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A Computational Framework for Mineralogical Thermodynamics

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Determining the compositional, thermodynamic and mechanical properties of the polycrystalline aggregates in the mantle is an essential tool for geodynamic and seismological applications. We have developed an efficient, object-oriented, extensible software framework to facilitate such computations: Taking a database of thermodynamic model parameters for different minerals, a stable phase assemblage can be determined using Gibbs energy minimization at any given pressure and temperature. The program also computes densities, elastic moduli, heat capacities and thermal expansivities to name a few possibilities. These outputs can be transferred to control parameters of the mass and energy balance equations of a mantle convection model or of the propagation equation for seismic waves.