

Known Problems with PMATCHC (Version 1.1, 31-08-2001)

1. If $\Delta_f G^\circ$ and $\Delta_f H^\circ$ are given for a secondary master species, product species, mineral or solid, or gas (calculation case 15, see documentation TM-44-01-07), PMATCHC calculates $\Delta_f G^\circ$ of the corresponding formation reaction but fails to calculate $\log K$. In the case of the Nagra/PSI TDB 01/01 that is distributed with PMATCHC (backup file NAPSI_290502w.BAC) this problem concerns the following secondary master species, product species, and minerals or solids:

Secondary Master Species	Product Species	Minerals or Solids
S2O3-2 SO3-2	As(OH)4- AsO4-3 H2AsO4- H3AsO4 HSO3-	Mo(cr) Tugarinovite Molybdite Nb2O5(s) NbO2(s)