A typical *Build* session for exercise 1

```
erdw-imp-nw-dock-dhcp-151:Low resolution copy markcaddick$ ./build


NO is the default (<cr>) answer to all Y/N prompts


Enter the name of the problem definition file to be created,
< 100 characters, left justified [default = in]:
input

Enter thermodynamic data file name, left justified, [default = hp02ver.dat]:
<cr>

Enter the computational option file name, left justified, [default =
perplex_option.dat]:
See: www.perplex.ethz.ch/perplex_options.html
<cr>

The current data base components are:
 NA2O  MGO   AL2O3 SIO2  K2O   CAO   TIO2  MNO   FEO   NIO   ZRO2  CL2
 O2    H2O   CO2
Transform them (Y/N)?
N

Calculations with a saturated phase (Y/N)?
The phase is:   FLUID
Its compositional variable is: Y(CO2), X(O), etc.
Y

Select the independent saturated phase components:
 H2O   CO2
Enter names, left justified, 1 per line, <cr> to finish:

For C-O-H fluids it is only necessary to select volatile species present in
the solids of interest. If the species listed here are H2O and CO2, then to
constrain O2 chemical potential to be consistent with C-O-H fluid speciation
treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

H2O

Calculations with saturated components (Y/N)?
N

Use chemical potentials, activities or fugacities as independent
variables (Y/N)?
N

Select thermodynamic components from the set:
 NA2O  MGO   AL2O3 SIO2  K2O   CAO   TIO2  MNO   FEO   NIO   ZRO2  CL2
 O2    CO2
Enter names, left justified, 1 per line, <cr> to finish:
K2O
FEO
MGO
AL2O3
SIO2

Select fluid equation of state:

   0 - X(CO2) Modified Redlich-Kwong (MRK/DeSantis/Holloway)
   1 - X(CO2) Kerrick & Jacobs 1981 (HSMRK)
   2 - X(CO2) Hybrid MRK/HSMRK
   3 - X(CO2) Saxena & Fei 1987 pseudo-virial expansion
   4 - Bottinga & Richet 1981 (CO2 RK)
   5 - X(CO2) Holland & Powell 1991, 1998 (CORK)
   6 - X(CO2) Hybrid Haar et al 1979/CORK (TRKMRK)
   7 - f(O2/CO2)-f(S2) Graphite buffered COHS MRK fluid
   8 - f(O2/CO2)-f(S2) Graphite buffered COHS hybrid-EoS fluid
   9 - Max X(H2O) GCOH fluid Cesare & Connolly 1993
  10 - X(O) GCOH-fluid hybrid-EoS Connolly & Cesare 1993
  11 - X(O) GCOH-fluid MRK Connolly & Cesare 1993
  12 - X(O)-f(S2) GCOHS-fluid hybrid-EoS Connolly & Cesare 1993
  13 - X(H2) H2-H2O hybrid-EoS
  14 - EoS Birch & Feeblebop (1993)
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  15 - X(H2) low T H2-H2O hybrid-EoS
  16 - X(O) H-O HSMRK/MRK hybrid-EoS
  17 - X(O) H-O-S HSMRK/MRK hybrid-EoS
  18 - X(CO2) Delany/HSMRK/MRK hybrid-EoS, for P > 10 kb
  19 - X(O)-X(S) COHS hybrid-EoS Connolly & Cesare 1993
  20 - X(O)-X(C) COHS hybrid-EoS Connolly & Cesare 1993
  21 - X(CO2) Halbach & Chatterjee 1982, P > 10 kb, hybrid-Eos
  22 - X(CO2) DHCORK, hybrid-Eos
  23 - Toop-Samis Silicate Melt
  24 - f(O2/CO2)-N/C Graphite saturated COHN MRK fluid
  25 - H2O-CO2-NaCl Aranovich and Haefner 2004
5

Specify computational mode:

     1 - Unconstrained minimization
     2 - Constrained minimization on a 2d grid [default]
     3 - Constrained minimization on a 1d grid
     4 - Output pseudocompound data
     5 - Phase fractionation calculations

Unconstrained optimization should be used for the calculation of composition,
mixed variable, and Schreinemakers diagrams. Gridded minimization can be used to
construct phase diagram sections.

2

The data base has P(bar)   and T(K)     as default independent potentials.
Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?
N

Select x-axis variable:
     1 - P(bar)
     2 - T(K)
     3 - Y(CO2)
     4 - Composition X(C1)* (user defined)

*Although only 1 component is specified for the saturated fluid phase, the
 equation of state permits fluid composition to vary through the variable Y(CO2)  .
 For pure fluids, specify the appropriate composition as a sectioning constraint.


*X(C1) can not be selected as the y-axis variable

2

Enter minimum and maximum values, respectively, for: T(K)
723
973

Select y-axis variable:
     2 - P(bar)
     3 - Y(CO2)

2

Enter minimum and maximum values, respectively, for: P(bar)
2000
15000

Specify sectioning value for: Y(CO2)
0

For gridded minimization, grid resolution is determined by the number of levels
(grid_levels) and the resolution at the lowest level in the X- and Y-directions
(x_nodes and y_nodes) these parameters are currently set for the exploratory and
autorefine cycles as follows:

stage        grid_levels  xnodes  ynodes    effective resolution
exploratory       1          20      20        20 x  20 nodes
auto-refine       2          60      60       473 x 473 nodes

To change these options edit or create the file perplex_option.dat
See: www.perplex.ethz.ch/perplex_options.html#grid_parameters


Specify component amounts by weight (Y/N)?
N
```

```
Enter molar  amounts of the components:
 K2O   FEO   MGO   AL2O3 SIO2
for the bulk composition of interest:
3.819
10.529
4.761
12.488
68.00

Do you want a print file (Y/N)?
Y
Enter the print file name, < 100 characters, left justified [default = pr]:
Print

Do you want a plot file (Y/N)?
Y
Enter the plot file name, < 100 characters, left justified [default = pl]:
Plot

Summary of valid make definitions:

          FEO   MGO   AL2O3 FEO   H2O
fbr       0.00  0.00  0.00  1.00  1.00
fchum     0.00  0.00  4.00  9.00  1.00
fphA      0.00  0.00  2.00  7.00  3.00
fper      0.00  0.00  0.00  1.00  0.00
fatg      0.00  0.00 34.00 48.00 31.00
sil8L     0.00  1.60  1.60  0.00  0.00
fo8L      4.00  0.00  2.00  0.00  0.00
fa8L      0.00  0.00  2.00  4.00  0.00
q8L       0.00  0.00  4.00  0.00  0.00
ged_dqf   5.00  2.00  6.00  0.00  1.00
fanth_dq  0.00  0.00  8.00  7.00  1.00



Exclude phases (Y/N)?
N

Do you want to treat solution phases (Y/N)?
Y
Enter solution model file name [default = solut_08.dat] left justified, < 100
characters:
solut_09.dat


**warning ver114** the following endmembers are missing for Bio(TCC)
  mfbit     ffbit     fbit      mtbit     ftbit     tbit      mts       mnbi

                        ..... LOTS MORE WARNINGS .....

**warning ver025** 0 endmembers for CF(stx8)   The solution will not be considered.

Select phases from the following list, enter 1 per line,
left justified, <cr> to finish

  Bio(TCC)    oAmph(DP)   cAmph(DP)   Bio(HP)     TiBio(WPH)  TiBio(HP)
  Chl(HP)     O(SG)       E(SG)       melt(HP)    pMELTS(G)   Pheng(HP)
  Sapp(HP)    Sapp(KWP)   Osm(HP)     GaHcSp      T           St(HP)
  Ctd(HP)     Carp        hCrd        Sud(Livi)   Sud         Cumm
  Anth        KN-Phen     Mica(CH1)   Mica(CH2)   O(HP)       Mont
  Sp(JR)      Sp(GS)      Sp(HP)      GrPyAlSp(B  GrPyAlSp(G  Gt(HP)
  Gt(EWHP)    Gt(WPH)     A-phase     Chum        Atg         B
  P           Mn-Opx      O(stx)      Sp(stx)     Gt(stx)     Opx(stx)
  o-Amph      CrGt        CrOpx(HP)   Opx(HP)     Opx(I)      CrSp
  O(stx7)     Sp(stx7)    Sp(WPH)     Sp(stx8)    O(stx8)     Opx(stx8)
  Gt(stx8)

Bio(HP)
Chl(HP)
St(HP)
Ctd(HP)
hCrd
Gt(HP)
Pheng(HP)


Enter calculation title:
My first calculation
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