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# Thermo-chemical and thermo-physical properties of the high-pressure phase anhydrous B ($Mg_{14}Si_5O_{24}$): An ab-initio all-electron investigation

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## Abstract

Using the hybrid B3LYP density functional method, we computed the ab-initio thermo-chemical and -physical properties of the mineral anhydrous B (Anh-B), which has been recently suggested as a potential phase responsible for the X-discontinuity in the Earth's mantle at ~300 km depth through the reaction forsterite + periclase = Anh-B, and also to likely split the 410 km discontinuity within the interior of a cold slab through the reaction wadsleyite/ringwoodite = Anh-B + stishovite. We first conducted an investigation of the static properties through a symmetry-preserving relaxation procedure and then computed, on the equilibrium structure, harmonic vibrational modes at the long-wavelength limit corresponding to the center of the Brillouin zone ($\mathbf{k} \rightarrow 0$). While optic modes are the eigenvectors of the Hessian matrix at Γ point, acoustic modes were obtained by solving the non-zero components of the strain matrix. Following the Kieffer model, acoustic branches were assumed to follow sine wave dispersion when traveling within the Brillouin zone. All thermodynamic properties that depend on vibrational frequencies namely, heat capacities, thermal expansion, thermal derivative of the bulk modulus, thermal correction to internal energy, enthalpy, Gibbs free energy, thermal pressure and Debye temperature, were computed on the basis of quasi-harmonic mode-gamma analysis of the volume effects on vibrational frequencies. Moreover, the strain tensor was used to calculate several thermo-physical properties of geophysical interest (transverse and longitudinal wave velocities, shear modulus, Young's modulus, and Poisson's ratio). The ab-initio results derived in this study and the available data on molar volumes were used to calculate the univariant equilibrium forsterite + periclase = Anh-B. The results are in satisfactory agreement with the reversed experimental data of Ganguly and Frost (2006).

**Keywords:** Anhydrous B, thermodynamic properties, ab-initio, density functional theory, X-discontinuity, subduction