

Test of the C++ program using the iso-C interface to OC

```
C:\Users\...\TQ4lib\Cpp\Matthias>linkmake
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM 160926 Bo Sundman update
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM 151210 Matthias original
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM You must have compiled the OC software
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM to obtain liboceq.a and liboceqplus.mod
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM These files are copied here together with
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM the F90 source library
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM the F90 source library liboctq.F90
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM liboctqisoc is the OCTQ library
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM that can be called from C++
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM The copy commands assume we are at
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM TQ4lib/Cpp/isoC-matthias/ below OC
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>copy ..\...\liboceq.a .
```

```
1 fil(er) kopierad(e).
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>copy ..\...\liboceqplus.mod .
```

```
1 fil(er) kopierad(e).
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM this is the same for library for F90 and C++
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>copy ..\...\liboctq.F90 .
```

```
1 fil(er) kopierad(e).
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>gfortran -c liboctq.F90
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM this library calls the F90 library,
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>gfortran -c liboctqisoc.F90
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>REM This is linking all together
```

```
C:\Users\...\TQ4lib\Cpp\Matthias>g++ -o tqcpptest1 -lstl -ltcmalloc tqcpptest1.cpp liboctqisoc.o lib
```

```
In file included from tqcpptest1.cpp:1:0:
```

```
tqintf.h: In function 'void ListConstituentFractions(std::vector<std::__cxx11::basic_string<char> >, std::vector<double>, std::vector<std::vector<double> >, void*)':
```

```
tqintf.h:378:30: warning: deprecated conversion from string constant to 'char*' [-Wwrite-strings]
```

```
char* statevar = "X";
```

```
^
```

```

C:\Users\..\TQ4lib\Cpp\Matthias>tqcpptest1.exe
tqini created: DEFAULT_EQUILIBRIUM
-> Adress of ceq-Storage: [0x28fca0]
-> Element Data: [CR, FE] [0x28fca8]
-> Phase Data: [LIQUID, BCC_A2, CBCC_A12, CHI_A12, CR3SI, CRSI2, CUB_A13, FCC_A1
, FE4N, HCP_A3, SIGMA] [0x28fca4]
-> Set Temperature to: [800] [0x28fca8]
-> Set Pressure to: [100000] [0x28fca8]
-> Set Moles to: [1] [0x28fca8]
-> Set Composition of CR to: [0.3] [0x28fca4]
-> Set Composition of FE to: [0.7] [0x28fca4]
3Y Gridmin:      99 points    0.00E+00 s and      0 clockcycles, T= 800.00
Equilibrium calculation  9 its,    0.0000E+00 s and      0 clockcycles
-> Calculated Equilibrium [0x28fd0c]
-> Phase Fractions: [LIQUID: 0, BCC_A2: 0.668213, CBCC_A12: 0, CHI_A12: 0, CR3SI
: 0, CRSI2: 0, CUB_A13: 0, FCC_A1: 0, FE4N: 0, HCP_A3: 0, SIGMA: 0.331787] [0x28
fca8]
-> Constituent Fractions for BCC_A2 [CR: 0.197577, FE: 0.802423] [0x28fcac]
-> Constituent Fractions for SIGMA [CR: 0.506278, FE: 0.493722] [0x28fcac]
-> Extended Constituent Fractions for BCC_A2 [1 moles of atoms/formula unit] [Co
nst. 0: 0.197577, Const. 1: 0.802423]_(1) [Const. 2: 1]_(3)
-> Set Constituents to: [0: 0.197577, 1: 0.802423, 2: 1]
-> Read Gibbs Data G: [-4.53418, -0.00921571, 1.09085e-009, -7.35275e-006, 4.579
45e-014, -6.38585e-021]
-> Read Gibbs Data dGdY: [-3.66577, -4.22737, -4.8013]
-> Read Gibbs Data d2GdYdT: [-0.00844687, -0.00662165, -0.00754981]
-> Read Gibbs Data d2GdYdP: [1.10191e-009, 1.08813e-009, 1.09085e-009]
-> Read Gibbs Data d2GdY2: [3.94308, -0.293516, -1.72288]

C:\Users\..\TQ4lib\Cpp\Matthias>

```