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An improved thermodynamic model for ultramafic minerals and melts up to 10 GPa in the KNCFMASTOCr system

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Since petrological phase equilibrium modelling was developed, it has provided key information on the evolution of a multitude of magmatic settings. Its flexibility to investigate a broader range of bulk compositions and environmental conditions, interpolating between sparse experiments, has led to a better understanding of plume and impact melting, as well as the magmatic processes under hot mantle conditions in the Archean, such as the generation of komatiites. Still, the lack of experimental constraints in the literature on anhydrous compositions set the modelling upper-pressure limit at 6 GPa, restraining the calculations at the shallow part of the upper mantle and preventing a further investigation of deep magmatic systems.

This work presents an improved and extended calibration of melt and key anhydrous ultramafic minerals, incorporating recent HPHT experimental data for fertile and depleted peridotites in the KNCFMASTOCr system. The updated database enables thermodynamic modelling of magmatic processes at depths of up to ~300 km (10 GPa) in the Earth's upper mantle. Specifically, the new calibration includes: (1) a revised melt model for pressures exceeding 6 GPa, (2) new endmembers for high-pressure phases such as majorite and clinoenstatite, and (3) refined element partitioning among clinopyroxene, orthopyroxene, garnet, and spinel, with a particular focus on Cr and K.

We demonstrate the accuracy of the new database by comparing pressure, temperature, and modal abundances obtained through modelling with results from traditional geothermobarometry applied to natural peridotites. We discuss how PT estimates derived from modelling can compensate for the absence of key minerals in the assemblage. For instance, in garnet-free peridotites, where traditional barometry is unavailable, thermodynamic calculations provide a viable and efficient alternative. In conclusion, this new model offers a valuable tool for exploring deep Earth processes under HPHT conditions.