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# Discrepancies of mineral volumes predicted by thermodynamic databases

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Thermodynamic databases are an essential tool to predict complex equilibrium mineral assemblages and mineral properties like mineral volumes. They consist of numerous thermodynamic data of various minerals, extracted from experiments. Each database follows its own methodology in calculating chemical and physical properties. Therefore a direct comparision between different database predictions was avoided, due to the contrasting methodolgies and philosophy. Here, we present a direct comparison between the databases of Berman [1] and Holland & Powell [2][3], focusing on mineral volumes [4]. For this propose, a reevaluation of the equation of states was nesscary. In this context, we identify an error also implemented in common thermodynamic softwares, concerning the calculation of excess volume. Even after treating the excess energy correctly, volumes show significant discrepancies between the different database predictions. These discrepancies impact geodynamic interpretations and geothermobarometrical estimations, due to the fact that the Gibbs free energy and rock density depends on mineral volumes.

The imagination that pressure can vary by 4 kbar, temperature by 150°C or rock-density up to 30 %, by changing the thermodynamic database is dramatic. These enormous differences must be considered keeping in mind that calculations were done for well studied minerals (e.g. quartz and forsterite). The results play an important role for studies of geodynamic interpretations extracted from thermobarometric software packages like Perple_X, Theriak-Domino or Thermocalc. It is important to estimate the influence of the thermodynamic database on Gibbs free energy, volume and rock density. Summarizing, more experimental data will lead to a better comprehension of these discrepancies.

[1] Berman (1988). Journal of Petrology 29, 445-522. [2] Holland & Powell (1998) Journal of Metamorphic Geology 16, 309–343. [3] Holland & Powell (2011) Journal of Metamorphic Geology 29, 333-383. [4] Duesterhoeft, Zaehle, De Capitani, Oberhänsli & Bousquet (2012, in prep.) Submitted to Contributions to Mineralogy and Petrology.