

This is the output expected when you compile and link the TQ1-crfe program and execute it for two different temperatures

```
C:\Users\...\TQ4lib\F90\test1>linktest1
```

```
C:\Users\...\TQ4lib\F90\test1>REM command file to create test program 1 for OCASI/TQ
C:\Users\...\TQ4lib\F90\test1>REM Either execute the commands below interactively or
```

```
C:\Users\...\TQ4lib\F90\test1>REM rename this file with extension .cmd and execute it as a batch
C:\Users\...\TQ4lib\F90\test1>REM YOU MUST HAVE COMPILED AND LINKED THE MAIN OC PROGRAM
```

```
C:\Users\...\TQ4lib\F90\test1>REM The copy commands assume you are on the directory TQ4lib/F90
C:\Users\...\TQ4lib\F90\test1>REM and have the main program three directories up
C:\Users\...\TQ4lib\F90\test1>REM as when you downloaded the zip file with the program
```

```
C:\Users\...\TQ4lib\F90\test1>copy ..\..\..\liboceq.a .
      1 file(s) copied
C:\Users\...\TQ4lib\F90\test1>copy ..\..\..\liboceqplus.mod .
      1 file(s) copied
C:\Users\...\TQ4lib\F90\test1>copy ..\..\liboctq.F90 .
      1 file(s) copied
C:\Users\...\TQ4lib\F90\test1>gfortran -c liboctq.F90
C:\Users\...\TQ4lib\F90\test1>gfortran -o tqex1 TQ1-crfe.F90 lib
octq.o liboceq.a
C:\Users\...\TQ4lib\F90\test1>tqex1
tqini created: DEFAULT_EQUILIBRIUM
```

System with 2 elements: CR, FE,
and 4 phases: LIQUID, BCC_A2, FCC_A1, SIGMA,

Give conditions:

Temperature: /800/:

Pressure: /100000/:

Mole fraction of CR: /0.25/:

```
3Y Composition set(s) created: 1
3Y Gridmin: 32 points 0.00E+00 s and 0 clockcycles, T= 800.00
Phase change: its/add/remove: 5 0 2
Phase change: its/add/remove: 10 4 0
Equilibrium calculation 19 its, 0.0000E+00 s and 0 clockcycles
3Y move results from tuple 5 to 2
3Y Removing unstable phase tuple(s) 6
```

Successful calculation

Amount of 4 phases: 0.0000 0.8302 0.0000 0.1698

Stable phase: BCC_A2, amount: 8.3018E-01, mole fractions:

CR : 0.197577, FE : 0.802423,

Stable phase: SIGMA, amount: 1.6982E-01, mole fractions:

CR : 0.506278, FE : 0.493722,

Component, mole fraction and chemical potential

CR 0.250000 -2.716211E+04

FE 0.750000 -3.089767E+04

Start debug output from TQLR:

1:T=800, 2:P=100000, 3:N=1, 4:X(CR)=0.25

Degrees of freedom are 0

T= 800.00 K (526.85 C), P= 1.0000E+05 Pa, V= 6.6465E-06 m3

N= 1.0000E+00 moles, B= 5.4884E+01 g, RT= 6.6516E+03 J/mol

G= -2.9964E+04 J, G/N= -2.9964E+04 J/mol, H= 1.9289E+04 J, S= 6.1566E+01 J/K

Component name Moles Mole-fr Chem.pot/RT Activities Ref.state

CR 2.5000E-01 0.25000 -4.0835E+00 1.6848E-02 SER (default)

FE 7.5000E-01 0.75000 -4.6451E+00 9.6082E-03 SER (default)

Name Status Moles Volume Form.Units At/FU dGm/RT Comp:

BCC_A2..... E 8.302E-01 6.02E-06 8.30E-01 1.00 0.00E+00 X:

FE 8.02423E-01 CR 1.97577E-01

SIGMA..... E 1.698E-01 6.23E-07 5.66E-03 30.00 0.00E+00 X:

CR 5.06278E-01 FE 4.93722E-01

End debug output from TQLR

Any more calculations? /N/: y

Give conditions:

Temperature: /800/: 600

Pressure: /100000/:

Mole fraction of CR: /0.25/:

3Y Composition set(s) created: 1

3Y Gridmin: 32 points 0.00E+00 s and 0 clockcycles, T= 600.00

Equilibrium calculation 15 its, 0.0000E+00 s and 0 clockcycles

Successful calculation

Amount of 5 phases: 0.0000 0.2157 0.0000 0.0000 0.7843

Stable phase: BCC_A2, amount: 2.1567E-01, mole fractions:

CR : 0.970535, FE : 0.029465,

Stable phase: BCC_A2_AUTO#2, amount: 7.8433E-01, mole fractions:

CR : 0.051867, FE : 0.948133,

Component, mole fraction and chemical potential

CR 0.250000 -1.718694E+04

FE 0.750000 -1.975398E+04

Start debug output from TQLR:

1:T=600, 2:P=100000, 3:N=1, 4:X(CR)=0.25

Degrees of freedom are 0

T= 600.00 K (326.85 C), P= 1.0000E+05 Pa, V= 7.2044E-06 m3

N= 1.0000E+00 moles, B= 5.4884E+01 g, RT= 4.9887E+03 J/mol

G= -1.9112E+04 J, G/N= -1.9112E+04 J/mol, H= 9.3417E+03 J, S= 4.7423E+01 J/K

Component name Moles Mole-fr Chem.pot/RT Activities Ref.state

CR 2.5000E-01 0.25000 -3.4452E+00 3.1899E-02 SER (default)

FE 7.5000E-01 0.75000 -3.9597E+00 1.9068E-02 SER (default)

Name	Status	Moles	Volume	Form.Units	At/FU	dGm/RT	Comp:
BCC_A2.....	E	2.157E-01	1.57E-06	2.16E-01	1.00	0.00E+00	X:
CR	9.70535E-01	FE	2.94648E-02				

BCC_A2_AUTO#2.....	E	7.843E-01	5.63E-06	7.84E-01	1.00	0.00E+00	X:
FE	9.48133E-01	CR	5.18667E-02				

End debug output from TQLR

Any more calculations? /N/:

Auf wiedersehen

C:\Users\..\TQ4lib\F90\test1>