The published version of the KLB-1 phase diagram section (Fig 1., Holland et a;., JPet, 2013) vs raw output from Perple_X 6.8.5 (computed with the klb-1_hhph.dat input file, originally compiled by Bob Myhill).

klb-1_hhph calculation: global_reach_increment = 2, auto_refine_factor_I = 2.5, x/y_nodes = [60 60], all other options default.

Computation time ~8 h.

A global_reach_increment of 2 was specified to reduce cosmetic flaws (spurious solvi near the lower boundary of the Ca-Ferrite structure phase). Without global_reach_increment computation time is reduced by > 2 orders of magnitude (< 20 min). The reduction in auto_refine_factor_I from its default value (3) is necessary to prevent VERTEX from exhausting memory during the auto_refine stage of the calculation.

The absence of a stability field for the NAl phase in the Perple_X calculation is the only notable discrepancy. The absence of the NAl in the KLB-1 section is consistent with the MORB calculation (see morb_hhph_benchmark) which indicates the NAl phase is less stable in Perple_X than indicated in the original publication. This discrepancy is likely due to a change, or transcription error, in the NAl phase data. The similarity of phase boundaries irrespective of the presence of the NAl phase suggests that the NAl phase has no significant influence on bulk properties in the original calculation.