```
C         0.032
Mn       2.02
Ni       7.23
Cr       0.47
Si       0.25
S      0.008
P       0.011
Mo       0.63
O (ppm)     380
N (ppm)    250
```

373 K, 473 K, 573 K, 673 K, 773 K, 873 K, 973 K

```
lqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqq
qk
  x  aa     aa    aaaaaaaaa    aaaaaaa        aaa      aaaaaaaaa      aaa
x
  x  aaa   aaa    aaaaaaaaa    aa     aa     aa    aa    aaaaaaaaa    aa   aa
x
  x  aa a a aa       aaa       aa     aaa    aa    aa       aaa       aa   aa
x
  x  aa  a  aa       aaa       aa     aaa   aaaaaaaaa       aaa
aaaaaaaaa  x
  x  aa     aa       aaa       aa     aa    aa      aa      aaa      aa
aa  x
  x  aa     aa       aaa       aaaaaaa      aa      aa      aaa      aa
aa  x

mqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqq
qj
```

- THERMODYNAMICS AND PROCESS MODELLING GROUP -
- NPL MATERIALS CENTRE -
- NATIONAL PHYSICAL LABORATORY -

Authorised for use by Dr H K D H Bhadeshia
at University of Cambridge
under the terms and conditions of NPL 79/199-3

```
lqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqk
x VERSION 4.73   FOR LNX RH 7.3 x
```

```
                        x          2002-11-15          x
                        mqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqqj
                         ******************************
                         * USING DEFAULT MTCONFIG FILE *
                         ******************************
                        17 of 18 DATABASES ARE AVAILABLE

 WHICH MODULE ? multiphase
 MULTIPHASE OPTION ? define data 'def.mpi' !
 Date and time of run 18-SEP-2004  17:35:22
 * DATAFILE = /asterix/users/hkdb/harry/mtdata/def.mpi -  CREATED 18:38:
44 19-JUN-2004
 * SYSTEM = C,Si,Mn,Cr,Mo,Ni,V,W,B,Nb,N,Fe,
 * NUMBER OF PHASES  =   85
 * NUMBER OF SPECIES =  297
 *

 MULTIPHASE OPTION ? lis sys ph !

 NUMBER    PHASE                    STATUS      MODEL
    1      BETA_RHOMBO_B            ABSENT      PURE SUBSTANCE
    2      LIQUID                   ABSENT      REDLICH-KISTER
    3      CR2B_ORTH                ABSENT      PURE SUBSTANCE
    4      CR3B4                    ABSENT      PURE SUBSTANCE
    5      CR5B3                    ABSENT      PURE SUBSTANCE
    6      CRB2                     ABSENT      PURE SUBSTANCE
    7      CRB4                     ABSENT      PURE SUBSTANCE
    8      CRB                      ABSENT      PURE SUBSTANCE
    9      BCC_A2                   NORMAL      SUBLATTICE
   10      FEB                      ABSENT      PURE SUBSTANCE
   11      M2B_TETR                 ABSENT      SUBLATTICE
   12      FCC_A1                   ABSENT      SUBLATTICE
   13      MO2B2                    ABSENT      PURE SUBSTANCE
   14      MO2B5                    ABSENT      PURE SUBSTANCE
   15      MOB4                     ABSENT      PURE SUBSTANCE
   16      MOB                      ABSENT      PURE SUBSTANCE
   17      NI3B                     ABSENT      PURE SUBSTANCE
   18      NI4B3                    ABSENT      PURE SUBSTANCE
   19      NIB                      ABSENT      PURE SUBSTANCE
   20      V2B3                     ABSENT      PURE SUBSTANCE
   21      V3B2                     ABSENT      PURE SUBSTANCE
 >>>>> Type return for more, Q to quit paging :
   22      V3B4                     ABSENT      PURE SUBSTANCE
   23      VB2                      ABSENT      PURE SUBSTANCE
   24      VB                       ABSENT      PURE SUBSTANCE
   25      DIAMOND_A4               ABSENT      REDLICH-KISTER
```

```
  26      GRAPHITE                  ABSENT      PURE SUBSTANCE
  27      GAS                       ABSENT      IDEAL GAS
  28      CEMENTITE                 NORMAL      SUBLATTICE
  29      HCP_A3                    ABSENT      SUBLATTICE
  30      KSI_CARBIDE               ABSENT      SUBLATTICE
  31      M3C2                      ABSENT      SUBLATTICE
  32      M7C3                      ABSENT      SUBLATTICE
  33      M23C6                     ABSENT      SUBLATTICE
  34      M6C                       ABSENT      SUBLATTICE
  35      CBCC_A12                  ABSENT      SUBLATTICE
  36      CUB_A13                   ABSENT      SUBLATTICE
  37      FE4N                      ABSENT      SUBLATTICE
  38      FECN_CHI                  ABSENT      REDLICH-KISTER
  39      M5C2                      ABSENT      SUBLATTICE
  40      V3C2                      ABSENT      SUBLATTICE
  41      FE8SI2C                   ABSENT      PURE SUBSTANCE
  42      MC_ETA                    ABSENT      SUBLATTICE
  43      MC_SHP                    ABSENT      REDLICH-KISTER
  44      SIC                       ABSENT      PURE SUBSTANCE
>>>>> Type return for more, Q to quit paging : q
  45      CR3SI                     ABSENT      SUBLATTICE
  46      CRSI2                     ABSENT      SUBLATTICE
  47      CHI_A12                   ABSENT      SUBLATTICE
  48      SIGMA                     ABSENT      SUBLATTICE
  49      LAVES_PHASE               ABSENT      SUBLATTICE
  50      MU_PHASE                  ABSENT      SUBLATTICE
  51      R_PHASE                   ABSENT      SUBLATTICE
  52      MONI_DELTA                ABSENT      SUBLATTICE
  53      P_PHASE                   ABSENT      SUBLATTICE
  54      CR3MN5                    ABSENT      PURE SUBSTANCE
  55      HIGH_SIGMA                ABSENT      SUBLATTICE
  56      CR5SI3                    ABSENT      PURE SUBSTANCE
  57      CRSI                      ABSENT      PURE SUBSTANCE
  58      AL5FE4                    ABSENT      PURE SUBSTANCE
  59      FE1SI1                    ABSENT      SUBLATTICE
  60      FE5SI3                    ABSENT      SUBLATTICE
  61      M3SI                      ABSENT      SUBLATTICE
  62      FE2SI                     ABSENT      PURE SUBSTANCE
  63      FESI2_H                   ABSENT      PURE SUBSTANCE
  64      FESI2_L                   ABSENT      PURE SUBSTANCE
  65      MN4N                      ABSENT      PURE SUBSTANCE
  66      MN6N4                     ABSENT      PURE SUBSTANCE
  67      MN6N5                     ABSENT      PURE SUBSTANCE
  68      MN2NI                     ABSENT      PURE SUBSTANCE
  69      MN3NI                     ABSENT      PURE SUBSTANCE
  70      MNNI2                     ABSENT      PURE SUBSTANCE
```

```
  71      MNNI3                   ABSENT      PURE SUBSTANCE
  72      MNNI                    ABSENT      PURE SUBSTANCE
  73      MN11SI19                ABSENT      PURE SUBSTANCE
  74      MN6SI                   ABSENT      PURE SUBSTANCE
  75      MN9SI2                  ABSENT      PURE SUBSTANCE
  76      MONI3_GAMMA             ABSENT      PURE SUBSTANCE
  77      MONI4_BETA              ABSENT      PURE SUBSTANCE
  78      AL3NI2                  ABSENT      PURE SUBSTANCE
  79      ALNI_B2                 ABSENT      SUBLATTICE
  80      CO3W                    ABSENT      PURE SUBSTANCE
  81      NI4W                    ABSENT      PURE SUBSTANCE
  82      NIW2                    ABSENT      PURE SUBSTANCE
  83      NIW                     ABSENT      PURE SUBSTANCE
  84      SI2W                    ABSENT      PURE SUBSTANCE
  85      SI3W5                   ABSENT      PURE SUBSTANCE

MULTIPHASE OPTION ? li sy com !

NUMBER    COMPONENT               STATUS      AMOUNT     DELTA    REF.P
   1      C                       NORMAL      2.66422
   2      Si                      NORMAL     undefined
   3      Mn                      NORMAL     undefined
   4      Cr                      NORMAL     undefined
   5      Mo                      NORMAL     undefined
   6      Ni                      NORMAL     undefined
   7      V                       ABSENT     undefined
   8      W                       ABSENT     undefined
   9      B                       ABSENT     undefined
  10      Nb                      ABSENT     undefined
  11      N                       NORMAL     undefined
  12      Fe                      NORMAL     undefined

MULTIPHASE OPTION ? set w(1)=0.032 w(2)=0.25 w(3)=2.02 !
MULTIPHASE OPTION ? set w(4)=0.47 w(5)=0.63 w(6)=7.23 !
MULTIPHASE OPTION ? set w(11)=0.025 !
MULTIPHASE OPTION ? li sy co !

NUMBER    COMPONENT               STATUS      AMOUNT     DELTA    REF.P
   1      C                       NORMAL      2.66422
   2      Si                      NORMAL      8.90139
   3      Mn                      NORMAL      36.7687
   4      Cr                      NORMAL      9.03916
   5      Mo                      NORMAL      6.56660
   6      Ni                      NORMAL      123.190
   7      V                       ABSENT     undefined
   8      W                       ABSENT     undefined
```

```
    9      B                        ABSENT     undefined
   10      Nb                       ABSENT     undefined
   11      N                        NORMAL      1.78486
   12      Fe                       # TO BAL    1599.78

 MULTIPHASE OPTION ? step tem 373 973 100 !
 MULTIPHASE OPTION ? compute pr br print mol !
 NUMBER OF STEPS =   7

     373.000
*** MULTIPHASE - Stage 1* Results ***

Temperature =   373.0000 K

Fixed pressure =  1.013250E+05 Pa,    1.000000E+00 atm

Component      Ref.Phase     Chem.Pot.    Activity     Amount/mol   Mass/kg
C                           -4.259288E+04 1.085115E
-06 2.664224E+00 3.200000E-02
Si                          -1.369136E+05 6.717408E
-20 8.901390E+00 2.500000E-01
Mn                          -1.625565E+04 5.292098E
-03 3.676872E+01 2.020000E+00
Cr                          -1.353777E+04 1.271241E
-02 9.039157E+00 4.700000E-01
Mo
1.896912E+03 1.843467E+00 6.566604E+00 6.300000E-01
Ni                          -1.206258E+04 2.045542E
-02 1.231896E+02 7.230000E+00
N                           -8.193701E+03 7.121790E
-02 1.784860E+00 2.500000E-02
Fe                          -1.068851E+04 3.185863E
-02 1.599782E+03 8.934300E+01
Total
1.788696E+03 1.000000E+02

Amount      Phase              Mole fraction of component within phase
compnt moles
                               C              Si             Mn
 1.7780E+03 BCC_A2            0.0000000      0.0050063      0.0196047
 1.0657E+01 CEMENTITE         0.2499999      0.0000000      0.1792957

                               Cr             Mo             Ni
 1.7780E+03 BCC_A2            0.0016665      0.0036931      0.0692820
 1.0657E+01 CEMENTITE         0.5701517      0.0000113      0.0003372
```

```
                                N               Fe
 1.7780E+03 BCC_A2             0.0010038       0.8997436
 1.0657E+01 CEMENTITE          0.0000001       0.0002042

Gibbs Energy = -2.0639652384E+07 J   System Enthalpy =  4.0174722320E+06 J
     473.000
*** MULTIPHASE - Stage 1* Results ***

Temperature =   473.0000 K

Fixed pressure =  1.013250E+05 Pa,    1.000000E+00 atm

Component      Ref.Phase     Chem.Pot.    Activity     Amount/mol   Mass/kg
C                           -3.205940E+04 2.881940E
-04 2.664224E+00 3.200000E-02
Si                          -1.416946E+05 2.252627E
-16 8.901390E+00 2.500000E-01
Mn                          -2.397344E+04 2.252249E
-03 3.676872E+01 2.020000E+00
Cr                          -2.171328E+04 4.001337E
-03 9.039157E+00 4.700000E-01
Mo                          -7.428176E+03 1.512543E
-01 6.566604E+00 6.300000E-01
Ni                          -1.853689E+04 8.973740E
-03 1.231896E+02 7.230000E+00
N                           -1.938165E+04 7.239140E
-03 1.784860E+00 2.500000E-02
Fe                          -1.441766E+04 2.557763E
-02 1.599782E+03 8.934300E+01
Total
1.788696E+03 1.000000E+02

Amount      Phase              Mole fraction of component within phase
compnt moles
                                C               Si              Mn
 1.7780E+03 BCC_A2             0.0000000       0.0050063       0.0191524
 1.0657E+01 CEMENTITE          0.2500000       0.0000000       0.2547616

                                Cr              Mo              Ni
 1.7780E+03 BCC_A2             0.0021637       0.0036919       0.0692661
 1.0657E+01 CEMENTITE          0.4871941       0.0002159       0.0029903

                                N               Fe
 1.7780E+03 BCC_A2             0.0010038       0.8997158
 1.0657E+01 CEMENTITE          0.0000000       0.0048382
```

```
Gibbs Energy = -2.7856454584E+07 J   System Enthalpy =  9.0029478059E+06 J
     573.000
*** MULTIPHASE - Stage 1* Results ***

Temperature =   573.0000 K

Fixed pressure =  1.013250E+05 Pa,    1.000000E+00 atm

Component      Ref.Phase     Chem.Pot.    Activity     Amount/mol   Mass/kg
C                           -2.286244E+04 8.239757E
-03 2.664224E+00 3.200000E-02
Si                          -1.470680E+05 3.923131E
-14 8.901390E+00 2.500000E-01
Mn                          -3.251279E+04 1.086954E
-03 3.676872E+01 2.020000E+00
Cr                          -3.034766E+04 1.712297E
-03 9.039157E+00 4.700000E-01
Mo                          -1.735923E+04 2.615617E
-02 6.566604E+00 6.300000E-01
Ni                          -2.566925E+04 4.571433E
-03 1.231896E+02 7.230000E+00
N                           -3.089809E+04 1.525468E
-03 1.784860E+00 2.500000E-02
Fe                          -1.875684E+04 1.950611E
-02 1.599782E+03 8.934300E+01
Total
1.788696E+03 1.000000E+02

Amount      Phase               Mole fraction of component within phase
compnt moles
                                 C               Si              Mn
 1.7780E+03 BCC_A2              0.0000000       0.0050063       0.0189297
 1.0657E+01 CEMENTITE           0.2500000       0.0000000       0.2919262

                                 Cr              Mo              Ni
 1.7780E+03 BCC_A2              0.0026299       0.0036851       0.0692196
 1.0657E+01 CEMENTITE           0.4094073       0.0013444       0.0107442

                                 N               Fe
 1.7780E+03 BCC_A2              0.0010038       0.8995256
 1.0657E+01 CEMENTITE           0.0000000       0.0365779

Gibbs Energy = -3.6178393625E+07 J   System Enthalpy =  1.4439354635E+07 J
     673.000
*** MULTIPHASE - Stage 1* Results ***
```

Temperature =   673.0000 K

Fixed pressure = 1.013250E+05 Pa,   1.000000E+00 atm

Component   Ref.Phase   Chem.Pot.   Activity   Amount/mol   Mass/kg
C   -1.634789E+04 5.385136E
-02 2.664224E+00 3.200000E-02
Si   -1.530090E+05 1.332187E
-12 8.901390E+00 2.500000E-01
Mn   -4.183924E+04 5.659068E
-04 3.676872E+01 2.020000E+00
Cr   -3.916720E+04 9.122830E
-04 9.039157E+00 4.700000E-01
Mo   -2.785303E+04 6.890518E
-03 6.566604E+00 6.300000E-01
Ni   -3.342401E+04 2.546089E
-03 1.231896E+02 7.230000E+00
N   -4.272568E+04 4.829986E
-04 1.784860E+00 2.500000E-02
Fe   -2.364316E+04 1.462147E
-02 1.599782E+03 8.934300E+01
Total
1.788696E+03 1.000000E+02

Amount   Phase   Mole fraction of component within phase
compnt moles
                                C   Si   Mn
 1.7780E+03 BCC_A2   0.0000002   0.0050063   0.0190346
 1.0655E+01 CEMENTITE   0.2500000   0.0000000   0.2744594

                                Cr   Mo   Ni
 1.7780E+03 BCC_A2   0.0032005   0.0036655   0.0691671
 1.0655E+01 CEMENTITE   0.3142603   0.0046092   0.0194906

                                N   Fe
 1.7780E+03 BCC_A2   0.0010038   0.8989219
 1.0655E+01 CEMENTITE   0.0000000   0.1371805

Gibbs Energy = -4.5498512821E+07 J   System Enthalpy = 2.0438822913E+07 J
     773.000
*** MULTIPHASE - Stage 1* Results ***

Temperature =   773.0000 K

Fixed pressure = 1.013250E+05 Pa,   1.000000E+00 atm

```
Component      Ref.Phase     Chem.Pot.    Activity     Amount/mol   Mass/kg
C                           -1.338386E+04 1.246301E
-01 2.664224E+00 3.200000E-02
Si                          -1.595315E+05 1.659977E
-11 8.901390E+00 2.500000E-01
Mn                          -5.201654E+04 3.055817E
-04 3.676872E+01 2.020000E+00
Cr                          -4.825296E+04 5.488333E
-04 9.039157E+00 4.700000E-01
Mo                          -3.888920E+04 2.355975E
-03 6.566604E+00 6.300000E-01
Ni                          -4.179006E+04 1.500214E
-03 1.231896E+02 7.230000E+00
N                           -5.481000E+04 1.978640E
-04 1.784860E+00 2.500000E-02
Fe                          -2.903899E+04 1.090864E
-02 1.599782E+03 8.934300E+01
Total
1.788696E+03 1.000000E+02

Amount      Phase               Mole fraction of component within phase
compnt moles
                                 C               Si              Mn
 1.7781E+03 BCC_A2              0.0000073       0.0050062       0.0194317
 1.0605E+01 CEMENTITE           0.2500000       0.0000000       0.2090809

                                 Cr              Mo              Ni
 1.7781E+03 BCC_A2              0.0038253       0.0036359       0.0691541
 1.0605E+01 CEMENTITE           0.2109725       0.0095839       0.0214426

                                 N               Fe
 1.7781E+03 BCC_A2              0.0010038       0.8979358
 1.0605E+01 CEMENTITE           0.0000000       0.2989201

Gibbs Energy = -5.5761829291E+07 J   System Enthalpy =  2.7151885712E+07 J
     873.000
*** MULTIPHASE - Stage 1* Results ***

Temperature =   873.0000 K

Fixed pressure =  1.013250E+05 Pa,    1.000000E+00 atm

Component      Ref.Phase     Chem.Pot.    Activity     Amount/mol   Mass/kg
C                           -1.323267E+04 1.615336E
-01 2.664224E+00 3.200000E-02
Si                          -1.667073E+05 1.060646E
```

```
-10 8.901390E+00 2.500000E-01
Mn                          -6.330313E+04 1.630978E
-04 3.676872E+01 2.020000E+00
Cr                          -5.794350E+04 3.412914E
-04 9.039157E+00 4.700000E-01
Mo                          -5.044919E+04 9.583511E
-04 6.566604E+00 6.300000E-01
Ni                          -5.079774E+04 9.134201E
-04 1.231896E+02 7.230000E+00
N                           -6.706416E+04 9.714455E
-05 1.784860E+00 2.500000E-02
Fe                          -3.492447E+04 8.135791E
-03 1.599782E+03 8.934300E+01
Total
1.788696E+03 1.000000E+02

Amount      Phase               Mole fraction of component within phase
compnt moles
                                C               Si              Mn
 1.7785E+03 BCC_A2             0.0000713       0.0050049       0.0198935
 1.0150E+01 CEMENTITE          0.2500000       0.0000000       0.1366726

                                Cr              Mo              Ni
 1.7785E+03 BCC_A2             0.0043059       0.0036193       0.0691517
 1.0150E+01 CEMENTITE          0.1360523       0.0127596       0.0197139

                                N               Fe
 1.7785E+03 BCC_A2             0.0010035       0.8969498
 1.0150E+01 CEMENTITE          0.0000000       0.4448016

Gibbs Energy = -6.6952164397E+07 J   System Enthalpy =  3.4834655603E+07 J
     973.000
*** MULTIPHASE - Stage 1* Results ***

Temperature =   973.0000 K

Fixed pressure =  1.013250E+05 Pa,    1.000000E+00 atm

Component      Ref.Phase     Chem.Pot.    Activity     Amount/mol   Mass/kg
C                           -1.466591E+04 1.631900E
-01 2.664224E+00 3.200000E-02
Si                          -1.747268E+05 4.170444E
-10 8.901390E+00 2.500000E-01
Mn                          -7.625491E+04 8.061688E
-05 3.676872E+01 2.020000E+00
Cr                          -6.827825E+04 2.160903E
```

-04 9.039157E+00 4.700000E-01
Mo -6.260543E+04 4.356804E
-04 6.566604E+00 6.300000E-01
Ni -6.058942E+04 5.589757E
-04 1.231896E+02 7.230000E+00
N -7.946796E+04 5.419271E
-05 1.784860E+00 2.500000E-02
Fe -4.130032E+04 6.065755E
-03 1.599782E+03 8.934300E+01
Total
1.788696E+03 1.000000E+02

Amount	Phase	Mole fraction of component within phase		
compnt moles				
		C	Si	Mn
1.7807E+03	BCC_A2	0.0003684	0.0049989	0.0202885
8.0331E+00	CEMENTITE	0.2499997	0.0000000	0.0798769
		Cr	Mo	Ni
1.7807E+03	BCC_A2	0.0046599	0.0036283	0.0691021
8.0331E+00	CEMENTITE	0.0923090	0.0131631	0.0176771
		N	Fe	
1.7807E+03	BCC_A2	0.0010024	0.8959515	
8.0331E+00	CEMENTITE	0.0000003	0.5469738	

Gibbs Energy = -7.9103794368E+07 J System Enthalpy = 4.4119728057E+07 J

MULTIPHASE OPTION ?

\bye