3.94815E-05   9.83979E-07
-6.00701    -1.03207    -7.03909
   MG++                 2.90891E-08   7.07011E-07   2.90570E-08
-7.53675    -1.03207    -8.56882
   AL+++                1.49161E-23   4.02458E-22   1.48996E-23
-22.82683    -2.32217   -25.14899
   H4SIO4(AQ)           1.18255E-02   1.13660E+00   1.18124E-02
-1.92766      .00000    -1.92766
   H+                   1.77922E-07   1.79328E-07   1.77726E-07
-6.75025     -.25802    -7.00827
   CL-                  4.52444E-01   1.60405E+01   4.51945E-01     -.
34491     -.25802     -.60293
   FE++                 2.37946E-10   1.32885E-08   2.37683E-10
-9.62400    -1.03207   -10.65608
   O2(AQ)               1.33479E-29   4.27117E-28   1.33332E-29
-28.87507      .00000   -28.87507
   H2(AQ)               3.20994E-03   6.47060E-03   3.20640E-03
-2.49398      .00000    -2.49398
   FE+++                1.46014E-23   8.15443E-22   1.45853E-23
-22.83609    -2.32217   -25.15825
   OH-                  1.54348E-01   2.62504E+00   1.54178E-01     -.
81198     -.25802    -1.07000
   H8SI3O10(AQ)         8.39509E-09   2.11820E-06   8.38582E-09
-8.07645      .00000    -8.07645
   H6SI2O7(AQ)          3.77852E-04   6.58272E-02   3.77435E-04
-3.42316      .00000    -3.42316
   AL(OH)3(AQ)          1.28089E-06   9.99135E-05   1.27947E-06
-5.89297      .00000    -5.89297
   AL(OH)4-             6.47426E-04   6.15124E-02   6.46711E-04
-3.18929     -.25802    -3.44731
   AL(OH)SI(OH)-        1.37817E-03   2.38576E-01   1.37665E-03
```

```
-2.86118     -.25802    -3.11919
   CACL+                1.84746E-06   1.39544E-04   1.84542E-06
-5.73390     -.25802    -5.99192
   CACL2(AQ)            3.15972E-08   3.50685E-06   3.15623E-08
-7.50083      .00000    -7.50083
   CA(OH)+              7.19963E-06   4.11007E-04   7.19168E-06
-5.14317     -.25802    -5.40119
   CA(H3SIO4)+          6.97798E-05   9.43331E-03   6.97028E-05
-4.15675     -.25802    -4.41477
   FE(OH)+              1.57708E-08   1.14897E-06   1.57533E-08
-7.80263     -.25802    -8.06065
   FE(OH)2              2.72432E-07   2.44812E-05   2.72131E-07
-6.56522      .00000    -6.56522
   FE(OH)3-             7.27343E-06   7.77304E-04   7.26540E-06
-5.13874     -.25802    -5.39676
   FECL+                2.34258E-10   2.13877E-08   2.33999E-10
-9.63079     -.25802    -9.88880
   FECL2(AQ)            5.13616E-09   6.51024E-07   5.13049E-09
-8.28984      .00000    -8.28984
   FE(H3SIO4)+          2.27186E-04   3.42946E-02   2.26935E-04
-3.64410     -.25802    -3.90212
   MGCL+                2.57721E-08   1.54009E-06   2.57436E-08
-7.58933     -.25802    -7.84735
   MG(OH)+              1.51075E-06   6.24124E-05   1.50908E-06
-5.82129     -.25802    -6.07931
   MG(OH)2(AQ)          2.48222E-01   1.44762E+01   2.47948E-01     -.
60564      .00000     -.60564
   MG(H3SIO4)+          6.14677E-09   7.33997E-07   6.13999E-09
-8.21183     -.25802    -8.46985
   NACL(AQ)             4.75537E-02   2.77917E+00   4.75012E-02
-1.32330      .00000    -1.32330
   NAOH(AQ)             5.02068E-02   2.00812E+00   5.01513E-02
-1.29972      .00000    -1.29972
   H3SIO4-              1.35573E-02   1.28939E+00   1.35423E-02
-1.86831     -.25802    -2.12632
   HCL(AQ)              2.10865E-07   7.68832E-06   2.10632E-07
-6.67648      .00000    -6.67648

           --- activity ratios of cations ---


           log (NA+   /h+**0)           6.5436111
           log (CA++  /h+**0)           6.9774482
           log (MG++  /h+**0)           5.4477131
           log (AL+++ /h+**0)          -4.1241885
           log (FE++  /h+**0)           3.3604600
           log (FE+++ /h+**0)          -4.1334487


           --- summary of solid product phases---
```

```
  product                          log moles        moles        grams
volume, cc

   MAGNETITE                     -2.2687037    5.38637E-03    1.24715E+00
2.39801E-01
   ANTIGORITE                    -3.4862114    3.26429E-04    7.40332E-01
2.84395E-01

   CLINOPYROXENE(SS)              -.3017263    4.99199E-01    1.09867E+02
3.29651E+01
   DIOPSIDE                       -.3737576    4.22905E-01    9.15810E+01
2.79963E+01
   HEDENBERGITE                  -1.2054107    6.23145E-02    1.54599E+01
4.12522E+00
   JADEITE                       -1.8544964    1.39799E-02    2.82588E+00
8.43546E-01

   CHLORITE(SS)                   -.0509538    8.89296E-01    1.01634E+02
3.76427E+01
   CLINOCHLORE                    -.0962921    8.01139E-01    8.90541E+01
3.38802E+01
   CHAMOSITE                     -1.0547452    8.81566E-02    1.25801E+01
3.76252E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member         log moles        moles        grams
volume, cc

   MAGNETITE                      1.9998747    9.99712E+01    2.31472E+04
4.45072E+03
   TREMOLITE                      1.9998739    9.99710E+01    8.12135E+04
2.72601E+04
   ANTIGORITE                    -3.4862114    3.26429E-04    7.40332E-01
2.84395E-01

   PLAGIOCLASE(SS)                1.9988453    9.97345E+01

   ALBITE                         1.7769966    5.98407E+01    1.56916E+04
6.03374E+03
   ANORTHITE                      1.6009053    3.98938E+01    1.10988E+04
4.01930E+03


   CLINOPYROXENE(SS)              2.0007775    1.00179E+02
```

```
   DIOPSIDE                   1.9039950    8.01669E+01    1.73603E+04
5.30705E+03
   HEDENBERGITE               1.3009933    1.99983E+01    4.96147E+03
1.32389E+03
   JADEITE                   -1.8544964    1.39799E-02    2.82588E+00
8.43546E-01


   CHLORITE(SS)               -.0509538    8.89296E-01

   CLINOCHLORE                -.0962921    8.01139E-01    8.90541E+01
3.38802E+01
   CHAMOSITE                 -1.0547452    8.81566E-02    1.25801E+01
3.76252E+00



                          mass, grams        volume, cc

              created        2.134885E+02       7.113194E+01
              destroyed      1.741566E+02       5.739044E+01
              net            3.933183E+01       1.374150E+01

             warning-- these volume totals may be incomplete because
             of missing partial molar volume data in the data base



              --- mineral saturation state summary ---


   mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-2.2471
 PERICLASE              -6.9342                BRUCITE
-3.1979
 DIASPORE               -6.3054                FORSTERITE
-1.0020
 FAYALITE               -1.3262                CHRYSOTILE
-.9995
 ENSTATITE-CL           -1.2987                ENSTATITE-OR
-1.3768
 ENSTATITE-PR           -1.7822                DIOPSIDE
-.2384
 HEDENBERGITE           -2.9903                JADEITE
-5.1381
 FERROSILITE            -2.5888                WOLLASTONITE
-4.6344
```

```
 PSEUDOWOLLASTONITE      -5.1205                TREMOLITE
-.1939
 ANTHOPHYLLITE           -8.2374                ALBITE
-6.3454
 ANTIGORITE                .0000  satd          TALC
-1.2877
 CLINOCHLORE              -.1500                CHAMOSITE
-3.3216
 PYROPE                  -6.3722                ALMANDINE
-5.4478
 GROSSULAR               -4.9719                QUARTZ-ALPHA
-2.6705
 QUARTZ-BETA             -2.9074                COESITE
-3.2668
 HALITE                  -9.5766                CRISTOBALITE-ALPHA
-3.9564
 CRISTOBALITE-BETA       -4.6698


                    --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -6.3441
     ALBITE                      -6.34409     .9991111     1.00000
     ANORTHITE                   -6.34409     .0008889     1.00000

 ORTHOPYROXENE(SS)          -.8625
     ENSTATITE-OR                 -.86254     .6991658     1.00000
     FERROSILITE                  -.86254     .3008342     1.00000

 GARNET(SS)                -3.9088
     PYROPE                      -3.90877     .1801101     1.00000
     ALMANDINE                   -3.90877     .3426871     1.00000
     GROSSULAR                   -3.90877     .4772028     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .8471663     1.00000
     HEDENBERGITE                  .00000     .1248290     1.00000
     JADEITE                       .00000     .0280046     1.00000

 CPX_SUBCALCIC(SS)          -.0408
     DIOPSIDE                     -.04082     .8715744     1.00000
     HEDENBERGITE                 -.04082     .1284256     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9008692     1.00000
     CHAMOSITE                     .00000     .0991308     1.00000
```

```
 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .8472    1.0000     .8472    -.0720     .0000    -.0720
     HEDENBERGITE
              .1248    1.0000     .1248    -.9037     .0000    -.9037
     JADEITE
              .0280    1.0000     .0280   -1.5528     .0000   -1.5528

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9009    1.0000     .9009    -.0453     .0000    -.0453
     CHAMOSITE
              .0991    1.0000     .0991   -1.0038     .0000   -1.0038


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -24.80017       1.58429E-25
   H2(G)                          1.27792       1.89635E+01
   H2O(G)                         3.80603       6.39785E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.6343E-01, delzi=  4.9387E-03, nord= 6
              ncycle=  0
 iter =    5
       1 supersaturated pure minerals
       0 supersaturated solid solutions

                         the most supersaturated phases     affinity,
kcal
```

```
                            1      32   TREMOLITE                .
01571197
 --- go back to reduce the extent of supersaturation ---
 --- cutting step size and trying again ---

 stepping to zi=  1.5972E-01, delzi=  1.2347E-03, nord= 6
               ncycle=  0
 steps completed =    64, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -3.5449

 stepping to zi=  1.6219E-01, delzi=  2.4693E-03, nord= 4
               ncycle=  0
 steps completed =    65, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -3.7015

 stepping to zi=  1.6327E-01, delzi=  1.0725E-03, nord= 5
               ncycle=  0
 iter =    4
       1 supersaturated pure minerals
       0 supersaturated solid solutions

                          the most supersaturated phases     affinity,
kcal

                            1      32   TREMOLITE                .
00906211


   attempted species assemblage no.   2

              1      1  H2O
              2      2  NA+
              3      4  CA++
              4      5  MG++
              5      6  AL+++
              6      7  H4SIO4(AQ)
              7     13  H+
              8     16  CL-
              9     21  FE++
             10     32  O2(G)
             11      1  MAGNETITE
             12     32  TREMOLITE
             13     39  ANTIGORITE
             14      1  CLINOPYRDIOPSIDE
             15      2  CLINOPYRHEDENBERGITE
             16      3  CLINOPYRJADEITE
             17      1  CHLORITECLINOCHLORE
             18      2  CHLORITECHAMOSITE

 steps completed =    66, iter = 11, ncorr = 0
```

- -

```
                    reaction progress        =  1.63265798963150E-01
                    log of reaction progress =       -.7871048

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000
```

change in the product phase assemblage

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.97265E+01	2.73519E-01	2.67883E+04	7.34720E+01
CLINOPYROXENE(SS)	9.96703E+01	3.29666E-01	2.22126E+04	7.34697E+01
MAGNETITE	9.99647E+01	3.52654E-02	2.31457E+04	8.16530E+00
TREMOLITE	9.99701E+01	2.99103E-02	8.12127E+04	2.42982E+01

```
               current total mass =  1.53359E+05 grams
               delta total mass   =  1.79405E+02 grams
               delta total volume =     59.12005 cc
```

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	9.1412	1.67530E+00
CLINOPYROXENE(SS)	.0779	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	.0000	0.00000E+00

affinity of the overall irreversible reaction=   15.314 kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.543520E+05	5.630983E+01	5.637069E+01
NA	1.570882E+04	7.205430E-01	7.213217E-01
CA	2.918975E+00	7.679868E-05	7.688168E-05
MG	5.408474E+03	2.346552E-01	2.349088E-01
AL	5.588234E+01	2.184031E-03	2.186392E-03
SI	8.022040E+02	3.011991E-02	3.015246E-02
H	1.068650E+05	1.118070E+02	1.119278E+02
CL	1.679202E+04	4.994602E-01	5.000000E-01
FE	1.265068E+01	2.388719E-04	2.391301E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	7.0085	.4732	3.2978E+00
modified nbs ph scale	6.7503	.5102	3.5560E+00
rational ph scale	6.7503	.5102	3.5560E+00

phcl = 7.6116

oxygen fugacity = 2.22734E-25
log oxygen fugacity = -24.65221

activity of water = .98386
log activity of water = -.00707

```
               alkalinity =  0.000000E+00 equiv/kg solvent
                                           (not def. for t.gt.50 c)

                    ionic strength =  6.230225E-01 molal
                 sum of molalities =    1.5944434680374
               osmotic coefficient =     .56641
                    equiv. stoich. ionic strength =  4.994602E-01
molal

                         mass of solution =   1.055651 kg
                         mass of solvent  =   1.001081 kg
                         mass of solutes  =    .054570 kg
                         conc of solutes  =   5.169296 per cent (w/w)


   species                moles         grams          conc         log
conc      log g      log act

   H2O                  5.55687E+01   1.00108E+03
   NA+                  6.23384E-01   1.43314E+01   6.22710E-01     -.
20571     -.25815     -.46387
   CA++                 8.86325E-07   3.55239E-05   8.85369E-07
-6.05288    -1.03261    -7.08548
   MG++                 2.75384E-08   6.69322E-07   2.75087E-08
-7.56053    -1.03261    -8.59314
   AL+++                1.52617E-23   4.11783E-22   1.52452E-23
-22.81687    -2.32337   -25.14023
   H4SIO4(AQ)           1.27819E-02   1.22853E+00   1.27681E-02
-1.89387      .00000    -1.89387
   H+                   1.77894E-07   1.79300E-07   1.77702E-07
-6.75031     -.25815    -7.00846
   CL-                  4.52379E-01   1.60382E+01   4.51891E-01     -.
34497     -.25815     -.60312
   FE++                 2.24885E-10   1.25592E-08   2.24642E-10
-9.64851    -1.03261   -10.68112
   O2(AQ)               1.87653E-29   6.00467E-28   1.87450E-29
-28.72711      .00000   -28.72711
   H2(AQ)               2.70714E-03   5.45705E-03   2.70421E-03
-2.56796      .00000    -2.56796
   FE+++                1.50432E-23   8.40118E-22   1.50270E-23
-22.82313    -2.32337   -25.14650
   OH-                  1.54459E-01   2.62693E+00   1.54293E-01     -.
81166     -.25815    -1.06981
   H8SI3O10(AQ)         1.06017E-08   2.67496E-06   1.05903E-08
-7.97509      .00000    -7.97509
   H6SI2O7(AQ)          4.41454E-04   7.69076E-02   4.40978E-04
-3.35558      .00000    -3.35558
   AL(OH)3(AQ)          1.30867E-06   1.02081E-04   1.30726E-06
-5.88364      .00000    -5.88364
   AL(OH)4-             6.61962E-04   6.28935E-02   6.61248E-04
```

```
-3.17964     -.25815    -3.43779
   AL(OH)SI(OH)-         1.52312E-03   2.63668E-01   1.52148E-03
-2.81773     -.25815    -3.07589
   CACL+                 1.66004E-06   1.25388E-04   1.65825E-06
-5.78035     -.25815    -6.03850
   CACL2(AQ)             2.83709E-08   3.14877E-06   2.83403E-08
-7.54760      .00000    -7.54760
   CA(OH)+               6.47482E-06   3.69630E-04   6.46783E-06
-5.18924     -.25815    -5.44739
   CA(H3SIO4)+           6.78321E-05   9.17001E-03   6.77589E-05
-4.16903     -.25815    -4.42719
   FE(OH)+               1.48979E-08   1.08538E-06   1.48819E-08
-7.82734     -.25815    -8.08549
   FE(OH)2               2.57388E-07   2.31293E-05   2.57110E-07
-6.58988      .00000    -6.58988
   FE(OH)3-              6.87691E-06   7.34928E-04   6.86948E-06
-5.16308     -.25815    -5.42123
   FECL+                 2.21102E-10   2.01866E-08   2.20863E-10
-9.65588     -.25815    -9.91403
   FECL2(AQ)             4.84416E-09   6.14012E-07   4.83893E-09
-8.31525      .00000    -8.31525
   FE(H3SIO4)+           2.31976E-04   3.50176E-02   2.31725E-04
-3.63503     -.25815    -3.89318
   MGCL+                 2.43654E-08   1.45603E-06   2.43391E-08
-7.61370     -.25815    -7.87185
   MG(OH)+               1.42952E-06   5.90569E-05   1.42798E-06
-5.84528     -.25815    -6.10343
   MG(OH)2(AQ)           2.34907E-01   1.36997E+01   2.34654E-01     -.
62957      .00000     -.62957
   MG(H3SIO4)+           6.28686E-09   7.50726E-07   6.28008E-09
-8.20204     -.25815    -8.46019
   NACL(AQ)              4.76190E-02   2.78299E+00   4.75676E-02
-1.32269      .00000    -1.32269
   NAOH(AQ)              5.03192E-02   2.01262E+00   5.02649E-02
-1.29874      .00000    -1.29874
   H3SIO4-               1.46647E-02   1.39471E+00   1.46489E-02
-1.83420     -.25815    -2.09235
   HCL(AQ)               2.10677E-07   7.68149E-06   2.10450E-07
-6.67685      .00000    -6.67685

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.5445931
           log (CA++  /h+**0)            6.9314342
           log (MG++  /h+**0)            5.4237805
           log (AL+++ /h+**0)           -4.1148576
           log (FE++  /h+**0)            3.3358014
           log (FE+++ /h+**0)           -4.1211191
```

```
           --- summary of solid product phases---


  product                       log moles        moles        grams
volume, cc

   MAGNETITE                   -2.2280243    5.91528E-03    1.36962E+00
2.63348E-01
   TREMOLITE                   -3.2994276    5.01848E-04    4.07687E-01
1.36844E-01
   ANTIGORITE                  -4.2861062    5.17480E-05    1.17363E-01
4.50844E-02

   CLINOPYROXENE(SS)            -.2872607    5.16106E-01    1.13532E+02
3.40649E+01
   DIOPSIDE                     -.3616637    4.34847E-01    9.41671E+01
2.87869E+01
   HEDENBERGITE                -1.1940428    6.39672E-02    1.58699E+01
4.23463E+00
   JADEITE                     -1.7621430    1.72925E-02    3.49548E+00
1.04343E+00

   CHLORITE(SS)                 -.0416165    9.08623E-01    1.03839E+02
3.84607E+01
   CLINOCHLORE                  -.0868829    8.18686E-01    9.10046E+01
3.46222E+01
   CHAMOSITE                   -1.0460620    8.99369E-02    1.28341E+01
3.83851E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member         log moles        moles        grams
volume, cc

   MAGNETITE                    1.9998725    9.99706E+01    2.31471E+04
4.45069E+03
   TREMOLITE                    1.9998723    9.99706E+01    8.12131E+04
2.72600E+04
   ANTIGORITE                  -4.2861062    5.17480E-05    1.17363E-01
4.50844E-02

   PLAGIOCLASE(SS)              1.9988105    9.97265E+01

   ALBITE                       1.7769617    5.98359E+01    1.56903E+04
6.03325E+03
   ANORTHITE                    1.6008705    3.98906E+01    1.10979E+04
4.01898E+03
```

```
   CLINOPYROXENE(SS)         2.0008089    1.00186E+02

   DIOPSIDE                  1.9040179    8.01711E+01    1.73612E+04
5.30733E+03
   HEDENBERGITE              1.3009873    1.99980E+01    4.96140E+03
1.32387E+03
   JADEITE                  -1.7621430    1.72925E-02    3.49548E+00
1.04343E+00


   CHLORITE(SS)              -.0416165    9.08623E-01

   CLINOCHLORE               -.0868829    8.18686E-01    9.10046E+01
3.46222E+01
   CHAMOSITE                -1.0460620    8.99369E-02    1.28341E+01
3.83851E+00


                        mass, grams        volume, cc

           created         2.192659E+02       7.297091E+01
           destroyed       1.794053E+02       5.912005E+01
           net             3.986060E+01       1.385086E+01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE              .0000  satd          HEMATITE
-2.1655
 PERICLASE            -7.0134                BRUCITE
-3.2771
 DIASPORE             -6.2745                FORSTERITE
-1.0253
 FAYALITE             -1.3519                CHRYSOTILE
-1.0135
 ENSTATITE-CL         -1.2661                ENSTATITE-OR
-1.3442
 ENSTATITE-PR         -1.7496                DIOPSIDE
-.2462
```

```
 HEDENBERGITE           -3.0006                JADEITE
-4.8804
 FERROSILITE            -2.5586                WOLLASTONITE
-4.6749
 PSEUDOWOLLASTONITE     -5.1610
TREMOLITE                .0000  satd
 ANTHOPHYLLITE          -7.8973                ALBITE
-5.9758
 ANTIGORITE               .0000  satd          TALC
-1.0781
 CLINOCHLORE             -.1498                CHAMOSITE
-3.3237
 PYROPE                 -6.3191                ALMANDINE
-5.3971
 GROSSULAR              -4.9920                QUARTZ-ALPHA
-2.5587
 QUARTZ-BETA            -2.7956                COESITE
-3.1550
 HALITE                 -9.5746                CRISTOBALITE-ALPHA
-3.8446
 CRISTOBALITE-BETA      -4.5580


                   --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -5.9748
     ALBITE                      -5.97475     .9992458     1.00000
     ANORTHITE                   -5.97475     .0007542     1.00000

 ORTHOPYROXENE(SS)          -.8307
     ENSTATITE-OR                 -.83065     .6995173     1.00000
     FERROSILITE                  -.83065     .3004827     1.00000

 GARNET(SS)                -3.8910
     PYROPE                      -3.89096     .1845868     1.00000
     ALMANDINE                   -3.89096     .3506175     1.00000
     GROSSULAR                   -3.89096     .4647957     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .8425525     1.00000
     HEDENBERGITE                  .00000     .1239418     1.00000
     JADEITE                       .00000     .0335056     1.00000

 CPX_SUBCALCIC(SS)          -.0490
     DIOPSIDE                     -.04898     .8717614     1.00000
     HEDENBERGITE                 -.04898     .1282386     1.00000
```

```
 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9010184     1.00000
     CHAMOSITE                     .00000     .0989816     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .8426    1.0000     .8426    -.0744     .0000    -.0744
     HEDENBERGITE
             .1239    1.0000     .1239    -.9068     .0000    -.9068
     JADEITE
             .0335    1.0000     .0335   -1.4749     .0000   -1.4749

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
             .9010    1.0000     .9010    -.0453     .0000    -.0453
     CHAMOSITE
             .0990    1.0000     .0990   -1.0044     .0000   -1.0044


           --- summary of gas species ---

           gas                 log fugacity         fugacity
partial pressure

   O2(G)                         -24.65221       2.22734E-25
   H2(G)                           1.20394       1.59934E+01
   H2O(G)                          3.80603       6.39785E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.6327E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =    67, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -4.2862
```

```
 stepping to zi=  1.6327E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =    68, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -4.2862

 stepping to zi=  1.6327E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =    69, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -4.2862

 stepping to zi=  1.6327E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =    70, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -4.2863

 stepping to zi=  1.6327E-01, delzi=  1.0000E-07, nord= 2
              ncycle=  0
 steps completed =    71, iter =  3, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -4.2867

 stepping to zi=  1.6327E-01, delzi=  1.0000E-06, nord= 2
              ncycle=  0
 steps completed =    72, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -4.2912

 stepping to zi=  1.6328E-01, delzi=  1.0000E-05, nord= 2
              ncycle=  0
 steps completed =    73, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ANTIGORITE        ) =     -4.3384

 stepping to zi=  1.6336E-01, delzi=  8.7040E-05, nord= 2
                    the phase to be dropped is ANTIGORITE
(   39)


   attempted species assemblage no.   2

             1      1  H2O
             2      2  NA+
             3      4  CA++
             4      5  MG++
             5      6  AL+++
             6      7  H4SIO4(AQ)
             7     13  H+
             8     16  CL-
             9     21  FE++
            10     32  O2(G)
            11      1  MAGNETITE
            12     32  TREMOLITE
            13      1  CLINOPYRDIOPSIDE
```

```
            14       2  CLINOPYRHEDENBERGITE
            15       3  CLINOPYRJADEITE
            16       1  CHLORITECLINOCHLORE
            17       2  CHLORITECHAMOSITE

 steps completed =    74, iter =  5, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  1.63363978726610E-01
                    log of reaction progress =       -.7868437

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 change in the product phase assemblage


                              --- reactant summary ---



        reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.97263E+01    2.73684E-01    2.67882E+04
7.35162E+01
   CLINOPYROXENE(SS)      9.96701E+01    3.29865E-01    2.22126E+04
7.35139E+01
   MAGNETITE              9.99647E+01    3.52866E-02    2.31457E+04
8.17021E+00
   TREMOLITE              9.99701E+01    2.99283E-02    8.12127E+04
2.43128E+01


               current total mass =  1.53359E+05 grams
               delta total mass   =  1.79513E+02 grams
               delta total volume =     59.15560 cc


        reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           9.1408    1.67530E+00
   CLINOPYROXENE(SS)          .0780    0.00000E+00
   MAGNETITE                  .0000    0.00000E+00
   TREMOLITE                  .0000    0.00000E+00
```

affinity of the overall irreversible reaction= 15.314 kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.543504E+05	5.630994E+01	5.637089E+01
NA	1.571078E+04	7.206360E-01	7.214161E-01
CA	2.917746E+00	7.676663E-05	7.684973E-05
MG	5.408368E+03	2.346515E-01	2.349055E-01
AL	5.590566E+01	2.184951E-03	2.187316E-03
SI	8.023906E+02	3.012704E-02	3.015965E-02
H	1.068647E+05	1.118071E+02	1.119281E+02
CL	1.679192E+04	4.994593E-01	5.000000E-01
FE	1.264652E+01	2.387942E-04	2.390527E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	7.0086	.4732	3.2976E+00
modified nbs ph scale	6.7505	.5102	3.5558E+00
rational ph scale	6.7505	.5102	3.5558E+00

phcl = 7.6118

oxygen fugacity = 2.22728E-25

```
          log oxygen fugacity = -24.65223



                    activity of water =    .98386
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                    ionic strength =  6.230881E-01 molal
                 sum of molalities =    1.5945987266673
               osmotic coefficient =     .56635
                    equiv. stoich. ionic strength =  4.994593E-01
molal

                         mass of solution =   1.055656 kg
                         mass of solvent  =   1.001082 kg
                         mass of solutes  =    .054574 kg
                         conc of solutes  =   5.169666 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55688E+01   1.00108E+03
   NA+                  6.23450E-01   1.43330E+01   6.22776E-01     -.
20567     -.25816     -.46383
   CA++                 8.85646E-07   3.54967E-05   8.84689E-07
-6.05321    -1.03263    -7.08584
   MG++                 2.75183E-08   6.68832E-07   2.74885E-08
-7.56085    -1.03263    -8.59348
   AL+++                1.52460E-23   4.11359E-22   1.52295E-23
-22.81732    -2.32343   -25.14074
   H4SIO4(AQ)           1.27822E-02   1.22856E+00   1.27684E-02
-1.89386      .00000    -1.89386
   H+                   1.77828E-07   1.79233E-07   1.77636E-07
-6.75047     -.25816    -7.00863
   CL-                  4.52376E-01   1.60381E+01   4.51887E-01     -.
34497     -.25816     -.60313
   FE++                 2.24725E-10   1.25502E-08   2.24482E-10
-9.64882    -1.03263   -10.68145
   O2(AQ)               1.87648E-29   6.00452E-28   1.87445E-29
-28.72713      .00000   -28.72713
   H2(AQ)               2.70718E-03   5.45713E-03   2.70425E-03
-2.56795      .00000    -2.56795
   FE+++                1.50277E-23   8.39250E-22   1.50114E-23
-22.82358    -2.32343   -25.14700
   OH-                  1.54522E-01   2.62800E+00   1.54355E-01     -.
81148     -.25816    -1.06964
   H8SI3O10(AQ)         1.06025E-08   2.67515E-06   1.05910E-08
```

```
-7.97506      .00000    -7.97506
   H6SI2O7(AQ)          4.41475E-04   7.69111E-02   4.40997E-04
-3.35556      .00000    -3.35556
   AL(OH)3(AQ)          1.30867E-06   1.02081E-04   1.30726E-06
-5.88364      .00000    -5.88364
   AL(OH)4-             6.62232E-04   6.29192E-02   6.61516E-04
-3.17946     -.25816    -3.43762
   AL(OH)SI(OH)-        1.52378E-03   2.63781E-01   1.52213E-03
-2.81755     -.25816    -3.07571
   CACL+                1.65865E-06   1.25283E-04   1.65686E-06
-5.78071     -.25816    -6.03887
   CACL2(AQ)            2.83461E-08   3.14602E-06   2.83154E-08
-7.54798      .00000    -7.54798
   CA(OH)+              6.47209E-06   3.69474E-04   6.46509E-06
-5.18943     -.25816    -5.44758
   CA(H3SIO4)+          6.78050E-05   9.16634E-03   6.77317E-05
-4.16921     -.25816    -4.42737
   FE(OH)+              1.48925E-08   1.08498E-06   1.48763E-08
-7.82750     -.25816    -8.08566
   FE(OH)2              2.57390E-07   2.31295E-05   2.57112E-07
-6.58988      .00000    -6.58988
   FE(OH)3-             6.87973E-06   7.35230E-04   6.87230E-06
-5.16290     -.25816    -5.42106
   FECL+                2.20929E-10   2.01708E-08   2.20690E-10
-9.65622     -.25816    -9.91438
   FECL2(AQ)            4.84018E-09   6.13508E-07   4.83495E-09
-8.31561      .00000    -8.31561
   FE(H3SIO4)+          2.31895E-04   3.50055E-02   2.31645E-04
-3.63518     -.25816    -3.89334
   MGCL+                2.43459E-08   1.45486E-06   2.43195E-08
-7.61404     -.25816    -7.87220
   MG(OH)+              1.42897E-06   5.90339E-05   1.42742E-06
-5.84545     -.25816    -6.10361
   MG(OH)2(AQ)          2.34904E-01   1.36995E+01   2.34650E-01      -.
62958      .00000     -.62958
   MG(H3SIO4)+          6.28456E-09   7.50451E-07   6.27776E-09
-8.20219     -.25816    -8.46035
   NACL(AQ)             4.76223E-02   2.78318E+00   4.75708E-02
-1.32266      .00000    -1.32266
   NAOH(AQ)             5.03434E-02   2.01359E+00   5.02890E-02
-1.29853      .00000    -1.29853
   H3SIO4-              1.46710E-02   1.39531E+00   1.46551E-02
-1.83401     -.25816    -2.09217
   HCL(AQ)              2.10591E-07   7.67832E-06   2.10363E-07
-6.67703      .00000    -6.67703

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.5448016
```

```
          log (CA++  /h+**0)            6.9314127
          log (MG++  /h+**0)            5.4237736
          log (AL+++ /h+**0)           -4.1148572
          log (FE++  /h+**0)            3.3358034
          log (FE+++ /h+**0)           -4.1211201


          --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                  -2.2264671    5.93653E-03    1.37454E+00
2.64294E-01
   TREMOLITE                  -3.1394077    7.25425E-04    5.89314E-01
1.97809E-01

   CLINOPYROXENE(SS)           -.2873809    5.15964E-01    1.13501E+02
3.40554E+01
   DIOPSIDE                    -.3617929    4.34717E-01    9.41391E+01
2.87783E+01
   HEDENBERGITE               -1.1941632    6.39494E-02    1.58655E+01
4.23345E+00
   JADEITE                    -1.7620349    1.72968E-02    3.49635E+00
1.04369E+00

   CHLORITE(SS)                -.0413477    9.09185E-01    1.03903E+02
3.84845E+01
   CLINOCHLORE                 -.0866149    8.19191E-01    9.10608E+01
3.46436E+01
   CHAMOSITE                  -1.0457852    8.99943E-02    1.28423E+01
3.84096E+00


               --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                   1.9998725    9.99706E+01    2.31471E+04
4.45069E+03
   TREMOLITE                   1.9998732    9.99708E+01    8.12133E+04
2.72600E+04

   PLAGIOCLASE(SS)             1.9988098    9.97263E+01

   ALBITE                      1.7769610    5.98358E+01    1.56903E+04
6.03324E+03
```

```
   ANORTHITE                  1.6008698    3.98905E+01    1.10979E+04
4.01897E+03


   CLINOPYROXENE(SS)          2.0008075    1.00186E+02

   DIOPSIDE                   1.9040164    8.01708E+01    1.73612E+04
5.30731E+03
   HEDENBERGITE               1.3009861    1.99980E+01    4.96139E+03
1.32387E+03
   JADEITE                   -1.7620349    1.72968E-02    3.49635E+00
1.04369E+00


   CHLORITE(SS)               -.0413477    9.09185E-01

   CLINOCHLORE                -.0866149    8.19191E-01    9.10608E+01
3.46436E+01
   CHAMOSITE                 -1.0457852    8.99943E-02    1.28423E+01
3.84096E+00



                        mass, grams        volume, cc

           created         2.193679E+02       7.300207E+01
           destroyed       1.795132E+02       5.915560E+01
           net             3.985470E+01       1.384647E+01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-2.1655
 PERICLASE              -7.0134                BRUCITE
-3.2771
 DIASPORE               -6.2745                FORSTERITE
-1.0253
 FAYALITE               -1.3518                CHRYSOTILE
-1.0135
 ENSTATITE-CL           -1.2661                ENSTATITE-OR
-1.3442
```

```
 ENSTATITE-PR           -1.7496                DIOPSIDE
-.2462
 HEDENBERGITE           -3.0006                JADEITE
-4.8797
 FERROSILITE            -2.5585                WOLLASTONITE
-4.6749
 PSEUDOWOLLASTONITE     -5.1610
TREMOLITE                .0000  satd
 ANTHOPHYLLITE          -7.8972                ALBITE
-5.9750
 ANTIGORITE               .0000  ssatd         TALC
-1.0780
 CLINOCHLORE             -.1498                CHAMOSITE
-3.3237
 PYROPE                 -6.3191                ALMANDINE
-5.3971
 GROSSULAR              -4.9920                QUARTZ-ALPHA
-2.5586
 QUARTZ-BETA            -2.7956                COESITE
-3.1549
 HALITE                 -9.5745                CRISTOBALITE-ALPHA
-3.8445
 CRISTOBALITE-BETA      -4.5579


                 --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -5.9740
     ALBITE                     -5.97396     .9992462     1.00000
     ANORTHITE                  -5.97396     .0007538     1.00000

 ORTHOPYROXENE(SS)         -.8306
     ENSTATITE-OR                -.83063     .6995131     1.00000
     FERROSILITE                 -.83063     .3004869     1.00000

 GARNET(SS)               -3.8910
     PYROPE                     -3.89096     .1845884     1.00000
     ALMANDINE                  -3.89096     .3506277     1.00000
     GROSSULAR                  -3.89096     .4647840     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .8425350     1.00000
     HEDENBERGITE                 .00000     .1239418     1.00000
     JADEITE                      .00000     .0335232     1.00000

 CPX_SUBCALCIC(SS)         -.0490
     DIOPSIDE                    -.04900     .8717592     1.00000
```

```
     HEDENBERGITE                    -.04900     .1282408     1.00000

 CHLORITE(SS)              .0000
saturated
     CLINOCHLORE                      .00000     .9010166     1.00000
     CHAMOSITE                        .00000     .0989834     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .8425    1.0000     .8425    -.0744     .0000    -.0744
     HEDENBERGITE
             .1239    1.0000     .1239    -.9068     .0000    -.9068
     JADEITE
             .0335    1.0000     .0335   -1.4747     .0000   -1.4747

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
             .9010    1.0000     .9010    -.0453     .0000    -.0453
     CHAMOSITE
             .0990    1.0000     .0990   -1.0044     .0000   -1.0044


          --- summary of gas species ---

          gas                  log fugacity         fugacity
partial pressure

   O2(G)                         -24.65223       2.22728E-25
   H2(G)                           1.20395       1.59936E+01
   H2O(G)                          3.80603       6.39785E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.6336E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =    75, iter =  3, ncorr = 0
```

```
 most rapidly changing is zvclg1(TREMOLITE         ) =    -3.1394

 stepping to zi=  1.6336E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =    76, iter =  3, ncorr = 0
 most rapidly changing is zvclg1(TREMOLITE         ) =    -3.1394

 stepping to zi=  1.6336E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =    77, iter =  3, ncorr = 0
 most rapidly changing is zvclg1(TREMOLITE         ) =    -3.1394

 stepping to zi=  1.6336E-01, delzi=  1.0000E-07, nord= 1
              ncycle=  0
 steps completed =    78, iter =  1, ncorr = 0
 most rapidly changing is zvclg1(TREMOLITE         ) =    -3.1394

 stepping to zi=  1.6337E-01, delzi=  1.0000E-06, nord= 2
              ncycle=  0
 steps completed =    79, iter =  3, ncorr = 0
 most rapidly changing is zvclg1(TREMOLITE         ) =    -3.1395

 stepping to zi=  1.6338E-01, delzi=  1.0000E-05, nord= 2
              ncycle=  0
 steps completed =    80, iter =  3, ncorr = 0
 most rapidly changing is zvclg1(TREMOLITE         ) =    -3.1402

 stepping to zi=  1.6348E-01, delzi=  1.0000E-04, nord= 2
              ncycle=  0
 steps completed =    81, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(TREMOLITE         ) =    -3.1469

 stepping to zi=  1.6448E-01, delzi=  1.0000E-03, nord= 3
              ncycle=  0
 steps completed =    82, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(TREMOLITE         ) =    -3.2225

 stepping to zi=  1.6567E-01, delzi=  1.1952E-03, nord= 4
              ncycle=  0
 steps completed =    83, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(TREMOLITE         ) =    -3.3387

 stepping to zi=  1.6912E-01, delzi=  3.4470E-03, nord= 4
              ncycle=  0
 steps completed =    84, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(TREMOLITE         ) =    -4.5753

 stepping to zi=  1.6932E-01, delzi=  2.0284E-04, nord= 5
                    the phase to be dropped is TREMOLITE
(   32)
```

```
   attempted species assemblage no.   2

                1      1  H2O
                2      2  NA+
                3      4  CA++
                4      5  MG++
                5      6  AL+++
                6      7  H4SIO4(AQ)
                7     13  H+
                8     16  CL-
                9     21  FE++
               10     32  O2(G)
               11      1  MAGNETITE
               12      1  CLINOPYRDIOPSIDE
               13      2  CLINOPYRHEDENBERGITE
               14      3  CLINOPYRJADEITE
               15      1  CHLORITECLINOCHLORE
               16      2  CHLORITECHAMOSITE

 steps completed =    85, iter =  5, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  1.69320170127289E-01
                    log of reaction progress =       -.7712913

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 change in the product phase assemblage


                              --- reactant summary ---



        reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.97163E+01    2.83662E-01    2.67856E+04
7.61966E+01
   CLINOPYROXENE(SS)      9.96581E+01    3.41891E-01    2.22099E+04
7.61942E+01
   MAGNETITE              9.99634E+01    3.65732E-02    2.31454E+04
```

```
8.46810E+00
   TREMOLITE              9.99690E+01    3.10195E-02    8.12118E+04
2.51993E+01


                current total mass =  1.53353E+05 grams
                delta total mass   =  1.86058E+02 grams
                delta total volume =     61.31240 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)            8.7395    1.67530E+00
   CLINOPYROXENE(SS)           .0908    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                   .0000    1.83200E-01

          affinity of the overall irreversible reaction=    14.641
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O         8.545935E+05        5.628377E+01        5.634425E+01
      NA        1.573626E+04        7.212636E-01        7.220387E-01
      CA        2.929644E+00        7.702193E-05        7.710469E-05
      MG        5.009677E+03        2.171908E-01        2.174241E-01
      AL        6.444409E+01        2.516771E-03        2.519475E-03
      SI        8.586279E+02        3.221440E-02        3.224902E-02
      H         1.069175E+05        1.117786E+02        1.118987E+02
      CL        1.680464E+04        4.994633E-01        5.000000E-01
      FE        1.244674E+01        2.348459E-04        2.350982E-04

      co3--                         0.000000E+00        0.000000E+00
      so4--                         0.000000E+00        0.000000E+00
      s--                           0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale
```

```
                                         ph            eh            pe

     internal ph scale              7.0072        .4809
3.3514E+00
     modified nbs ph scale          6.7490        .5179
3.6096E+00
     rational ph scale              6.7490        .5179
3.6096E+00

   phcl =      7.6104



          oxygen fugacity =  3.60603E-25
          log oxygen fugacity = -24.44297



                              activity of water =    .98386
               log activity of water =   -.00707
               alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                    ionic strength =  6.237942E-01 molal
                 sum of molalities =    1.5787668421890
               osmotic coefficient =     .57204
                    equiv. stoich. ionic strength =  4.994633E-01
molal

                         mass of solution =   1.054857 kg
                         mass of solvent  =   1.001075 kg
                         mass of solutes  =    .053783 kg
                         conc of solutes  =   5.098577 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.55683E+01   1.00107E+03
   NA+                  6.24156E-01   1.43492E+01   6.23486E-01     -.
20517     -.25823     -.46340
   CA++                 8.44114E-07   3.38321E-05   8.43208E-07
-6.07407    -1.03292    -7.10698
   MG++                 2.56561E-08   6.23572E-07   2.56286E-08
-7.59128    -1.03292    -8.62419
   AL+++                1.70563E-23   4.60204E-22   1.70380E-23
-22.76858    -2.32406   -25.09265
   H4SIO4(AQ)           1.36017E-02   1.30732E+00   1.35871E-02
```

```
-1.86687       .00000    -1.86687
   H+                    1.78445E-07   1.79854E-07   1.78253E-07
-6.74896     -.25823    -7.00719
   CL-                   4.52341E-01   1.60368E+01   4.51855E-01     -.
34500     -.25823     -.60323
   FE++                  2.08895E-10   1.16661E-08   2.08670E-10
-9.68054    -1.03292   -10.71346
   O2(AQ)                3.03805E-29   9.72141E-28   3.03479E-29
-28.51787       .00000   -28.51787
   H2(AQ)                2.12758E-03   4.28878E-03   2.12530E-03
-2.67258       .00000    -2.67258
   FE+++                 1.58224E-23   8.83632E-22   1.58054E-23
-22.80119    -2.32406   -25.12526
   OH-                   1.54036E-01   2.61973E+00   1.53870E-01     -.
81284     -.25823    -1.07107
   H8SI3O10(AQ)          1.27755E-08   3.22343E-06   1.27618E-08
-7.89409       .00000    -7.89409
   H6SI2O7(AQ)           4.99902E-04   8.70900E-02   4.99366E-04
-3.30158       .00000    -3.30158
   AL(OH)3(AQ)           1.44749E-06   1.12909E-04   1.44594E-06
-5.83985       .00000    -5.83985
   AL(OH)4-              7.30178E-04   6.93748E-02   7.29394E-04
-3.13704     -.25823    -3.39527
   AL(OH)SI(OH)-         1.78785E-03   3.09495E-01   1.78593E-03
-2.74814     -.25823    -3.00636
   CACL+                 1.57973E-06   1.19322E-04   1.57804E-06
-5.80188     -.25823    -6.06011
   CACL2(AQ)             2.69867E-08   2.99514E-06   2.69577E-08
-7.56932       .00000    -7.56932
   CA(OH)+               6.14521E-06   3.50814E-04   6.13862E-06
-5.21193     -.25823    -5.47016
   CA(H3SIO4)+           6.85086E-05   9.26146E-03   6.84351E-05
-4.16472     -.25823    -4.42295
   FE(OH)+               1.37909E-08   1.00473E-06   1.37761E-08
-7.86087     -.25823    -8.11910
   FE(OH)2               2.37527E-07   2.13445E-05   2.37272E-07
-6.62475       .00000    -6.62475
   FE(OH)3-              6.32888E-06   6.76361E-04   6.32209E-06
-5.19914     -.25823    -5.45737
   FECL+                 2.05218E-10   1.87364E-08   2.04998E-10
-9.68825     -.25823    -9.94648
   FECL2(AQ)             4.49421E-09   5.69654E-07   4.48938E-09
-8.34781       .00000    -8.34781
   FE(H3SIO4)+           2.28513E-04   3.44949E-02   2.28268E-04
-3.64156     -.25823    -3.89978
   MGCL+                 2.26820E-08   1.35543E-06   2.26577E-08
-7.64478     -.25823    -7.90301
   MG(OH)+               1.32722E-06   5.48306E-05   1.32580E-06
-5.87752     -.25823    -6.13575
   MG(OH)2(AQ)           2.17423E-01   1.26800E+01   2.17189E-01     -.
```

```
66316      .00000     -.66316
   MG(H3SIO4)+          6.21138E-09   7.41712E-07   6.20471E-09
-8.20728    -.25823    -8.46551
   NACL(AQ)             4.76573E-02   2.78523E+00   4.76062E-02
-1.32234     .00000    -1.32234
   NAOH(AQ)             5.02258E-02   2.00888E+00   5.01719E-02
-1.29954     .00000    -1.29954
   H3SIO4-              1.55626E-02   1.48011E+00   1.55459E-02
-1.80838    -.25823    -2.06661
   HCL(AQ)              2.11237E-07   7.70191E-06   2.11011E-07
-6.67570     .00000    -6.67570

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.5437891
           log (CA++  /h+**0)            6.9074017
           log (MG++  /h+**0)            5.3901918
           log (AL+++ /h+**0)           -4.0710697
           log (FE++  /h+**0)            3.3009277
           log (FE+++ /h+**0)           -4.1036821


           --- summary of solid product phases---


  product                    log moles        moles        grams
volume, cc

   MAGNETITE                -2.1776048    6.64347E-03    1.53822E+00
2.95767E-01

   CLINOPYROXENE(SS)         -.2668194    5.40979E-01    1.18915E+02
3.56800E+01
   DIOPSIDE                  -.3448415    4.52021E-01    9.78862E+01
2.99238E+01
   HEDENBERGITE             -1.1785057    6.62971E-02    1.64479E+01
4.38887E+00
   JADEITE                  -1.6447157    2.26613E-02    4.58072E+00
1.36738E+00

   CHLORITE(SS)              -.0315787    9.29868E-01    1.06259E+02
3.93599E+01
   CLINOCHLORE               -.0767181    8.38073E-01    9.31597E+01
3.54421E+01
   CHAMOSITE                -1.0371822    9.17947E-02    1.30992E+01
3.91780E+00


                --- grand summary of solid phases (e.s.+p.r.s.
```

```
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 1.9998700    9.99701E+01    2.31469E+04
4.45067E+03
   TREMOLITE                 1.9998653    9.99690E+01    8.12118E+04
2.72595E+04

   PLAGIOCLASE(SS)           1.9987663    9.97163E+01

   ALBITE                    1.7769176    5.98298E+01    1.56888E+04
6.03264E+03
   ANORTHITE                 1.6008263    3.98865E+01    1.10968E+04
4.01857E+03


   CLINOPYROXENE(SS)         2.0008638    1.00199E+02

   DIOPSIDE                  1.9040580    8.01785E+01    1.73628E+04
5.30782E+03
   HEDENBERGITE              1.3009848    1.99979E+01    4.96137E+03
1.32386E+03
   JADEITE                  -1.6447157    2.26613E-02    4.58072E+00
1.36738E+00


   CHLORITE(SS)              -.0315787    9.29868E-01

   CLINOCHLORE               -.0767181    8.38073E-01    9.31597E+01
3.54421E+01
   CHAMOSITE                -1.0371822    9.17947E-02    1.30992E+01
3.91780E+00


                           mass, grams        volume, cc

                created         2.267120E+02       7.533571E+01
                destroyed       1.860582E+02       6.131240E+01
                net             4.065386E+01       1.402331E+01

               warning-- these volume totals may be incomplete because
               of missing partial molar volume data in the data base



                --- mineral saturation state summary ---
```

```
   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          HEMATITE
-2.0501
 PERICLASE              -7.1246                BRUCITE
-3.3882
 DIASPORE               -6.1296                FORSTERITE
-1.0918
 FAYALITE               -1.4226                CHRYSOTILE
-1.1682
 ENSTATITE-CL           -1.2879                ENSTATITE-OR
-1.3660
 ENSTATITE-PR           -1.7714                DIOPSIDE
-.2582
 HEDENBERGITE           -3.0168                JADEITE
-4.5595
 FERROSILITE            -2.5846                WOLLASTONITE
-4.6651
 PSEUDOWOLLASTONITE     -5.1512
TREMOLITE                .0000
 ANTHOPHYLLITE          -7.9606                ALBITE
-5.5656
 ANTIGORITE             -1.1486                TALC
-1.0541
 CLINOCHLORE             -.1494                CHAMOSITE
-3.3276
 PYROPE                 -6.2445                ALMANDINE
-5.3268
 GROSSULAR              -4.8858                QUARTZ-ALPHA
-2.4693
 QUARTZ-BETA            -2.7063                COESITE
-3.0656
 HALITE                 -9.5734                CRISTOBALITE-ALPHA
-3.7552
 CRISTOBALITE-BETA      -4.4686


                      --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -5.5645
     ALBITE                      -5.56449     .9992569     1.00000
     ANORTHITE                   -5.56449     .0007431     1.00000

 ORTHOPYROXENE(SS)          -.8537
     ENSTATITE-OR                 -.85373     .7001389     1.00000
     FERROSILITE                  -.85373     .2998611     1.00000
```

```
 GARNET(SS)                -3.8030
     PYROPE                      -3.80305     .1828834     1.00000
     ALMANDINE                   -3.80305     .3463546     1.00000
     GROSSULAR                   -3.80305     .4707620     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .8355605     1.00000
     HEDENBERGITE                  .00000     .1225501     1.00000
     JADEITE                       .00000     .0418894     1.00000

 CPX_SUBCALCIC(SS)          -.0615
     DIOPSIDE                     -.06150     .8720919     1.00000
     HEDENBERGITE                 -.06150     .1279081     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9012820     1.00000
     CHAMOSITE                     .00000     .0987180     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .8356    1.0000     .8356    -.0780     .0000    -.0780
     HEDENBERGITE
              .1226    1.0000     .1226    -.9117     .0000    -.9117
     JADEITE
              .0419    1.0000     .0419   -1.3779     .0000   -1.3779

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9013    1.0000     .9013    -.0451     .0000    -.0451
     CHAMOSITE
              .0987    1.0000     .0987   -1.0056     .0000   -1.0056


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure
```

```
  O2(G)                          -24.44297       3.60603E-25
  H2(G)                            1.09932       1.25695E+01
  H2O(G)                           3.80603       6.39785E+03


- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


stepping to zi=  1.6932E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =    86, iter =  3, ncorr = 0
most rapidly changing is zvclg1(O2(G)             ) =    -24.4430

stepping to zi=  1.6932E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =    87, iter =  3, ncorr = 0
most rapidly changing is zvclg1(O2(G)             ) =    -24.4430

stepping to zi=  1.6932E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =    88, iter =  3, ncorr = 0
most rapidly changing is zvclg1(O2(G)             ) =    -24.4430

stepping to zi=  1.6932E-01, delzi=  1.0000E-07, nord= 1
              ncycle=  0
steps completed =    89, iter =  1, ncorr = 0
most rapidly changing is zvclg1(O2(G)             ) =    -24.4430

stepping to zi=  1.6932E-01, delzi=  1.0000E-06, nord= 1
              ncycle=  0
steps completed =    90, iter =  2, ncorr = 0
most rapidly changing is zvclg1(O2(G)             ) =    -24.4429

stepping to zi=  1.6933E-01, delzi=  1.0000E-05, nord= 2
              ncycle=  0
steps completed =    91, iter =  3, ncorr = 0
most rapidly changing is zvclg1(O2(G)             ) =    -24.4425

stepping to zi=  1.6943E-01, delzi=  1.0000E-04, nord= 2
              ncycle=  0
steps completed =    92, iter =  3, ncorr = 0
most rapidly changing is zvclg1(O2(G)             ) =    -24.4388

stepping to zi=  1.7043E-01, delzi=  1.0000E-03, nord= 3
              ncycle=  0
steps completed =    93, iter =  4, ncorr = 0
most rapidly changing is zvclg1(O2(G)             ) =    -24.4009
```

```
 stepping to zi=  1.7212E-01, delzi=  1.6901E-03, nord= 4
               ncycle=  0
 steps completed =    94, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(O2(G)             ) =    -24.3374

 stepping to zi=  1.7541E-01, delzi=  3.2910E-03, nord= 4
               ncycle=  0
 steps completed =    95, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(O2(G)             ) =    -24.2153

 stepping to zi=  1.8405E-01, delzi=  8.6339E-03, nord= 5
               ncycle=  0
 steps completed =    96, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(O2(G)             ) =    -23.9101

 stepping to zi=  1.9786E-01, delzi=  1.3811E-02, nord= 6
               ncycle=  0
 steps completed =    97, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(O2(G)             ) =    -23.4763

 stepping to zi=  2.1237E-01, delzi=  1.4516E-02, nord= 6
               ncycle=  0
 steps completed =    98, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(O2(G)             ) =    -23.0890

 stepping to zi=  2.2754E-01, delzi=  1.5168E-02, nord= 6
               ncycle=  0
 steps completed =    99, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(O2(G)             ) =    -22.7442

 stepping to zi=  2.4342E-01, delzi=  1.5877E-02, nord= 6
               ncycle=  0
 steps completed =   100, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -21.2229

 stepping to zi=  2.4689E-01, delzi=  3.4735E-03, nord= 6
               ncycle=  0
 iter =    6
       0 supersaturated pure minerals
       1 supersaturated solid solutions

                          the most supersaturated phases     affinity,
kcal

                            1   50600   GARNET(SS)               .
00610875


   attempted species assemblage no.   2
```

```
                 1      1  H2O
                 2      2  NA+
                 3      4  CA++
                 4      5  MG++
                 5      6  AL+++
                 6      7  H4SIO4(AQ)
                 7     13  H+
                 8     16  CL-
                 9     21  FE++
                10     32  O2(G)
                11      1  MAGNETITE
                12      1  GARNET(SPYROPE
                13      2  GARNET(SALMANDINE
                14      3  GARNET(SGROSSULAR
                15      1  CLINOPYRDIOPSIDE
                16      2  CLINOPYRHEDENBERGITE
                17      3  CLINOPYRJADEITE
                18      1  CHLORITECLINOCHLORE
                19      2  CHLORITECHAMOSITE

 steps completed =   101, iter =  9, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                   reaction progress        =  2.46892271710351E-01
                   log of reaction progress =       -.6074925

                   temperature    =    450.000 degrees c
                   total pressure =    500.000 bars

                   computing units remaining =       .000


 change in the product phase assemblage


                             --- reactant summary ---



        reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.95864E+01    4.13619E-01    2.67506E+04
1.11105E+02
   CLINOPYROXENE(SS)      9.95015E+01    4.98525E-01    2.21750E+04
1.11102E+02
   MAGNETITE              9.99467E+01    5.33287E-02    2.31415E+04
```

1.23477E+01
TREMOLITE 9.99548E+01 4.52307E-02 8.12003E+04
3.67441E+01

current total mass = 1.53267E+05 grams
delta total mass = 2.71299E+02 grams
delta total volume = 89.40197 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	4.4165	1.67530E+00
CLINOPYROXENE(SS)	.2713	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	7.6788	1.83200E-01

affinity of the overall irreversible reaction= 8.806
kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.569338E+05	5.605676E+01	5.615668E+01
NA	1.503694E+04	6.845565E-01	6.857767E-01
CA	1.656090E+01	4.324547E-04	4.332255E-04
MG	2.328414E+03	1.002649E-01	1.004436E-01
AL	6.327131E+02	2.454282E-02	2.458657E-02
SI	7.206717E+02	2.685590E-02	2.690377E-02
H	1.074203E+05	1.115459E+02	1.117447E+02
CL	1.690694E+04	4.991103E-01	5.000000E-01
FE	3.653711E+00	6.847291E-05	6.859496E-05
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

```
                                             ph            eh            pe

     internal ph scale                     6.8944         .5716
3.9835E+00
     modified nbs ph scale                 6.6384         .6083
4.2394E+00
     rational ph scale                     6.6384         .6083
4.2394E+00

   phcl =      7.4945



          oxygen fugacity =  4.30597E-23
          log oxygen fugacity = -22.36593




                                 activity of water =    .98387
               log activity of water =   -.00706
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  6.011677E-01 molal
                 sum of molalities =    1.3936011122603
               osmotic coefficient =     .64758
                    equiv. stoich. ionic strength =  4.991103E-01
molal

                         mass of solution =   1.048474 kg
                         mass of solvent  =   1.001783 kg
                         mass of solutes  =    .046692 kg
                         conc of solutes  =   4.453323 per cent (w/w)


   species                moles         grams          conc         log
conc      log g      log act

   H2O                  5.56076E+01   1.00178E+03
   NA+                  6.01718E-01   1.38333E+01   6.00647E-01     -.
22138     -.25592     -.47730
   CA++                 1.07309E-05   4.30095E-04   1.07118E-05
-4.97014    -1.02368    -5.99382
   MG++                 1.95079E-08   4.74139E-07   1.94732E-08
-7.71056    -1.02368    -8.73424
   AL+++                6.99652E-22   1.88777E-20   6.98407E-22
-21.15589    -2.30328   -23.45917
   H4SIO4(AQ)           6.78842E-03   6.52467E-01   6.77634E-03
```

```
-2.16900      .00000    -2.16900
   H+                   2.30318E-07   2.32138E-07   2.29908E-07
-6.63845     -.25592    -6.89437
   CL-                  4.53461E-01   1.60766E+01   4.52654E-01     -.
34423     -.25592     -.60015
   FE++                 1.55050E-10   8.65906E-09   1.54774E-10
-9.81030    -1.02368   -10.83398
   O2(AQ)               3.63031E-27   1.16166E-25   3.62386E-27
-26.44083      .00000   -26.44083
   H2(AQ)               1.94840E-04   3.92758E-04   1.94493E-04
-3.71110      .00000    -3.71110
   FE+++                4.90176E-23   2.73749E-21   4.89304E-23
-22.31042    -2.30328   -24.61370
   OH-                  1.18249E-01   2.01110E+00   1.18039E-01     -.
92798     -.25592    -1.18390
   H8SI3O10(AQ)         1.58592E-09   4.00149E-07   1.58310E-09
-8.80049      .00000    -8.80049
   H6SI2O7(AQ)          1.24430E-04   2.16775E-02   1.24209E-04
-3.90585      .00000    -3.90585
   AL(OH)3(AQ)          2.85716E-05   2.22868E-03   2.85208E-05
-4.54484      .00000    -4.54484
   AL(OH)4-             1.10565E-02   1.05048E+00   1.10368E-02
-1.95716     -.25592    -2.21308
   AL(OH)SI(OH)-        1.35015E-02   2.33725E+00   1.34775E-02
-1.87039     -.25592    -2.12631
   CACL+                2.05506E-05   1.55225E-03   2.05140E-05
-4.68795     -.25592    -4.94387
   CACL2(AQ)            3.55448E-07   3.94498E-05   3.54816E-07
-6.45000      .00000    -6.45000
   CA(OH)+              6.12181E-05   3.49477E-03   6.11091E-05
-4.21389     -.25592    -4.46981
   CA(H3SIO4)+          3.40371E-04   4.60136E-02   3.39765E-04
-3.46882     -.25592    -3.72474
   FE(OH)+              8.02129E-09   5.84386E-07   8.00702E-09
-8.09653     -.25592    -8.35245
   FE(OH)2              1.07115E-07   9.62553E-06   1.06924E-07
-6.97092      .00000    -6.97092
   FE(OH)3-             2.18945E-06   2.33984E-04   2.18555E-06
-5.66044     -.25592    -5.91636
   FECL+                1.55871E-10   1.42310E-08   1.55593E-10
-9.80801     -.25592   -10.06393
   FECL2(AQ)            3.45612E-09   4.38073E-07   3.44997E-09
-8.46219      .00000    -8.46219
   FE(H3SIO4)+          6.62866E-05   1.00062E-02   6.61687E-05
-4.17935     -.25592    -4.43527
   MGCL+                1.76484E-08   1.05464E-06   1.76170E-08
-7.75407     -.25592    -8.00999
   MG(OH)+              7.90806E-07   3.26700E-05   7.89399E-07
-6.10270     -.25592    -6.35862
   MG(OH)2(AQ)          1.00443E-01   5.85778E+00   1.00264E-01     -.
```

```
99885      .00000     -.99885
   MG(H3SIO4)+          1.84577E-09   2.20407E-07   1.84249E-09
-8.73460     -.25592    -8.99052
   NACL(AQ)             4.65174E-02   2.71861E+00   4.64347E-02
-1.33316      .00000    -1.33316
   NAOH(AQ)             3.75417E-02   1.50156E+00   3.74749E-02
-1.42626      .00000    -1.42626
   H3SIO4-              5.95830E-03   5.66675E-01   5.94770E-03
-2.22565     -.25592    -2.48157
   HCL(AQ)              2.76046E-07   1.00649E-05   2.75555E-07
-6.55979      .00000    -6.55979

           --- activity ratios of cations ---


           log (NA+   /h+**0)           6.4170647
           log (CA++  /h+**0)           7.7949149
           log (MG++  /h+**0)           5.0544884
           log (AL+++ /h+**0)          -2.7760728
           log (FE++  /h+**0)           2.9547490
           log (FE+++ /h+**0)          -3.9306029


           --- summary of solid product phases---


  product                     log moles        moles        grams
volume, cc

   MAGNETITE                 -1.6682427    2.14663E-02    4.97028E+00
9.55680E-01

   GARNET(SS)                -4.2651308    5.43087E-05    8.17149E-03
2.25729E-03
   PYROPE                    -5.9279571    1.18044E-06    1.58630E-04
4.45261E-05
   ALMANDINE                 -5.6610962    2.18225E-06    3.62156E-04
8.37328E-05
   GROSSULAR                 -4.2928900    5.09460E-05    7.65071E-03
2.12903E-03

   CLINOPYROXENE(SS)          -.0497098    8.91847E-01    1.94141E+02
5.82380E+01
   DIOPSIDE                   -.1801940    6.60398E-01    1.43011E+02
4.37184E+01
   HEDENBERGITE              -1.0243335    9.45511E-02    2.34576E+01
6.25928E+00
   JADEITE                    -.8636055    1.36897E-01    2.76722E+01
8.26038E+00
```

```
   CHLORITE(SS)                .0186455    1.04387E+00    1.19216E+02
4.41845E+01
   CLINOCHLORE               -.0254708    9.43038E-01    1.04828E+02
3.98811E+01
   CHAMOSITE                 -.9964103    1.00830E-01    1.43886E+01
4.30342E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 1.9998616    9.99681E+01    2.31465E+04
4.45058E+03
   TREMOLITE                 1.9998035    9.99548E+01    8.12003E+04
2.72557E+04

   PLAGIOCLASE(SS)           1.9982000    9.95864E+01

   ALBITE                    1.7763512    5.97518E+01    1.56683E+04
6.02478E+03
   ANORTHITE                 1.6002599    3.98346E+01    1.10823E+04
4.01333E+03


   GARNET(SS)               -4.2651308    5.43087E-05

   PYROPE                   -5.9279571    1.18044E-06    1.58630E-04
4.45261E-05
   ALMANDINE                -5.6610962    2.18225E-06    3.62156E-04
8.37328E-05
   GROSSULAR                -4.2928900    5.09460E-05    7.65071E-03
2.12903E-03


   CLINOPYROXENE(SS)         2.0017048    1.00393E+02

   DIOPSIDE                  1.9045077    8.02616E+01    1.73808E+04
5.31332E+03
   HEDENBERGITE              1.3009181    1.99948E+01    4.96061E+03
1.32366E+03
   JADEITE                   -.8636055    1.36897E-01    2.76722E+01
8.26038E+00


   CHLORITE(SS)               .0186455    1.04387E+00

   CLINOCHLORE               -.0254708    9.43038E-01    1.04828E+02
```

```
3.98811E+01
   CHAMOSITE                 -.9964103    1.00830E-01    1.43886E+01
4.30342E+00



                           mass, grams        volume, cc

           created         3.183352E+02       1.033805E+02
           destroyed       2.712986E+02       8.940197E+01
           net             4.703664E+01       1.397849E+01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE              .0000  satd          CORUNDUM
-4.3680
 HEMATITE              -.9046                PERICLASE
-8.2354
 SPINEL               -6.6333                BRUCITE
-4.4990
 DIASPORE             -1.8444                ANDALUSITE
-7.9529
 KYANITE              -6.7339                SILLIMANITE
-7.7167
 LAWSONITE            -3.8843                PUMPELLYITE
-5.8744
 ZOISITE              -2.2520                CLINOZOISITE
-2.9624
 FORSTERITE           -2.7025                FAYALITE
-3.0680
 CHRYSOTILE           -6.5002                ENSTATITE-CL
-3.3985
 ENSTATITE-OR         -3.4766                ENSTATITE-PR
-3.8820
 DIOPSIDE              -.4318                HEDENBERGITE
-3.2250
 JADEITE              -2.6932                FERROSILITE
-4.7299
 WOLLASTONITE         -2.7280                PSEUDOWOLLASTONITE
-3.2141
 TREMOLITE            -7.6788                ALBITE
```

```
-4.6991
 ANORTHITE               -6.4107                TALC
-8.3857
 PARAGONITE              -4.8420                MARGARITE
-6.8461
 PREHNITE                -4.7300                CLINOCHLORE
-.1460
 CHAMOSITE               -3.3588                PYROPE
-5.5023
 ALMANDINE               -4.6193                GROSSULAR
-.0919
 QUARTZ-ALPHA            -3.4691                QUARTZ-BETA
-3.7060
 COESITE                 -4.0654                HALITE
-9.6092
 CRISTOBALITE-ALPHA      -4.7550                CRISTOBALITE-BETA
-5.4684


                         --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -4.3177
     ALBITE                      -4.31771     .7669266     1.00000
     ANORTHITE                   -4.31771     .2330734     1.00000

 ORTHOPYROXENE(SS)         -2.9747
     ENSTATITE-OR                -2.97465     .7051783     1.00000
     FERROSILITE                 -2.97465     .2948217     1.00000

 GARNET(SS)                  .0000
saturated
     PYROPE                        .00000     .0217357     1.00000
     ALMANDINE                     .00000     .0401823     1.00000
     GROSSULAR                     .00000     .9380820     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .7404842     1.00000
     HEDENBERGITE                  .00000     .1060172     1.00000
     JADEITE                       .00000     .1534986     1.00000

 CPX_SUBCALCIC(SS)          -.2395
     DIOPSIDE                     -.23948     .8747584     1.00000
     HEDENBERGITE                 -.23948     .1252416     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9034073     1.00000
```

```
    CHAMOSITE                     .00000     .0965927     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   GARNET(SS)
 ideal solution

    PYROPE
             .0217    1.0000     .0217   -1.6628     .0000   -1.6628
    ALMANDINE
             .0402    1.0000     .0402   -1.3960     .0000   -1.3960
    GROSSULAR
             .9381    1.0000     .9381    -.0278     .0000    -.0278

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
             .7405    1.0000     .7405    -.1305     .0000    -.1305
    HEDENBERGITE
             .1060    1.0000     .1060    -.9746     .0000    -.9746
    JADEITE
             .1535    1.0000     .1535    -.8139     .0000    -.8139

   CHLORITE(SS)
 ideal solution

    CLINOCHLORE
             .9034    1.0000     .9034    -.0441     .0000    -.0441
    CHAMOSITE
             .0966    1.0000     .0966   -1.0151     .0000   -1.0151


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                       -22.36593       4.30597E-23
   H2(G)                          .06080       1.15028E+00
   H2O(G)                        3.80604       6.39793E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
stepping to zi=  2.4689E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   102, iter =  4, ncorr = 0
most rapidly changing is zvclg1(PYROPE           ) =    -5.9279

stepping to zi=  2.4689E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   103, iter =  4, ncorr = 0
most rapidly changing is zvclg1(PYROPE           ) =    -5.9279

stepping to zi=  2.4689E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   104, iter =  4, ncorr = 0
most rapidly changing is zvclg1(PYROPE           ) =    -5.9279

stepping to zi=  2.4689E-01, delzi=  1.4223E-08, nord= 1
              ncycle=  0
steps completed =   105, iter =  1, ncorr = 0
most rapidly changing is zvclg1(PYROPE           ) =    -5.9278

stepping to zi=  2.4689E-01, delzi=  1.4223E-07, nord= 2
              ncycle=  0
steps completed =   106, iter =  3, ncorr = 0
most rapidly changing is zvclg1(PYROPE           ) =    -5.9274

stepping to zi=  2.4689E-01, delzi=  1.4223E-06, nord= 2
              ncycle=  0
steps completed =   107, iter =  3, ncorr = 0
most rapidly changing is zvclg1(PYROPE           ) =    -5.9231

stepping to zi=  2.4691E-01, delzi=  1.4223E-05, nord= 2
              ncycle=  0
steps completed =   108, iter =  4, ncorr = 0
most rapidly changing is zvclg1(PYROPE           ) =    -5.8821

stepping to zi=  2.4702E-01, delzi=  1.1646E-04, nord= 3
              ncycle=  0
steps completed =   109, iter =  4, ncorr = 0
most rapidly changing is zvclg1(PYROPE           ) =    -5.6422

stepping to zi=  2.4819E-01, delzi=  1.1646E-03, nord= 3
              ncycle=  0
steps completed =   110, iter =  5, ncorr = 0
most rapidly changing is zvclg1(PYROPE           ) =    -4.9204

stepping to zi=  2.5119E-01, delzi=  2.9995E-03, nord= 4
              ncycle=  0
steps completed =   111, iter =  4, ncorr = 0
```

```
 most rapidly changing is zvclg1(PYROPE            ) =     -4.4254
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  2.51188643150955E-01
                    log of reaction progress =       -.6000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



        reactant             moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.95792E+01    4.20816E-01    2.67487E+04
1.13039E+02
   CLINOPYROXENE(SS)      9.94928E+01    5.07200E-01    2.21730E+04
1.13035E+02
   MAGNETITE              9.99457E+01    5.42567E-02    2.31413E+04
1.25625E+01
   TREMOLITE              9.99540E+01    4.60178E-02    8.11997E+04
3.73835E+01


               current total mass =  1.53263E+05 grams
               delta total mass   =  2.76020E+02 grams
               delta total volume =     90.95773 cc


        reactant            affinity     rel. rate

   PLAGIOCLASE(SS)            4.3452    1.67530E+00
   CLINOPYROXENE(SS)           .2803    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                  7.6487    1.83200E-01

          affinity of the overall irreversible reaction=     8.681
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included
```

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.570182E+05	5.605111E+01	5.615248E+01
NA	1.496441E+04	6.811188E-01	6.823506E-01
CA	1.669714E+01	4.359256E-04	4.367140E-04
MG	2.285218E+03	9.838522E-02	9.856316E-02
AL	6.352651E+02	2.463691E-02	2.468146E-02
SI	7.305384E+02	2.721816E-02	2.726739E-02
H	1.074361E+05	1.115400E+02	1.117417E+02
CL	1.690987E+04	4.990974E-01	5.000000E-01
FE	3.737227E+00	7.002411E-05	7.015075E-05
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.8850	.5747	4.0053E+00
modified nbs ph scale	6.6293	.6114	4.2610E+00
rational ph scale	6.6293	.6114	4.2610E+00

phcl = 7.4848

oxygen fugacity = 4.82801E-23
log oxygen fugacity = -22.31623

activity of water = .98387

```
                 log activity of water =   -.00706
                 alkalinity =  0.000000E+00 equiv/kg solvent
                                            (not def. for t.gt.50 c)

                      ionic strength =  5.987822E-01 molal
                   sum of molalities =    1.3860530815006
                 osmotic coefficient =     .65109
                      equiv. stoich. ionic strength =  4.990974E-01
molal

                           mass of solution =   1.048293 kg
                           mass of solvent  =   1.001809 kg
                           mass of solutes  =    .046484 kg
                           conc of solutes  =   4.434288 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.56091E+01   1.00181E+03
   NA+                  5.99338E-01   1.37786E+01   5.98256E-01     -.
22311     -.25567     -.47878
   CA++                 1.08235E-05   4.33806E-04   1.08040E-05
-4.96642    -1.02268    -5.98910
   MG++                 1.99422E-08   4.84696E-07   1.99062E-08
-7.70101    -1.02268    -8.72370
   AL+++                7.52807E-22   2.03119E-20   7.51448E-22
-21.12410    -2.30104   -23.42514
   H4SIO4(AQ)           6.94338E-03   6.67360E-01   6.93084E-03
-2.15921      .00000    -2.15921
   H+                   2.35220E-07   2.37078E-07   2.34795E-07
-6.62931     -.25567    -6.88498
   CL-                  4.53581E-01   1.60808E+01   4.52762E-01     -.
34413     -.25567     -.59980
   FE++                 1.58479E-10   8.85056E-09   1.58193E-10
-9.80081    -1.02268   -10.82350
   O2(AQ)               4.07055E-27   1.30253E-25   4.06320E-27
-26.39113      .00000   -26.39113
   H2(AQ)               1.84009E-04   3.70926E-04   1.83677E-04
-3.73594      .00000    -3.73594
   FE+++                5.25311E-23   2.93371E-21   5.24363E-23
-22.28037    -2.30104   -24.58141
   OH-                  1.15658E-01   1.96704E+00   1.15450E-01     -.
93761     -.25567    -1.19328
   H8SI3O10(AQ)         1.69693E-09   4.28158E-07   1.69387E-09
-8.77112      .00000    -8.77112
   H6SI2O7(AQ)          1.30172E-04   2.26778E-02   1.29937E-04
-3.88627      .00000    -3.88627
   AL(OH)3(AQ)          2.89617E-05   2.25911E-03   2.89094E-05
-4.53896      .00000    -4.53896
```

```
   AL(OH)4-              1.09616E-02   1.04147E+00   1.09418E-02
-1.96091     -.25567    -2.21658
   AL(OH)SI(OH)-         1.36909E-02   2.37003E+00   1.36662E-02
-1.86435     -.25567    -2.12002
   CACL+                 2.07803E-05   1.56960E-03   2.07428E-05
-4.68313     -.25567    -4.93880
   CACL2(AQ)             3.59919E-07   3.99460E-05   3.59270E-07
-6.44458      .00000    -6.44458
   CA(OH)+               6.05304E-05   3.45551E-03   6.04211E-05
-4.21881     -.25567    -4.47448
   CA(H3SIO4)+           3.44220E-04   4.65340E-02   3.43598E-04
-3.46395     -.25567    -3.71962
   FE(OH)+               8.03725E-09   5.85548E-07   8.02274E-09
-8.09568     -.25567    -8.35135
   FE(OH)2               1.05094E-07   9.44394E-06   1.04905E-07
-6.97921      .00000    -6.97921
   FE(OH)3-              2.10103E-06   2.24534E-04   2.09723E-06
-5.67835     -.25567    -5.93402
   FECL+                 1.59721E-10   1.45825E-08   1.59433E-10
-9.79742     -.25567   -10.05309
   FECL2(AQ)             3.54639E-09   4.49516E-07   3.53999E-09
-8.45100      .00000    -8.45100
   FE(H3SIO4)+           6.79327E-05   1.02547E-02   6.78101E-05
-4.16871     -.25567    -4.42438
   MGCL+                 1.80871E-08   1.08085E-06   1.80544E-08
-7.74342     -.25567    -7.99909
   MG(OH)+               7.92494E-07   3.27398E-05   7.91064E-07
-6.10179     -.25567    -6.35746
   MG(OH)2(AQ)           9.85623E-02   5.74812E+00   9.83844E-02
-1.00707      .00000    -1.00707
   MG(H3SIO4)+           1.89188E-09   2.25913E-07   1.88847E-09
-8.72389     -.25567    -8.97956
   NACL(AQ)              4.63976E-02   2.71160E+00   4.63138E-02
-1.33429      .00000    -1.33429
   NAOH(AQ)              3.66150E-02   1.46449E+00   3.65489E-02
-1.43713      .00000    -1.43713
   H3SIO4-               5.96063E-03   5.66897E-01   5.94987E-03
-2.22549     -.25567    -2.48116
   HCL(AQ)               2.82311E-07   1.02933E-05   2.81801E-07
-6.55006      .00000    -6.55006

           --- activity ratios of cations ---


           log (NA+   /h+**0)            6.4061980
           log (CA++  /h+**0)            7.7808626
           log (MG++  /h+**0)            5.0462689
           log (AL+++ /h+**0)           -2.7701948
           log (FE++  /h+**0)            2.9464659
           log (FE+++ /h+**0)           -3.9264617
```

```
          --- summary of solid product phases---


  product                          log moles        moles        grams
volume, cc

   MAGNETITE                      -1.6500722    2.23835E-02    5.18264E+00
9.96513E-01

   GARNET(SS)                     -2.7680276    1.70597E-03    2.56694E-01
7.09024E-02
   PYROPE                         -4.4253764    3.75512E-05    5.04621E-03
1.41643E-03
   ALMANDINE                      -4.1585792    6.94098E-05    1.15189E-02
2.66325E-03
   GROSSULAR                      -2.7961480    1.59901E-03    2.40128E-01
6.68227E-02

   CLINOPYROXENE(SS)               -.0404022    9.11167E-01    1.98258E+02
5.94716E+01
   DIOPSIDE                        -.1735777    6.70536E-01    1.45206E+02
4.43895E+01
   HEDENBERGITE                   -1.0177807    9.59885E-02    2.38142E+01
6.35444E+00
   JADEITE                         -.8397060    1.44642E-01    2.92377E+01
8.72769E+00

   CHLORITE(SS)                     .0198268    1.04671E+00    1.19540E+02
4.43048E+01
   CLINOCHLORE                     -.0242835    9.45620E-01    1.05115E+02
3.99903E+01
   CHAMOSITE                       -.9952865    1.01091E-01    1.44259E+01
4.31457E+00


               --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member         log moles        moles        grams
volume, cc

   MAGNETITE                       1.9998616    9.99681E+01    2.31465E+04
4.45058E+03
   TREMOLITE                       1.9998001    9.99540E+01    8.11997E+04
2.72555E+04

   PLAGIOCLASE(SS)                 1.9981686    9.95792E+01
```

```
   ALBITE                     1.7763198    5.97475E+01    1.56672E+04
6.02434E+03
   ANORTHITE                  1.6002286    3.98317E+01    1.10815E+04
4.01304E+03


   GARNET(SS)                -2.7680276    1.70597E-03

   PYROPE                    -4.4253764    3.75512E-05    5.04621E-03
1.41643E-03
   ALMANDINE                 -4.1585792    6.94098E-05    1.15189E-02
2.66325E-03
   GROSSULAR                 -2.7961480    1.59901E-03    2.40128E-01
6.68227E-02


   CLINOPYROXENE(SS)          2.0017509    1.00404E+02

   DIOPSIDE                   1.9045250    8.02648E+01    1.73815E+04
5.31353E+03
   HEDENBERGITE               1.3009116    1.99945E+01    4.96054E+03
1.32364E+03
   JADEITE                    -.8397060    1.44642E-01    2.92377E+01
8.72769E+00


   CHLORITE(SS)                .0198268    1.04671E+00

   CLINOCHLORE                -.0242835    9.45620E-01    1.05115E+02
3.99903E+01
   CHAMOSITE                  -.9952865    1.01091E-01    1.44259E+01
4.31457E+00



                           mass, grams        volume, cc

           created         3.232379E+02       1.048439E+02
           destroyed       2.760197E+02       9.095773E+01
           net             4.721823E+01       1.388615E+01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
```

```
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-4.3291
 HEMATITE                -.8772                PERICLASE
-8.2626
 SPINEL                 -6.6215                BRUCITE
-4.5262
 DIASPORE               -1.8250                ANDALUSITE
-7.8816
 KYANITE                -6.6626                SILLIMANITE
-7.6454
 LAWSONITE              -3.8271                PUMPELLYITE
-5.7960
 ZOISITE                -2.1895                CLINOZOISITE
-2.8999
 FORSTERITE             -2.7135                FAYALITE
-3.0792
 CHRYSOTILE             -6.5170                ENSTATITE-CL
-3.3933
 ENSTATITE-OR           -3.4714                ENSTATITE-PR
-3.8768
 DIOPSIDE                -.4407                HEDENBERGITE
-3.2342
 JADEITE                -2.6449                FERROSILITE
-4.7249
 WOLLASTONITE           -2.7422                PSEUDOWOLLASTONITE
-3.2282
 TREMOLITE              -7.6487                ALBITE
-4.6184
 ANORTHITE              -6.3535                TALC
-8.3378
 PARAGONITE             -4.7224                MARGARITE
-6.7500
 PREHNITE               -4.6869                CLINOCHLORE
-.1460
 CHAMOSITE              -3.3590                PYROPE
-5.4842
 ALMANDINE              -4.6014                GROSSULAR
-.0931
 QUARTZ-ALPHA           -3.4367                QUARTZ-BETA
-3.6736
 COESITE                -4.0330                HALITE
-9.6130
 CRISTOBALITE-ALPHA     -4.7226                CRISTOBALITE-BETA
-5.4360


                     --- summary of solid solutions  ---
```

```
 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -4.2425
     ALBITE                      -4.24247     .7698351     1.00000
     ANORTHITE                   -4.24247     .2301649     1.00000

 ORTHOPYROXENE(SS)         -2.9695
     ENSTATITE-OR                -2.96952     .7052087     1.00000
     FERROSILITE                 -2.96952     .2947913     1.00000

 GARNET(SS)                  .0000
saturated
     PYROPE                        .00000     .0220116     1.00000
     ALMANDINE                     .00000     .0406863     1.00000
     GROSSULAR                     .00000     .9373021     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .7359096     1.00000
     HEDENBERGITE                  .00000     .1053468     1.00000
     JADEITE                       .00000     .1587436     1.00000

 CPX_SUBCALCIC(SS)          -.2484
     DIOPSIDE                     -.24841     .8747744     1.00000
     HEDENBERGITE                 -.24841     .1252256     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9034201     1.00000
     CHAMOSITE                     .00000     .0965799     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   GARNET(SS)
 ideal solution

     PYROPE
              .0220    1.0000     .0220   -1.6573     .0000   -1.6573
     ALMANDINE
              .0407    1.0000     .0407   -1.3906     .0000   -1.3906
     GROSSULAR
              .9373    1.0000     .9373    -.0281     .0000    -.0281

   CLINOPYROXENE(SS)
 ideal solution
```

```
    DIOPSIDE
             .7359    1.0000     .7359    -.1332     .0000    -.1332
    HEDENBERGITE
             .1053    1.0000     .1053    -.9774     .0000    -.9774
    JADEITE
             .1587    1.0000     .1587    -.7993     .0000    -.7993

  CHLORITE(SS)
 ideal solution

    CLINOCHLORE
             .9034    1.0000     .9034    -.0441     .0000    -.0441
    CHAMOSITE
             .0966    1.0000     .0966   -1.0151     .0000   -1.0151


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

  O2(G)                          -22.31623       4.82801E-23
  H2(G)                             .03596       1.08631E+00
  H2O(G)                           3.80604       6.39793E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  2.5905E-01, delzi=  7.8575E-03, nord= 4
               ncycle=  0
 steps completed =   112, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(PYROPE            ) =     -3.9680

 stepping to zi=  2.7592E-01, delzi=  1.6876E-02, nord= 5
               ncycle=  0
 steps completed =   113, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(PYROPE            ) =     -3.5632

 stepping to zi=  3.0075E-01, delzi=  2.4827E-02, nord= 6
               ncycle=  0
 steps completed =   114, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(PYROPE            ) =     -3.2556

 stepping to zi=  3.2588E-01, delzi=  2.5132E-02, nord= 6
               ncycle=  0
 steps completed =   115, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -20.4492
```

```
 stepping to zi=  3.5079E-01, delzi=  2.4905E-02, nord= 6
              ncycle=  0
 steps completed =   116, iter =  7, ncorr = 0
 most rapidly changing is zvclg1(AL+++            ) =    -20.1382

 stepping to zi=  3.7476E-01, delzi=  2.3972E-02, nord= 6
              ncycle=  0
 steps completed =   117, iter =  7, ncorr = 0
 most rapidly changing is zvclg1(AL+++            ) =    -19.7632

 stepping to zi=  3.9713E-01, delzi=  2.2376E-02, nord= 6
              ncycle=  0
 steps completed =   118, iter =  7, ncorr = 0
 most rapidly changing is zvclg1(AL+++            ) =    -19.3095

 stepping to zi=  3.9811E-01, delzi=  9.7236E-04, nord= 6
              ncycle=  0
 steps completed =   119, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(AL+++            ) =    -19.2867
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  3.98107170553492E-01
                    log of reaction progress =       -.4000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.93331E+01    6.66949E-01    2.66826E+04
1.79154E+02
   CLINOPYROXENE(SS)       9.91961E+01    8.03858E-01    2.21069E+04
1.79148E+02
   MAGNETITE               9.99140E+01    8.59911E-02    2.31339E+04
1.99103E+01
   TREMOLITE               9.99271E+01    7.29332E-02    8.11778E+04
```

5.92488E+01

current total mass = 1.53101E+05 grams
delta total mass = 4.37462E+02 grams
delta total volume = 144.15828 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	2.4504	1.67530E+00
CLINOPYROXENE(SS)	.4782	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	6.1716	1.83200E-01

affinity of the overall irreversible reaction= 5.236 kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.601219E+05	5.583247E+01	5.600118E+01
NA	1.224874E+04	5.533340E-01	5.550060E-01
CA	4.571422E+01	1.184552E-03	1.188131E-03
MG	1.209199E+03	5.166930E-02	5.182543E-02
AL	4.089599E+02	1.574144E-02	1.578901E-02
SI	8.942699E+02	3.306869E-02	3.316861E-02
H	1.080381E+05	1.113243E+02	1.116607E+02
CL	1.701697E+04	4.984937E-01	5.000000E-01
FE	1.609595E+01	2.993279E-04	3.002324E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

```
                                             ph           eh           pe

     internal ph scale              6.2989        .7195
5.0147E+00
     modified nbs ph scale          6.0538        .7547
5.2598E+00
     rational ph scale              6.0538        .7547
5.2598E+00

   phcl =      6.8840



          oxygen fugacity =  2.38303E-21
          log oxygen fugacity = -20.62287



                         activity of water =    .98389
               log activity of water =   -.00705
               alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                    ionic strength =  5.053922E-01 molal
                 sum of molalities =    1.1281104992157
               osmotic coefficient =     .79898
                    equiv. stoich. ionic strength =  4.984937E-01
molal

                         mass of solution =   1.041696 kg
                         mass of solvent  =   1.003022 kg
                         mass of solutes  =    .038674 kg
                         conc of solutes  =   3.712594 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.56764E+01   1.00302E+03
   NA+                  5.05334E-01   1.16175E+01   5.03811E-01     -.
29773     -.24507     -.54280
   CA++                 4.81896E-05   1.93144E-03   4.80444E-05
-4.31836     -.98026    -5.29862
   MG++                 1.41360E-07   3.43575E-06   1.40934E-07
-6.85098     -.98026    -7.83125
   AL+++                5.16811E-20   1.39444E-18   5.15254E-20
-19.28798    -2.20559   -21.49357
   H4SIO4(AQ)           1.56010E-02   1.49948E+00   1.55540E-02
-1.80816      .00000    -1.80816
   H+                   8.86097E-07   8.93098E-07   8.83428E-07
```

```
-6.05383     -.24507    -6.29889
   CL-                  4.58425E-01   1.62525E+01   4.57044E-01     -.
34004     -.24507     -.58511
   FE++                 1.11690E-09   6.23754E-08   1.11353E-09
-8.95330     -.98026    -9.93356
   O2(AQ)               2.01159E-25   6.43684E-24   2.00553E-25
-24.69777      .00000   -24.69777
   H2(AQ)               2.62237E-05   5.28617E-05   2.61447E-05
-4.58262      .00000    -4.58262
   FE+++                3.34853E-21   1.87005E-19   3.33844E-21
-20.47646    -2.20559   -22.68204
   OH-                  2.93101E-02   4.98486E-01   2.92218E-02
-1.53429     -.24507    -1.77936
   H8SI3O10(AQ)         1.92016E-08   4.84484E-06   1.91438E-08
-7.71797      .00000    -7.71797
   H6SI2O7(AQ)          6.56364E-04   1.14348E-01   6.54387E-04
-3.18417      .00000    -3.18417
   AL(OH)3(AQ)          4.32202E-05   3.37133E-03   4.30900E-05
-4.36562      .00000    -4.36562
   AL(OH)4-             4.14050E-03   3.93392E-01   4.12803E-03
-2.38426     -.24507    -2.62932
   AL(OH)SI(OH)-        1.16053E-02   2.00899E+00   1.15703E-02
-1.93665     -.24507    -2.18172
   CACL+                1.02979E-04   7.77834E-03   1.02669E-04
-3.98856     -.24507    -4.23363
   CACL2(AQ)            1.89061E-06   2.09832E-04   1.88492E-06
-5.72471      .00000    -5.72471
   CA(OH)+              7.52138E-05   4.29375E-03   7.49872E-05
-4.12501     -.24507    -4.37008
   CA(H3SIO4)+          9.59858E-04   1.29760E-01   9.56966E-04
-3.01910     -.24507    -3.26417
   FE(OH)+              1.58084E-08   1.15171E-06   1.57608E-08
-7.80242     -.24507    -8.04749
   FE(OH)2              5.49398E-08   4.93697E-06   5.47742E-08
-7.26142      .00000    -7.26142
   FE(OH)3-             2.78006E-07   2.97102E-05   2.77168E-07
-6.55726     -.24507    -6.80232
   FECL+                1.25290E-09   1.14390E-07   1.24913E-09
-8.90339     -.24507    -9.14846
   FECL2(AQ)            2.94877E-08   3.73765E-06   2.93988E-08
-7.53167      .00000    -7.53167
   FE(H3SIO4)+          2.99852E-04   4.52638E-02   2.98948E-04
-3.52440     -.24507    -3.76947
   MGCL+                1.42702E-07   8.52760E-06   1.42272E-07
-6.84688     -.24507    -7.09194
   MG(OH)+              1.56778E-06   6.47687E-05   1.56306E-06
-5.80602     -.24507    -6.05109
   MG(OH)2(AQ)          5.18236E-02   3.02233E+00   5.16674E-02
-1.28678      .00000    -1.28678
   MG(H3SIO4)+          8.39907E-09   1.00295E-06   8.37377E-09
```

```
-8.07708     -.24507    -8.32214
   NACL(AQ)             4.14669E-02   2.42344E+00   4.13420E-02
-1.38361      .00000    -1.38361
   NAOH(AQ)             8.20526E-03   3.28186E-01   8.18054E-03
-2.08722      .00000    -2.08722
   H3SIO4-              3.38984E-03   3.22397E-01   3.37963E-03
-2.47113     -.24507    -2.71620
   HCL(AQ)              1.12729E-06   4.11020E-05   1.12389E-06
-5.94928      .00000    -5.94928

           --- activity ratios of cations ---


           log (NA+   /h+**0)            5.7560969
           log (CA++  /h+**0)            7.2991705
           log (MG++  /h+**0)            4.7665424
           log (AL+++ /h+**0)           -2.5968835
           log (FE++  /h+**0)            2.6642305
           log (FE+++ /h+**0)           -3.7853613


           --- summary of solid product phases---


  product                      log moles       moles        grams
volume, cc

   MAGNETITE                  -1.2679272    5.39601E-02    1.24938E+01
2.40230E+00

   GARNET(SS)                 -1.1618001    6.88969E-02    1.03772E+01
2.85508E+00
   PYROPE                     -2.6326743    2.32984E-03    3.13089E-01
8.78815E-02
   ALMANDINE                  -2.3683885    4.28165E-03    7.10565E-01
1.64287E-01
   GROSSULAR                  -1.2056134    6.22854E-02    9.35358E+00
2.60291E+00

   CLINOPYROXENE(SS)            .1969038    1.57363E+00    3.39260E+02
1.01715E+02
   DIOPSIDE                     .0044033    1.01019E+00    2.18759E+02
6.68746E+01
   HEDENBERGITE                -.8423086    1.43778E-01    3.56704E+01
9.51808E+00
   JADEITE                     -.3770962    4.19666E-01    8.48307E+01
2.53226E+01

   CHLORITE(SS)                 .0534522    1.13097E+00    1.29146E+02
4.78712E+01
```

```
   CLINOCHLORE                  .0095836    1.02231E+00    1.13640E+02
4.32336E+01
   CHAMOSITE                   -.9639283    1.08660E-01    1.55060E+01
4.63763E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                   1.9998609    9.99680E+01    2.31464E+04
4.45057E+03
   TREMOLITE                   1.9996831    9.99271E+01    8.11778E+04
2.72481E+04

   PLAGIOCLASE(SS)             1.9970938    9.93331E+01

   ALBITE                      1.7752450    5.95998E+01    1.56284E+04
6.00945E+03
   ANORTHITE                   1.5991538    3.97332E+01    1.10542E+04
4.00312E+03


   GARNET(SS)                 -1.1618001    6.88969E-02

   PYROPE                     -2.6326743    2.32984E-03    3.13089E-01
8.78815E-02
   ALMANDINE                  -2.3683885    4.28165E-03    7.10565E-01
1.64287E-01
   GROSSULAR                  -1.2056134    6.22854E-02    9.35358E+00
2.60291E+00


   CLINOPYROXENE(SS)           2.0033303    1.00770E+02

   DIOPSIDE                    1.9050783    8.03671E+01    1.74037E+04
5.32030E+03
   HEDENBERGITE                1.3006608    1.99830E+01    4.95767E+03
1.32288E+03
   JADEITE                     -.3770962    4.19666E-01    8.48307E+01
2.53226E+01


   CHLORITE(SS)                 .0534522    1.13097E+00

   CLINOCHLORE                  .0095836    1.02231E+00    1.13640E+02
4.32336E+01
   CHAMOSITE                   -.9639283    1.08660E-01    1.55060E+01
```

```
4.63763E+00



                           mass, grams        volume, cc

           created         4.912771E+02       1.548439E+02
           destroyed       4.374617E+02       1.441583E+02
           net             5.381540E+01       1.068566E+01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-3.1820
 HEMATITE                 .0567  ssatd         PERICLASE
-9.1882
 SPINEL                 -6.4001                BRUCITE
-5.4518
 DIASPORE               -1.2514                ANDALUSITE
-5.5730
 KYANITE                -4.3539                SILLIMANITE
-5.3367
 LAWSONITE              -1.9507                PUMPELLYITE
-3.2599
 ZOISITE                 -.1719                CLINOZOISITE
-.8823
 FORSTERITE             -3.0583                FAYALITE
-3.4323
 CHRYSOTILE             -6.9706                ENSTATITE-CL
-3.1573
 ENSTATITE-OR           -3.2354                ENSTATITE-PR
-3.6408
 DIOPSIDE                -.6370                HEDENBERGITE
-3.4388
 JADEITE                -1.8994                FERROSILITE
-4.4972
 WOLLASTONITE           -3.1745                PSEUDOWOLLASTONITE
-3.6606
 TREMOLITE              -6.1716                ALBITE
-2.7113
 ANORTHITE              -4.4771                KAOLINITE
```

```
-7.9252
 TALC                      -6.4681                PARAGONITE
-1.6682
 MARGARITE                 -3.7266                PREHNITE
-3.2428
 CLINOCHLORE                -.1452                CHAMOSITE
-3.3665
 PYROPE                    -4.8671                ALMANDINE
-3.9926
 GROSSULAR                  -.1450                QUARTZ-ALPHA
-2.2751
 QUARTZ-BETA               -2.5121                COESITE
-2.8714
 HALITE                    -9.7762                CRISTOBALITE-ALPHA
-3.5610
 CRISTOBALITE-BETA         -4.2744


                       --- summary of solid solutions  ---

 mineral                  aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)            -2.3424
     ALBITE                       -2.34237     .7736077     1.00000
     ANORTHITE                    -2.34237     .2263923     1.00000

 ORTHOPYROXENE(SS)          -2.7360
     ENSTATITE-OR                 -2.73596     .7064082     1.00000
     FERROSILITE                  -2.73596     .2935918     1.00000

 GARNET(SS)                   .0000
saturated
     PYROPE                         .00000     .0338163     1.00000
     ALMANDINE                      .00000     .0621458     1.00000
     GROSSULAR                      .00000     .9040379     1.00000

 CLINOPYROXENE(SS)            .0000
saturated
     DIOPSIDE                       .00000     .6419475     1.00000
     HEDENBERGITE                   .00000     .0913666     1.00000
     JADEITE                        .00000     .2666859     1.00000

 CPX_SUBCALCIC(SS)           -.4458
     DIOPSIDE                      -.44576     .8754059     1.00000
     HEDENBERGITE                  -.44576     .1245941     1.00000

 CHLORITE(SS)                 .0000
saturated
     CLINOCHLORE                    .00000     .9039230     1.00000
     CHAMOSITE                      .00000     .0960770     1.00000
```

```
 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   GARNET(SS)
 ideal solution

     PYROPE
             .0338    1.0000     .0338   -1.4709     .0000   -1.4709
     ALMANDINE
             .0621    1.0000     .0621   -1.2066     .0000   -1.2066
     GROSSULAR
             .9040    1.0000     .9040    -.0438     .0000    -.0438

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .6419    1.0000     .6419    -.1925     .0000    -.1925
     HEDENBERGITE
             .0914    1.0000     .0914   -1.0392     .0000   -1.0392
     JADEITE
             .2667    1.0000     .2667    -.5740     .0000    -.5740

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
             .9039    1.0000     .9039    -.0439     .0000    -.0439
     CHAMOSITE
             .0961    1.0000     .0961   -1.0174     .0000   -1.0174


           --- summary of gas species ---

           gas                 log fugacity         fugacity
partial pressure

   O2(G)                         -20.62287       2.38303E-21
   H2(G)                           -.81072       1.54626E-01
   H2O(G)                          3.80605       6.39806E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
 stepping to zi=  4.0783E-01, delzi=  9.7236E-03, nord= 5
              ncycle=  0
 iter =    7
       1 supersaturated pure minerals
       0 supersaturated solid solutions

                          the most supersaturated phases     affinity,
kcal

                            1      15   ZOISITE                  .
02161083
 --- go back to reduce the extent of supersaturation ---
 --- cutting step size and trying again ---

 stepping to zi=  4.0054E-01, delzi=  2.4309E-03, nord= 5
              ncycle=  0
 steps completed =   120, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(AL+++            ) =    -19.2284

 stepping to zi=  4.0540E-01, delzi=  4.8618E-03, nord= 5
              ncycle=  0
 steps completed =   121, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(AL+++            ) =    -19.1058

 stepping to zi=  4.0719E-01, delzi=  1.7870E-03, nord= 6
              ncycle=  0
 iter =    5
       1 supersaturated pure minerals
       0 supersaturated solid solutions

                          the most supersaturated phases     affinity,
kcal

                            1      15   ZOISITE                  .
00818524


   attempted species assemblage no.   2

             1      1  H2O
             2      2  NA+
             3      4  CA++
             4      5  MG++
             5      6  AL+++
             6      7  H4SIO4(AQ)
             7     13  H+
             8     16  CL-
             9     21  FE++
            10     32  O2(G)
```

```
              11      1  MAGNETITE
              12     15  ZOISITE
              13      1  GARNET(SPYROPE
              14      2  GARNET(SALMANDINE
              15      3  GARNET(SGROSSULAR
              16      1  CLINOPYRDIOPSIDE
              17      2  CLINOPYRHEDENBERGITE
              18      3  CLINOPYRJADEITE
              19      1  CHLORITECLINOCHLORE
              20      2  CHLORITECHAMOSITE

 steps completed =   122, iter = 12, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                   reaction progress        =  4.07186894212364E-01
                   log of reaction progress =       -.3902062

                   temperature    =    450.000 degrees c
                   total pressure =    500.000 bars

                   computing units remaining =       .000


 change in the product phase assemblage


                             --- reactant summary ---



        reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.93178E+01    6.82160E-01    2.66785E+04
1.83240E+02
   CLINOPYROXENE(SS)      9.91778E+01    8.22192E-01    2.21028E+04
1.83234E+02
   MAGNETITE              9.99120E+01    8.79524E-02    2.31335E+04
2.03644E+01
   TREMOLITE              9.99254E+01    7.45966E-02    8.11764E+04
6.06001E+01


                current total mass =  1.53091E+05 grams
                delta total mass   =  4.47439E+02 grams
                delta total volume =    147.44613 cc
```

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	2.3065	1.67530E+00
CLINOPYROXENE(SS)	.4854	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.9907	1.83200E-01

affinity of the overall irreversible reaction= 4.962 kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.603056E+05	5.581990E+01	5.599185E+01
NA	1.208932E+04	5.458926E-01	5.475742E-01
CA	5.277155E+01	1.366823E-03	1.371033E-03
MG	1.140926E+03	4.873059E-02	4.888071E-02
AL	3.793592E+02	1.459567E-02	1.464063E-02
SI	9.154630E+02	3.383753E-02	3.394177E-02
H	1.080739E+05	1.113124E+02	1.116553E+02
CL	1.702344E+04	4.984645E-01	5.000000E-01
FE	1.925016E+01	3.578282E-04	3.589304E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	6.2285	.7352	5.1239E+00
modified nbs ph scale	5.9841	.7702	5.3683E+00
rational ph scale	5.9841	.7702	5.3683E+00

```
   phcl =      6.8126



          oxygen fugacity =  3.40542E-21
          log oxygen fugacity = -20.46783



                              activity of water =    .98389
               log activity of water =   -.00705
               alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                    ionic strength =  4.998323E-01 molal
                  sum of molalities =    1.1137655980080
               osmotic coefficient =     .80922
                    equiv. stoich. ionic strength =  4.984645E-01
molal

                         mass of solution =   1.041300 kg
                         mass of solvent  =   1.003081 kg
                         mass of solutes  =    .038219 kg
                         conc of solutes  =   3.670348 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.56797E+01   1.00308E+03
   NA+                  4.99522E-01   1.14839E+01   4.97988E-01     -.
30278     -.24437     -.54716
   CA++                 5.98185E-05   2.39752E-03   5.96348E-05
-4.22450     -.97749    -5.20199
   MG++                 1.83227E-07   4.45332E-06   1.82664E-07
-6.73835     -.97749    -7.71584
   AL+++                8.53874E-20   2.30388E-18   8.51252E-20
-19.06994    -2.19936   -21.26930
   H4SIO4(AQ)           1.68641E-02   1.62089E+00   1.68124E-02
-1.77437      .00000    -1.77437
   H+                   1.04048E-06   1.04870E-06   1.03729E-06
-5.98410     -.24437    -6.22847
   CL-                  4.58720E-01   1.62630E+01   4.57311E-01     -.
33979     -.24437     -.58416
   FE++                 1.44634E-09   8.07739E-08   1.44190E-09
-8.84106     -.97749    -9.81856
   O2(AQ)               2.87479E-25   9.19898E-24   2.86596E-25
-24.54273      .00000   -24.54273
   H2(AQ)               2.19381E-05   4.42228E-05   2.18707E-05
```

```
-4.66014      .00000    -4.66014
   FE+++                5.53137E-21   3.08910E-19   5.51438E-21
-20.25850    -2.19936   -22.45786
   OH-                  2.48847E-02   4.23221E-01   2.48083E-02
-1.60540     -.24437    -1.84978
   H8SI3O10(AQ)         2.42507E-08   6.11879E-06   2.41762E-08
-7.61661      .00000    -7.61661
   H6SI2O7(AQ)          7.66910E-04   1.33607E-01   7.64555E-04
-3.11659      .00000    -3.11659
   AL(OH)3(AQ)          4.45365E-05   3.47400E-03   4.43998E-05
-4.35262      .00000    -4.35262
   AL(OH)4-             3.62219E-03   3.44147E-01   3.61106E-03
-2.44236     -.24437    -2.68674
   AL(OH)SI(OH)-        1.09739E-02   1.89969E+00   1.09402E-02
-1.96097     -.24437    -2.20535
   CACL+                1.28722E-04   9.72276E-03   1.28327E-04
-3.89168     -.24437    -4.13606
   CACL2(AQ)            2.37215E-06   2.63276E-04   2.36487E-06
-5.62619      .00000    -5.62619
   CA(OH)+              7.97692E-05   4.55381E-03   7.95242E-05
-4.09950     -.24437    -4.34387
   CA(H3SIO4)+          1.10035E-03   1.48753E-01   1.09697E-03
-2.95980     -.24437    -3.20418
   FE(OH)+              1.74905E-08   1.27426E-06   1.74368E-08
-7.75853     -.24437    -8.00291
   FE(OH)2              5.17693E-08   4.65207E-06   5.16103E-08
-7.28726      .00000    -7.28726
   FE(OH)3-             2.22397E-07   2.37673E-05   2.21714E-07
-6.65421     -.24437    -6.89858
   FECL+                1.63378E-09   1.49164E-07   1.62877E-09
-8.78814     -.24437    -9.03251
   FECL2(AQ)            3.85973E-08   4.89232E-06   3.84787E-08
-7.41478      .00000    -7.41478
   FE(H3SIO4)+          3.58597E-04   5.41316E-02   3.57496E-04
-3.44673     -.24437    -3.69110
   MGCL+                1.86258E-07   1.11304E-05   1.85686E-07
-6.73122     -.24437    -6.97559
   MG(OH)+              1.73622E-06   7.17273E-05   1.73089E-06
-5.76173     -.24437    -6.00610
   MG(OH)2(AQ)          4.88786E-02   2.85058E+00   4.87285E-02
-1.31222      .00000    -1.31222
   MG(H3SIO4)+          1.00540E-08   1.20056E-06   1.00231E-08
-7.99900     -.24437    -8.24337
   NACL(AQ)             4.11448E-02   2.40462E+00   4.10184E-02
-1.38702      .00000    -1.38702
   NAOH(AQ)             6.90781E-03   2.76292E-01   6.88660E-03
-2.16200      .00000    -2.16200
   H3SIO4-              3.11086E-03   2.95864E-01   3.10131E-03
-2.50845     -.24437    -2.75283
   HCL(AQ)              1.32870E-06   4.84455E-05   1.32462E-06
```

```
-5.87791      .00000    -5.87791

           --- activity ratios of cations ---


           log (NA+   /h+**0)            5.6813193
           log (CA++  /h+**0)            7.2549542
           log (MG++  /h+**0)            4.7411074
           log (AL+++ /h+**0)           -2.5838809
           log (FE++  /h+**0)            2.6383898
           log (FE+++ /h+**0)           -3.7724418


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                  -1.2524558    5.59170E-02    1.29470E+01
2.48943E+00
   ZOISITE                    -3.2357806    5.81058E-04    2.64010E-01
7.89542E-02

   GARNET(SS)                 -1.1424897    7.20295E-02    1.08503E+01
2.98390E+00
   PYROPE                     -2.5963773    2.53293E-03    3.40380E-01
9.55420E-02
   ALMANDINE                  -2.3324976    4.65053E-03    7.71782E-01
1.78441E-01
   GROSSULAR                  -1.1881166    6.48460E-02    9.73812E+00
2.70992E+00

   CLINOPYROXENE(SS)            .2079115    1.61403E+00    3.47859E+02
1.04292E+02
   DIOPSIDE                     .0133334    1.03118E+00    2.23304E+02
6.82640E+01
   HEDENBERGITE                -.8337842    1.46628E-01    3.63775E+01
9.70675E+00
   JADEITE                     -.3602898    4.36225E-01    8.81779E+01
2.63218E+01

   CHLORITE(SS)                 .0554215    1.13611E+00    1.29730E+02
4.80888E+01
   CLINOCHLORE                  .0115919    1.02705E+00    1.14166E+02
4.34340E+01
   CHAMOSITE                   -.9623257    1.09062E-01    1.55633E+01
4.65477E+00
```

--- grand summary of solid phases (e.s.+p.r.s. +reactants) ---

phase/end-member	log moles	moles	grams	volume, cc
MAGNETITE	1.9998609	9.99680E+01	2.31464E+04	4.45057E+03
ZOISITE	-3.2357806	5.81058E-04	2.64010E-01	7.89542E-02
TREMOLITE	1.9996759	9.99254E+01	8.11764E+04	2.72477E+04
PLAGIOCLASE(SS)	1.9970273	9.93178E+01		
ALBITE	1.7751785	5.95907E+01	1.56261E+04	6.00853E+03
ANORTHITE	1.5990873	3.97271E+01	1.10525E+04	4.00251E+03
GARNET(SS)	-1.1424897	7.20295E-02		
PYROPE	-2.5963773	2.53293E-03	3.40380E-01	9.55420E-02
ALMANDINE	-2.3324976	4.65053E-03	7.71782E-01	1.78441E-01
GROSSULAR	-1.1881166	6.48460E-02	9.73812E+00	2.70992E+00
CLINOPYROXENE(SS)	2.0034254	1.00792E+02		
DIOPSIDE	1.9051125	8.03734E+01	1.74051E+04	5.32072E+03
HEDENBERGITE	1.3006431	1.99822E+01	4.95747E+03	1.32282E+03
JADEITE	-.3602898	4.36225E-01	8.81779E+01	2.63218E+01
CHLORITE(SS)	.0554215	1.13611E+00		
CLINOCHLORE	.0115919	1.02705E+00	1.14166E+02	4.34340E+01
CHAMOSITE	-.9623257	1.09062E-01	1.55633E+01	4.65477E+00

```
                        mass, grams        volume, cc

           created         5.016503E+02       1.579335E+02
           destroyed       4.474390E+02       1.474461E+02
           net             5.421129E+01       1.048740E+01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-3.0960
 HEMATITE                 .1422  ssatd         PERICLASE
-9.2723
 SPINEL                 -6.3982                BRUCITE
-5.5360
 DIASPORE               -1.2084                ANDALUSITE
-5.3751
 KYANITE                -4.1561                SILLIMANITE
-5.1389
 LAWSONITE              -1.7874                PUMPELLYITE
-3.0434
 ZOISITE                  .0000  satd          CLINOZOISITE
-.7104
 FORSTERITE             -3.0866                FAYALITE
-3.4619
 CHRYSOTILE             -6.9995                ENSTATITE-CL
-3.1297
 ENSTATITE-OR           -3.2078                ENSTATITE-PR
-3.6132
 DIOPSIDE                -.6439                HEDENBERGITE
-3.4470
 JADEITE                -1.8802                FERROSILITE
-4.4709
 WOLLASTONITE           -3.2090                PSEUDOWOLLASTONITE
-3.6951
 TREMOLITE              -5.9907                ALBITE
-2.5803
 ANORTHITE              -4.3138                KAOLINITE
-7.6156
 TALC                   -6.2734                PARAGONITE
-1.4511
 MARGARITE              -3.4772                PREHNITE
```

```
-3.1140
 CLINOCHLORE            -.1450              CHAMOSITE
-3.3677
 PYROPE                -4.8109              ALMANDINE
-3.9378
 GROSSULAR              -.1510              QUARTZ-ALPHA
-2.1633
 QUARTZ-BETA           -2.4003              COESITE
-2.7596
 HALITE                -9.7875              CRISTOBALITE-ALPHA
-3.4492
 CRISTOBALITE-BETA     -4.1626


                    --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)          -2.2040
     ALBITE                     -2.20399     .7696401     1.00000
     ANORTHITE                  -2.20399     .2303599     1.00000

 ORTHOPYROXENE(SS)        -2.7087
     ENSTATITE-OR               -2.70872     .7066020     1.00000
     FERROSILITE                -2.70872     .2933980     1.00000

 GARNET(SS)                 .0000
saturated
     PYROPE                       .00000     .0351651     1.00000
     ALMANDINE                    .00000     .0645643     1.00000
     GROSSULAR                    .00000     .9002706     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .6388838     1.00000
     HEDENBERGITE                 .00000     .0908457     1.00000
     JADEITE                      .00000     .2702705     1.00000

 CPX_SUBCALCIC(SS)         -.4528
     DIOPSIDE                    -.45280     .8755077     1.00000
     HEDENBERGITE                -.45280     .1244923     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9040041     1.00000
     CHAMOSITE                    .00000     .0959959     1.00000


 solid solution product phases
```

```
            xbar     lambda   activity  log xbar  log lambda log
activity

   GARNET(SS)
 ideal solution

     PYROPE
              .0352    1.0000     .0352   -1.4539     .0000   -1.4539
     ALMANDINE
              .0646    1.0000     .0646   -1.1900     .0000   -1.1900
     GROSSULAR
              .9003    1.0000     .9003    -.0456     .0000    -.0456

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6389    1.0000     .6389    -.1946     .0000    -.1946
     HEDENBERGITE
              .0908    1.0000     .0908   -1.0417     .0000   -1.0417
     JADEITE
              .2703    1.0000     .2703    -.5682     .0000    -.5682

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9040    1.0000     .9040    -.0438     .0000    -.0438
     CHAMOSITE
              .0960    1.0000     .0960   -1.0177     .0000   -1.0177


           --- summary of gas species ---

           gas                 log fugacity         fugacity
partial pressure

   O2(G)                         -20.46783       3.40542E-21
   H2(G)                           -.88824       1.29349E-01
   H2O(G)                          3.80605       6.39806E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  4.0719E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =   123, iter =  4, ncorr = 0
```

```
 most rapidly changing is zvclg1(ZOISITE           ) =    -3.2358

 stepping to zi=  4.0719E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =   124, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =    -3.2358

 stepping to zi=  4.0719E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
 steps completed =   125, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =    -3.2357

 stepping to zi=  4.0719E-01, delzi=  3.9474E-08, nord= 1
              ncycle=  0
 steps completed =   126, iter =  2, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =    -3.2357

 stepping to zi=  4.0719E-01, delzi=  3.9474E-07, nord= 2
              ncycle=  0
 steps completed =   127, iter =  2, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =    -3.2353

 stepping to zi=  4.0719E-01, delzi=  3.9474E-06, nord= 2
              ncycle=  0
 steps completed =   128, iter =  2, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =    -3.2310

 stepping to zi=  4.0723E-01, delzi=  3.9474E-05, nord= 2
              ncycle=  0
 steps completed =   129, iter =  3, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =    -3.1900

 stepping to zi=  4.0763E-01, delzi=  3.9474E-04, nord= 2
              ncycle=  0
 steps completed =   130, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =    -2.9112

 stepping to zi=  4.1157E-01, delzi=  3.9474E-03, nord= 3
              ncycle=  0
 steps completed =   131, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =    -2.1522

 stepping to zi=  4.2380E-01, delzi=  1.2231E-02, nord= 4
                    the phase to be dropped is GARNET(SS)
(50600)


   attempted species assemblage no.   2

             1      1  H2O
```

```
          2      2  NA+
          3      4  CA++
          4      5  MG++
          5      6  AL+++
          6      7  H4SIO4(AQ)
          7     13  H+
          8     16  CL-
          9     21  FE++
         10     32  O2(G)
         11      1  MAGNETITE
         12     15  ZOISITE
         13      1  CLINOPYRDIOPSIDE
         14      2  CLINOPYRHEDENBERGITE
         15      3  CLINOPYRJADEITE
         16      1  CHLORITECLINOCHLORE
         17      2  CHLORITECHAMOSITE

 steps completed =   132, iter =  5, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  4.23804024333403E-01
                    log of reaction progress =       -.3728349

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 change in the product phase assemblage


                              --- reactant summary ---



        reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.92900E+01    7.09999E-01    2.66710E+04
1.90718E+02
   CLINOPYROXENE(SS)      9.91443E+01    8.55745E-01    2.20954E+04
1.90712E+02
   MAGNETITE              9.99085E+01    9.15417E-02    2.31327E+04
2.11954E+01
   TREMOLITE              9.99224E+01    7.76409E-02    8.11740E+04
6.30732E+01
```

current total mass = 1.53073E+05 grams
delta total mass = 4.65699E+02 grams
delta total volume = 153.46335 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	2.3095	1.67530E+00
CLINOPYROXENE(SS)	.4776	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	5.9688	1.83200E-01

affinity of the overall irreversible reaction= 4.963 kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.603313E+05	5.581773E+01	5.598975E+01
NA	1.206818E+04	5.449007E-01	5.465800E-01
CA	5.392449E+01	1.396588E-03	1.400893E-03
MG	1.135846E+03	4.851030E-02	4.865980E-02
AL	3.727368E+02	1.433988E-02	1.438408E-02
SI	9.139617E+02	3.377971E-02	3.388382E-02
H	1.080794E+05	1.113104E+02	1.116534E+02
CL	1.702458E+04	4.984638E-01	5.000000E-01
FE	2.001198E+01	3.719635E-04	3.731099E-04
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

ph eh pe

```
     internal ph scale              6.2198         .7352
5.1243E+00
     modified nbs ph scale          5.9755         .7703
5.3685E+00
     rational ph scale              5.9755         .7703
5.3685E+00

   phcl =      6.8038



          oxygen fugacity =  3.15452E-21
          log oxygen fugacity = -20.50107




                              activity of water =    .98389
               log activity of water =   -.00705
               alkalinity =  0.000000E+00 equiv/kg solvent
                                            (not def. for t.gt.50 c)

                    ionic strength =  4.990787E-01 molal
                 sum of molalities =    1.1119574122703
               osmotic coefficient =     .81053
                    equiv. stoich. ionic strength =  4.984638E-01
molal

                         mass of solution =   1.041230 kg
                         mass of solvent  =   1.003082 kg
                         mass of solutes  =    .038148 kg
                         conc of solutes  =   3.663717 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.56798E+01   1.00308E+03
   NA+                  4.98718E-01   1.14654E+01   4.97186E-01     -.
30348     -.24428     -.54776
   CA++                 6.18300E-05   2.47815E-03   6.16401E-05
-4.21014     -.97712    -5.18725
   MG++                 1.89674E-07   4.61002E-06   1.89091E-07
-6.72333     -.97712    -7.70045
   AL+++                9.02876E-20   2.43610E-18   9.00102E-20
-19.04571    -2.19851   -21.24422
   H4SIO4(AQ)           1.69698E-02   1.63105E+00   1.69177E-02
-1.77166      .00000    -1.77166
   H+                   1.06126E-06   1.06965E-06   1.05800E-06
-5.97551     -.24428    -6.21979
   CL-                  4.58760E-01   1.62644E+01   4.57351E-01     -.
```

```
33975     -.24428     -.58403
   FE++                    1.52334E-09   8.50741E-08   1.51866E-09
-8.81854     -.97712    -9.79566
   O2(AQ)                  2.66299E-25   8.52125E-24   2.65481E-25
-24.57597      .00000   -24.57597
   H2(AQ)                  2.27939E-05   4.59479E-05   2.27239E-05
-4.64352      .00000    -4.64352
   FE+++                   5.82452E-21   3.25282E-19   5.80663E-21
-20.23608    -2.19851   -22.43459
   OH-                     2.43869E-02   4.14755E-01   2.43120E-02
-1.61418     -.24428    -1.85846
   H8SI3O10(AQ)            2.47093E-08   6.23450E-06   2.46334E-08
-7.60848      .00000    -7.60848
   H6SI2O7(AQ)             7.76549E-04   1.35286E-01   7.74163E-04
-3.11117      .00000    -3.11117
   AL(OH)3(AQ)             4.44379E-05   3.46631E-03   4.43014E-05
-4.35358      .00000    -4.35358
   AL(OH)4-                3.54187E-03   3.36515E-01   3.53098E-03
-2.45210     -.24428    -2.69638
   AL(OH)SI(OH)-           1.07978E-02   1.86920E+00   1.07646E-02
-1.96800     -.24428    -2.21228
   CACL+                   1.33178E-04   1.00593E-02   1.32769E-04
-3.87690     -.24428    -4.12118
   CACL2(AQ)               2.45554E-06   2.72531E-04   2.44800E-06
-5.61119      .00000    -5.61119
   CA(OH)+                 8.08724E-05   4.61679E-03   8.06239E-05
-4.09354     -.24428    -4.33782
   CA(H3SIO4)+             1.12256E-03   1.51755E-01   1.11911E-03
-2.95113     -.24428    -3.19541
   FE(OH)+                 1.80688E-08   1.31639E-06   1.80133E-08
-7.74441     -.24428    -7.98869
   FE(OH)2                 5.24339E-08   4.71180E-06   5.22728E-08
-7.28172      .00000    -7.28172
   FE(OH)3-                2.20746E-07   2.35908E-05   2.20067E-07
-6.65744     -.24428    -6.90172
   FECL+                   1.72241E-09   1.57256E-07   1.71712E-09
-8.76520     -.24428    -9.00948
   FECL2(AQ)               4.07121E-08   5.16039E-06   4.05871E-08
-7.39161      .00000    -7.39161
   FE(H3SIO4)+             3.72775E-04   5.62717E-02   3.71629E-04
-3.42989     -.24428    -3.67417
   MGCL+                   1.92996E-07   1.15331E-05   1.92403E-07
-6.71579     -.24428    -6.96007
   MG(OH)+                 1.76289E-06   7.28290E-05   1.75747E-06
-5.75511     -.24428    -5.99939
   MG(OH)2(AQ)             4.86576E-02   2.83769E+00   4.85081E-02
-1.31419      .00000    -1.31419
   MG(H3SIO4)+             1.02723E-08   1.22664E-06   1.02408E-08
-7.98967     -.24428    -8.23395
   NACL(AQ)                4.11000E-02   2.40200E+00   4.09737E-02
```

```
-1.38749       .00000    -1.38749
   NAOH(AQ)              6.76167E-03   2.70447E-01   6.74090E-03
-2.17128       .00000    -2.17128
   H3SIO4-               3.06773E-03   2.91762E-01   3.05830E-03
-2.51452      -.24428    -2.75880
   HCL(AQ)               1.35594E-06   4.94388E-05   1.35177E-06
-5.86910       .00000    -5.86910

           --- activity ratios of cations ---


           log (NA+   /h+**0)            5.6720321
           log (CA++  /h+**0)            7.2523311
           log (MG++  /h+**0)            4.7391392
           log (AL+++ /h+**0)           -2.5848440
           log (FE++  /h+**0)            2.6439293
           log (FE+++ /h+**0)           -3.7752116


           --- summary of solid product phases---


  product                     log moles        moles        grams
volume, cc

   MAGNETITE                 -1.2254305    5.95072E-02    1.37782E+01
2.64926E+00
   ZOISITE                   -1.5997416    2.51338E-02    1.14198E+01
3.41518E+00

   CLINOPYROXENE(SS)           .2300093    1.69828E+00    3.66185E+02
1.09766E+02
   DIOPSIDE                    .0362635    1.08709E+00    2.35411E+02
7.19650E+01
   HEDENBERGITE               -.8033463    1.57273E-01    3.90185E+01
1.04115E+01
   JADEITE                    -.3430187    4.53922E-01    9.17552E+01
2.73897E+01

   CHLORITE(SS)                .0514341    1.12573E+00    1.28598E+02
4.76499E+01
   CLINOCHLORE                 .0068781    1.01596E+00    1.12934E+02
4.29651E+01
   CHAMOSITE                  -.9595318    1.09766E-01    1.56638E+01
4.68482E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---
```

```
      phase/end-member        log moles        moles        grams
volume, cc

   MAGNETITE                  1.9998609    9.99680E+01    2.31464E+04
4.45057E+03
   ZOISITE                   -1.5997416    2.51338E-02    1.14198E+01
3.41518E+00
   TREMOLITE                  1.9996627    9.99224E+01    8.11740E+04
2.72468E+04

   PLAGIOCLASE(SS)            1.9969055    9.92900E+01

   ALBITE                     1.7750568    5.95740E+01    1.56217E+04
6.00685E+03
   ANORTHITE                  1.5989655    3.97160E+01    1.10494E+04
4.00139E+03


   CLINOPYROXENE(SS)          2.0036438    1.00843E+02

   DIOPSIDE                   1.9052695    8.04025E+01    1.74114E+04
5.32264E+03
   HEDENBERGITE               1.3007286    1.99861E+01    4.95845E+03
1.32308E+03
   JADEITE                    -.3430187    4.53922E-01    9.17552E+01
2.73897E+01


   CHLORITE(SS)                .0514341    1.12573E+00

   CLINOCHLORE                 .0068781    1.01596E+00    1.12934E+02
4.29651E+01
   CHAMOSITE                  -.9595318    1.09766E-01    1.56638E+01
4.68482E+00



                          mass, grams        volume, cc

           created        5.199803E+02       1.634805E+02
           destroyed      4.656988E+02       1.534633E+02
           net            5.428155E+01       1.001716E+01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---
```

mineral	affinity, kcal	state	mineral	affinity, kcal	state
MAGNETITE	.0000	satd	CORUNDUM	-3.1023	
HEMATITE	.1238	ssatd	PERICLASE	-9.2789	
SPINEL	-6.4111		BRUCITE	-5.5425	
DIASPORE	-1.2116		ANDALUSITE	-5.3725	
KYANITE	-4.1535		SILLIMANITE	-5.1363	
LAWSONITE	-1.7845		PUMPELLYITE	-3.0467	
ZOISITE	.0000	satd	CLINOZOISITE	-.7104	
FORSTERITE	-3.0886		FAYALITE	-3.4391	
CHRYSOTILE	-7.0011		ENSTATITE-CL	-3.1272	
ENSTATITE-OR	-3.2053		ENSTATITE-PR	-3.6107	
DIOPSIDE	-.6411		HEDENBERGITE	-3.4194	
JADEITE	-1.8962		FERROSILITE	-4.4436	
WOLLASTONITE	-3.2087		PSEUDOWOLLASTONITE	-3.6948	
TREMOLITE	-5.9688		ALBITE	-2.5873	
ANORTHITE	-4.3109		KAOLINITE	-7.6040	
TALC	-6.2571		PARAGONITE	-1.4645	
MARGARITE	-3.4807		PREHNITE	-3.1108	
CLINOCHLORE	-.1474		CHAMOSITE	-3.3453	
PYROPE	-4.8106		ALMANDINE	-3.9126	
GROSSULAR	-.1528		QUARTZ-ALPHA	-2.1544	
QUARTZ-BETA	-2.3913		COESITE	-2.7506	
HALITE	-9.7890		CRISTOBALITE-ALPHA	-3.4402	
CRISTOBALITE-BETA	-4.1537				

```
                    --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -2.2087
     ALBITE                      -2.20871     .7684175     1.00000
     ANORTHITE                   -2.20871     .2315825     1.00000

 ORTHOPYROXENE(SS)         -2.6989
     ENSTATITE-OR                -2.69892     .7030053     1.00000
     FERROSILITE                 -2.69892     .2969947     1.00000

 GARNET(SS)                  .0000
     PYROPE                        .00000     .0351733     1.00000
     ALMANDINE                     .00000     .0657064     1.00000
     GROSSULAR                     .00000     .8991203     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .6401095     1.00000
     HEDENBERGITE                  .00000     .0926071     1.00000
     JADEITE                       .00000     .2672834     1.00000

 CPX_SUBCALCIC(SS)          -.4469
     DIOPSIDE                     -.44693     .8736113     1.00000
     HEDENBERGITE                 -.44693     .1263887     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9024934     1.00000
     CHAMOSITE                     .00000     .0975066     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6401    1.0000     .6401    -.1937     .0000    -.1937
     HEDENBERGITE
              .0926    1.0000     .0926   -1.0334     .0000   -1.0334
     JADEITE
              .2673    1.0000     .2673    -.5730     .0000    -.5730

   CHLORITE(SS)
```

```
 ideal solution

     CLINOCHLORE
              .9025    1.0000     .9025    -.0446     .0000    -.0446
     CHAMOSITE
              .0975    1.0000     .0975   -1.0110     .0000   -1.0110


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                         -20.50107       3.15452E-21
   H2(G)                           -.87162       1.34395E-01
   H2O(G)                          3.80605       6.39806E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  4.2380E-01, delzi=  1.0000E-08, nord= 0
               ncycle=  0
 steps completed =   133, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -19.0444

 stepping to zi=  4.2380E-01, delzi=  1.0000E-08, nord= 0
               ncycle=  0
 steps completed =   134, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -19.0444

 stepping to zi=  4.2380E-01, delzi=  1.0000E-08, nord= 0
               ncycle=  0
 steps completed =   135, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -19.0444

 stepping to zi=  4.2380E-01, delzi=  1.0000E-07, nord= 1
               ncycle=  0
 steps completed =   136, iter =  1, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -19.0444

 stepping to zi=  4.2381E-01, delzi=  1.0000E-06, nord= 1
               ncycle=  0
 steps completed =   137, iter =  2, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -19.0443

 stepping to zi=  4.2382E-01, delzi=  1.0000E-05, nord= 2
               ncycle=  0
```

```
steps completed =   138, iter =  3, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -19.0441

stepping to zi=  4.2392E-01, delzi=  1.0000E-04, nord= 2
              ncycle=  0
steps completed =   139, iter =  3, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -19.0419

stepping to zi=  4.2492E-01, delzi=  1.0000E-03, nord= 3
              ncycle=  0
steps completed =   140, iter =  4, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -19.0197

stepping to zi=  4.2740E-01, delzi=  2.4801E-03, nord= 4
              ncycle=  0
steps completed =   141, iter =  5, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -18.9635

stepping to zi=  4.3082E-01, delzi=  3.4260E-03, nord= 4
              ncycle=  0
steps completed =   142, iter =  5, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -18.8828

stepping to zi=  4.3694E-01, delzi=  6.1144E-03, nord= 5
              ncycle=  0
steps completed =   143, iter =  5, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -18.7302

stepping to zi=  4.4629E-01, delzi=  9.3499E-03, nord= 6
              ncycle=  0
steps completed =   144, iter =  6, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -18.4739

stepping to zi=  4.5612E-01, delzi=  9.8316E-03, nord= 6
              ncycle=  0
steps completed =   145, iter =  6, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -18.1748

stepping to zi=  4.6643E-01, delzi=  1.0313E-02, nord= 6
              ncycle=  0
steps completed =   146, iter =  6, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -17.8344

stepping to zi=  4.7738E-01, delzi=  1.0952E-02, nord= 6
              ncycle=  0
steps completed =   147, iter =  6, ncorr = 0
most rapidly changing is zvclg1(AL+++             ) =    -17.4586

stepping to zi=  4.8950E-01, delzi=  1.2123E-02, nord= 6
              ncycle=  0
```

```
 steps completed =   148, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -17.0527

 stepping to zi=  4.9889E-01, delzi=  9.3825E-03, nord= 6
               ncycle=  0
 steps completed =   149, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -16.7617

 stepping to zi=  5.0272E-01, delzi=  3.8341E-03, nord= 6
               ncycle=  0
 steps completed =   150, iter =  6, ncorr = 0
 most rapidly changing is zvclg1(AL+++             ) =    -16.6504

 stepping to zi=  5.0330E-01, delzi=  5.7512E-04, nord= 6
               ncycle=  0
 iter =    4
       1 supersaturated pure minerals
       0 supersaturated solid solutions

                            the most supersaturated phases     affinity,
kcal

                              1      42   PARAGONITE               .
00884193


   attempted species assemblage no.   2

              1      1  H2O
              2      2  NA+
              3      4  CA++
              4      5  MG++
              5      6  AL+++
              6      7  H4SIO4(AQ)
              7     13  H+
              8     16  CL-
              9     21  FE++
             10     32  O2(G)
             11      1  MAGNETITE
             12     15  ZOISITE
             13     42  PARAGONITE
             14      1  CLINOPYRDIOPSIDE
             15      2  CLINOPYRHEDENBERGITE
             16      3  CLINOPYRJADEITE
             17      1  CHLORITECLINOCHLORE
             18      2  CHLORITECHAMOSITE

 steps completed =   151, iter =  9, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
                    reaction progress        =  5.03296205375839E-01
                    log of reaction progress =       -.2981763

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 change in the product phase assemblage


                              --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.91568E+01    8.43172E-01    2.66353E+04
2.26491E+02
   CLINOPYROXENE(SS)       9.89837E+01    1.01626E+00    2.20596E+04
2.26484E+02
   MAGNETITE               9.98913E+01    1.08712E-01    2.31287E+04
2.51710E+01
   TREMOLITE               9.99078E+01    9.22039E-02    8.11621E+04
7.49037E+01


                current total mass =  1.52986E+05 grams
                delta total mass   =  5.53049E+02 grams
                delta total volume =    182.24820 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)           1.0756    1.67530E+00
   CLINOPYROXENE(SS)          .5158    0.00000E+00
   MAGNETITE                  .0000    0.00000E+00
   TREMOLITE                 2.7044    1.83200E-01

          affinity of the overall irreversible reaction=     2.297
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included
```

```
     --- element totals for the aqueous phase ---

  element         mg/kg soln.         molal conc.          moles

     O          8.606879E+05        5.587054E+01        5.598682E+01
     NA         1.101200E+04        4.974764E-01        4.985118E-01
     CA         2.565198E+02        6.647129E-03        6.660963E-03
     MG         6.217873E+02        2.656973E-02        2.662502E-02
     AL         1.281166E+02        4.931506E-03        4.941770E-03
     SI         1.993034E+03        7.370101E-02        7.385439E-02
     H          1.080693E+05        1.113591E+02        1.115909E+02
     CL         1.703253E+04        4.989616E-01        5.000000E-01
     FE         1.988292E+02        3.697610E-03        3.705306E-03

     co3--                          0.000000E+00        0.000000E+00
     so4--                          0.000000E+00        0.000000E+00
     s--                            0.000000E+00        0.000000E+00

   warning-- co3--, so4--, and s-- totals require that routine comp1
   have the names of non-carbonate carbon, sulfide sulfur,
   and non-sulfate sulfur aqueous species


  single ion activities and activity coefficients are here defined
  with respect to the internal ph scale



                                          ph           eh           pe

    internal ph scale                   5.4022        .9095
6.3386E+00
    modified nbs ph scale               5.1617        .9440
6.5790E+00
    rational ph scale                   5.1617        .9440
6.5790E+00

  phcl =      5.9808



         oxygen fugacity =  1.21830E-19
         log oxygen fugacity = -18.91424



                             activity of water =    .98388
              log activity of water =   -.00706
              alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)
```

```
                    ionic strength =  4.694801E-01 molal
                 sum of molalities =    1.0569518981082
               osmotic coefficient =     .85358
                    equiv. stoich. ionic strength =  4.989616E-01
molal

                         mass of solution =   1.040744 kg
                         mass of solvent  =   1.002081 kg
                         mass of solutes  =    .038663 kg
                         conc of solutes  =   3.714899 per cent (w/w)


   species                moles        grams          conc         log
conc      log g      log act

   H2O                  5.56242E+01   1.00208E+03
   NA+                  4.58922E-01   1.05505E+01   4.57969E-01     -.
33916     -.24046     -.57962
   CA++                 5.81666E-04   2.33132E-02   5.80458E-04
-3.23623     -.96183    -4.19806
   MG++                 4.32353E-06   1.05083E-04   4.31455E-06
-5.36506     -.96183    -6.32690
   AL+++                2.26961E-17   6.12375E-16   2.26490E-17
-16.64495    -2.16413   -18.80908
   H4SIO4(AQ)           4.75989E-02   4.57495E+00   4.75000E-02
-1.32331      .00000    -1.32331
   H+                   6.90516E-06   6.95971E-06   6.89082E-06
-5.16173     -.24046    -5.40219
   CL-                  4.59999E-01   1.63083E+01   4.59043E-01     -.
33815     -.24046     -.57860
   FE++                 3.45007E-08   1.92676E-06   3.44291E-08
-7.46307     -.96183    -8.42491
   O2(AQ)               1.02744E-23   3.28770E-22   1.02531E-23
-22.98914      .00000   -22.98914
   H2(AQ)               3.66409E-06   7.38608E-06   3.65648E-06
-5.43694      .00000    -5.43694
   FE+++                2.06776E-18   1.15478E-16   2.06347E-18
-17.68540    -2.16413   -19.84953
   OH-                  3.67528E-03   6.25065E-02   3.66764E-03
-2.43561     -.24046    -2.67607
   H8SI3O10(AQ)         5.46389E-07   1.37862E-04   5.45255E-07
-6.26340      .00000    -6.26340
   H6SI2O7(AQ)          6.11575E-03   1.06545E+00   6.10305E-03
-2.21445      .00000    -2.21445
   AL(OH)3(AQ)          4.26214E-05   3.32461E-03   4.25329E-05
-4.37128      .00000    -4.37128
   AL(OH)4-             5.12475E-04   4.86906E-02   5.11411E-04
-3.29123     -.24046    -3.53169
   AL(OH)SI(OH)-        4.38667E-03   7.59378E-01   4.37756E-03
```

```
-2.35877     -.24046    -2.59923
   CACL+                1.30255E-03   9.83852E-02   1.29984E-03
-2.88611     -.24046    -3.12657
   CACL2(AQ)            2.45332E-05   2.72285E-03   2.44823E-05
-4.61115      .00000    -4.61115
   CA(OH)+              1.18884E-04   6.78679E-03   1.18637E-04
-3.92578     -.24046    -4.16624
   CA(H3SIO4)+          4.63333E-03   6.26365E-01   4.62371E-03
-2.33501     -.24046    -2.57547
   FE(OH)+              6.39455E-08   4.65870E-06   6.38127E-08
-7.19509     -.24046    -7.43555
   FE(OH)2              2.84906E-08   2.56021E-06   2.84314E-08
-7.54620      .00000    -7.54620
   FE(OH)3-             1.80946E-08   1.93375E-06   1.80570E-08
-7.74335     -.24046    -7.98381
   FECL+                4.05559E-08   3.70275E-06   4.04716E-08
-7.39285     -.24046    -7.63331
   FECL2(AQ)            9.79236E-07   1.24121E-04   9.77202E-07
-6.01002      .00000    -6.01002
   FE(H3SIO4)+          3.70414E-03   5.59154E-01   3.69645E-03
-2.43222     -.24046    -2.67267
   MGCL+                4.57369E-06   2.73315E-04   4.56419E-06
-5.34064     -.24046    -5.58109
   MG(OH)+              6.27922E-06   2.59409E-04   6.26618E-06
-5.20300     -.24046    -5.44346
   MG(OH)2(AQ)          2.66097E-02   1.55187E+00   2.65545E-02
-1.57586      .00000    -1.57586
   MG(H3SIO4)+          1.02733E-07   1.22675E-05   1.02520E-07
-6.98919     -.24046    -7.22965
   NACL(AQ)             3.86342E-02   2.25789E+00   3.85539E-02
-1.41393      .00000    -1.41393
   NAOH(AQ)             9.55315E-04   3.82098E-02   9.53331E-04
-3.02076      .00000    -3.02076
   H3SIO4-              1.29811E-03   1.23459E-01   1.29541E-03
-2.88759     -.24046    -3.12805
   HCL(AQ)              9.01233E-06   3.28598E-04   8.99361E-06
-5.04607      .00000    -5.04607

           --- activity ratios of cations ---


           log (NA+   /h+**0)            4.8225651
           log (CA++  /h+**0)            6.6063119
           log (MG++  /h+**0)            4.4774766
           log (AL+++ /h+**0)           -2.6025157
           log (FE++  /h+**0)            2.3794661
           log (FE+++ /h+**0)           -3.6429657


           --- summary of solid product phases---
```

```
  product                          log moles        moles        grams
volume, cc

   MAGNETITE                      -1.1154404    7.66584E-02    1.77494E+01
3.41283E+00
   ZOISITE                        -1.3860294    4.11122E-02    1.86798E+01
5.58632E+00
   PARAGONITE                     -3.1490427    7.09508E-04    2.71174E-01
9.37686E-02

   CLINOPYROXENE(SS)                .3077595    2.03123E+00    4.37239E+02
1.31062E+02
   DIOPSIDE                         .1030533    1.26781E+00    2.74547E+02
8.39288E+01
   HEDENBERGITE                    -.7393572    1.82240E-01    4.52126E+01
1.20643E+01
   JADEITE                         -.2356858    5.81185E-01    1.17480E+02
3.50687E+01

   CHLORITE(SS)                     .0689743    1.17213E+00    1.33877E+02
4.96135E+01
   CLINOCHLORE                      .0246906    1.05850E+00    1.17662E+02
4.47639E+01
   CHAMOSITE                       -.9445199    1.13627E-01    1.62147E+01
4.84958E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                       1.9998608    9.99679E+01    2.31464E+04
4.45057E+03
   ZOISITE                        -1.3860294    4.11122E-02    1.86798E+01
5.58632E+00
   TREMOLITE                       1.9995994    9.99078E+01    8.11621E+04
2.72429E+04
   PARAGONITE                     -3.1490427    7.09508E-04    2.71174E-01
9.37686E-02

   PLAGIOCLASE(SS)                 1.9963226    9.91568E+01

   ALBITE                          1.7744739    5.94941E+01    1.56007E+04
5.99879E+03
   ANORTHITE                       1.5983826    3.96627E+01    1.10345E+04
3.99602E+03
```

```
   CLINOPYROXENE(SS)          2.0043858    1.01015E+02

   DIOPSIDE                   1.9055520    8.04548E+01    1.74227E+04
5.32611E+03
   HEDENBERGITE               1.3005735    1.99790E+01    4.95668E+03
1.32261E+03
   JADEITE                    -.2356858    5.81185E-01    1.17480E+02
3.50687E+01


   CHLORITE(SS)                .0689743    1.17213E+00

   CLINOCHLORE                 .0246906    1.05850E+00    1.17662E+02
4.47639E+01
   CHAMOSITE                  -.9445199    1.13627E-01    1.62147E+01
4.84958E+00



                            mass, grams        volume, cc

           created         6.078164E+02       1.897682E+02
           destroyed       5.530491E+02       1.822482E+02
           net             5.476736E+01       7.520042E+00

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE               .0000  satd          CORUNDUM
-3.2194
 HEMATITE                .9990  ssatd         SPINEL
-7.3940
 BRUCITE               -6.4084                DIASPORE
-1.2701
 ANDALUSITE            -4.0059                KYANITE
-2.7868
 SILLIMANITE           -3.7696                GLAUCOPHANE
-6.7654
 LAWSONITE             -1.0720                PUMPELLYITE
-3.8541
```

```
 ZOISITE                    .0000  satd           CLINOZOISITE
-.7104
 FORSTERITE               -3.2126                 FAYALITE
-3.5724
 CHRYSOTILE               -6.6314                 ENSTATITE-CL
-2.5095
 ENSTATITE-OR             -2.5876                 ENSTATITE-PR
-2.9929
 DIOPSIDE                  -.6774                 HEDENBERGITE
-3.4649
 JADEITE                  -1.7983                 FERROSILITE
-3.8351
 WOLLASTONITE             -3.8627                 PSEUDOWOLLASTONITE
-4.3488
 TREMOLITE                -2.7044                 ALBITE
-1.0057
 ANORTHITE                -3.5983                 KAOLINITE
-4.7537
 PYROPHYLLITE             -5.0218                 TALC
-2.9201
 PARAGONITE                 .0000  satd           MARGARITE
-2.8851
 PREHNITE                 -3.0523                 CLINOCHLORE
-.1465
 CHAMOSITE                -3.3537                 PYROPE
-4.2327
 ALMANDINE                -3.3439                 GROSSULAR
-.8480
 QUARTZ-ALPHA              -.6707                 QUARTZ-BETA
-.9076
 COESITE                  -1.2670                 HALITE
-9.8765
 CRISTOBALITE-ALPHA       -1.9566                 CRISTOBALITE-BETA
-2.6700


                    --- summary of solid solutions  ---

 mineral                  aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)              -.7867
     ALBITE                        -.78671     .8586436     1.00000
     ANORTHITE                     -.78671     .1413564     1.00000

 ORTHOPYROXENE(SS)           -2.0839
     ENSTATITE-OR                 -2.08388     .7043499     1.00000
     FERROSILITE                  -2.08388     .2956501     1.00000

 GARNET(SS)                   -.5034
     PYROPE                        -.50341     .0746456     1.00000
```

```
    ALMANDINE                           -.50341     .1385466     1.00000
    GROSSULAR                           -.50341     .7868077     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
    DIOPSIDE                             .00000     .6241569     1.00000
    HEDENBERGITE                         .00000     .0897188     1.00000
    JADEITE                              .00000     .2861243     1.00000

 CPX_SUBCALCIC(SS)          -.4844
    DIOPSIDE                            -.48437     .8743216     1.00000
    HEDENBERGITE                        -.48437     .1256784     1.00000

 CHLORITE(SS)                .0000
saturated
    CLINOCHLORE                          .00000     .9030594     1.00000
    CHAMOSITE                            .00000     .0969406     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

    DIOPSIDE
             .6242    1.0000     .6242    -.2047     .0000    -.2047
    HEDENBERGITE
             .0897    1.0000     .0897   -1.0471     .0000   -1.0471
    JADEITE
             .2861    1.0000     .2861    -.5434     .0000    -.5434

   CHLORITE(SS)
 ideal solution

    CLINOCHLORE
             .9031    1.0000     .9031    -.0443     .0000    -.0443
    CHAMOSITE
             .0969    1.0000     .0969   -1.0135     .0000   -1.0135


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                          -18.91424       1.21830E-19
   H2(G)                           -1.66504       2.16254E-02
```

```
  H2O(G)                          3.80604      6.39796E+03


 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


stepping to zi=  5.0330E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   152, iter =  3, ncorr = 0
most rapidly changing is zvclg1(PARAGONITE        ) =     -3.1490

stepping to zi=  5.0330E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   153, iter =  3, ncorr = 0
most rapidly changing is zvclg1(PARAGONITE        ) =     -3.1490

stepping to zi=  5.0330E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   154, iter =  3, ncorr = 0
most rapidly changing is zvclg1(PARAGONITE        ) =     -3.1490

stepping to zi=  5.0330E-01, delzi=  5.3296E-08, nord= 1
              ncycle=  0
steps completed =   155, iter =  1, ncorr = 0
most rapidly changing is zvclg1(PARAGONITE        ) =     -3.1490

stepping to zi=  5.0330E-01, delzi=  5.3296E-07, nord= 2
              ncycle=  0
steps completed =   156, iter =  2, ncorr = 0
most rapidly changing is zvclg1(PARAGONITE        ) =     -3.1485

stepping to zi=  5.0330E-01, delzi=  5.3296E-06, nord= 2
              ncycle=  0
steps completed =   157, iter =  3, ncorr = 0
most rapidly changing is zvclg1(PARAGONITE        ) =     -3.1442

stepping to zi=  5.0336E-01, delzi=  5.3296E-05, nord= 2
              ncycle=  0
steps completed =   158, iter =  3, ncorr = 0
most rapidly changing is zvclg1(PARAGONITE        ) =     -3.1033

stepping to zi=  5.0389E-01, delzi=  5.3296E-04, nord= 2
              ncycle=  0
steps completed =   159, iter =  3, ncorr = 0
most rapidly changing is zvclg1(PARAGONITE        ) =     -2.8245

stepping to zi=  5.0831E-01, delzi=  4.4211E-03, nord= 3
              ncycle=  0
```

```
 steps completed =   160, iter =  3, ncorr = 0
 most rapidly changing is zvclg1(PARAGONITE        ) =     -2.1320

 stepping to zi=  5.2192E-01, delzi=  1.3614E-02, nord= 4
              ncycle=  0
 steps completed =   161, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(PARAGONITE        ) =     -1.5947

 stepping to zi=  5.4324E-01, delzi=  2.1312E-02, nord= 5
              ncycle=  0
 steps completed =   162, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(PARAGONITE        ) =     -1.2719

 stepping to zi=  5.8847E-01, delzi=  4.5232E-02, nord= 5
              ncycle=  0
 steps completed =   163, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =     -2.0276

 stepping to zi=  6.1465E-01, delzi=  2.6186E-02, nord= 6
                    the phase to be dropped is ZOISITE
(   15)


   attempted species assemblage no.   2

             1      1  H2O
             2      2  NA+
             3      4  CA++
             4      5  MG++
             5      6  AL+++
             6      7  H4SIO4(AQ)
             7     13  H+
             8     16  CL-
             9     21  FE++
            10     32  O2(G)
            11      1  MAGNETITE
            12     42  PARAGONITE
            13      1  CLINOPYRDIOPSIDE
            14      2  CLINOPYRHEDENBERGITE
            15      3  CLINOPYRJADEITE
            16      1  CHLORITECLINOCHLORE
            17      2  CHLORITECHAMOSITE

 steps completed =   164, iter =  6, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  6.14653847029671E-01
                    log of reaction progress =      -.2113694
```

```
                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


  change in the product phase assemblage


                              --- reactant summary ---



         reactant            moles       delta moles      grams
 delta grams

    PLAGIOCLASE(SS)        9.89703E+01    1.02973E+00    2.65851E+04
 2.76603E+02
    CLINOPYROXENE(SS)      9.87589E+01    1.24111E+00    2.20095E+04
 2.76595E+02
    MAGNETITE              9.98672E+01    1.32765E-01    2.31231E+04
 3.07403E+01
    TREMOLITE              9.98874E+01    1.12605E-01    8.11456E+04
 9.14766E+01


                 current total mass =  1.52863E+05 grams
                 delta total mass   =  6.75415E+02 grams
                 delta total volume =    222.57183 cc


         reactant           affinity     rel. rate

    PLAGIOCLASE(SS)            .9106    1.67530E+00
    CLINOPYROXENE(SS)          .4160    0.00000E+00
    MAGNETITE                  .0000    0.00000E+00
    TREMOLITE                 1.4294    1.83200E-01

          affinity of the overall irreversible reaction=     1.787
 kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



       --- element totals for the aqueous phase ---

    element         mg/kg soln.         molal conc.          moles
```

```
   O          8.600473E+05        5.598732E+01        5.601872E+01
   NA         1.052826E+04        4.769721E-01        4.772395E-01
   CA         5.579579E+02        1.449922E-02        1.450735E-02
   MG         5.280412E+02        2.262785E-02        2.264053E-02
   AL         7.809584E+01        3.014618E-03        3.016308E-03
   SI         2.919540E+03        1.082688E-01        1.083295E-01
   H          1.078648E+05        1.114636E+02        1.115261E+02
   CL         1.701016E+04        4.997198E-01        5.000000E-01
   FE         4.659282E+02        8.689409E-03        8.694282E-03

   co3--                          0.000000E+00        0.000000E+00
   so4--                          0.000000E+00        0.000000E+00
   s--                            0.000000E+00        0.000000E+00

 warning-- co3--, so4--, and s-- totals require that routine comp1
 have the names of non-carbonate carbon, sulfide sulfur,
 and non-sulfate sulfur aqueous species


single ion activities and activity coefficients are here defined
with respect to the internal ph scale



                                    ph           eh            pe

  internal ph scale               5.0887        .9707
6.7652E+00
  modified nbs ph scale           4.8487       1.0051
7.0052E+00
  rational ph scale               4.8487       1.0051
7.0052E+00

phcl =      5.6672



       oxygen fugacity =  3.45427E-19
       log oxygen fugacity = -18.46164



                        activity of water =    .98385
            log activity of water =   -.00707
            alkalinity =  0.000000E+00 equiv/kg solvent
                                     (not def. for t.gt.50 c)

                 ionic strength =  4.660245E-01 molal
              sum of molalities =    1.0630721660655
            osmotic coefficient =     .84997
```

```
                    equiv. stoich. ionic strength =  4.997198E-01
molal

                         mass of solution =   1.042112 kg
                         mass of solvent  =   1.000561 kg
                         mass of solutes  =    .041552 kg
                         conc of solutes  =   3.987247 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.55398E+01   1.00056E+03
   NA+                  4.39723E-01   1.01091E+01   4.39477E-01     -.
35706     -.24000     -.59706
   CA++                 1.67347E-03   6.70726E-02   1.67253E-03
-2.77663     -.95999    -3.73661
   MG++                 1.54854E-05   3.76373E-04   1.54767E-05
-4.81032     -.95999    -5.77031
   AL+++                1.85490E-16   5.00480E-15   1.85386E-16
-15.73192    -2.15997   -17.89190
   H4SIO4(AQ)           6.46230E-02   6.21122E+00   6.45868E-02
-1.18986      .00000    -1.18986
   H+                   1.41742E-05   1.42862E-05   1.41663E-05
-4.84874     -.24000    -5.08874
   CL-                  4.58984E-01   1.62724E+01   4.58727E-01     -.
33845     -.24000     -.57844
   FE++                 1.22121E-07   6.82010E-06   1.22053E-07
-6.91345     -.95999    -7.87344
   O2(AQ)               2.90871E-23   9.30751E-22   2.90708E-23
-22.53654      .00000   -22.53654
   H2(AQ)               2.17268E-06   4.37969E-06   2.17146E-06
-5.66325      .00000    -5.66325
   FE+++                1.94428E-17   1.08582E-15   1.94319E-17
-16.71149    -2.15997   -18.87146
   OH-                  1.78120E-03   3.02934E-02   1.78020E-03
-2.74953     -.24000    -2.98953
   H8SI3O10(AQ)         1.37156E-06   3.46063E-04   1.37079E-06
-5.86303      .00000    -5.86303
   H6SI2O7(AQ)          1.12902E-02   1.96691E+00   1.12839E-02
-1.94754      .00000    -1.94754
   AL(OH)3(AQ)          4.03441E-05   3.14698E-03   4.03215E-05
-4.39446      .00000    -4.39446
   AL(OH)4-             2.35455E-04   2.23707E-02   2.35323E-04
-3.62834     -.24000    -3.86833
   AL(OH)SI(OH)-        2.74051E-03   4.74410E-01   2.73897E-03
-2.56241     -.24000    -2.80241
   CACL+                3.76083E-03   2.84066E-01   3.75872E-03
-2.42496     -.24000    -2.66496
   CACL2(AQ)            7.09363E-05   7.87294E-03   7.08966E-05
```

```
-4.14937       .00000    -4.14937
   CA(OH)+               1.66723E-04   9.51779E-03   1.66630E-04
-3.77825     -.24000    -4.01824
   CA(H3SIO4)+           8.83540E-03   1.19443E+00   8.83045E-03
-2.05402     -.24000    -2.29401
   FE(OH)+               1.10332E-07   8.03814E-06   1.10270E-07
-6.95754     -.24000    -7.19754
   FE(OH)2               2.39110E-08   2.14868E-06   2.38976E-08
-7.62165       .00000    -7.62165
   FE(OH)3-              7.37101E-09   7.87731E-07   7.36688E-09
-8.13272     -.24000    -8.37271
   FECL+                 1.44066E-07   1.31533E-05   1.43986E-07
-6.84168     -.24000    -7.08168
   FECL2(AQ)             3.48353E-06   4.41548E-04   3.48158E-06
-5.45822       .00000    -5.45822
   FE(H3SIO4)+           8.69039E-03   1.31185E+00   8.68552E-03
-2.06120     -.24000    -2.30120
   MGCL+                 1.64398E-05   9.82412E-04   1.64306E-05
-4.78435     -.24000    -5.02434
   MG(OH)+               1.09627E-05   4.52896E-04   1.09566E-05
-4.96032     -.24000    -5.20032
   MG(OH)2(AQ)           2.25974E-02   1.31787E+00   2.25847E-02
-1.64618       .00000    -1.64618
   MG(H3SIO4)+           2.43884E-07   2.91227E-05   2.43748E-07
-6.61306     -.24000    -6.85306
   NACL(AQ)              3.70711E-02   2.16654E+00   3.70503E-02
-1.43121       .00000    -1.43121
   NAOH(AQ)              4.45238E-04   1.78082E-02   4.44988E-04
-3.35165       .00000    -3.35165
   H3SIO4-               8.55451E-04   8.13592E-02   8.54971E-04
-3.06805     -.24000    -3.30805
   HCL(AQ)               1.85261E-05   6.75480E-04   1.85158E-05
-4.73246       .00000    -4.73246

           --- activity ratios of cations ---


           log (NA+   /h+**0)            4.4916809
           log (CA++  /h+**0)            6.4408702
           log (MG++  /h+**0)            4.4071756
           log (AL+++ /h+**0)           -2.6256710
           log (FE++  /h+**0)            2.3040434
           log (FE+++ /h+**0)           -3.6052327


           --- summary of solid product phases---


  product                    log moles       moles       grams
volume, cc
```

```
   MAGNETITE                  -.9969268    1.00710E-01    2.33183E+01
4.48362E+00
   PARAGONITE                 -.8383710    1.45087E-01    5.54522E+01
1.91747E+01

   CLINOPYROXENE(SS)           .3864484    2.43472E+00    5.26344E+02
1.57838E+02
   DIOPSIDE                    .2129212    1.63276E+00    3.53577E+02
1.08088E+02
   HEDENBERGITE               -.6346110    2.31947E-01    5.75448E+01
1.53549E+01
   JADEITE                    -.2441147    5.70014E-01    1.15222E+02
3.43946E+01

   CHLORITE(SS)                .0347596    1.08333E+00    1.23699E+02
4.58544E+01
   CLINOCHLORE                -.0090302    9.79422E-01    1.08872E+02
4.14198E+01
   CHAMOSITE                  -.9833624    1.03905E-01    1.48274E+01
4.43468E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  1.9998608    9.99679E+01    2.31464E+04
4.45057E+03
   TREMOLITE                  1.9995107    9.98874E+01    8.11456E+04
2.72373E+04
   PARAGONITE                 -.8383710    1.45087E-01    5.54522E+01
1.91747E+01

   PLAGIOCLASE(SS)            1.9955048    9.89703E+01

   ALBITE                     1.7736560    5.93822E+01    1.55714E+04
5.98750E+03
   ANORTHITE                  1.5975647    3.95881E+01    1.10138E+04
3.98850E+03


   CLINOPYROXENE(SS)          2.0051531    1.01194E+02

   DIOPSIDE                   1.9065498    8.06399E+01    1.74628E+04
5.33836E+03
   HEDENBERGITE               1.3006765    1.99837E+01    4.95785E+03
1.32292E+03
```

```
   JADEITE                   -.2441147    5.70014E-01    1.15222E+02
3.43946E+01


   CHLORITE(SS)               .0347596    1.08333E+00

   CLINOCHLORE               -.0090302    9.79422E-01    1.08872E+02
4.14198E+01
   CHAMOSITE                 -.9833624    1.03905E-01    1.48274E+01
4.43468E+00



                          mass, grams        volume, cc

           created        7.288137E+02       2.273507E+02
           destroyed      6.754149E+02       2.225718E+02
           net            5.339880E+01       4.778885E+00

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-3.3727
 HEMATITE                1.2486  ssatd         SPINEL
-7.7800
 BRUCITE                -6.6411                DIASPORE
-1.3468
 ANDALUSITE             -3.7176                KYANITE
-2.4985
 SILLIMANITE            -3.4813                GLAUCOPHANE
-6.2734
 LAWSONITE               -.8895                PUMPELLYITE
-4.0102
 ZOISITE                  .0000                CLINOZOISITE
-.7105
 FORSTERITE             -3.2245                FAYALITE
-3.6012
 CHRYSOTILE             -6.4461                ENSTATITE-CL
-2.3005
 ENSTATITE-OR           -2.3786                ENSTATITE-PR
-2.7839
```

```
 DIOPSIDE                 -.5742                HEDENBERGITE
-3.3787
 JADEITE                 -2.0865                FERROSILITE
-3.6430
 WOLLASTONITE            -3.9686                PSEUDOWOLLASTONITE
-4.4547
 TREMOLITE               -1.4294                ALBITE
-.8523
 ANORTHITE               -3.4158                KAOLINITE
-4.0238
 PYROPHYLLITE            -3.4086                TALC
-1.8515
 PARAGONITE                .0000  satd          MARGARITE
-2.8560
 PREHNITE                -2.9757                CLINOCHLORE
-.1449
 CHAMOSITE               -3.3690                PYROPE
-4.0750
 ALMANDINE               -3.2031                GROSSULAR
-1.0054
 QUARTZ-ALPHA             -.2290                QUARTZ-BETA
-.4660
 COESITE                  -.8253                HALITE
-9.9337
 CRISTOBALITE-ALPHA      -1.5149                CRISTOBALITE-BETA
-2.2283


                     --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -.6292
     ALBITE                      -.62917     .8561681     1.00000
     ANORTHITE                   -.62917     .1438319     1.00000

 ORTHOPYROXENE(SS)        -1.8799
     ENSTATITE-OR               -1.87988     .7067998     1.00000
     FERROSILITE                -1.87988     .2932002     1.00000

 GARNET(SS)                -.5904
     PYROPE                      -.59039     .0885010     1.00000
     ALMANDINE                   -.59039     .1623354     1.00000
     GROSSULAR                   -.59039     .7491636     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .6706142     1.00000
     HEDENBERGITE                 .00000     .0952666     1.00000
     JADEITE                      .00000     .2341192     1.00000
```

```
 CPX_SUBCALCIC(SS)          -.3833
     DIOPSIDE                     -.38331     .8756117     1.00000
     HEDENBERGITE                 -.38331     .1243883     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9040869     1.00000
     CHAMOSITE                     .00000     .0959131     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6706    1.0000     .6706    -.1735     .0000    -.1735
     HEDENBERGITE
              .0953    1.0000     .0953   -1.0211     .0000   -1.0211
     JADEITE
              .2341    1.0000     .2341    -.6306     .0000    -.6306

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9041    1.0000     .9041    -.0438     .0000    -.0438
     CHAMOSITE
              .0959    1.0000     .0959   -1.0181     .0000   -1.0181


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                         -18.46164       3.45427E-19
   H2(G)                          -1.89135       1.28426E-02
   H2O(G)                          3.80603       6.39780E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
stepping to zi=  6.1465E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   165, iter =  3, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.7317

stepping to zi=  6.1465E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   166, iter =  3, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.7317

stepping to zi=  6.1465E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   167, iter =  3, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.7317

stepping to zi=  6.1465E-01, delzi=  1.0000E-07, nord= 1
              ncycle=  0
steps completed =   168, iter =  1, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.7317

stepping to zi=  6.1465E-01, delzi=  1.0000E-06, nord= 1
              ncycle=  0
steps completed =   169, iter =  1, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.7317

stepping to zi=  6.1466E-01, delzi=  1.0000E-05, nord= 2
              ncycle=  0
steps completed =   170, iter =  2, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.7316

stepping to zi=  6.1476E-01, delzi=  1.0000E-04, nord= 2
              ncycle=  0
steps completed =   171, iter =  3, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.7305

stepping to zi=  6.1576E-01, delzi=  1.0000E-03, nord= 3
              ncycle=  0
steps completed =   172, iter =  4, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.7199

stepping to zi=  6.2221E-01, delzi=  6.4431E-03, nord= 3
              ncycle=  0
steps completed =   173, iter =  3, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.6535

stepping to zi=  6.3096E-01, delzi=  8.7492E-03, nord= 4
              ncycle=  0
steps completed =   174, iter =  4, ncorr = 0
most rapidly changing is zvclg1(AL+++            ) =    -15.5688
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
                    reaction progress        =  6.30957344480185E-01
                    log of reaction progress =       -.2000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



        reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.89430E+01    1.05704E+00    2.65778E+04
2.83940E+02
   CLINOPYROXENE(SS)      9.87260E+01    1.27403E+00    2.20021E+04
2.83931E+02
   MAGNETITE              9.98637E+01    1.36287E-01    2.31223E+04
3.15557E+01
   TREMOLITE              9.98844E+01    1.15591E-01    8.11431E+04
9.39030E+01


               current total mass =  1.52845E+05 grams
               delta total mass   =  6.93330E+02 grams
               delta total volume =    228.47548 cc


        reactant           affinity     rel. rate

   PLAGIOCLASE(SS)            .8604    1.67530E+00
   CLINOPYROXENE(SS)          .4149    0.00000E+00
   MAGNETITE                  .0000    0.00000E+00
   TREMOLITE                 1.0365    1.83200E-01

         affinity of the overall irreversible reaction=     1.631
kcal
         contributions from irreversible reactions
         with no thermodynamic data are not included
```

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.597634E+05	5.603708E+01	5.604104E+01
NA	1.041512E+04	4.724219E-01	4.724553E-01
CA	6.161855E+02	1.603187E-02	1.603300E-02
MG	5.074616E+02	2.177248E-02	2.177401E-02
AL	7.074801E+01	2.734310E-03	2.734503E-03
SI	3.286881E+03	1.220400E-01	1.220486E-01
H	1.077769E+05	1.115086E+02	1.115165E+02
CL	1.699778E+04	4.999647E-01	5.000000E-01
FE	5.655231E+02	1.055968E-02	1.056043E-02
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	5.0275	.9835	6.8543E+00
modified nbs ph scale	4.7876	1.0179	7.0943E+00
rational ph scale	4.7876	1.0179	7.0943E+00

phcl = 5.6059

oxygen fugacity = 4.46765E-19
log oxygen fugacity = -18.34992

activity of water = .98385
log activity of water = -.00707
alkalinity = 0.000000E+00 equiv/kg solvent

(not def. for t.gt.50 c)

ionic strength = 4.657479E-01 molal
sum of molalities = 1.0695465028041
osmotic coefficient = .84525
equiv. stoich. ionic strength = 4.999647E-01 molal

mass of solution = 1.042872 kg
mass of solvent = 1.000071 kg
mass of solutes = .042801 kg
conc of solutes = 4.104166 per cent (w/w)

species	moles	grams	conc	log conc	log g	log act
H2O	5.55126E+01	1.00007E+03				
NA+	4.35360E-01	1.00088E+01	4.35329E-01	-.36118	-.23996	-.60114
CA++	1.90179E-03	7.62238E-02	1.90166E-03	-2.72087	-.95984	-3.68071
MG++	1.97269E-05	4.79463E-04	1.97255E-05	-4.70497	-.95984	-5.66481
AL+++	2.69869E-16	7.28148E-15	2.69850E-16	-15.56888	-2.15964	-17.72852
H4SIO4(AQ)	7.11627E-02	6.83978E+00	7.11577E-02	-1.14778	.00000	-1.14778
H+	1.63109E-05	1.64397E-05	1.63097E-05	-4.78755	-.23996	-5.02751
CL-	4.58799E-01	1.62658E+01	4.58767E-01	-.33841	-.23996	-.57837
FE++	1.54978E-07	8.65508E-06	1.54967E-07	-6.80976	-.95984	-7.76960
O2(AQ)	3.76019E-23	1.20321E-21	3.75992E-23	-22.42482	.00000	-22.42482
H2(AQ)	1.90949E-06	3.84916E-06	1.90936E-06	-5.71911	.00000	-5.71911
FE+++	3.02841E-17	1.69127E-15	3.02819E-17	-16.51882	-2.15964	-18.67846
OH-	1.54607E-03	2.62946E-02	1.54597E-03	-2.81080	-.23996	-3.05076
H8SI3O10(AQ)	1.83333E-06	4.62575E-04	1.83321E-06	-5.73679	.00000	-5.73679
H6SI2O7(AQ)	1.36977E-02	2.38633E+00	1.36967E-02	-1.86338	.00000	-1.86338
AL(OH)3(AQ)	3.84813E-05	3.00167E-03	3.84785E-05	-4.41478	.00000	-4.41478
AL(OH)4-	1.95033E-04	1.85302E-02	1.95019E-04	-3.70992	-.23996	-3.94988

```
   AL(OH)SI(OH)-          2.50099E-03   4.32947E-01   2.50081E-03
-2.60192     -.23996    -2.84188
   CACL+                  4.27577E-03   3.22962E-01   4.27547E-03
-2.36902     -.23996    -2.60898
   CACL2(AQ)              8.06698E-05   8.95322E-03   8.06641E-05
-4.09332      .00000    -4.09332
   CA(OH)+                1.64596E-04   9.39636E-03   1.64585E-04
-3.78361     -.23996    -4.02357
   CA(H3SIO4)+            9.61017E-03   1.29917E+00   9.60949E-03
-2.01730     -.23996    -2.25726
   FE(OH)+                1.21635E-07   8.86165E-06   1.21627E-07
-6.91497     -.23996    -7.15493
   FE(OH)2                2.28961E-08   2.05748E-06   2.28945E-08
-7.64027      .00000    -7.64027
   FE(OH)3-               6.12943E-09   6.55046E-07   6.12900E-09
-8.21261     -.23996    -8.45257
   FECL+                  1.82906E-07   1.66994E-05   1.82893E-07
-6.73780     -.23996    -6.97776
   FECL2(AQ)              4.42382E-06   5.60733E-04   4.42351E-06
-5.35423      .00000    -5.35423
   FE(H3SIO4)+            1.05555E-02   1.59339E+00   1.05548E-02
-1.97655     -.23996    -2.21651
   MGCL+                  2.09517E-05   1.25203E-03   2.09502E-05
-4.67881     -.23996    -4.91877
   MG(OH)+                1.21320E-05   5.01202E-04   1.21312E-05
-4.91610     -.23996    -5.15606
   MG(OH)2(AQ)            2.17209E-02   1.26675E+00   2.17194E-02
-1.66315      .00000    -1.66315
   MG(H3SIO4)+            2.97358E-07   3.55081E-05   2.97337E-07
-6.52675     -.23996    -6.76671
   NACL(AQ)               3.67127E-02   2.14559E+00   3.67101E-02
-1.43521      .00000    -1.43521
   NAOH(AQ)               3.82882E-04   1.53142E-02   3.82855E-04
-3.41697      .00000    -3.41697
   H3SIO4-                8.18076E-04   7.78046E-02   8.18018E-04
-3.08724     -.23996    -3.32720
   HCL(AQ)                2.13243E-05   7.77505E-04   2.13228E-05
-4.67115      .00000    -4.67115

           --- activity ratios of cations ---


           log (NA+   /h+**0)            4.4263706
           log (CA++  /h+**0)            6.3743182
           log (MG++  /h+**0)            4.3902148
           log (AL+++ /h+**0)           -2.6459785
           log (FE++  /h+**0)            2.2854266
           log (FE+++ /h+**0)           -3.5959172
```

```
          --- summary of solid product phases---


  product                     log moles       moles       grams
volume, cc

   MAGNETITE                  -.9820013   1.04231E-01   2.41336E+01
4.64038E+00
   PARAGONITE                 -.8123416   1.54049E-01   5.88774E+01
2.03591E+01

   CLINOPYROXENE(SS)           .3971089   2.49522E+00   5.39434E+02
1.61772E+02
   DIOPSIDE                    .2242313   1.67584E+00   3.62906E+02
1.10940E+02
   HEDENBERGITE               -.6249570   2.37161E-01   5.88383E+01
1.57001E+01
   JADEITE                    -.2349097   5.82224E-01   1.17690E+02
3.51314E+01

   CHLORITE(SS)                .0341828   1.08189E+00   1.23524E+02
4.57934E+01
   CLINOCHLORE                -.0094485   9.78479E-01   1.08767E+02
4.13799E+01
   CHAMOSITE                  -.9854368   1.03410E-01   1.47568E+01
4.41355E+00


               --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member        log moles       moles       grams
volume, cc

   MAGNETITE                  1.9998608   9.99679E+01   2.31464E+04
4.45057E+03
   TREMOLITE                  1.9994977   9.98844E+01   8.11431E+04
2.72365E+04
   PARAGONITE                 -.8123416   1.54049E-01   5.88774E+01
2.03591E+01

   PLAGIOCLASE(SS)            1.9953849   9.89430E+01

   ALBITE                     1.7735361   5.93658E+01   1.55671E+04
5.98585E+03
   ANORTHITE                  1.5974449   3.95772E+01   1.10107E+04
3.98740E+03


   CLINOPYROXENE(SS)          2.0052714   1.01221E+02
```

```
   DIOPSIDE                   1.9066400    8.06566E+01    1.74664E+04
5.33947E+03
   HEDENBERGITE               1.3006467    1.99824E+01    4.95751E+03
1.32283E+03
   JADEITE                    -.2349097    5.82224E-01    1.17690E+02
3.51314E+01


   CHLORITE(SS)                .0341828    1.08189E+00

   CLINOCHLORE                -.0094485    9.78479E-01    1.08767E+02
4.13799E+01
   CHAMOSITE                  -.9854368    1.03410E-01    1.47568E+01
4.41355E+00



                          mass, grams        volume, cc

           created        7.459694E+02       2.325646E+02
           destroyed      6.933300E+02       2.284755E+02
           net            5.263933E+01       4.089172E+00

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-3.5071
 HEMATITE                1.3102  ssatd         SPINEL
-7.9705
 BRUCITE                -6.6972                DIASPORE
-1.4140
 ANDALUSITE             -3.7127                KYANITE
-2.4937
 SILLIMANITE            -3.4765                GLAUCOPHANE
-5.8944
 LAWSONITE               -.9657                PUMPELLYITE
-4.4479
 ZOISITE                 -.2244                CLINOZOISITE
-.9348
 FORSTERITE             -3.2110                FAYALITE
```

```
-3.5931
 CHRYSOTILE               -6.3361                ENSTATITE-CL
-2.2173
 ENSTATITE-OR             -2.2954                ENSTATITE-PR
-2.7008
 DIOPSIDE                  -.5721                HEDENBERGITE
-3.3820
 JADEITE                  -2.0914                FERROSILITE
-3.5654
 WOLLASTONITE             -4.0495                PSEUDOWOLLASTONITE
-4.5356
 TREMOLITE                -1.0365                ALBITE
-.7179
 ANORTHITE                -3.4920                KAOLINITE
-3.8798
 PYROPHYLLITE             -2.9860                TALC
-1.4628
 PARAGONITE                 .0000  satd          MARGARITE
-3.0666
 PREHNITE                 -3.1328                CLINOCHLORE
-.1444
 CHAMOSITE                -3.3739                PYROPE
-4.0367
 ALMANDINE                -3.1703                GROSSULAR
-1.1314
 QUARTZ-ALPHA              -.0898                QUARTZ-BETA
-.3267
 COESITE                   -.6861                HALITE
-9.9469
 CRISTOBALITE-ALPHA       -1.3757                CRISTOBALITE-BETA
-2.0891


                     --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)            -.5232
     ALBITE                       -.52318     .8732893     1.00000
     ANORTHITE                    -.52318     .1267107     1.00000

 ORTHOPYROXENE(SS)         -1.7984
     ENSTATITE-OR                -1.79836     .7075894     1.00000
     FERROSILITE                 -1.79836     .2924106     1.00000

 GARNET(SS)                 -.6743
     PYROPE                       -.67432     .0963577     1.00000
     ALMANDINE                    -.67432     .1760734     1.00000
     GROSSULAR                    -.67432     .7275689     1.00000
```

```
 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .6716181     1.00000
     HEDENBERGITE                 .00000     .0950461     1.00000
     JADEITE                      .00000     .2333358     1.00000

 CPX_SUBCALCIC(SS)         -.3818
     DIOPSIDE                    -.38184     .8760265     1.00000
     HEDENBERGITE                -.38184     .1239735     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9044170     1.00000
     CHAMOSITE                    .00000     .0955830     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6716    1.0000     .6716    -.1729     .0000    -.1729
     HEDENBERGITE
              .0950    1.0000     .0950   -1.0221     .0000   -1.0221
     JADEITE
              .2333    1.0000     .2333    -.6320     .0000    -.6320

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9044    1.0000     .9044    -.0436     .0000    -.0436
     CHAMOSITE
              .0956    1.0000     .0956   -1.0196     .0000   -1.0196


           --- summary of gas species ---

           gas                 log fugacity         fugacity
partial pressure

   O2(G)                         -18.34992       4.46765E-19
   H2(G)                          -1.94721       1.12924E-02
   H2O(G)                          3.80603       6.39775E+03
```

```
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  6.4372E-01, delzi=  1.2766E-02, nord= 5
               ncycle=  0
 iter =    5
       1 supersaturated pure minerals
       0 supersaturated solid solutions

                          the most supersaturated phases     affinity,
kcal

                            1      50   QUARTZ-ALPHA             .
00771143


   attempted species assemblage no.   2

             1      1  H2O
             2      2  NA+
             3      4  CA++
             4      5  MG++
             5      6  AL+++
             6      7  H4SIO4(AQ)
             7     13  H+
             8     16  CL-
             9     21  FE++
            10     32  O2(G)
            11      1  MAGNETITE
            12     42  PARAGONITE
            13     50  QUARTZ-ALPHA
            14      1  CLINOPYRDIOPSIDE
            15      2  CLINOPYRHEDENBERGITE
            16      3  CLINOPYRJADEITE
            17      1  CHLORITECLINOCHLORE
            18      2  CHLORITECHAMOSITE

 steps completed =   175, iter =  8, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  6.43723141210064E-01
                    log of reaction progress =       -.1913009

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars
```

computing units remaining = .000

change in the product phase assemblage

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.89216E+01	1.07843E+00	2.65721E+04	2.89685E+02
CLINOPYROXENE(SS)	9.87002E+01	1.29981E+00	2.19964E+04	2.89676E+02
MAGNETITE	9.98610E+01	1.39044E-01	2.31217E+04	3.21941E+01
TREMOLITE	9.98821E+01	1.17930E-01	8.11412E+04	9.58029E+01

current total mass = 1.52831E+05 grams
delta total mass = 7.07358E+02 grams
delta total volume = 233.09809 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	.8280	1.67530E+00
CLINOPYROXENE(SS)	.4138	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	.7830	1.83200E-01

affinity of the overall irreversible reaction= 1.531 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.595520E+05	5.607361E+01	5.605722E+01
NA	1.033367E+04	4.691483E-01	4.690111E-01
CA	6.580318E+02	1.713599E-02	1.713098E-02
MG	4.945217E+02	2.123635E-02	2.123014E-02

```
      AL         6.638572E+01       2.568018E-03       2.567267E-03
      SI         3.553927E+03       1.320737E-01       1.320351E-01
      H          1.077120E+05       1.115415E+02       1.115089E+02
      CL         1.698869E+04       5.001463E-01       5.000000E-01
      FE         6.408558E+02       1.197707E-02       1.197357E-02

      co3--                         0.000000E+00       0.000000E+00
      so4--                         0.000000E+00       0.000000E+00
      s--                           0.000000E+00       0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                            ph            eh            pe

     internal ph scale                    4.9877          .9918
6.9124E+00
     modified nbs ph scale                4.7478        1.0262
7.1524E+00
     rational ph scale                    4.7478        1.0262
7.1524E+00

   phcl =      5.5661



          oxygen fugacity =  5.28767E-19
          log oxygen fugacity = -18.27674



                               activity of water =    .98384
               log activity of water =   -.00708
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                    ionic strength =  4.656235E-01 molal
                 sum of molalities =    1.0743741129109
               osmotic coefficient =     .84176
                    equiv. stoich. ionic strength =  5.001463E-01
molal

                         mass of solution =   1.043429 kg
```

mass of solvent = .999708 kg
mass of solutes = .043722 kg
conc of solutes = 4.190211 per cent (w/w)

species	moles	grams	conc	log conc	log g	log act
H2O	5.54924E+01	9.99708E+02				
NA+	4.32212E-01	9.93645E+00	4.32338E-01	-.36418	-.23994	-.60412
CA++	2.06924E-03	8.29351E-02	2.06984E-03	-2.68406	-.95977	-3.64384
MG++	2.30878E-05	5.61150E-04	2.30946E-05	-4.63649	-.95977	-5.59626
AL+++	3.44594E-16	9.29767E-15	3.44694E-16	-15.46257	-2.15949	-17.62206
H4SIO4(AQ)	7.57219E-02	7.27799E+00	7.57441E-02	-1.12065	.00000	-1.12065
H+	1.78683E-05	1.80094E-05	1.78735E-05	-4.74779	-.23994	-4.98773
CL-	4.58660E-01	1.62609E+01	4.58795E-01	-.33838	-.23994	-.57832
FE++	1.80888E-07	1.01021E-05	1.80941E-07	-6.74246	-.95977	-7.70224
O2(AQ)	4.44874E-23	1.42354E-21	4.45004E-23	-22.35164	.00000	-22.35164
H2(AQ)	1.75455E-06	3.53682E-06	1.75506E-06	-5.75571	.00000	-5.75571
FE+++	4.03967E-17	2.25604E-15	4.04085E-17	-16.39353	-2.15949	-18.55302
OH-	1.41018E-03	2.39833E-02	1.41059E-03	-2.85060	-.23994	-3.09054
H8SI3O10(AQ)	2.21040E-06	5.57714E-04	2.21104E-06	-5.65540	.00000	-5.65540
H6SI2O7(AQ)	1.55148E-02	2.70290E+00	1.55193E-02	-1.80913	.00000	-1.80913
AL(OH)3(AQ)	3.73430E-05	2.91288E-03	3.73539E-05	-4.42766	.00000	-4.42766
AL(OH)4-	1.72690E-04	1.64074E-02	1.72741E-04	-3.76260	-.23994	-4.00255
AL(OH)SI(OH)-	2.35723E-03	4.08061E-01	2.35792E-03	-2.62747	-.23994	-2.86741
CACL+	4.65324E-03	3.51473E-01	4.65460E-03	-2.33212	-.23994	-2.57206
CACL2(AQ)	8.78036E-05	9.74497E-03	8.78293E-05	-4.05636	.00000	-4.05636
CA(OH)+	1.63432E-04	9.32988E-03	1.63480E-04	-3.78654	-.23994	-4.02648
CA(H3SIO4)+	1.01573E-02	1.37313E+00	1.01602E-02			

```
-1.99310     -.23994    -2.23304
   FE(OH)+              1.29559E-07   9.43891E-06   1.29597E-07
-6.88741     -.23994    -7.12735
   FE(OH)2              2.22537E-08   1.99976E-06   2.22603E-08
-7.65247      .00000    -7.65247
   FE(OH)3-             5.43581E-09   5.80919E-07   5.43740E-09
-8.26461     -.23994    -8.50455
   FECL+                2.13531E-07   1.94954E-05   2.13594E-07
-6.67041     -.23994    -6.91036
   FECL2(AQ)            5.16523E-06   6.54708E-04   5.16674E-06
-5.28678      .00000    -5.28678
   FE(H3SIO4)+          1.19678E-02   1.80659E+00   1.19714E-02
-1.92186     -.23994    -2.16180
   MGCL+                2.45266E-05   1.46566E-03   2.45337E-05
-4.61024     -.23994    -4.85018
   MG(OH)+              1.29576E-05   5.35310E-04   1.29614E-05
-4.88735     -.23994    -5.12729
   MG(OH)2(AQ)          2.11692E-02   1.23458E+00   2.11754E-02
-1.67417      .00000    -1.67417
   MG(H3SIO4)+          3.38066E-07   4.03691E-05   3.38165E-07
-6.47087     -.23994    -6.71081
   NACL(AQ)             3.64523E-02   2.13037E+00   3.64629E-02
-1.43815      .00000    -1.43815
   NAOH(AQ)             3.46856E-04   1.38732E-02   3.46957E-04
-3.45972      .00000    -3.45972
   H3SIO4-              7.94269E-04   7.55403E-02   7.94501E-04
-3.09991     -.23994    -3.33985
   HCL(AQ)              2.33636E-05   8.51859E-04   2.33705E-05
-4.63133      .00000    -4.63133

           --- activity ratios of cations ---


           log (NA+   /h+**0)           4.3836144
           log (CA++  /h+**0)           6.3316323
           log (MG++  /h+**0)           4.3792048
           log (AL+++ /h+**0)          -2.6588535
           log (FE++  /h+**0)           2.2732316
           log (FE+++ /h+**0)          -3.5898145


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                  -.9706621    1.06989E-01    2.47720E+01
4.76314E+00
   PARAGONITE                 -.7925626    1.61227E-01    6.16208E+01
```

```
2.13077E+01
   QUARTZ-ALPHA              -2.9525491    1.11545E-03    6.70211E-02
2.53074E-02

   CLINOPYROXENE(SS)           .4052147    2.54223E+00    5.49613E+02
1.64830E+02
   DIOPSIDE                    .2329005    1.70962E+00    3.70223E+02
1.13177E+02
   HEDENBERGITE               -.6174728    2.41283E-01    5.98610E+01
1.59730E+01
   JADEITE                    -.2281757    5.91322E-01    1.19529E+02
3.56804E+01

   CHLORITE(SS)                .0336568    1.08058E+00    1.23366E+02
4.57379E+01
   CLINOCHLORE                -.0098613    9.77549E-01    1.08664E+02
4.13406E+01
   CHAMOSITE                  -.9870345    1.03030E-01    1.47026E+01
4.39734E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  1.9998608    9.99679E+01    2.31464E+04
4.45057E+03
   TREMOLITE                  1.9994875    9.98821E+01    8.11412E+04
2.72358E+04
   PARAGONITE                 -.7925626    1.61227E-01    6.16208E+01
2.13077E+01
   QUARTZ-ALPHA              -2.9525491    1.11545E-03    6.70211E-02
2.53074E-02

   PLAGIOCLASE(SS)            1.9952910    9.89216E+01

   ALBITE                     1.7734423    5.93529E+01    1.55637E+04
5.98456E+03
   ANORTHITE                  1.5973510    3.95686E+01    1.10084E+04
3.98654E+03


   CLINOPYROXENE(SS)          2.0053625    1.01242E+02

   DIOPSIDE                   1.9067109    8.06698E+01    1.74692E+04
5.34034E+03
   HEDENBERGITE               1.3006242    1.99813E+01    4.95725E+03
1.32276E+03
```

```
   JADEITE                      -.2281757    5.91322E-01    1.19529E+02
3.56804E+01


   CHLORITE(SS)                  .0336568    1.08058E+00

   CLINOCHLORE                  -.0098613    9.77549E-01    1.08664E+02
4.13406E+01
   CHAMOSITE                    -.9870345    1.03030E-01    1.47026E+01
4.39734E+00



                           mass, grams        volume, cc

           created         7.594395E+02       2.366645E+02
           destroyed       7.073578E+02       2.330981E+02
           net             5.208168E+01       3.566412E+00

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral         affinity, kcal    state         mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-3.5924
 HEMATITE                1.3506  ssatd         SPINEL
-8.0922
 BRUCITE                -6.7337                DIASPORE
-1.4566
 ANDALUSITE             -3.7082                KYANITE
-2.4892
 SILLIMANITE            -3.4719                GLAUCOPHANE
-5.6537
 LAWSONITE              -1.0127                PUMPELLYITE
-4.7238
 ZOISITE                 -.3654                CLINOZOISITE
-1.0758
 FORSTERITE             -3.2025                FAYALITE
-3.5886
 CHRYSOTILE             -6.2658                ENSTATITE-CL
-2.1640
 ENSTATITE-OR           -2.2421                ENSTATITE-PR
-2.6474
```

DIOPSIDE	-.5702		HEDENBERGITE	-3.3841
JADEITE	-2.0959		FERROSILITE	-3.5160
WOLLASTONITE	-4.1010		PSEUDOWOLLASTONITE	-4.5871
TREMOLITE	-.7830		ALBITE	-.6327
ANORTHITE	-3.5389		KAOLINITE	-3.7855
PYROPHYLLITE	-2.7121		TALC	-1.2130
PARAGONITE	.0000	satd	MARGARITE	-3.1988
PREHNITE	-3.2312		CLINOCHLORE	-.1440
CHAMOSITE	-3.3775		PYROPE	-4.0117
ALMANDINE	-3.1493		GROSSULAR	-1.2114
QUARTZ-ALPHA	.0000	satd	QUARTZ-BETA	-.2369
COESITE	-.5963		HALITE	-9.9566
CRISTOBALITE-ALPHA	-1.2859		CRISTOBALITE-BETA	-1.9993

--- summary of solid solutions ---

mineral	aff. kcal/mol	mole frac.	lambda	state
PLAGIOCLASE(SS)	-.4540			
ALBITE	-.45403	.8831218	1.00000	
ANORTHITE	-.45403	.1168782	1.00000	
ORTHOPYROXENE(SS)	-1.7462			
ENSTATITE-OR	-1.74616	.7081536	1.00000	
FERROSILITE	-1.74616	.2918464	1.00000	
GARNET(SS)	-.7257			
PYROPE	-.72569	.1016118	1.00000	
ALMANDINE	-.72569	.1851676	1.00000	
GROSSULAR	-.72569	.7132207	1.00000	
CLINOPYROXENE(SS)	.0000			saturated
DIOPSIDE	.00000	.6724899	1.00000	
HEDENBERGITE	.00000	.0949101	1.00000	
JADEITE	.00000	.2325999	1.00000	

```
 CPX_SUBCALCIC(SS)          -.3805
     DIOPSIDE                     -.38046     .8763225     1.00000
     HEDENBERGITE                 -.38046     .1236775     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .9046526     1.00000
     CHAMOSITE                     .00000     .0953474     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6725    1.0000     .6725    -.1723     .0000    -.1723
     HEDENBERGITE
              .0949    1.0000     .0949   -1.0227     .0000   -1.0227
     JADEITE
              .2326    1.0000     .2326    -.6334     .0000    -.6334

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9047    1.0000     .9047    -.0435     .0000    -.0435
     CHAMOSITE
              .0953    1.0000     .0953   -1.0207     .0000   -1.0207


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                          -18.27674       5.28767E-19
   H2(G)                           -1.98381       1.03799E-02
   H2O(G)                           3.80602       6.39771E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
stepping to zi=  6.4372E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   176, iter =  2, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -2.9525

stepping to zi=  6.4372E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   177, iter =  2, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -2.9525

stepping to zi=  6.4372E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   178, iter =  2, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -2.9525

stepping to zi=  6.4372E-01, delzi=  1.0000E-07, nord= 1
              ncycle=  0
steps completed =   179, iter =  2, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -2.9525

stepping to zi=  6.4372E-01, delzi=  1.0000E-06, nord= 2
              ncycle=  0
steps completed =   180, iter =  2, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -2.9521

stepping to zi=  6.4373E-01, delzi=  1.0000E-05, nord= 2
              ncycle=  0
steps completed =   181, iter =  2, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -2.9480

stepping to zi=  6.4383E-01, delzi=  1.0000E-04, nord= 2
              ncycle=  0
steps completed =   182, iter =  3, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -2.9090

stepping to zi=  6.4483E-01, delzi=  1.0000E-03, nord= 2
              ncycle=  0
steps completed =   183, iter =  3, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -2.6399

stepping to zi=  6.5483E-01, delzi=  1.0000E-02, nord= 3
              ncycle=  0
steps completed =   184, iter =  4, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -1.8902

stepping to zi=  6.9677E-01, delzi=  4.1939E-02, nord= 3
              ncycle=  0
steps completed =   185, iter =  4, ncorr = 0
most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =     -1.2416
```

```
 stepping to zi=  8.0741E-01, delzi=  1.1064E-01, nord= 4
              ncycle=  0
 steps completed =   186, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(QUARTZ-ALPHA      ) =      -.7570

 stepping to zi=  8.2705E-01, delzi=  1.9641E-02, nord= 5
              ncycle=  0
 iter =    4
       1 supersaturated pure minerals
       0 supersaturated solid solutions

                           the most supersaturated phases     affinity,
kcal

                             1      15   ZOISITE                  .
00757748


   attempted species assemblage no.   2

               1      1  H2O
               2      2  NA+
               3      4  CA++
               4      5  MG++
               5      6  AL+++
               6      7  H4SIO4(AQ)
               7     13  H+
               8     16  CL-
               9     21  FE++
              10     32  O2(G)
              11      1  MAGNETITE
              12     15  ZOISITE
              13     42  PARAGONITE
              14     50  QUARTZ-ALPHA
              15      1  CLINOPYRDIOPSIDE
              16      2  CLINOPYRHEDENBERGITE
              17      3  CLINOPYRJADEITE
              18      1  CHLORITECLINOCHLORE
              19      2  CHLORITECHAMOSITE

 steps completed =   187, iter = 14, ncorr = 0
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  8.27052527104739E-01
                     log of reaction progress =       -.0824669

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars
```

computing units remaining =   .000

change in the product phase assemblage

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.86144E+01	1.38556E+00	2.64896E+04	3.72186E+02
CLINOPYROXENE(SS)	9.83300E+01	1.66998E+00	2.19139E+04	3.72174E+02
MAGNETITE	9.98214E+01	1.78643E-01	2.31125E+04	4.13628E+01
TREMOLITE	9.98485E+01	1.51516E-01	8.11140E+04	1.23087E+02

current total mass = 1.52630E+05 grams
delta total mass   = 9.08810E+02 grams
delta total volume =   299.48335 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	.8292	1.67530E+00
CLINOPYROXENE(SS)	.3700	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	.7994	1.83200E-01

affinity of the overall irreversible reaction=   1.536 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.594202E+05	5.608558E+01	5.599080E+01
NA	1.013605E+04	4.603450E-01	4.595670E-01
CA	8.379249E+02	2.182864E-02	2.179176E-02

```
      MG         4.839003E+02        2.078786E-02        2.075273E-02
      AL         6.109793E+01        2.364336E-03        2.360340E-03
      SI         3.644855E+03        1.355026E-01        1.352736E-01
      H          1.076807E+05        1.115501E+02        1.113616E+02
      CL         1.700623E+04        5.008464E-01        5.000000E-01
      FE         7.290774E+02        1.363086E-02        1.360782E-02

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                             ph            eh            pe


     internal ph scale               4.9285       1.0010
6.9762E+00
     modified nbs ph scale           4.6886       1.0354
7.2161E+00
     rational ph scale               4.6886       1.0354
7.2161E+00

   phcl =      5.5072



          oxygen fugacity =  5.51493E-19
          log oxygen fugacity = -18.25846



                        activity of water =    .98382
               log activity of water =   -.00709
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  4.654956E-01 molal
                 sum of molalities =    1.0705508362916
               osmotic coefficient =     .84596
                    equiv. stoich. ionic strength =  5.008464E-01
molal
```

mass of solution = 1.042353 kg
mass of solvent = .998310 kg
mass of solutes = .044043 kg
conc of solutes = 4.225346 per cent (w/w)

species	moles	grams	conc	log conc	log g	log act
H2O	5.54149E+01	9.98310E+02				
NA+	4.23577E-01	9.73795E+00	4.24294E-01	-.37233	-.23993	-.61226
CA++	2.85173E-03	1.14297E-01	2.85655E-03	-2.54416	-.95970	-3.50386
MG++	2.96174E-05	7.19850E-04	2.96675E-05	-4.52772	-.95970	-5.48742
AL+++	5.45341E-16	1.47141E-14	5.46264E-16	-15.26260	-2.15933	-17.42193
H4SIO4(AQ)	7.56126E-02	7.26748E+00	7.57406E-02	-1.12067	.00000	-1.12067
H+	2.04491E-05	2.06107E-05	2.04837E-05	-4.68859	-.23993	-4.92852
CL-	4.57586E-01	1.62228E+01	4.58360E-01	-.33879	-.23993	-.57872
FE++	2.35576E-07	1.31562E-05	2.35975E-07	-6.62713	-.95970	-7.58684
O2(AQ)	4.63346E-23	1.48265E-21	4.64130E-23	-22.33336	.00000	-22.33336
H2(AQ)	1.71558E-06	3.45826E-06	1.71848E-06	-5.76486	.00000	-5.76486
FE+++	6.09218E-17	3.40230E-15	6.10249E-17	-16.21449	-2.15933	-18.37383
OH-	1.22864E-03	2.08958E-02	1.23071E-03	-2.90984	-.23993	-3.14977
H8SI3O10(AQ)	2.20710E-06	5.56882E-04	2.21084E-06	-5.65544	.00000	-5.65544
H6SI2O7(AQ)	1.54920E-02	2.69893E+00	1.55183E-02	-1.80916	.00000	-1.80916
AL(OH)3(AQ)	3.92684E-05	3.06307E-03	3.93349E-05	-4.40522	.00000	-4.40522
AL(OH)4-	1.58438E-04	1.50533E-02	1.58706E-04	-3.79941	-.23993	-4.03933
AL(OH)SI(OH)-	2.16263E-03	3.74374E-01	2.16630E-03	-2.66428	-.23993	-2.90421
CACL+	6.40781E-03	4.84001E-01	6.41866E-03	-2.19256	-.23993	-2.43248
CACL2(AQ)	1.20806E-04	1.34078E-02	1.21011E-04	-3.91718	.00000	-3.91718
CA(OH)+	1.96543E-04	1.12201E-02	1.96876E-04	-3.70581	-.23993	-3.94573

```
   CA(H3SIO4)+          1.22149E-02   1.65129E+00   1.22355E-02
-1.91238     -.23993    -2.15230
   FE(OH)+              1.47236E-07   1.07267E-05   1.47485E-07
-6.83125     -.23993    -7.07118
   FE(OH)2              2.20668E-08   1.98296E-06   2.21042E-08
-7.65553      .00000    -7.65553
   FE(OH)3-             4.70280E-09   5.02583E-07   4.71076E-09
-8.32691     -.23993    -8.56683
   FECL+                2.77869E-07   2.53694E-05   2.78339E-07
-6.55543     -.23993    -6.79535
   FECL2(AQ)            6.71570E-06   8.51236E-04   6.72707E-06
-5.17217      .00000    -5.17217
   FE(H3SIO4)+          1.36004E-02   2.05303E+00   1.36234E-02
-1.86571     -.23993    -2.10564
   MGCL+                3.14382E-05   1.87868E-03   3.14914E-05
-4.50181     -.23993    -4.74173
   MG(OH)+              1.45049E-05   5.99229E-04   1.45294E-05
-4.83775     -.23993    -5.07768
   MG(OH)2(AQ)          2.06768E-02   1.20586E+00   2.07118E-02
-1.68378      .00000    -1.68378
   MG(H3SIO4)+          3.78425E-07   4.51884E-05   3.79065E-07
-6.42129     -.23993    -6.66121
   NACL(AQ)             3.56930E-02   2.08600E+00   3.57534E-02
-1.44668      .00000    -1.44668
   NAOH(AQ)             2.96603E-04   1.18632E-02   2.97105E-04
-3.52709      .00000    -3.52709
   H3SIO4-              6.92000E-04   6.58139E-02   6.93171E-04
-3.15916     -.23993    -3.39909
   HCL(AQ)              2.67150E-05   9.74054E-04   2.67602E-05
-4.57251      .00000    -4.57251

           --- activity ratios of cations ---


           log (NA+   /h+**0)           4.3162582
           log (CA++  /h+**0)           6.3531720
           log (MG++  /h+**0)           4.3696104
           log (AL+++ /h+**0)          -2.6363814
           log (FE++  /h+**0)           2.2701957
           log (FE+++ /h+**0)          -3.5882765


           --- summary of solid product phases---


  product                    log moles       moles        grams
volume, cc

   MAGNETITE                 -.8339022    1.46588E-01    3.39407E+01
6.52609E+00
```

```
   ZOISITE                     -3.0470663    8.97292E-04    4.07695E-01
1.21924E-01
   PARAGONITE                   -.5505613    2.81474E-01    1.07579E+02
3.71996E+01
   QUARTZ-ALPHA                 -.7040795    1.97661E-01    1.18763E+01
4.48453E+00

   CLINOPYROXENE(SS)             .5009843    3.16945E+00    6.86671E+02
2.05922E+02
   DIOPSIDE                      .3405953    2.19076E+00    4.74415E+02
1.45028E+02
   HEDENBERGITE                 -.5032195    3.13892E-01    7.78749E+01
2.07797E+01
   JADEITE                      -.1773103    6.64798E-01    1.34381E+02
4.01139E+01

   CHLORITE(SS)                  .0268533    1.06378E+00    1.21493E+02
4.50275E+01
   CLINOCHLORE                  -.0172945    9.60960E-01    1.06820E+02
4.06390E+01
   CHAMOSITE                    -.9879093    1.02823E-01    1.46730E+01
4.38849E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member        log moles        moles         grams
volume, cc

   MAGNETITE                    1.9998608    9.99679E+01    2.31464E+04
4.45057E+03
   ZOISITE                     -3.0470663    8.97292E-04    4.07695E-01
1.21924E-01
   TREMOLITE                    1.9993415    9.98485E+01    8.11140E+04
2.72267E+04
   PARAGONITE                   -.5505613    2.81474E-01    1.07579E+02
3.71996E+01
   QUARTZ-ALPHA                 -.7040795    1.97661E-01    1.18763E+01
4.48453E+00

   PLAGIOCLASE(SS)              1.9939405    9.86144E+01

   ALBITE                       1.7720918    5.91687E+01    1.55154E+04
5.96598E+03
   ANORTHITE                    1.5960005    3.94458E+01    1.09742E+04
3.97416E+03


   CLINOPYROXENE(SS)            2.0064638    1.01499E+02
```

```
   DIOPSIDE                    1.9077057    8.08548E+01    1.75093E+04
5.35259E+03
   HEDENBERGITE                1.3005932    1.99799E+01    4.95690E+03
1.32267E+03
   JADEITE                     -.1773103    6.64798E-01    1.34381E+02
4.01139E+01


   CHLORITE(SS)                 .0268533    1.06378E+00

   CLINOCHLORE                 -.0172945    9.60960E-01    1.06820E+02
4.06390E+01
   CHAMOSITE                   -.9879093    1.02823E-01    1.46730E+01
4.38849E+00



                          mass, grams        volume, cc

           created        9.619680E+02       2.992817E+02
           destroyed      9.088100E+02       2.994833E+02
           net            5.315800E+01      -2.016120E-01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE               .0000  satd          CORUNDUM
-3.4438
 HEMATITE               1.3606  ssatd         SPINEL
-7.9754
 BRUCITE               -6.7655                DIASPORE
-1.3824
 ANDALUSITE            -3.5596                KYANITE
-2.3405
 SILLIMANITE           -3.3233                GLAUCOPHANE
-6.0462
 LAWSONITE              -.7929                PUMPELLYITE
-4.0991
 ZOISITE                 .0000  satd          CLINOZOISITE
-.7104
 FORSTERITE            -3.2343                FAYALITE
```

```
-3.5987
 CHRYSOTILE               -6.3612                ENSTATITE-CL
-2.1958
 ENSTATITE-OR             -2.2739                ENSTATITE-PR
-2.6792
 DIOPSIDE                  -.5307                HEDENBERGITE
-3.3229
 JADEITE                  -2.2445                FERROSILITE
-3.5261
 WOLLASTONITE             -4.0298                PSEUDOWOLLASTONITE
-4.5159
 TREMOLITE                 -.7994                ALBITE
-.7812
 ANORTHITE                -3.3191                KAOLINITE
-3.6369
 PYROPHYLLITE             -2.5635                TALC
-1.3084
 PARAGONITE                 .0000  satd          MARGARITE
-2.8303
 PREHNITE                 -2.9402                CLINOCHLORE
-.1461
 CHAMOSITE                -3.3579                PYROPE
-3.9941
 ALMANDINE                -3.1099                GROSSULAR
-1.0906
 QUARTZ-ALPHA               .0000  satd          QUARTZ-BETA
-.2369
 COESITE                   -.5963                HALITE
-9.9849
 CRISTOBALITE-ALPHA       -1.2859                CRISTOBALITE-BETA
-1.9993


                     --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)            -.5544
     ALBITE                       -.55435     .8539523     1.00000
     ANORTHITE                    -.55435     .1460477     1.00000

 ORTHOPYROXENE(SS)         -1.7716
     ENSTATITE-OR                -1.77158     .7050228     1.00000
     FERROSILITE                 -1.77158     .2949772     1.00000

 GARNET(SS)                 -.6299
     PYROPE                       -.62987     .0962340     1.00000
     ALMANDINE                    -.62987     .1780386     1.00000
     GROSSULAR                    -.62987     .7257274     1.00000
```

```
 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .6912116     1.00000
     HEDENBERGITE                 .00000     .0990367     1.00000
     JADEITE                      .00000     .2097517     1.00000

 CPX_SUBCALCIC(SS)         -.3383
     DIOPSIDE                    -.33830     .8746764     1.00000
     HEDENBERGITE                -.33830     .1253236     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9033421     1.00000
     CHAMOSITE                    .00000     .0966579     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6912    1.0000     .6912    -.1604     .0000    -.1604
     HEDENBERGITE
              .0990    1.0000     .0990   -1.0042     .0000   -1.0042
     JADEITE
              .2098    1.0000     .2098    -.6783     .0000    -.6783

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .9033    1.0000     .9033    -.0441     .0000    -.0441
     CHAMOSITE
              .0967    1.0000     .0967   -1.0148     .0000   -1.0148


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                          -18.25846       5.51493E-19
   H2(G)                           -1.99296       1.01635E-02
   H2O(G)                           3.80601       6.39756E+03
```

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


stepping to zi=  8.2705E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   188, iter =  2, ncorr = 0
most rapidly changing is zvclg1(ZOISITE           ) =    -3.0471

stepping to zi=  8.2705E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   189, iter =  2, ncorr = 0
most rapidly changing is zvclg1(ZOISITE           ) =    -3.0471

stepping to zi=  8.2705E-01, delzi=  1.0000E-08, nord= 0
              ncycle=  0
steps completed =   190, iter =  2, ncorr = 0
most rapidly changing is zvclg1(ZOISITE           ) =    -3.0471

stepping to zi=  8.2705E-01, delzi=  1.0000E-07, nord= 1
              ncycle=  0
steps completed =   191, iter =  1, ncorr = 0
most rapidly changing is zvclg1(ZOISITE           ) =    -3.0471

stepping to zi=  8.2705E-01, delzi=  1.0000E-06, nord= 2
              ncycle=  0
steps completed =   192, iter =  2, ncorr = 0
most rapidly changing is zvclg1(ZOISITE           ) =    -3.0470

stepping to zi=  8.2706E-01, delzi=  1.0000E-05, nord= 2
              ncycle=  0
steps completed =   193, iter =  2, ncorr = 0
most rapidly changing is zvclg1(ZOISITE           ) =    -3.0460

stepping to zi=  8.2716E-01, delzi=  1.0000E-04, nord= 2
              ncycle=  0
steps completed =   194, iter =  2, ncorr = 0
most rapidly changing is zvclg1(ZOISITE           ) =    -3.0362

stepping to zi=  8.2816E-01, delzi=  1.0000E-03, nord= 2
              ncycle=  0
steps completed =   195, iter =  3, ncorr = 0
most rapidly changing is zvclg1(ZOISITE           ) =    -2.9493

stepping to zi=  8.3816E-01, delzi=  1.0000E-02, nord= 2
              ncycle=  0
steps completed =   196, iter =  5, ncorr = 0
most rapidly changing is zvclg1(ZOISITE           ) =    -2.5000
```

```
 stepping to zi=  8.8668E-01, delzi=  4.8517E-02, nord= 3
              ncycle=  0
 steps completed =   197, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE          ) =    -1.8843

 stepping to zi=  9.8747E-01, delzi=  1.0079E-01, nord= 4
              ncycle=  0
 steps completed =   198, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE          ) =    -1.4736

 stepping to zi=  1.0000E+00, delzi=  1.2534E-02, nord= 5
              ncycle=  0
 steps completed =   199, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE          ) =    -1.4418
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  9.99999999999987E-01
                    log of reaction progress =        .0000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reaction summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)         9.83247E+01    1.67530E+00    2.64117E+04
4.50015E+02
   CLINOPYROXENE(SS)       9.79808E+01    2.01920E+00    2.18361E+04
4.50001E+02
   MAGNETITE               9.97840E+01    2.16000E-01    2.31038E+04
5.00123E+01
   TREMOLITE               9.98168E+01    1.83200E-01    8.10882E+04
1.48826E+02


               current total mass =  1.52440E+05 grams
               delta total mass   =  1.09885E+03 grams
               delta total volume =    362.10923 cc
```

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	.8295	1.67530E+00
CLINOPYROXENE(SS)	.3680	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	.8132	1.83200E-01

affinity of the overall irreversible reaction= 1.539
kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.593763E+05	5.608646E+01	5.591238E+01
NA	1.014405E+04	4.607393E-01	4.593092E-01
CA	8.395757E+02	2.187311E-02	2.180522E-02
MG	4.830029E+02	2.075069E-02	2.068628E-02
AL	6.104115E+01	2.362296E-03	2.354964E-03
SI	3.651070E+03	1.357427E-01	1.353213E-01
H	1.076741E+05	1.115507E+02	1.112045E+02
CL	1.702922E+04	5.015568E-01	5.000000E-01
FE	7.416331E+02	1.386653E-02	1.382349E-02
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	4.9280	.9996	6.9665E+00
modified nbs ph scale	4.6880	1.0340	7.2065E+00

```
     rational ph scale               4.6880       1.0340
7.2065E+00

   phcl =      5.5062



          oxygen fugacity =  5.01750E-19
          log oxygen fugacity = -18.29951



                          activity of water =    .98379
               log activity of water =   -.00710
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  4.661236E-01 molal
                 sum of molalities =    1.0718032802662
               osmotic coefficient =     .84619
                    equiv. stoich. ionic strength =  5.015568E-01
molal

                         mass of solution =   1.040946 kg
                         mass of solvent  =    .996896 kg
                         mass of solutes  =    .044050 kg
                         conc of solutes  =   4.231738 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.53364E+01   9.96896E+02
   NA+                  4.23308E-01   9.73176E+00   4.24626E-01     -.
37199     -.24001     -.61200
   CA++                 2.85597E-03   1.14467E-01   2.86486E-03
-2.54290     -.96004    -3.50294
   MG++                 2.96184E-05   7.19874E-04   2.97106E-05
-4.52709     -.96004    -5.48713
   AL+++                5.47652E-16   1.47765E-14   5.49357E-16
-15.26015    -2.16009   -17.42024
   H4SIO4(AQ)           7.55019E-02   7.25685E+00   7.57370E-02
-1.12069      .00000    -1.12069
   H+                   2.04489E-05   2.06105E-05   2.05126E-05
-4.68798     -.24001    -4.92799
   CL-                  4.57559E-01   1.62219E+01   4.58984E-01     -.
33820     -.24001     -.57821
   FE++                 2.39751E-07   1.33894E-05   2.40497E-07
-6.61889     -.96004    -7.57893
   O2(AQ)               4.20957E-23   1.34701E-21   4.22267E-23
```

```
-22.37441       .00000   -22.37441
   H2(AQ)                1.79602E-06   3.62041E-06   1.80161E-06
-5.74434       .00000    -5.74434
   FE+++                 6.06865E-17   3.38916E-15   6.08755E-17
-16.21556    -2.16009    -18.37565
   OH-                   1.22561E-03   2.08444E-02   1.22943E-03
-2.91030     -.24001     -3.15031
   H8SI3O10(AQ)          2.20377E-06   5.56042E-04   2.21063E-06
-5.65548      .00000     -5.65548
   H6SI2O7(AQ)           1.54690E-02   2.69492E+00   1.55172E-02
-1.80919      .00000     -1.80919
   AL(OH)3(AQ)           3.92201E-05   3.05930E-03   3.93422E-05
-4.40514      .00000     -4.40514
   AL(OH)4-              1.58078E-04   1.50191E-02   1.58570E-04
-3.79978     -.24001     -4.03979
   AL(OH)SI(OH)-         2.15767E-03   3.73514E-01   2.16438E-03
-2.66467     -.24001     -2.90468
   CACL+                 6.42109E-03   4.85005E-01   6.44109E-03
-2.19104     -.24001     -2.43105
   CACL2(AQ)             1.21174E-04   1.34487E-02   1.21552E-04
-3.91524      .00000     -3.91524
   CA(OH)+               1.96478E-04   1.12164E-02   1.97089E-04
-3.70534     -.24001     -3.94535
   CA(H3SIO4)+           1.22105E-02   1.65070E+00   1.22485E-02
-1.91192     -.24001     -2.15193
   FE(OH)+               1.49572E-07   1.08970E-05   1.50038E-07
-6.82380     -.24001     -7.06381
   FE(OH)2               2.23849E-08   2.01155E-06   2.24546E-08
-7.64869      .00000     -7.64869
   FE(OH)3-              4.76562E-09   5.09296E-07   4.78046E-09
-8.32053     -.24001     -8.56054
   FECL+                 2.82958E-07   2.58341E-05   2.83839E-07
-6.54693     -.24001     -6.78694
   FECL2(AQ)             6.84536E-06   8.67670E-04   6.86667E-06
-5.16325      .00000     -5.16325
   FE(H3SIO4)+           1.38159E-02   2.08557E+00   1.38590E-02
-1.85827     -.24001     -2.09828
   MGCL+                 3.14576E-05   1.87984E-03   3.15556E-05
-4.50092     -.24001     -4.74093
   MG(OH)+               1.44790E-05   5.98160E-04   1.45241E-05
-4.83791     -.24001     -5.07792
   MG(OH)2(AQ)           2.06103E-02   1.20199E+00   2.06745E-02
-1.68456      .00000     -1.68456
   MG(H3SIO4)+           3.77741E-07   4.51067E-05   3.78917E-07
-6.42146     -.24001     -6.66147
   NACL(AQ)              3.57050E-02   2.08670E+00   3.58162E-02
-1.44592      .00000     -1.44592
   NAOH(AQ)              2.95990E-04   1.18387E-02   2.96912E-04
-3.52737      .00000     -3.52737
   H3SIO4-               6.90282E-04   6.56505E-02   6.92431E-04
```

```
-3.15962     -.24001    -3.39963
   HCL(AQ)              2.67408E-05   9.74993E-04   2.68240E-05
-4.57148      .00000    -4.57148

           --- activity ratios of cations ---


           log (NA+   /h+**0)            4.3159858
           log (CA++  /h+**0)            6.3530408
           log (MG++  /h+**0)            4.3688486
           log (AL+++ /h+**0)           -2.6362702
           log (FE++  /h+**0)            2.2770479
           log (FE+++ /h+**0)           -3.5916822


           --- summary of solid product phases---


  product                     log moles        moles        grams
volume, cc

   MAGNETITE                  -.7353131    1.83945E-01    4.25903E+01
8.18921E+00
   ZOISITE                   -1.4417835    3.61590E-02    1.64293E+01
4.91329E+00
   PARAGONITE                 -.4756788    3.34442E-01    1.27824E+02
4.41999E+01
   QUARTZ-ALPHA               -.3465261    4.50271E-01    2.70542E+01
1.02157E+01

   CLINOPYROXENE(SS)           .5738608    3.74853E+00    8.12316E+02
2.43547E+02
   DIOPSIDE                    .4125584    2.58558E+00    5.59914E+02
1.71166E+02
   HEDENBERGITE               -.4236423    3.77014E-01    9.35351E+01
2.49583E+01
   JADEITE                    -.1046154    7.85931E-01    1.58867E+02
4.74231E+01

   CHLORITE(SS)                .0466229    1.11333E+00    1.27205E+02
4.71253E+01
   CLINOCHLORE                 .0017333    1.00400E+00    1.11604E+02
4.24591E+01
   CHAMOSITE                  -.9612674    1.09328E-01    1.56013E+01
4.66613E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---
```

phase/end-member	log moles	moles	grams	volume, cc
MAGNETITE	1.9998608	9.99679E+01	2.31464E+04	4.45057E+03
ZOISITE	-1.4417835	3.61590E-02	1.64293E+01	4.91329E+00
TREMOLITE	1.9992036	9.98168E+01	8.10882E+04	2.72180E+04
PARAGONITE	-.4756788	3.34442E-01	1.27824E+02	4.41999E+01
QUARTZ-ALPHA	-.3465261	4.50271E-01	2.70542E+01	1.02157E+01
PLAGIOCLASE(SS)	1.9926626	9.83247E+01		
ALBITE	1.7708139	5.89948E+01	1.54698E+04	5.94845E+03
ANORTHITE	1.5947226	3.93299E+01	1.09419E+04	3.96249E+03
CLINOPYROXENE(SS)	2.0074462	1.01729E+02		
DIOPSIDE	1.9083253	8.09702E+01	1.75343E+04	5.36023E+03
HEDENBERGITE	1.3004471	1.99732E+01	4.95523E+03	1.32222E+03
JADEITE	-.1046154	7.85931E-01	1.58867E+02	4.74231E+01
CHLORITE(SS)	.0466229	1.11333E+00		
CLINOCHLORE	.0017333	1.00400E+00	1.11604E+02	4.24591E+01
CHAMOSITE	-.9612674	1.09328E-01	1.56013E+01	4.66613E+00

	mass, grams	volume, cc
created	1.153419E+03	3.581904E+02
destroyed	1.098854E+03	3.621092E+02
net	5.456492E+01	-3.918842E+00

warning-- these volume totals may be incomplete because of missing partial molar volume data in the data base

--- mineral saturation state summary ---

mineral	affinity, kcal	state	mineral	affinity, kcal	state
MAGNETITE	.0000	satd	CORUNDUM	-3.4431	
HEMATITE	1.3380	ssatd	SPINEL	-7.9773	
BRUCITE	-6.7681		DIASPORE	-1.3820	
ANDALUSITE	-3.5589		KYANITE	-2.3399	
SILLIMANITE	-3.3227		GLAUCOPHANE	-6.0551	
LAWSONITE	-.7928		PUMPELLYITE	-4.1021	
ZOISITE	.0000	satd	CLINOZOISITE	-.7104	
FORSTERITE	-3.2369		FAYALITE	-3.5760	
CHRYSOTILE	-6.3690		ENSTATITE-CL	-2.1983	
ENSTATITE-OR	-2.2764		ENSTATITE-PR	-2.6818	
DIOPSIDE	-.5338		HEDENBERGITE	-3.3008	
JADEITE	-2.2451		FERROSILITE	-3.5034	
WOLLASTONITE	-4.0302		PSEUDOWOLLASTONITE	-4.5163	
TREMOLITE	-.8132		ALBITE	-.7818	
ANORTHITE	-3.3189		KAOLINITE	-3.6363	
PYROPHYLLITE	-2.5629		TALC	-1.3161	
PARAGONITE	.0000	satd	MARGARITE	-2.8296	
PREHNITE	-2.9405		CLINOCHLORE	-.1485	
CHAMOSITE	-3.3351		PYROPE	-3.9964	
ALMANDINE	-3.0871		GROSSULAR	-1.0908	
QUARTZ-ALPHA	.0000	satd	QUARTZ-BETA	-.2369	

```
 COESITE                  -.5963              HALITE
-9.9824
 CRISTOBALITE-ALPHA      -1.2859              CRISTOBALITE-BETA
-1.9993


                     --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -.5548
     ALBITE                      -.55484     .8538857     1.00000
     ANORTHITE                   -.55484     .1461143     1.00000

 ORTHOPYROXENE(SS)        -1.7667
     ENSTATITE-OR               -1.76665     .7013637     1.00000
     FERROSILITE                -1.76665     .2986363     1.00000

 GARNET(SS)                -.6262
     PYROPE                      -.62618     .0958307     1.00000
     ALMANDINE                   -.62618     .1804315     1.00000
     GROSSULAR                   -.62618     .7237378     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .6897594     1.00000
     HEDENBERGITE                 .00000     .1005766     1.00000
     JADEITE                      .00000     .2096640     1.00000

 CPX_SUBCALCIC(SS)         -.3381
     DIOPSIDE                    -.33814     .8727420     1.00000
     HEDENBERGITE                -.33814     .1272580     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .9018004     1.00000
     CHAMOSITE                    .00000     .0981996     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6898    1.0000     .6898    -.1613     .0000    -.1613
     HEDENBERGITE
```

```
              .1006    1.0000     .1006    -.9975     .0000    -.9975
     JADEITE
              .2097    1.0000     .2097    -.6785     .0000    -.6785

   CHLORITE(SS)
  ideal solution

     CLINOCHLORE
              .9018    1.0000     .9018    -.0449     .0000    -.0449
     CHAMOSITE
              .0982    1.0000     .0982   -1.0079     .0000   -1.0079


           --- summary of gas species ---

           gas                log fugacity         fugacity
 partial pressure

   O2(G)                        -18.29951       5.01750E-19
   H2(G)                         -1.97244       1.06552E-02
   H2O(G)                         3.80600       6.39741E+03



  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



  stepping to zi=  1.1253E+00, delzi=  1.2534E-01, nord= 5
                ncycle=  0
  steps completed =   200, iter =  4, ncorr = 0
  most rapidly changing is zvclg1(ZOISITE          ) =     -1.2095

  stepping to zi=  1.3520E+00, delzi=  2.2661E-01, nord= 6
                ncycle=  0
  steps completed =   201, iter =  5, ncorr = 0
  most rapidly changing is zvclg1(ZOISITE          ) =      -.9667

  stepping to zi=  1.5849E+00, delzi=  2.3294E-01, nord= 6
                ncycle=  0
  steps completed =   202, iter =  5, ncorr = 0
  most rapidly changing is zvclg1(ZOISITE          ) =      -.8082
  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                      reaction progress        =  1.58489319246109E+00
                      log of reaction progress =        .2000000

                      temperature    =    450.000 degrees c
```

total pressure =   500.000 bars

computing units remaining =   .000

step size is limited by the print requirement

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	9.73448E+01	2.65517E+00	2.61485E+04	7.13226E+02
CLINOPYROXENE(SS)	9.67998E+01	3.20022E+00	2.15729E+04	7.13203E+02
MAGNETITE	9.96577E+01	3.42337E-01	2.30746E+04	7.92642E+01
TREMOLITE	9.97096E+01	2.90352E-01	8.10012E+04	2.35874E+02

current total mass = 1.51797E+05 grams
delta total mass   = 1.74157E+03 grams
delta total volume =   573.90445 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	.8301	1.67530E+00
CLINOPYROXENE(SS)	.3641	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	.8417	1.83200E-01

affinity of the overall irreversible reaction=   1.545 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.592387E+05	5.608842E+01	5.564618E+01
NA	1.017786E+04	4.623647E-01	4.587191E-01

```
      CA         8.453265E+02        2.202723E-02        2.185355E-02
      MG         4.811131E+02        2.067353E-02        2.051052E-02
      AL         6.084548E+01        2.355183E-03        2.336613E-03
      SI         3.664684E+03        1.362754E-01        1.352009E-01
      H          1.076545E+05        1.115521E+02        1.106726E+02
      CL         1.710794E+04        5.039737E-01        5.000000E-01
      FE         7.690255E+02        1.438149E-02        1.426810E-02

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species


   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                             ph            eh            pe

     internal ph scale              4.9263        .9968
6.9474E+00
     modified nbs ph scale          4.6860       1.0313
7.1877E+00
     rational ph scale              4.6860       1.0313
7.1877E+00

   phcl =      5.5028



          oxygen fugacity =  4.14194E-19
          log oxygen fugacity = -18.38280



                           activity of water =    .98372
               log activity of water =   -.00713
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  4.682393E-01 molal
                 sum of molalities =    1.0760925007860
               osmotic coefficient =     .84693
                    equiv. stoich. ionic strength =  5.039737E-01
molal
```

mass of solution = 1.036156 kg
mass of solvent = .992115 kg
mass of solutes = .044041 kg
conc of solutes = 4.250404 per cent (w/w)

species	moles	grams	conc	log conc	log g	log act
H2O	5.50710E+01	9.92115E+02				
NA+	4.22658E-01	9.71681E+00	4.26017E-01	-.37057	-.24029	-.61087
CA++	2.87039E-03	1.15045E-01	2.89320E-03	-2.53862	-.96117	-3.49979
MG++	2.96790E-05	7.21348E-04	2.99149E-05	-4.52411	-.96117	-5.48529
AL+++	5.55054E-16	1.49762E-14	5.59465E-16	-15.25223	-2.16264	-17.41487
H4SIO4(AQ)	7.51279E-02	7.22089E+00	7.57249E-02	-1.12076	.00000	-1.12076
H+	2.04442E-05	2.06057E-05	2.06067E-05	-4.68599	-.24029	-4.92628
CL-	4.57449E-01	1.62179E+01	4.61085E-01	-.33622	-.24029	-.57651
FE++	2.48960E-07	1.39037E-05	2.50938E-07	-6.60043	-.96117	-7.56161
O2(AQ)	3.45832E-23	1.10662E-21	3.48581E-23	-22.45770	.00000	-22.45770
H2(AQ)	1.96712E-06	3.96531E-06	1.98275E-06	-5.70273	.00000	-5.70273
FE+++	6.05029E-17	3.37891E-15	6.09838E-17	-16.21479	-2.16264	-18.37742
OH-	1.21565E-03	2.06750E-02	1.22531E-03	-2.91175	-.24029	-3.15205
H8SI3O10(AQ)	2.19250E-06	5.53198E-04	2.20993E-06	-5.65562	.00000	-5.65562
H6SI2O7(AQ)	1.53911E-02	2.68135E+00	1.55135E-02	-1.80929	.00000	-1.80929
AL(OH)3(AQ)	3.90459E-05	3.04571E-03	3.93562E-05	-4.40499	.00000	-4.40499
AL(OH)4-	1.56848E-04	1.49023E-02	1.58095E-04	-3.80108	-.24029	-4.04138
AL(OH)SI(OH)-	2.14072E-03	3.70580E-01	2.15773E-03	-2.66600	-.24029	-2.90630
CACL+	6.46618E-03	4.88410E-01	6.51757E-03	-2.18591	-.24029	-2.42621
CACL2(AQ)	1.22424E-04	1.35874E-02	1.23397E-04	-3.90869	.00000	-3.90869
CA(OH)+	1.96296E-04	1.12060E-02	1.97856E-04			

```
-3.70365     -.24029    -3.94394
   CA(H3SIO4)+          1.21983E-02   1.64904E+00   1.22952E-02
-1.91026     -.24029    -2.15056
   FE(OH)+              1.54395E-07   1.12483E-05   1.55622E-07
-6.80793     -.24029    -7.04822
   FE(OH)2              2.29993E-08   2.06675E-06   2.31821E-08
-7.63485      .00000    -7.63485
   FE(OH)3-             4.88001E-09   5.21521E-07   4.91880E-09
-8.30814     -.24029    -8.54843
   FECL+                2.94404E-07   2.68790E-05   2.96743E-07
-6.52762     -.24029    -6.76791
   FECL2(AQ)            7.14553E-06   9.05717E-04   7.20232E-06
-5.14253      .00000    -5.14253
   FE(H3SIO4)+          1.42602E-02   2.15264E+00   1.43736E-02
-1.84244     -.24029    -2.08273
   MGCL+                3.15839E-05   1.88739E-03   3.18349E-05
-4.49710     -.24029    -4.73739
   MG(OH)+              1.44224E-05   5.95823E-04   1.45370E-05
-4.83752     -.24029    -5.07782
   MG(OH)2(AQ)          2.04345E-02   1.19173E+00   2.05969E-02
-1.68620      .00000    -1.68620
   MG(H3SIO4)+          3.76235E-07   4.49269E-05   3.79225E-07
-6.42110     -.24029    -6.66140
   NACL(AQ)             3.57668E-02   2.09031E+00   3.60510E-02
-1.44308      .00000    -1.44308
   NAOH(AQ)             2.94162E-04   1.17656E-02   2.96500E-04
-3.52797      .00000    -3.52797
   H3SIO4-              6.84616E-04   6.51117E-02   6.90057E-04
-3.16111     -.24029    -3.40141
   HCL(AQ)              2.68220E-05   9.77955E-04   2.70352E-05
-4.56807      .00000    -4.56807

          --- activity ratios of cations ---


          log (NA+   /h+**0)            4.3154185
          log (CA++  /h+**0)            6.3527745
          log (MG++  /h+**0)            4.3672836
          log (AL+++ /h+**0)           -2.6360118
          log (FE++  /h+**0)            2.2909633
          log (FE+++ /h+**0)           -3.5985706


          --- summary of solid product phases---


  product                     log moles       moles        grams
volume, cc

   MAGNETITE                  -.5082439    3.10282E-01    7.18422E+01
```

```
1.38137E+01
   ZOISITE                  -.8082347    1.55512E-01    7.06588E+01
2.11310E+01
   PARAGONITE               -.2894799    5.13476E-01    1.96250E+02
6.78610E+01
   QUARTZ-ALPHA              .1157315    1.30536E+00    7.84319E+01
2.96161E+01

   CLINOPYROXENE(SS)         .7563715    5.70652E+00    1.23721E+03
3.70767E+02
   DIOPSIDE                  .5931685    3.91894E+00    8.48656E+02
2.59434E+02
   HEDENBERGITE             -.2275518    5.92172E-01    1.46915E+02
3.92018E+01
   JADEITE                   .0775171    1.19541E+00    2.41639E+02
7.21311E+01

   CHLORITE(SS)              .1076583    1.28132E+00    1.46529E+02
5.42378E+01
   CLINOCHLORE               .0612238    1.15139E+00    1.27988E+02
4.86924E+01
   CHAMOSITE                -.8862965    1.29928E-01    1.85409E+01
5.54534E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles         grams
volume, cc

   MAGNETITE                1.9998608    9.99679E+01    2.31464E+04
4.45057E+03
   ZOISITE                  -.8082347    1.55512E-01    7.06588E+01
2.11310E+01
   TREMOLITE                1.9987372    9.97096E+01    8.10012E+04
2.71888E+04
   PARAGONITE               -.2894799    5.13476E-01    1.96250E+02
6.78610E+01
   QUARTZ-ALPHA              .1157315    1.30536E+00    7.84319E+01
2.96161E+01

   PLAGIOCLASE(SS)          1.9883129    9.73448E+01

   ALBITE                   1.7664641    5.84069E+01    1.53156E+04
5.88917E+03
   ANORTHITE                1.5903729    3.89379E+01    1.08329E+04
3.92300E+03
```

```
   CLINOPYROXENE(SS)         2.0107506    1.02506E+02

   DIOPSIDE                  1.9104044    8.13588E+01    1.76184E+04
5.38595E+03
   HEDENBERGITE              1.2999892    1.99521E+01    4.95001E+03
1.32083E+03
   JADEITE                    .0775171    1.19541E+00    2.41639E+02
7.21311E+01


   CHLORITE(SS)               .1076583    1.28132E+00

   CLINOCHLORE                .0612238    1.15139E+00    1.27988E+02
4.86924E+01
   CHAMOSITE                 -.8862965    1.29928E-01    1.85409E+01
5.54534E+00



                       mass, grams        volume, cc

           created        1.800921E+03       5.574263E+02
           destroyed      1.741566E+03       5.739044E+02
           net            5.935502E+01      -1.647818E+01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base



           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-3.4418
 HEMATITE                1.2921  ssatd         SPINEL
-7.9812
 BRUCITE                -6.7735                DIASPORE
-1.3814
 ANDALUSITE             -3.5576                KYANITE
-2.3385
 SILLIMANITE            -3.3213                GLAUCOPHANE
-6.0736
 LAWSONITE               -.7926                PUMPELLYITE
-4.1084
 ZOISITE                  .0000  satd          CLINOZOISITE
-.7104
```

```
 FORSTERITE            -3.2422                FAYALITE
-3.5301
 CHRYSOTILE            -6.3851                ENSTATITE-CL
-2.2036
 ENSTATITE-OR          -2.2817                ENSTATITE-PR
-2.6871
 DIOPSIDE               -.5400                HEDENBERGITE
-3.2558
 JADEITE               -2.2463                FERROSILITE
-3.4575
 WOLLASTONITE          -4.0312                PSEUDOWOLLASTONITE
-4.5173
 TREMOLITE              -.8417                ALBITE
-.7831
 ANORTHITE             -3.3185                KAOLINITE
-3.6352
 PYROPHYLLITE          -2.5617                TALC
-1.3321
 PARAGONITE              .0000  satd          MARGARITE
-2.8279
 PREHNITE              -2.9412                CLINOCHLORE
-.1537
 CHAMOSITE             -3.2890                PYROPE
-4.0012
 ALMANDINE             -3.0406                GROSSULAR
-1.0914
 QUARTZ-ALPHA            .0000  satd          QUARTZ-BETA
-.2369
 COESITE                -.5963                HALITE
-9.9730
 CRISTOBALITE-ALPHA    -1.2859                CRISTOBALITE-BETA
-1.9993


                          --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)             -.5559
     ALBITE                        -.55586     .8537448     1.00000
     ANORTHITE                     -.55586     .1462552     1.00000

 ORTHOPYROXENE(SS)          -1.7565
     ENSTATITE-OR                 -1.75646     .6938446     1.00000
     FERROSILITE                  -1.75646     .3061554     1.00000

 GARNET(SS)                  -.6185
     PYROPE                        -.61854     .0950020     1.00000
     ALMANDINE                     -.61854     .1853685     1.00000
     GROSSULAR                     -.61854     .7196295     1.00000
```

```
 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                     .00000     .6867474     1.00000
     HEDENBERGITE                 .00000     .1037712     1.00000
     JADEITE                      .00000     .2094815     1.00000

 CPX_SUBCALCIC(SS)         -.3378
     DIOPSIDE                    -.33781     .8687302     1.00000
     HEDENBERGITE                -.33781     .1312698     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .8985983     1.00000
     CHAMOSITE                    .00000     .1014017     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6867    1.0000     .6867    -.1632     .0000    -.1632
     HEDENBERGITE
              .1038    1.0000     .1038    -.9839     .0000    -.9839
     JADEITE
              .2095    1.0000     .2095    -.6789     .0000    -.6789

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .8986    1.0000     .8986    -.0464     .0000    -.0464
     CHAMOSITE
              .1014    1.0000     .1014    -.9940     .0000    -.9940


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                        -18.38280       4.14194E-19
   H2(G)                         -1.93083       1.17265E-02
   H2O(G)                         3.80597       6.39690E+03
```

```
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  1.8499E+00, delzi=  2.6504E-01, nord= 6
               ncycle=  0
 steps completed =   203, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.6786

 stepping to zi=  2.1480E+00, delzi=  2.9803E-01, nord= 6
               ncycle=  0
 steps completed =   204, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.5679

 stepping to zi=  2.4889E+00, delzi=  3.4097E-01, nord= 6
               ncycle=  0
 steps completed =   205, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.4684

 stepping to zi=  2.5119E+00, delzi=  2.2951E-02, nord= 6
               ncycle=  0
 steps completed =   206, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.4624
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                     reaction progress        =  2.51188643150955E+00
                     log of reaction progress =        .4000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.57918E+01    4.20816E+00    2.57314E+04
1.13039E+03
```

```
   CLINOPYROXENE(SS)       9.49280E+01    5.07200E+00    2.11557E+04
1.13035E+03
   MAGNETITE               9.94574E+01    5.42567E-01    2.30282E+04
1.25625E+02
   TREMOLITE               9.95398E+01    4.60178E-01    8.08632E+04
3.73835E+02


                current total mass =  1.50779E+05 grams
                delta total mass   =  2.76020E+03 grams
                delta total volume =    909.57725 cc


         reactant           affinity     rel. rate

   PLAGIOCLASE(SS)             .8305    1.67530E+00
   CLINOPYROXENE(SS)           .3613    0.00000E+00
   MAGNETITE                   .0000    0.00000E+00
   TREMOLITE                   .8633    1.83200E-01

          affinity of the overall irreversible reaction=     1.550
kcal
          contributions from irreversible reactions
          with no thermodynamic data are not included



      --- element totals for the aqueous phase ---

   element         mg/kg soln.         molal conc.          moles

      O          8.590336E+05        5.609017E+01        5.522301E+01
      NA         1.024078E+04        4.653491E-01        4.581547E-01
      CA         8.547599E+02        2.227905E-02        2.193462E-02
      MG         4.796274E+02        2.061525E-02        2.029654E-02
      AL         6.053011E+01        2.343608E-03        2.307376E-03
      SI         3.676514E+03        1.367522E-01        1.346380E-01
      H          1.076267E+05        1.115534E+02        1.098287E+02
      CL         1.723492E+04        5.078514E-01        5.000000E-01
      FE         7.925921E+02        1.482621E-02        1.459700E-02

      co3--                          0.000000E+00        0.000000E+00
      so4--                          0.000000E+00        0.000000E+00
      s--                            0.000000E+00        0.000000E+00

    warning-- co3--, so4--, and s-- totals require that routine comp1
    have the names of non-carbonate carbon, sulfide sulfur,
    and non-sulfate sulfur aqueous species
```

```
   single ion activities and activity coefficients are here defined
   with respect to the internal ph scale



                                    ph            eh            pe

     internal ph scale            4.9237         .9950
6.9347E+00
     modified nbs ph scale        4.6829        1.0295
7.1754E+00
     rational ph scale            4.6829        1.0295
7.1754E+00

   phcl =      5.4975



          oxygen fugacity =  3.59630E-19
          log oxygen fugacity = -18.44414



                              activity of water =    .98359
               log activity of water =   -.00719
               alkalinity =  0.000000E+00 equiv/kg solvent
                                          (not def. for t.gt.50 c)

                    ionic strength =  4.716048E-01 molal
                 sum of molalities =    1.0830097114112
               osmotic coefficient =     .84809
                    equiv. stoich. ionic strength =  5.078514E-01
molal

                         mass of solution =   1.028522 kg
                         mass of solvent  =    .984540 kg
                         mass of solutes  =    .043982 kg
                         conc of solutes  =   4.276251 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.46505E+01   9.84540E+02
   NA+                  4.21970E-01   9.70099E+00   4.28596E-01     -.
36795    -.24074     -.60869
   CA++                 2.89351E-03   1.15972E-01   2.93894E-03
-2.53181     -.96296    -3.49477
   MG++                 2.98525E-05   7.25566E-04   3.03213E-05
-4.51825     -.96296    -5.48121
```

```
   AL+++                    5.66377E-16   1.52817E-14   5.75271E-16
-15.24013    -2.16666   -17.40679
   H4SIO4(AQ)               7.45351E-02   7.16392E+00   7.57055E-02
-1.12087      .00000    -1.12087
   H+                       2.04313E-05   2.05927E-05   2.07521E-05
-4.68294     -.24074    -4.92368
   CL-                      4.57245E-01   1.62107E+01   4.64425E-01     -.
33308     -.24074     -.57382
   FE++                     2.57088E-07   1.43576E-05   2.61125E-07
-6.58315     -.96296    -7.54611
   O2(AQ)                   2.97982E-23   9.53506E-22   3.02661E-23
-22.51904      .00000   -22.51904
   H2(AQ)                   2.09469E-06   4.22247E-06   2.12758E-06
-5.67211      .00000    -5.67211
   FE+++                    6.09906E-17   3.40614E-15   6.19483E-17
-16.20797    -2.16666   -18.37463
   OH-                      1.20023E-03   2.04127E-02   1.21908E-03
-2.91397     -.24074    -3.15471
   H8SI3O10(AQ)             2.17465E-06   5.48693E-04   2.20879E-06
-5.65584      .00000    -5.65584
   H6SI2O7(AQ)              1.52677E-02   2.65986E+00   1.55075E-02
-1.80946      .00000    -1.80946
   AL(OH)3(AQ)              3.87556E-05   3.02307E-03   3.93642E-05
-4.40490      .00000    -4.40490
   AL(OH)4-                 1.54891E-04   1.47163E-02   1.57323E-04
-3.80321     -.24074    -4.04395
   AL(OH)SI(OH)-            2.11373E-03   3.65908E-01   2.14692E-03
-2.66818     -.24074    -2.90892
   CACL+                    6.53850E-03   4.93872E-01   6.64117E-03
-2.17776     -.24074    -2.41850
   CACL2(AQ)                1.24434E-04   1.38104E-02   1.26388E-04
-3.89830      .00000    -3.89830
   CA(OH)+                  1.96062E-04   1.11926E-02   1.99140E-04
-3.70084     -.24074    -3.94158
   CA(H3SIO4)+              1.21821E-02   1.64686E+00   1.23734E-02
-1.90751     -.24074    -2.14825
   FE(OH)+                  1.57972E-07   1.15090E-05   1.60453E-07
-6.79465     -.24074    -7.03539
   FE(OH)2                  2.33644E-08   2.09956E-06   2.37313E-08
-7.62468      .00000    -7.62468
   FE(OH)3-                 4.93227E-09   5.27106E-07   5.00972E-09
-8.30019     -.24074    -8.54093
   FECL+                    3.04959E-07   2.78428E-05   3.09748E-07
-6.50899     -.24074    -6.74973
   FECL2(AQ)                7.44001E-06   9.43044E-04   7.55684E-06
-5.12166      .00000    -5.12166
   FE(H3SIO4)+              1.45888E-02   2.20224E+00   1.48179E-02
-1.82921     -.24074    -2.06995
   MGCL+                    3.18672E-05   1.90432E-03   3.23676E-05
-4.48989     -.24074    -4.73063
```

```
   MG(OH)+               1.43736E-05   5.93808E-04   1.45993E-05
-4.83567     -.24074    -5.07641
   MG(OH)2(AQ)           2.02201E-02   1.17923E+00   2.05376E-02
-1.68745      .00000    -1.68745
   MG(H3SIO4)+           3.74914E-07   4.47692E-05   3.80802E-07
-6.41930     -.24074    -6.66004
   NACL(AQ)              3.58932E-02   2.09770E+00   3.64568E-02
-1.43822      .00000    -1.43822
   NAOH(AQ)              2.91589E-04   1.16627E-02   2.96167E-04
-3.52846      .00000    -3.52846
   H3SIO4-               6.75847E-04   6.42777E-02   6.86460E-04
-3.16338     -.24074    -3.40413
   HCL(AQ)               2.69437E-05   9.82390E-04   2.73668E-05
-4.56278      .00000    -4.56278

           --- activity ratios of cations ---


           log (NA+   /h+**0)             4.3149862
           log (CA++  /h+**0)             6.3525862
           log (MG++  /h+**0)             4.3661431
           log (AL+++ /h+**0)            -2.6357564
           log (FE++  /h+**0)             2.3012434
           log (FE+++ /h+**0)            -3.6035994


           --- summary of solid product phases---


  product                     log moles        moles        grams
volume, cc

   MAGNETITE                 -.2919938    5.10512E-01    1.18203E+02
2.27280E+01
   ZOISITE                   -.4624270    3.44805E-01    1.56666E+02
4.68520E+01
   PARAGONITE                -.0984865    7.97101E-01    3.04652E+02
1.05345E+02
   QUARTZ-ALPHA               .4251469    2.66163E+00    1.59922E+02
6.03870E+01

   CLINOPYROXENE(SS)          .9449376    8.80922E+00    1.91058E+03
5.72364E+02
   DIOPSIDE                   .7802945    6.02968E+00    1.30574E+03
3.99165E+02
   HEDENBERGITE              -.0290052    9.35395E-01    2.32066E+02
6.19231E+01
   JADEITE                    .2657950    1.84414E+00    3.72773E+02
1.11276E+02
```

```
   CHLORITE(SS)                .1898132    1.54815E+00    1.77161E+02
6.55340E+01
   CLINOCHLORE                 .1422069    1.38742E+00    1.54224E+02
5.86739E+01
   CHAMOSITE                  -.7938928    1.60734E-01    2.29369E+01
6.86012E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                  1.9998608    9.99679E+01    2.31464E+04
4.45057E+03
   ZOISITE                    -.4624270    3.44805E-01    1.56666E+02
4.68520E+01
   TREMOLITE                  1.9979969    9.95398E+01    8.08632E+04
2.71425E+04
   PARAGONITE                 -.0984865    7.97101E-01    3.04652E+02
1.05345E+02
   QUARTZ-ALPHA                .4251469    2.66163E+00    1.59922E+02
6.03870E+01

   PLAGIOCLASE(SS)            1.9813285    9.57918E+01

   ALBITE                     1.7594798    5.74751E+01    1.50713E+04
5.79521E+03
   ANORTHITE                  1.5833885    3.83167E+01    1.06601E+04
3.86041E+03


   CLINOPYROXENE(SS)          2.0159346    1.03737E+02

   DIOPSIDE                   1.9136660    8.19721E+01    1.77513E+04
5.42655E+03
   HEDENBERGITE               1.2993110    1.99210E+01    4.94229E+03
1.31877E+03
   JADEITE                     .2657950    1.84414E+00    3.72773E+02
1.11276E+02


   CHLORITE(SS)                .1898132    1.54815E+00

   CLINOCHLORE                 .1422069    1.38742E+00    1.54224E+02
5.86739E+01
   CHAMOSITE                  -.7938928    1.60734E-01    2.29369E+01
6.86012E+00
```

	mass, grams	volume, cc
created	2.827186E+03	8.732097E+02
destroyed	2.760197E+03	9.095773E+02
net	6.698905E+01	-3.636753E+01

warning-- these volume totals may be incomplete because of missing partial molar volume data in the data base

--- mineral saturation state summary ---

mineral	affinity, kcal	state	mineral	affinity, kcal	state
MAGNETITE	.0000	satd	CORUNDUM	-3.4406	
HEMATITE	1.2582	ssatd	SPINEL	-7.9840	
BRUCITE	-6.7776		DIASPORE	-1.3809	
ANDALUSITE	-3.5564		KYANITE	-2.3374	
SILLIMANITE	-3.3202		GLAUCOPHANE	-6.0876	
LAWSONITE	-.7927		PUMPELLYITE	-4.1133	
ZOISITE	.0000	satd	CLINOZOISITE	-.7104	
FORSTERITE	-3.2461		FAYALITE	-3.4963	
CHRYSOTILE	-6.3973		ENSTATITE-CL	-2.2076	
ENSTATITE-OR	-2.2857		ENSTATITE-PR	-2.6910	
DIOPSIDE	-.5448		HEDENBERGITE	-3.2228	
JADEITE	-2.2473		FERROSILITE	-3.4236	
WOLLASTONITE	-4.0320		PSEUDOWOLLASTONITE	-4.5181	
TREMOLITE	-.8633		ALBITE	-.7840	
ANORTHITE	-3.3182		KAOLINITE	-3.6344	
PYROPHYLLITE	-2.5607		TALC		

```
-1.3442
 PARAGONITE                .0000  satd          MARGARITE
-2.8267
 PREHNITE                -2.9419                CLINOCHLORE
-.1575
 CHAMOSITE               -3.2551                PYROPE
-4.0048
 ALMANDINE               -3.0064                GROSSULAR
-1.0918
 QUARTZ-ALPHA              .0000  satd          QUARTZ-BETA
-.2369
 COESITE                  -.5963                HALITE
-9.9569
 CRISTOBALITE-ALPHA      -1.2859                CRISTOBALITE-BETA
-1.9993


                     --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)            -.5566
     ALBITE                      -.55662     .8536332     1.00000
     ANORTHITE                   -.55662     .1463668     1.00000

 ORTHOPYROXENE(SS)         -1.7487
     ENSTATITE-OR               -1.74874     .6882302     1.00000
     FERROSILITE                -1.74874     .3117698     1.00000

 GARNET(SS)                 -.6128
     PYROPE                      -.61278     .0943861     1.00000
     ALMANDINE                   -.61278     .1890790     1.00000
     GROSSULAR                   -.61278     .7165349     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                     .00000     .6844739     1.00000
     HEDENBERGITE                 .00000     .1061836     1.00000
     JADEITE                      .00000     .2093425     1.00000

 CPX_SUBCALCIC(SS)          -.3376
     DIOPSIDE                    -.33756     .8657022     1.00000
     HEDENBERGITE                -.33756     .1342978     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                  .00000     .8961769     1.00000
     CHAMOSITE                    .00000     .1038231     1.00000
```

```
 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6845    1.0000     .6845    -.1646     .0000    -.1646
     HEDENBERGITE
              .1062    1.0000     .1062    -.9739     .0000    -.9739
     JADEITE
              .2093    1.0000     .2093    -.6791     .0000    -.6791

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .8962    1.0000     .8962    -.0476     .0000    -.0476
     CHAMOSITE
              .1038    1.0000     .1038    -.9837     .0000    -.9837


           --- summary of gas species ---

           gas                 log fugacity         fugacity
partial pressure

   O2(G)                          -18.44414       3.59630E-19
   H2(G)                           -1.90021       1.25830E-02
   H2O(G)                           3.80591       6.39608E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



 stepping to zi=  2.7414E+00, delzi=  2.2951E-01, nord= 4
               ncycle=  0
 steps completed =   207, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.4071

 stepping to zi=  3.2684E+00, delzi=  5.2701E-01, nord= 6
               ncycle=  0
 steps completed =   208, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.3016

 stepping to zi=  3.8742E+00, delzi=  6.0578E-01, nord= 6
```

```
              ncycle=  0
 steps completed =   209, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.2055

 stepping to zi=  3.9811E+00, delzi=  1.0689E-01, nord= 6
              ncycle=  0
 steps completed =   210, iter =  4, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.1905
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    reaction progress        =  3.98107170553492E+00
                    log of reaction progress =        .6000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


 step size is limited by the print requirement


                              --- reactant summary ---



        reactant            moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        9.33305E+01    6.66949E+00    2.50702E+04
1.79154E+03
   CLINOPYROXENE(SS)      9.19614E+01    8.03858E+00    2.04946E+04
1.79148E+03
   MAGNETITE              9.91401E+01    8.59911E-01    2.29548E+04
1.99103E+02
   TREMOLITE              9.92707E+01    7.29332E-01    8.06446E+04
5.92488E+02


               current total mass =  1.49164E+05 grams
               delta total mass   =  4.37462E+03 grams
               delta total volume =   1441.58279 cc


        reactant           affinity     rel. rate

   PLAGIOCLASE(SS)             .8308    1.67530E+00
   CLINOPYROXENE(SS)           .3594    0.00000E+00
```

MAGNETITE .0000 0.00000E+00
TREMOLITE .8786 1.83200E-01

affinity of the overall irreversible reaction= 1.553 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.587148E+05	5.609190E+01	5.455134E+01
NA	1.034937E+04	4.704723E-01	4.575508E-01
CA	8.702574E+02	2.269211E-02	2.206887E-02
MG	4.784695E+02	2.057375E-02	2.000869E-02
AL	6.002492E+01	2.324983E-03	2.261127E-03
SI	3.687572E+03	1.372187E-01	1.334500E-01
H	1.075846E+05	1.115546E+02	1.084907E+02
CL	1.744066E+04	5.141203E-01	5.000000E-01
FE	8.142714E+02	1.523787E-02	1.481936E-02
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	4.9196	.9940	6.9280E+00
modified nbs ph scale	4.6781	1.0287	7.1695E+00
rational ph scale	4.6781	1.0287	7.1695E+00

phcl = 5.4891

oxygen fugacity = 3.25646E-19
log oxygen fugacity = -18.48725

activity of water = .98339
log activity of water = -.00728
alkalinity = 0.000000E+00 equiv/kg solvent
(not def. for t.gt.50 c)

ionic strength = 4.770188E-01 molal
sum of molalities = 1.0942145748174
osmotic coefficient = .84991
equiv. stoich. ionic strength = 5.141203E-01 molal

mass of solution = 1.016389 kg
mass of solvent = .972535 kg
mass of solutes = .043854 kg
conc of solutes = 4.314718 per cent (w/w)

species	moles	grams	conc	log conc	log g	log act
H2O	5.39841E+01	9.72535E+02				
NA+	4.21144E-01	9.68201E+00	4.33038E-01	-.36347	-.24145	-.60493
CA++	2.93086E-03	1.17469E-01	3.01363E-03	-2.52091	-.96581	-3.48672
MG++	3.01945E-05	7.33877E-04	3.10472E-05	-4.50798	-.96581	-5.47379
AL+++	5.84411E-16	1.57683E-14	6.00915E-16	-15.22119	-2.17308	-17.39427
H4SIO4(AQ)	7.35958E-02	7.07364E+00	7.56742E-02	-1.12105	.00000	-1.12105
H+	2.04061E-05	2.05673E-05	2.09824E-05	-4.67815	-.24145	-4.91960
CL-	4.56895E-01	1.61983E+01	4.69798E-01	-.32809	-.24145	-.56954
FE++	2.64874E-07	1.47924E-05	2.72354E-07	-6.56487	-.96581	-7.53068
O2(AQ)	2.66533E-23	8.52874E-22	2.74060E-23	-22.56215	.00000	-22.56215
H2(AQ)	2.17398E-06	4.38231E-06	2.23538E-06	-5.65065	.00000	-5.65065
FE+++	6.23926E-17	3.48444E-15	6.41546E-17	-16.19277	-2.17308	-18.36585
OH-	1.17620E-03	2.00040E-02	1.20942E-03			

```
-2.91742     -.24145    -3.15888
   H8SI3O10(AQ)         2.14635E-06   5.41554E-04   2.20697E-06
-5.65620      .00000    -5.65620
   H6SI2O7(AQ)          1.50722E-02   2.62579E+00   1.54979E-02
-1.80973      .00000    -1.80973
   AL(OH)3(AQ)          3.82844E-05   2.98631E-03   3.93655E-05
-4.40488      .00000    -4.40488
   AL(OH)4-             1.51795E-04   1.44221E-02   1.56081E-04
-3.80665     -.24145    -4.04810
   AL(OH)SI(OH)-        2.07105E-03   3.58520E-01   2.12954E-03
-2.67172     -.24145    -2.91317
   CACL+                6.65566E-03   5.02722E-01   6.84362E-03
-2.16471     -.24145    -2.40617
   CACL2(AQ)            1.27709E-04   1.41739E-02   1.31315E-04
-3.88169      .00000    -3.88169
   CA(OH)+              1.95729E-04   1.11736E-02   2.01256E-04
-3.69625     -.24145    -3.93770
   CA(H3SIO4)+          1.21589E-02   1.64372E+00   1.25023E-02
-1.90301     -.24145    -2.14446
   FE(OH)+              1.60410E-07   1.16865E-05   1.64940E-07
-6.78268     -.24145    -7.02413
   FE(OH)2              2.34596E-08   2.10812E-06   2.41221E-08
-7.61758      .00000    -7.61758
   FE(OH)3-             4.91312E-09   5.25060E-07   5.05187E-09
-8.29655     -.24145    -8.53800
   FECL+                3.15749E-07   2.88279E-05   3.24666E-07
-6.48856     -.24145    -6.73002
   FECL2(AQ)            7.76681E-06   9.84467E-04   7.98615E-06
-5.09766      .00000    -5.09766
   FE(H3SIO4)+          1.48108E-02   2.23575E+00   1.52291E-02
-1.81733     -.24145    -2.05878
   MGCL+                3.23916E-05   1.93566E-03   3.33064E-05
-4.47747     -.24145    -4.71893
   MG(OH)+              1.43286E-05   5.91948E-04   1.47333E-05
-4.83170     -.24145    -5.07315
   MG(OH)2(AQ)          1.99314E-02   1.16239E+00   2.04943E-02
-1.68837      .00000    -1.68837
   MG(H3SIO4)+          3.73663E-07   4.46197E-05   3.84215E-07
-6.41543     -.24145    -6.65688
   NACL(AQ)             3.61186E-02   2.11087E+00   3.71386E-02
-1.43017      .00000    -1.43017
   NAOH(AQ)             2.87765E-04   1.15098E-02   2.95891E-04
-3.52887      .00000    -3.52887
   H3SIO4-              6.62177E-04   6.29776E-02   6.80878E-04
-3.16693     -.24145    -3.40838
   HCL(AQ)              2.71325E-05   9.89275E-04   2.78987E-05
-4.55442      .00000    -4.55442

           --- activity ratios of cations ---
```

```
           log (NA+   /h+**0)            4.3146714
           log (CA++  /h+**0)            6.3524738
           log (MG++  /h+**0)            4.3654064
           log (AL+++ /h+**0)           -2.6354715
           log (FE++  /h+**0)            2.3085184
           log (FE+++ /h+**0)           -3.6070570


           --- summary of solid product phases---


  product                      log moles        moles        grams
volume, cc

   MAGNETITE                   -.0820450    8.27856E-01    1.91681E+02
3.68562E+01
   ZOISITE                     -.1905064    6.44902E-01    2.93018E+02
8.76293E+01
   PARAGONITE                   .0957067    1.24654E+00    4.76427E+02
1.64743E+02
   QUARTZ-ALPHA                 .6823210    4.81195E+00    2.89123E+02
1.09173E+02

   CLINOPYROXENE(SS)           1.1375526    1.37263E+01    2.97778E+03
8.91849E+02
   DIOPSIDE                     .9718805    9.37304E+00    2.02975E+03
6.20495E+02
   HEDENBERGITE                 .1705925    1.48113E+00    3.67459E+02
9.80507E+01
   JADEITE                      .4582002    2.87210E+00    5.80563E+02
1.73303E+02

   CHLORITE(SS)                 .2947920    1.97148E+00    2.25712E+02
8.34550E+01
   CLINOCHLORE                  .2463471    1.76338E+00    1.96017E+02
7.45735E+01
   CHAMOSITE                   -.6817409    2.08094E-01    2.96953E+01
8.88144E+00


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member         log moles        moles        grams
volume, cc

   MAGNETITE                   1.9998608    9.99679E+01    2.31464E+04
4.45057E+03
   ZOISITE                     -.1905064    6.44902E-01    2.93018E+02
```

```
8.76293E+01
   TREMOLITE                1.9968209    9.92707E+01    8.06446E+04
2.70691E+04
   PARAGONITE                .0957067    1.24654E+00    4.76427E+02
1.64743E+02
   QUARTZ-ALPHA              .6823210    4.81195E+00    2.89123E+02
1.09173E+02

   PLAGIOCLASE(SS)          1.9700236    9.33305E+01

   ALBITE                   1.7481749    5.59983E+01    1.46840E+04
5.64631E+03
   ANORTHITE                1.5720836    3.73322E+01    1.03862E+04
3.76122E+03


   CLINOPYROXENE(SS)        2.0240244    1.05688E+02

   DIOPSIDE                 1.9187754    8.29422E+01    1.79613E+04
5.49077E+03
   HEDENBERGITE             1.2982724    1.98734E+01    4.93048E+03
1.31562E+03
   JADEITE                   .4582002    2.87210E+00    5.80563E+02
1.73303E+02


   CHLORITE(SS)              .2947920    1.97148E+00

   CLINOCHLORE               .2463471    1.76338E+00    1.96017E+02
7.45735E+01
   CHAMOSITE                -.6817409    2.08094E-01    2.96953E+01
8.88144E+00


                          mass, grams        volume, cc

           created        4.453738E+03       1.373705E+03
           destroyed      4.374617E+03       1.441583E+03
           net            7.912170E+01      -6.787730E+01

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base


           --- mineral saturation state summary ---


   mineral        affinity, kcal    state        mineral
```

```
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-3.4396
 HEMATITE                1.2345  ssatd         SPINEL
-7.9858
 BRUCITE                -6.7807                DIASPORE
-1.3806
 ANDALUSITE             -3.5554                KYANITE
-2.3364
 SILLIMANITE            -3.3192                GLAUCOPHANE
-6.0975
 LAWSONITE               -.7929                PUMPELLYITE
-4.1173
 ZOISITE                  .0000  satd          CLINOZOISITE
-.7104
 FORSTERITE             -3.2489                FAYALITE
-3.4725
 CHRYSOTILE             -6.4061                ENSTATITE-CL
-2.2103
 ENSTATITE-OR           -2.2884                ENSTATITE-PR
-2.6938
 DIOPSIDE                -.5482                HEDENBERGITE
-3.1997
 JADEITE                -2.2480                FERROSILITE
-3.3999
 WOLLASTONITE           -4.0327                PSEUDOWOLLASTONITE
-4.5188
 TREMOLITE               -.8786                ALBITE
-.7847
 ANORTHITE              -3.3179                KAOLINITE
-3.6340
 PYROPHYLLITE           -2.5600                TALC
-1.3527
 PARAGONITE               .0000  satd          MARGARITE
-2.8256
 PREHNITE               -2.9425                CLINOCHLORE
-.1603
 CHAMOSITE              -3.2314                PYROPE
-4.0072
 ALMANDINE              -2.9822                GROSSULAR
-1.0921
 QUARTZ-ALPHA             .0000  satd          QUARTZ-BETA
-.2369
 COESITE                 -.5963                HALITE
-9.9303
 CRISTOBALITE-ALPHA     -1.2859                CRISTOBALITE-BETA
-1.9993
```

```
                    --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)            -.5572
     ALBITE                       -.55717     .8535448     1.00000
     ANORTHITE                    -.55717     .1464552     1.00000

 ORTHOPYROXENE(SS)         -1.7432
     ENSTATITE-OR                -1.74316     .6842582     1.00000
     FERROSILITE                 -1.74316     .3157418     1.00000

 GARNET(SS)                 -.6087
     PYROPE                       -.60865     .0939580     1.00000
     ALMANDINE                    -.60865     .1917295     1.00000
     GROSSULAR                    -.60865     .7143125     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .6828540     1.00000
     HEDENBERGITE                  .00000     .1079046     1.00000
     JADEITE                       .00000     .2092414     1.00000

 CPX_SUBCALCIC(SS)          -.3374
     DIOPSIDE                     -.33737     .8635429     1.00000
     HEDENBERGITE                 -.33737     .1364571     1.00000

 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .8944478     1.00000
     CHAMOSITE                     .00000     .1055522     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .6829    1.0000     .6829    -.1657     .0000    -.1657
     HEDENBERGITE
             .1079    1.0000     .1079    -.9670     .0000    -.9670
     JADEITE
             .2092    1.0000     .2092    -.6794     .0000    -.6794

   CHLORITE(SS)
 ideal solution
```

```
    CLINOCHLORE
              .8944    1.0000     .8944    -.0484     .0000    -.0484
    CHAMOSITE
              .1056    1.0000     .1056    -.9765     .0000    -.9765


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                       -18.48725       3.25646E-19
   H2(G)                        -1.87875       1.32206E-02
   H2O(G)                        3.80582       6.39475E+03



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 stepping to zi=  4.7744E+00, delzi=  7.9330E-01, nord= 6
               ncycle=  0
 steps completed =   211, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.0932

 stepping to zi=  5.6763E+00, delzi=  9.0193E-01, nord= 6
               ncycle=  0
 steps completed =   212, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =      -.0038

 stepping to zi=  6.3096E+00, delzi=  6.3327E-01, nord= 6
               ncycle=  0
 steps completed =   213, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE           ) =       .0494
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                     reaction progress        =  6.30957344480185E+00
                     log of reaction progress =       .8000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement
```

--- reactant summary ---

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	8.94296E+01	1.05704E+01	2.40223E+04	2.83940E+03
CLINOPYROXENE(SS)	8.72597E+01	1.27403E+01	1.94468E+04	2.83931E+03
MAGNETITE	9.86371E+01	1.36287E+00	2.28383E+04	3.15557E+02
TREMOLITE	9.88441E+01	1.15591E+00	8.02980E+04	9.39030E+02

current total mass = 1.46605E+05 grams
delta total mass = 6.93330E+03 grams
delta total volume = 2284.75475 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	.8310	1.67530E+00
CLINOPYROXENE(SS)	.3581	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	.8889	1.83200E-01

affinity of the overall irreversible reaction= 1.555 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.582031E+05	5.609388E+01	5.348607E+01
NA	1.053183E+04	4.790691E-01	4.567972E-01
CA	8.960237E+02	2.337873E-02	2.229185E-02
MG	4.775116E+02	2.054553E-02	1.959037E-02
AL	5.921733E+01	2.295150E-03	2.188449E-03
SI	3.699576E+03	1.377523E-01	1.313482E-01
H	1.075180E+05	1.115560E+02	1.063697E+02
CL	1.777742E+04	5.243784E-01	5.000000E-01

```
     FE          8.373437E+02        1.567953E-02        1.495059E-02

     co3--                           0.000000E+00        0.000000E+00
     so4--                           0.000000E+00        0.000000E+00
     s--                             0.000000E+00        0.000000E+00

   warning-- co3--, so4--, and s-- totals require that routine comp1
   have the names of non-carbonate carbon, sulfide sulfur,
   and non-sulfate sulfur aqueous species


  single ion activities and activity coefficients are here defined
  with respect to the internal ph scale



                                               ph            eh            pe

     internal ph scale               4.9131         .9939
6.9272E+00
     modified nbs ph scale           4.6705        1.0287
7.1698E+00
     rational ph scale               4.6705        1.0287
7.1698E+00

  phcl =      5.4758



         oxygen fugacity =  3.04309E-19
         log oxygen fugacity = -18.51669



                           activity of water =    .98305
              log activity of water =   -.00742
              alkalinity =  0.000000E+00 equiv/kg solvent
                                        (not def. for t.gt.50 c)

                   ionic strength =  4.858484E-01 molal
                sum of molalities =    1.1125499125547
              osmotic coefficient =     .85284
                   equiv. stoich. ionic strength =  5.243784E-01
molal

                        mass of solution =    .997136 kg
                        mass of solvent  =    .953510 kg
                        mass of solutes  =    .043626 kg
                        conc of solutes  =   4.375121 per cent (w/w)
```

```
   species                moles        grams          conc        log
conc      log g      log act

   H2O                 5.29281E+01   9.53510E+02
   NA+                 4.20015E-01   9.65605E+00   4.40494E-01     -.
35606     -.24260     -.59866
   CA++                2.99191E-03   1.19916E-01   3.13778E-03
-2.50338     -.97040    -3.47378
   MG++                3.08000E-05   7.48593E-04   3.23017E-05
-4.49078     -.97040    -5.46117
   AL+++               6.14194E-16   1.65719E-14   6.44140E-16
-15.19102    -2.18340   -17.37442
   H4SIO4(AQ)          7.21071E-02   6.93056E+00   7.56228E-02
-1.12135      .00000    -1.12135
   H+                  2.03620E-05   2.05228E-05   2.13547E-05
-4.67051     -.24260    -4.91311
   CL-                 4.56308E-01   1.61775E+01   4.78556E-01     -.
32007     -.24260     -.56267
   FE++                2.73580E-07   1.52786E-05   2.86919E-07
-6.54224     -.97040    -7.51264
   O2(AQ)              2.44197E-23   7.81400E-22   2.56103E-23
-22.59159      .00000   -22.59159
   H2(AQ)              2.20417E-06   4.44316E-06   2.31163E-06
-5.63608      .00000    -5.63608
   FE+++               6.51806E-17   3.64014E-15   6.83586E-17
-16.16521    -2.18340   -18.34860
   OH-                 1.13869E-03   1.93661E-02   1.19421E-03
-2.92292     -.24260    -3.16552
   H8SI3O10(AQ)        2.10151E-06   5.30239E-04   2.20397E-06
-5.65679      .00000    -5.65679
   H6SI2O7(AQ)         1.47623E-02   2.57181E+00   1.54821E-02
-1.81017      .00000    -1.81017
   AL(OH)3(AQ)         3.75292E-05   2.92741E-03   3.93590E-05
-4.40496      .00000    -4.40496
   AL(OH)4-            1.46930E-04   1.39599E-02   1.54093E-04
-3.81222     -.24260    -4.05482
   AL(OH)SI(OH)-       2.00399E-03   3.46911E-01   2.10170E-03
-2.67743     -.24260    -2.92003
   CACL+               6.84828E-03   5.17271E-01   7.18218E-03
-2.14374     -.24260    -2.38634
   CACL2(AQ)           1.33150E-04   1.47777E-02   1.39642E-04
-3.85499      .00000    -3.85499
   CA(OH)+             1.95222E-04   1.11447E-02   2.04740E-04
-3.68880     -.24260    -3.93140
   CA(H3SIO4)+         1.21233E-02   1.63891E+00   1.27144E-02
-1.89570     -.24260    -2.13830
   FE(OH)+             1.61881E-07   1.17937E-05   1.69774E-07
-6.77013     -.24260    -7.01273
   FE(OH)2             2.32541E-08   2.08965E-06   2.43879E-08
```

```
-7.61283      .00000    -7.61283
   FE(OH)3-             4.80884E-09   5.13915E-07   5.04330E-09
-8.29729     -.24260    -8.53988
   FECL+                3.28719E-07   3.00120E-05   3.44746E-07
-6.46250     -.24260    -6.70510
   FECL2(AQ)            8.19322E-06   1.03851E-03   8.59269E-06
-5.06587      .00000    -5.06587
   FE(H3SIO4)+          1.49416E-02   2.25549E+00   1.56701E-02
-1.80493     -.24260    -2.04753
   MGCL+                3.33037E-05   1.99016E-03   3.49275E-05
-4.45683     -.24260    -4.69943
   MG(OH)+              1.42806E-05   5.89965E-04   1.49769E-05
-4.82458     -.24260    -5.06718
   MG(OH)2(AQ)          1.95116E-02   1.13791E+00   2.04629E-02
-1.68903      .00000    -1.68903
   MG(H3SIO4)+          3.72285E-07   4.44552E-05   3.90436E-07
-6.40845     -.24260    -6.65105
   NACL(AQ)             3.65001E-02   2.13317E+00   3.82797E-02
-1.41703      .00000    -1.41703
   NAOH(AQ)             2.81893E-04   1.12749E-02   2.95637E-04
-3.52924      .00000    -3.52924
   H3SIO4-              6.40843E-04   6.09485E-02   6.72089E-04
-3.17257     -.24260    -3.41517
   HCL(AQ)              2.74334E-05   1.00025E-03   2.87709E-05
-4.54105      .00000    -4.54105

           --- activity ratios of cations ---


           log (NA+   /h+**0)            4.3144453
           log (CA++  /h+**0)            6.3524344
           log (MG++  /h+**0)            4.3650364
           log (AL+++ /h+**0)           -2.6351014
           log (FE++  /h+**0)            2.3135710
           log (FE+++ /h+**0)           -3.6092885


           --- summary of solid product phases---


  product                    log moles        moles         grams
volume, cc

   MAGNETITE                   .1241170    1.33081E+00    3.08135E+02
5.92478E+01
   ZOISITE                     .0494327    1.12055E+00    5.09136E+02
1.52261E+02
   PARAGONITE                  .2920038    1.95886E+00    7.48676E+02
2.58883E+02
   QUARTZ-ALPHA                .9148983    8.22050E+00    4.93923E+02
```

```
1.86507E+02

   CLINOPYROXENE(SS)         1.3328219    2.15190E+01    4.66915E+03
1.39818E+03
   DIOPSIDE                  1.1664457    1.46705E+01    3.17694E+03
9.71189E+02
   HEDENBERGITE               .3705803    2.34736E+00    5.82368E+02
1.55395E+02
   JADEITE                    .6533187    4.50110E+00    9.09847E+02
2.71596E+02

   CHLORITE(SS)               .4220415    2.64266E+00    3.02654E+02
1.11868E+02
   CLINOCHLORE                .3730210    2.36059E+00    2.62402E+02
9.98294E+01
   CHAMOSITE                 -.5496445    2.82069E-01    4.02517E+01
1.20387E+01


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member       log moles        moles        grams
volume, cc

   MAGNETITE                 1.9998608    9.99679E+01    2.31464E+04
4.45057E+03
   ZOISITE                    .0494327    1.12055E+00    5.09136E+02
1.52261E+02
   TREMOLITE                 1.9949507    9.88441E+01    8.02980E+04
2.69528E+04
   PARAGONITE                 .2920038    1.95886E+00    7.48676E+02
2.58883E+02
   QUARTZ-ALPHA               .9148983    8.22050E+00    4.93923E+02
1.86507E+02

   PLAGIOCLASE(SS)           1.9514812    8.94296E+01

   ALBITE                    1.7296324    5.36577E+01    1.40703E+04
5.41031E+03
   ANORTHITE                 1.5535411    3.57718E+01    9.95205E+03
3.60401E+03


   CLINOPYROXENE(SS)         2.0365439    1.08779E+02

   DIOPSIDE                  1.9267451    8.44783E+01    1.82940E+04
5.59246E+03
   HEDENBERGITE              1.2966499    1.97993E+01    4.91210E+03
1.31071E+03
```

```
   JADEITE                      .6533187    4.50110E+00    9.09847E+02
2.71596E+02


   CHLORITE(SS)                 .4220415    2.64266E+00

   CLINOCHLORE                  .3730210    2.36059E+00    2.62402E+02
9.98294E+01
   CHAMOSITE                   -.5496445    2.82069E-01    4.02517E+01
1.20387E+01



                           mass, grams        volume, cc

              created         7.031676E+03       2.166947E+03
              destroyed       6.933300E+03       2.284755E+03
              net             9.837530E+01      -1.178073E+02

             warning-- these volume totals may be incomplete because
             of missing partial molar volume data in the data base



              --- mineral saturation state summary ---


   mineral         affinity, kcal    state        mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-3.4386
 HEMATITE                1.2182  ssatd         SPINEL
-7.9865
 BRUCITE                -6.7829                DIASPORE
-1.3804
 ANDALUSITE             -3.5545                KYANITE
-2.3354
 SILLIMANITE            -3.3182                GLAUCOPHANE
-6.1041
 LAWSONITE               -.7935                PUMPELLYITE
-4.1207
 ZOISITE                  .0000  satd          CLINOZOISITE
-.7104
 FORSTERITE             -3.2506                FAYALITE
-3.4563
 CHRYSOTILE             -6.4122                ENSTATITE-CL
-2.2120
 ENSTATITE-OR           -2.2901                ENSTATITE-PR
-2.6955
```

```
 DIOPSIDE                  -.5505                HEDENBERGITE
-3.1841
 JADEITE                  -2.2485                FERROSILITE
-3.3836
 WOLLASTONITE             -4.0333                PSEUDOWOLLASTONITE
-4.5194
 TREMOLITE                 -.8889                ALBITE
-.7852
 ANORTHITE                -3.3175                KAOLINITE
-3.6340
 PYROPHYLLITE             -2.5595                TALC
-1.3583
 PARAGONITE                 .0000  satd          MARGARITE
-2.8248
 PREHNITE                 -2.9433                CLINOCHLORE
-.1622
 CHAMOSITE                -3.2153                PYROPE
-4.0086
 ALMANDINE                -2.9657                GROSSULAR
-1.0924
 QUARTZ-ALPHA               .0000  satd          QUARTZ-BETA
-.2369
 COESITE                   -.5963                HALITE
-9.8868
 CRISTOBALITE-ALPHA       -1.2859                CRISTOBALITE-BETA
-1.9993


                    --- summary of solid solutions  ---

 mineral                 aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)             -.5575
     ALBITE                        -.55754     .8534693     1.00000
     ANORTHITE                     -.55754     .1465307     1.00000

 ORTHOPYROXENE(SS)          -1.7392
     ENSTATITE-OR                 -1.73918     .6815545     1.00000
     FERROSILITE                  -1.73918     .3184455     1.00000

 GARNET(SS)                  -.6058
     PYROPE                        -.60580     .0936811     1.00000
     ALMANDINE                     -.60580     .1935687     1.00000
     GROSSULAR                     -.60580     .7127502     1.00000

 CLINOPYROXENE(SS)            .0000
saturated
     DIOPSIDE                       .00000     .6817479     1.00000
     HEDENBERGITE                   .00000     .1090833     1.00000
     JADEITE                        .00000     .2091688     1.00000
```

```
 CPX_SUBCALCIC(SS)         -.3372
     DIOPSIDE                    -.33724     .8620650     1.00000
     HEDENBERGITE                -.33724     .1379350     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                  .00000     .8932632     1.00000
     CHAMOSITE                    .00000     .1067368     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
              .6817    1.0000     .6817    -.1664     .0000    -.1664
     HEDENBERGITE
              .1091    1.0000     .1091    -.9622     .0000    -.9622
     JADEITE
              .2092    1.0000     .2092    -.6795     .0000    -.6795

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
              .8933    1.0000     .8933    -.0490     .0000    -.0490
     CHAMOSITE
              .1067    1.0000     .1067    -.9717     .0000    -.9717


           --- summary of gas species ---

           gas                log fugacity         fugacity
partial pressure

   O2(G)                         -18.51669       3.04309E-19
   H2(G)                          -1.86418       1.36716E-02
   H2O(G)                          3.80568       6.39258E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
 stepping to zi=  7.5098E+00, delzi=  1.2002E+00, nord= 6
               ncycle=  0
 steps completed =   214, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE          ) =      .1354

 stepping to zi=  8.9262E+00, delzi=  1.4165E+00, nord= 6
               ncycle=  0
 steps completed =   215, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE          ) =      .2188

 stepping to zi=  1.0000E+01, delzi=  1.0738E+00, nord= 6
               ncycle=  0
 steps completed =   216, iter =  5, ncorr = 0
 most rapidly changing is zvclg1(ZOISITE          ) =      .2728
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                     reaction progress        =  9.99999999999987E+00
                     log of reaction progress =       1.0000000

                     temperature    =    450.000 degrees c
                     total pressure =    500.000 bars

                     computing units remaining =       .000


 step size is limited by the print requirement


                               --- reactant summary ---



         reactant             moles       delta moles      grams
delta grams

   PLAGIOCLASE(SS)        8.32470E+01    1.67530E+01    2.23616E+04
4.50015E+03
   CLINOPYROXENE(SS)      7.98080E+01    2.01920E+01    1.77861E+04
4.50001E+03
   MAGNETITE              9.78400E+01    2.16000E+00    2.26537E+04
5.00123E+02
   TREMOLITE              9.81680E+01    1.83200E+00    7.97488E+04
1.48826E+03


                 current total mass =  1.42550E+05 grams
                 delta total mass   =  1.09885E+04 grams
                 delta total volume =   3621.09225 cc
```

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	.8310	1.67530E+00
CLINOPYROXENE(SS)	.3573	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	.8954	1.83200E-01

affinity of the overall irreversible reaction= 1.556 kcal

contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.573573E+05	5.609658E+01	5.179725E+01
NA	1.083875E+04	4.935405E-01	4.557148E-01
CA	9.399550E+02	2.455035E-02	2.266877E-02
MG	4.765930E+02	2.052723E-02	1.895399E-02
AL	5.792480E+01	2.247378E-03	2.075135E-03
SI	3.715144E+03	1.384751E-01	1.278622E-01
H	1.074087E+05	1.115578E+02	1.030079E+02
CL	1.833895E+04	5.415016E-01	5.000000E-01
FE	8.667637E+02	1.624722E-02	1.500201E-02
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

warning-- co3--, so4--, and s-- totals require that routine comp1
have the names of non-carbonate carbon, sulfide sulfur,
and non-sulfate sulfur aqueous species

single ion activities and activity coefficients are here defined
with respect to the internal ph scale

	ph	eh	pe
internal ph scale	4.9026	.9947	6.9329E+00
modified nbs ph scale	4.6582	1.0298	7.1773E+00

```
     rational ph scale               4.6582       1.0298
7.1773E+00

   phcl =      5.4541



          oxygen fugacity =  2.90656E-19
          log oxygen fugacity = -18.53662



                    activity of water =    .98249
               log activity of water =   -.00767
               alkalinity =  0.000000E+00 equiv/kg solvent
                                           (not def. for t.gt.50 c)

                    ionic strength =  5.005389E-01 molal
                 sum of molalities =    1.1431080751464
               osmotic coefficient =     .85758
                    equiv. stoich. ionic strength =  5.415016E-01
molal

                         mass of solution =    .966604 kg
                         mass of solvent  =    .923358 kg
                         mass of solutes  =    .043246 kg
                         conc of solutes  =   4.473973 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.12544E+01   9.23358E+02
   NA+                  4.18304E-01   9.61672E+00   4.53025E-01     -.
34388     -.24446     -.58834
   CA++                 3.09356E-03   1.23990E-01   3.35034E-03
-2.47491     -.97785    -3.45276
   MG++                 3.18427E-05   7.73937E-04   3.44857E-05
-4.46236     -.97785    -5.44021
   AL+++                6.65466E-16   1.79553E-14   7.20702E-16
-15.14224    -2.20016   -17.34240
   H4SIO4(AQ)           6.97478E-02   6.70379E+00   7.55371E-02
-1.12184      .00000    -1.12184
   H+                   2.02869E-05   2.04472E-05   2.19708E-05
-4.65815     -.24446    -4.90262
   CL-                  4.55324E-01   1.61426E+01   4.93118E-01     -.
30705     -.24446     -.55151
   FE++                 2.85184E-07   1.59267E-05   3.08855E-07
-6.51024     -.97785    -7.48809
   O2(AQ)               2.25865E-23   7.22741E-22   2.44613E-23
```

```
-22.61152       .00000   -22.61152
   H2(AQ)                2.18279E-06   4.40006E-06   2.36396E-06
-5.62636       .00000    -5.62636
   FE+++                 7.03231E-17   3.92734E-15   7.61602E-17
-16.11827    -2.20016    -18.31843
   OH-                   1.08038E-03   1.83744E-02   1.17006E-03
-2.93179     -.24446     -3.17625
   H8SI3O10(AQ)          2.03044E-06   5.12309E-04   2.19898E-06
-5.65778      .00000     -5.65778
   H6SI2O7(AQ)           1.42712E-02   2.48625E+00   1.54558E-02
-1.81091      .00000     -1.81091
   AL(OH)3(AQ)           3.63266E-05   2.83360E-03   3.93418E-05
-4.40515      .00000     -4.40515
   AL(OH)4-              1.39345E-04   1.32393E-02   1.50911E-04
-3.82128     -.24446     -4.06574
   AL(OH)SI(OH)-         1.89946E-03   3.28817E-01   2.05712E-03
-2.68674     -.24446     -2.93120
   CACL+                 7.17234E-03   5.41748E-01   7.76767E-03
-2.10971     -.24446     -2.35417
   CACL2(AQ)             1.42467E-04   1.58118E-02   1.54292E-04
-3.81166      .00000     -3.81166
   CA(OH)+               1.94409E-04   1.10983E-02   2.10546E-04
-3.67665     -.24446     -3.92112
   CA(H3SIO4)+           1.20660E-02   1.63116E+00   1.30675E-02
-1.88381     -.24446     -2.12827
   FE(OH)+               1.62523E-07   1.18405E-05   1.76013E-07
-6.75446     -.24446     -6.99892
   FE(OH)2               2.26788E-08   2.03795E-06   2.45612E-08
-7.60975      .00000     -7.60975
   FE(OH)3-              4.59503E-09   4.91066E-07   4.97643E-09
-8.30308     -.24446     -8.54754
   FECL+                 3.47084E-07   3.16887E-05   3.75893E-07
-6.42494     -.24446     -6.66940
   FECL2(AQ)             8.83808E-06   1.12025E-03   9.57166E-06
-5.01901      .00000     -5.01901
   FE(H3SIO4)+           1.49923E-02   2.26315E+00   1.62368E-02
-1.78950     -.24446     -2.03396
   MGCL+                 3.48756E-05   2.08409E-03   3.77703E-05
-4.42285     -.24446     -4.66731
   MG(OH)+               1.42195E-05   5.87441E-04   1.53998E-05
-4.81249     -.24446     -5.05695
   MG(OH)2(AQ)           1.88727E-02   1.10065E+00   2.04392E-02
-1.68954      .00000     -1.68954
   MG(H3SIO4)+           3.70482E-07   4.42399E-05   4.01233E-07
-6.39660     -.24446     -6.64107
   NACL(AQ)              3.71377E-02   2.17043E+00   4.02202E-02
-1.39556      .00000     -1.39556
   NAOH(AQ)              2.72718E-04   1.09079E-02   2.95355E-04
-3.52966      .00000     -3.52966
   H3SIO4-               6.07683E-04   5.77948E-02   6.58123E-04
```

```
-3.18169     -.24446    -3.42615
   HCL(AQ)              2.79234E-05   1.01811E-03   3.02412E-05
-4.51940      .00000    -4.51940

           --- activity ratios of cations ---


           log (NA+   /h+**0)            4.3142764
           log (CA++  /h+**0)            6.3524731
           log (MG++  /h+**0)            4.3650244
           log (AL+++ /h+**0)           -2.6345524
           log (FE++  /h+**0)            2.3171400
           log (FE+++ /h+**0)           -3.6105803


           --- summary of solid product phases---


  product                        log moles        moles        grams
volume, cc

   MAGNETITE                      .3279604    2.12794E+00    4.92701E+02
9.47361E+01
   ZOISITE                        .2728464    1.87433E+00    8.51624E+02
2.54684E+02
   PARAGONITE                     .4896758    3.08799E+00    1.18023E+03
4.08109E+02
   QUARTZ-ALPHA                  1.1342684    1.36229E+01    8.18520E+02
3.09076E+02

   CLINOPYROXENE(SS)             1.5298084    3.38695E+01    7.34980E+03
2.20065E+03
   DIOPSIDE                      1.3629662    2.30657E+01    4.99493E+03
1.52695E+03
   HEDENBERGITE                   .5706818    3.72119E+00    9.23206E+02
2.46343E+02
   JADEITE                        .8501926    7.08260E+00    1.43167E+03
4.27364E+02

   CHLORITE(SS)                   .5689533    3.70641E+00    4.24573E+02
1.56899E+02
   CLINOCHLORE                    .5195492    3.30788E+00    3.67701E+02
1.39890E+02
   CHAMOSITE                     -.3995353    3.98533E-01    5.68713E+01
1.70094E+01


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---
```

phase/end-member	log moles	moles	grams	volume, cc
MAGNETITE	1.9998608	9.99679E+01	2.31464E+04	4.45057E+03
ZOISITE	.2728464	1.87433E+00	8.51624E+02	2.54684E+02
TREMOLITE	1.9919699	9.81680E+01	7.97488E+04	2.67685E+04
PARAGONITE	.4896758	3.08799E+00	1.18023E+03	4.08109E+02
QUARTZ-ALPHA	1.1342684	1.36229E+01	8.18520E+02	3.09076E+02
PLAGIOCLASE(SS)	1.9203686	8.32470E+01		
ALBITE	1.6985198	4.99482E+01	1.30976E+04	5.03628E+03
ANORTHITE	1.5224286	3.32988E+01	9.26404E+03	3.35485E+03
CLINOPYROXENE(SS)	2.0556744	1.13677E+02		
DIOPSIDE	1.9390801	8.69121E+01	1.88210E+04	5.75358E+03
HEDENBERGITE	1.2940866	1.96828E+01	4.88319E+03	1.30300E+03
JADEITE	.8501926	7.08260E+00	1.43167E+03	4.27364E+02
CHLORITE(SS)	.5689533	3.70641E+00		
CLINOCHLORE	.5195492	3.30788E+00	3.67701E+02	1.39890E+02
CHAMOSITE	-.3995353	3.98533E-01	5.68713E+01	1.70094E+01

	mass, grams	volume, cc
created	1.111745E+04	3.424159E+03
destroyed	1.098854E+04	3.621092E+03
net	1.289072E+02	-1.969336E+02

warning-- these volume totals may be incomplete because
of missing partial molar volume data in the data base

--- mineral saturation state summary ---

mineral	affinity, kcal	state	mineral	affinity, kcal	state
MAGNETITE	.0000	satd	CORUNDUM	-3.4375	
HEMATITE	1.2072	ssatd	SPINEL	-7.9862	
BRUCITE	-6.7845		DIASPORE	-1.3802	
ANDALUSITE	-3.5533		KYANITE	-2.3342	
SILLIMANITE	-3.3170		GLAUCOPHANE	-6.1082	
LAWSONITE	-.7947		PUMPELLYITE	-4.1242	
ZOISITE	.0000	satd	CLINOZOISITE	-.7104	
FORSTERITE	-3.2514		FAYALITE	-3.4453	
CHRYSOTILE	-6.4164		ENSTATITE-CL	-2.2129	
ENSTATITE-OR	-2.2910		ENSTATITE-PR	-2.6963	
DIOPSIDE	-.5521		HEDENBERGITE	-3.1738	
JADEITE	-2.2489		FERROSILITE	-3.3726	
WOLLASTONITE	-4.0340		PSEUDOWOLLASTONITE	-4.5201	
TREMOLITE	-.8954		ALBITE	-.7856	
ANORTHITE	-3.3170		KAOLINITE	-3.6345	
PYROPHYLLITE	-2.5591		TALC	-1.3617	
PARAGONITE	.0000	satd	MARGARITE	-2.8239	
PREHNITE	-2.9443		CLINOCHLORE	-.1635	
CHAMOSITE	-3.2047		PYROPE	-4.0091	
ALMANDINE	-2.9543		GROSSULAR	-1.0927	
QUARTZ-ALPHA	.0000	satd	QUARTZ-BETA	-.2369	

```
 COESITE                  -.5963                HALITE
-9.8157
 CRISTOBALITE-ALPHA     -1.2859                CRISTOBALITE-BETA
-1.9993


                    --- summary of solid solutions  ---

 mineral               aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)           -.5578
     ALBITE                     -.55778     .8533933     1.00000
     ANORTHITE                  -.55778     .1466067     1.00000

 ORTHOPYROXENE(SS)        -1.7362
     ENSTATITE-OR              -1.73625     .6797622     1.00000
     FERROSILITE               -1.73625     .3202378     1.00000

 GARNET(SS)                -.6038
     PYROPE                     -.60384     .0935233     1.00000
     ALMANDINE                  -.60384     .1948442     1.00000
     GROSSULAR                  -.60384     .7116326     1.00000

 CLINOPYROXENE(SS)          .0000
saturated
     DIOPSIDE                    .00000     .6810169     1.00000
     HEDENBERGITE                .00000     .1098686     1.00000
     JADEITE                     .00000     .2091146     1.00000

 CPX_SUBCALCIC(SS)         -.3371
     DIOPSIDE                   -.33714     .8610816     1.00000
     HEDENBERGITE               -.33714     .1389184     1.00000

 CHLORITE(SS)               .0000
saturated
     CLINOCHLORE                 .00000     .8924745     1.00000
     CHAMOSITE                   .00000     .1075255     1.00000


 solid solution product phases

            xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .6810    1.0000     .6810    -.1668     .0000    -.1668
     HEDENBERGITE
```

```
            .1099    1.0000     .1099    -.9591     .0000    -.9591
     JADEITE
            .2091    1.0000     .2091    -.6796     .0000    -.6796

   CHLORITE(SS)
  ideal solution

     CLINOCHLORE
            .8925    1.0000     .8925    -.0494     .0000    -.0494
     CHAMOSITE
            .1075    1.0000     .1075    -.9685     .0000    -.9685


          --- summary of gas species ---

          gas                log fugacity         fugacity
 partial pressure

   O2(G)                       -18.53662       2.90656E-19
   H2(G)                        -1.85446       1.39811E-02
   H2O(G)                        3.80543       6.38896E+03



  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



  stepping to zi=  1.0000E+01, delzi=  1.2612E-13, nord= 6
  steps completed =   217, iter =  1, ncorr = 0
  most rapidly changing is zvclg1(MG++              ) =     -4.4970
  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


                    reaction progress        =  1.00000000000000E+01
                    log of reaction progress =       1.0000000

                    temperature    =    450.000 degrees c
                    total pressure =    500.000 bars

                    computing units remaining =       .000


  maximum value of reaction progress


                              --- reactant summary ---
```

reactant	moles	delta moles	grams	delta grams
PLAGIOCLASE(SS)	8.32470E+01	1.67530E+01	2.23616E+04	4.50015E+03
CLINOPYROXENE(SS)	7.98080E+01	2.01920E+01	1.77861E+04	4.50001E+03
MAGNETITE	9.78400E+01	2.16000E+00	2.26537E+04	5.00123E+02
TREMOLITE	9.81680E+01	1.83200E+00	7.97488E+04	1.48826E+03

current total mass = 1.42550E+05 grams
delta total mass = 1.09885E+04 grams
delta total volume = 3621.09225 cc

reactant	affinity	rel. rate
PLAGIOCLASE(SS)	.8310	1.67530E+00
CLINOPYROXENE(SS)	.3573	0.00000E+00
MAGNETITE	.0000	0.00000E+00
TREMOLITE	.8954	1.83200E-01

affinity of the overall irreversible reaction= 1.556 kcal
contributions from irreversible reactions
with no thermodynamic data are not included

--- element totals for the aqueous phase ---

element	mg/kg soln.	molal conc.	moles
O	8.573573E+05	5.609658E+01	5.179725E+01
NA	1.083875E+04	4.935405E-01	4.557148E-01
CA	9.399550E+02	2.455035E-02	2.266877E-02
MG	4.765930E+02	2.052723E-02	1.895399E-02
AL	5.792480E+01	2.247378E-03	2.075135E-03
SI	3.715144E+03	1.384751E-01	1.278622E-01
H	1.074087E+05	1.115578E+02	1.030079E+02
CL	1.833895E+04	5.415016E-01	5.000000E-01
FE	8.667637E+02	1.624722E-02	1.500201E-02
co3--		0.000000E+00	0.000000E+00
so4--		0.000000E+00	0.000000E+00
s--		0.000000E+00	0.000000E+00

```
 warning-- co3--, so4--, and s-- totals require that routine comp1
 have the names of non-carbonate carbon, sulfide sulfur,
 and non-sulfate sulfur aqueous species


single ion activities and activity coefficients are here defined
with respect to the internal ph scale



                                    ph            eh            pe

     internal ph scale            4.9026         .9947
6.9329E+00
     modified nbs ph scale        4.6582        1.0298
7.1773E+00
     rational ph scale            4.6582        1.0298
7.1773E+00

   phcl =      5.4541



          oxygen fugacity =  2.90656E-19
          log oxygen fugacity = -18.53662



                           activity of water =    .98249
               log activity of water =   -.00767
               alkalinity =  0.000000E+00 equiv/kg solvent
                                         (not def. for t.gt.50 c)

                    ionic strength =  5.005389E-01 molal
                 sum of molalities =    1.1431080751478
               osmotic coefficient =     .85758
                    equiv. stoich. ionic strength =  5.415016E-01
molal

                         mass of solution =    .966604 kg
                         mass of solvent  =    .923358 kg
                         mass of solutes  =    .043246 kg
                         conc of solutes  =   4.473973 per cent (w/w)


   species                moles        grams          conc        log
conc      log g      log act

   H2O                  5.12544E+01   9.23358E+02
```

```
   NA+                       4.18304E-01   9.61672E+00   4.53025E-01      -.
34388     -.24446     -.58834
   CA++                      3.09356E-03   1.23990E-01   3.35034E-03
-2.47491     -.97785    -3.45276
   MG++                      3.18427E-05   7.73937E-04   3.44857E-05
-4.46236     -.97785    -5.44021
   AL+++                     6.65466E-16   1.79553E-14   7.20702E-16
-15.14224    -2.20016   -17.34240
   H4SIO4(AQ)                6.97478E-02   6.70379E+00   7.55371E-02
-1.12184      .00000    -1.12184
   H+                        2.02869E-05   2.04472E-05   2.19708E-05
-4.65815     -.24446    -4.90262
   CL-                       4.55324E-01   1.61426E+01   4.93118E-01      -.
30705     -.24446     -.55151
   FE++                      2.85184E-07   1.59267E-05   3.08855E-07
-6.51024     -.97785    -7.48809
   O2(AQ)                    2.25865E-23   7.22741E-22   2.44613E-23
-22.61152      .00000   -22.61152
   H2(AQ)                    2.18279E-06   4.40006E-06   2.36396E-06
-5.62636      .00000    -5.62636
   FE+++                     7.03231E-17   3.92734E-15   7.61602E-17
-16.11827    -2.20016   -18.31843
   OH-                       1.08038E-03   1.83744E-02   1.17006E-03
-2.93179     -.24446    -3.17625
   H8SI3O10(AQ)              2.03044E-06   5.12309E-04   2.19898E-06
-5.65778      .00000    -5.65778
   H6SI2O7(AQ)               1.42712E-02   2.48625E+00   1.54558E-02
-1.81091      .00000    -1.81091
   AL(OH)3(AQ)               3.63266E-05   2.83360E-03   3.93418E-05
-4.40515      .00000    -4.40515
   AL(OH)4-                  1.39345E-04   1.32393E-02   1.50911E-04
-3.82128     -.24446    -4.06574
   AL(OH)SI(OH)-             1.89946E-03   3.28817E-01   2.05712E-03
-2.68674     -.24446    -2.93120
   CACL+                     7.17234E-03   5.41748E-01   7.76767E-03
-2.10971     -.24446    -2.35417
   CACL2(AQ)                 1.42467E-04   1.58118E-02   1.54292E-04
-3.81166      .00000    -3.81166
   CA(OH)+                   1.94409E-04   1.10983E-02   2.10546E-04
-3.67665     -.24446    -3.92112
   CA(H3SIO4)+               1.20660E-02   1.63116E+00   1.30675E-02
-1.88381     -.24446    -2.12827
   FE(OH)+                   1.62523E-07   1.18405E-05   1.76013E-07
-6.75446     -.24446    -6.99892
   FE(OH)2                   2.26788E-08   2.03795E-06   2.45612E-08
-7.60975      .00000    -7.60975
   FE(OH)3-                  4.59503E-09   4.91066E-07   4.97643E-09
-8.30308     -.24446    -8.54754
   FECL+                     3.47084E-07   3.16887E-05   3.75893E-07
-6.42494     -.24446    -6.66940
```

```
   FECL2(AQ)             8.83808E-06   1.12025E-03   9.57166E-06
-5.01901      .00000    -5.01901
   FE(H3SIO4)+           1.49923E-02   2.26315E+00   1.62368E-02
-1.78950     -.24446    -2.03396
   MGCL+                 3.48756E-05   2.08409E-03   3.77703E-05
-4.42285     -.24446    -4.66731
   MG(OH)+               1.42195E-05   5.87441E-04   1.53998E-05
-4.81249     -.24446    -5.05695
   MG(OH)2(AQ)           1.88727E-02   1.10065E+00   2.04392E-02
-1.68954      .00000    -1.68954
   MG(H3SIO4)+           3.70482E-07   4.42399E-05   4.01233E-07
-6.39660     -.24446    -6.64107
   NACL(AQ)              3.71377E-02   2.17043E+00   4.02202E-02
-1.39556      .00000    -1.39556
   NAOH(AQ)              2.72718E-04   1.09079E-02   2.95355E-04
-3.52966      .00000    -3.52966
   H3SIO4-               6.07683E-04   5.77948E-02   6.58123E-04
-3.18169     -.24446    -3.42615
   HCL(AQ)               2.79234E-05   1.01811E-03   3.02412E-05
-4.51940      .00000    -4.51940

           --- activity ratios of cations ---


           log (NA+   /h+**0)            4.3142764
           log (CA++  /h+**0)            6.3524731
           log (MG++  /h+**0)            4.3650244
           log (AL+++ /h+**0)           -2.6345524
           log (FE++  /h+**0)            2.3171400
           log (FE+++ /h+**0)           -3.6105803


           --- summary of solid product phases---


  product                    log moles       moles        grams
volume, cc

   MAGNETITE                  .3279604    2.12794E+00    4.92701E+02
9.47361E+01
   ZOISITE                    .2728464    1.87433E+00    8.51624E+02
2.54684E+02
   PARAGONITE                 .4896758    3.08799E+00    1.18023E+03
4.08109E+02
   QUARTZ-ALPHA              1.1342684    1.36229E+01    8.18520E+02
3.09076E+02

   CLINOPYROXENE(SS)         1.5298084    3.38695E+01    7.34980E+03
2.20065E+03
   DIOPSIDE                  1.3629662    2.30657E+01    4.99493E+03
```

```
1.52695E+03
   HEDENBERGITE                 .5706818    3.72119E+00    9.23206E+02
2.46343E+02
   JADEITE                      .8501926    7.08260E+00    1.43167E+03
4.27364E+02

   CHLORITE(SS)                 .5689533    3.70641E+00    4.24573E+02
1.56899E+02
   CLINOCHLORE                  .5195492    3.30788E+00    3.67701E+02
1.39890E+02
   CHAMOSITE                   -.3995353    3.98533E-01    5.68713E+01
1.70094E+01


                --- grand summary of solid phases (e.s.+p.r.s.
+reactants) ---

      phase/end-member        log moles        moles        grams
volume, cc

   MAGNETITE                   1.9998608    9.99679E+01    2.31464E+04
4.45057E+03
   ZOISITE                      .2728464    1.87433E+00    8.51624E+02
2.54684E+02
   TREMOLITE                   1.9919699    9.81680E+01    7.97488E+04
2.67685E+04
   PARAGONITE                   .4896758    3.08799E+00    1.18023E+03
4.08109E+02
   QUARTZ-ALPHA                1.1342684    1.36229E+01    8.18520E+02
3.09076E+02

   PLAGIOCLASE(SS)             1.9203686    8.32470E+01

   ALBITE                      1.6985198    4.99482E+01    1.30976E+04
5.03628E+03
   ANORTHITE                   1.5224286    3.32988E+01    9.26404E+03
3.35485E+03


   CLINOPYROXENE(SS)           2.0556744    1.13677E+02

   DIOPSIDE                    1.9390801    8.69121E+01    1.88210E+04
5.75358E+03
   HEDENBERGITE                1.2940866    1.96828E+01    4.88319E+03
1.30300E+03
   JADEITE                      .8501926    7.08260E+00    1.43167E+03
4.27364E+02


   CHLORITE(SS)                 .5689533    3.70641E+00
```

```
   CLINOCHLORE                .5195492    3.30788E+00    3.67701E+02
1.39890E+02
   CHAMOSITE                 -.3995353    3.98533E-01    5.68713E+01
1.70094E+01


                           mass, grams        volume, cc

           created         1.111745E+04       3.424159E+03
           destroyed       1.098854E+04       3.621092E+03
           net             1.289072E+02      -1.969336E+02

          warning-- these volume totals may be incomplete because
          of missing partial molar volume data in the data base


           --- mineral saturation state summary ---


   mineral        affinity, kcal    state         mineral
affinity, kcal    state

 MAGNETITE                .0000  satd          CORUNDUM
-3.4375
 HEMATITE                1.2072  ssatd         SPINEL
-7.9862
 BRUCITE                -6.7845                DIASPORE
-1.3802
 ANDALUSITE             -3.5533                KYANITE
-2.3342
 SILLIMANITE            -3.3170                GLAUCOPHANE
-6.1082
 LAWSONITE               -.7947                PUMPELLYITE
-4.1242
 ZOISITE                  .0000  satd          CLINOZOISITE
-.7104
 FORSTERITE             -3.2514                FAYALITE
-3.4453
 CHRYSOTILE             -6.4164                ENSTATITE-CL
-2.2129
 ENSTATITE-OR           -2.2910                ENSTATITE-PR
-2.6963
 DIOPSIDE                -.5521                HEDENBERGITE
-3.1738
 JADEITE                -2.2489                FERROSILITE
-3.3726
 WOLLASTONITE           -4.0340                PSEUDOWOLLASTONITE
```

```
-4.5201
 TREMOLITE              -.8954               ALBITE
-.7856
 ANORTHITE             -3.3170               KAOLINITE
-3.6345
 PYROPHYLLITE          -2.5591               TALC
-1.3617
 PARAGONITE              .0000  satd         MARGARITE
-2.8239
 PREHNITE              -2.9443               CLINOCHLORE
-.1635
 CHAMOSITE             -3.2047               PYROPE
-4.0091
 ALMANDINE             -2.9543               GROSSULAR
-1.0927
 QUARTZ-ALPHA            .0000  satd         QUARTZ-BETA
-.2369
 COESITE                -.5963               HALITE
-9.8157
 CRISTOBALITE-ALPHA    -1.2859               CRISTOBALITE-BETA
-1.9993


                    --- summary of solid solutions  ---

 mineral                aff. kcal/mol  mole frac.    lambda      state

 PLAGIOCLASE(SS)            -.5578
     ALBITE                       -.55778     .8533933     1.00000
     ANORTHITE                    -.55778     .1466067     1.00000

 ORTHOPYROXENE(SS)         -1.7362
     ENSTATITE-OR                -1.73625     .6797622     1.00000
     FERROSILITE                 -1.73625     .3202378     1.00000

 GARNET(SS)                 -.6038
     PYROPE                       -.60384     .0935233     1.00000
     ALMANDINE                    -.60384     .1948442     1.00000
     GROSSULAR                    -.60384     .7116326     1.00000

 CLINOPYROXENE(SS)           .0000
saturated
     DIOPSIDE                      .00000     .6810169     1.00000
     HEDENBERGITE                  .00000     .1098686     1.00000
     JADEITE                       .00000     .2091146     1.00000

 CPX_SUBCALCIC(SS)          -.3371
     DIOPSIDE                     -.33714     .8610816     1.00000
     HEDENBERGITE                 -.33714     .1389184     1.00000
```

```
 CHLORITE(SS)                .0000
saturated
     CLINOCHLORE                   .00000     .8924745     1.00000
     CHAMOSITE                     .00000     .1075255     1.00000


 solid solution product phases

           xbar     lambda   activity  log xbar  log lambda log
activity

   CLINOPYROXENE(SS)
 ideal solution

     DIOPSIDE
             .6810    1.0000     .6810    -.1668     .0000    -.1668
     HEDENBERGITE
             .1099    1.0000     .1099    -.9591     .0000    -.9591
     JADEITE
             .2091    1.0000     .2091    -.6796     .0000    -.6796

   CHLORITE(SS)
 ideal solution

     CLINOCHLORE
             .8925    1.0000     .8925    -.0494     .0000    -.0494
     CHAMOSITE
             .1075    1.0000     .1075    -.9685     .0000    -.9685


          --- summary of gas species ---

          gas                log fugacity         fugacity
partial pressure

   O2(G)                       -18.53662       2.90656E-19
   H2(G)                        -1.85446       1.39811E-02
   H2O(G)                        3.80543       6.38896E+03



 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -



                    --- maximum value of reaction progress ---

 ---  the reaction path has terminated normally ---
```

```
     217 steps were taken
   zi increased from
           0.00000E+00 to  1.00000E+01
   the average value of delzi was  4.60829E-02
   the average matrix dimension was   17


      start time =
        end time =

       user time =       .000
        cpu time =       .000

--- no further input found ---
```