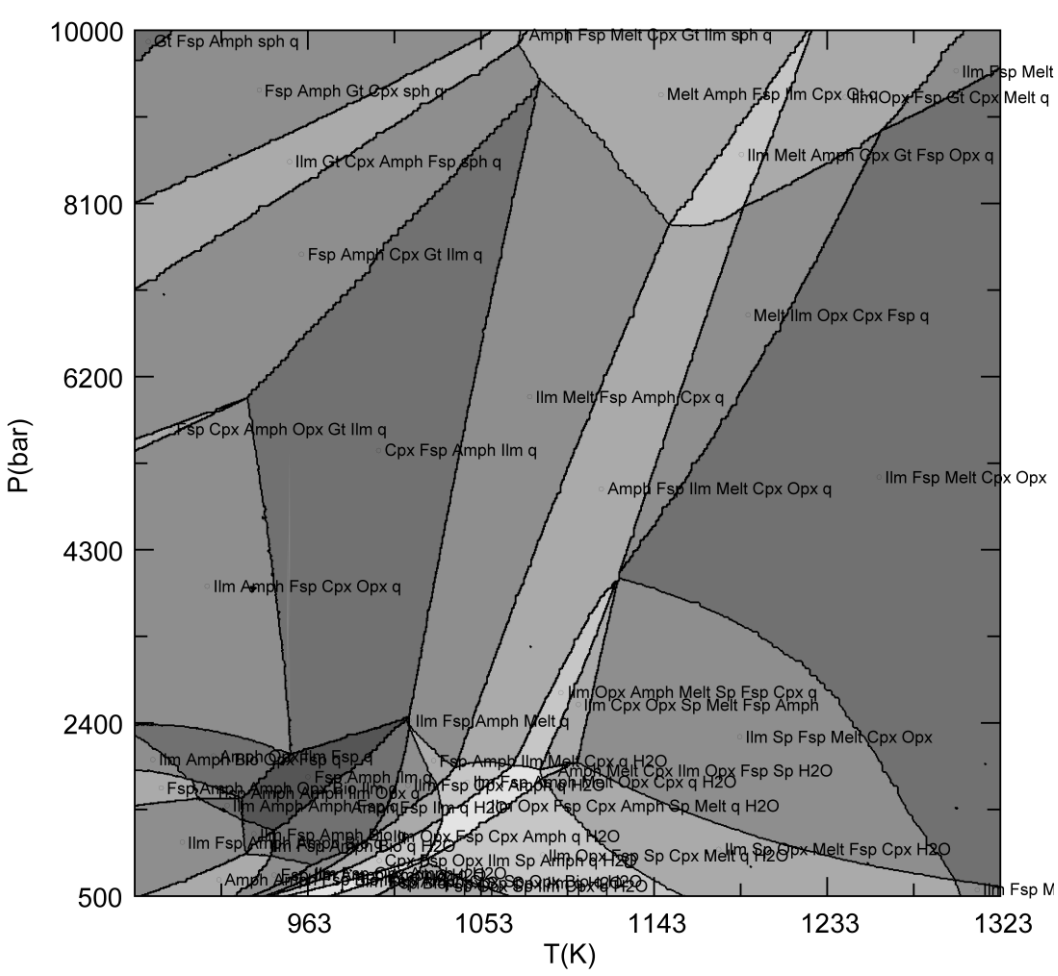
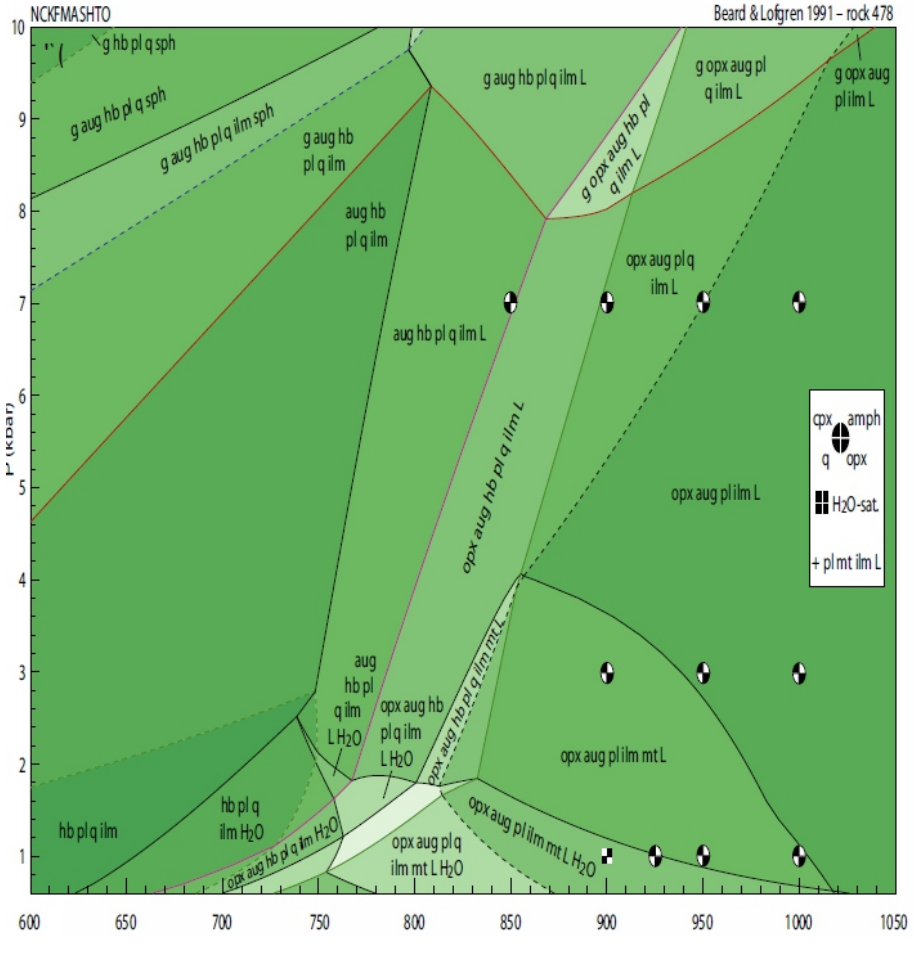
The published bl478 phase diagram section of Green et al. (Fig 4a, 2016) computed with THERMOCALC vs raw Perple_X 6.9.1 output computed from the bl478.dat input file (at www.perplex.ethz.ch/perplex/examples) with all Perple_X options set to **default** except:

```
grid_levels         1 5    | default: [1 4]
x_nodes             10 60  | default: [10 40]
y_nodes             10 60  | default: [10 40]
```

Computation time ~44 minutes. When all options are set to **default** the result on the following page is obtained in ~20 minutes.

The reasons for the discrepancies between the sections are: 1) biotite was not considered in the THERMOCALC section; 2) the low-temperature Opx field has been overlooked in the THERMOCALC section; 3) The spinel model (White et al. 2004) used in the THERMOCALC computation is an invalid equipartition model (Holland & Powell 2007), the implementation of such models in Perple_X is approximate.





Bl478 benchmark phase diagram section: Perple_X 6.9.1 (left) vs 6.9.0 (right), red boundaries are traced from the THERMOCALC result.

Computation time for the 6.9.1 calculation was 20 minutes with all options set to **default**.

Computation time for the 6.9.0 calculation was > 24 h, with

intial_resolution 1/10 1/16 | default: [1/16 1/48]

and all other options set to **default**.

The high-pressure low-temperature Ep-field in the 6.9.0 section is metastable with respect to the Ep-free stability fields of the 691 and THERMOCALC sections, likewise in the 6.9.0 section, the Cpx+Amph+Gt+Fsp+sph+q field extends metastably into the Cpx+Amph+Gt+Fsp+sph+q+ilm field. That the 6.9.0 phase fields are metastable can be verified by comparing the bulk Gibbs energies computed with 6.9.0 and 6.9.1 in the discrepant phase fields. The reasons for the discrepancies with the THERMOCALC computed phase field boundaries are listed on the previous page.