

Structural Compression and Phonon Dispersion of Diaspore from Experiment and Theory

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Knowledge about the strength of hydrogen bonds and their stability at elevated p,T-conditions is important for the construction of model systems concerning hydrogen-transport into the Earth's mantle. High-pressure studies of minerals with hydrogen bonds of intermediate strength, like diaspore, will deepen our understanding of the potential of high pressure to induce or strengthen hydrogen bonds, and of the resultant change of the physical properties of these materials.

We have performed quantum-mechanical calculations using density functional theory in order to obtain information on the response of the hydrogen bond geometry and phonon dispersion relations of diaspore when under compression. Our calculations were subsequently confirmed by experiments. Structural data were obtained by single-crystal synchrotron X-ray diffraction at ambient temperature and pressures up to 50 GPa using D3 at HASYLAB, while the dynamics of the hydrogen bond were measured by inelastic X-ray scattering at ambient conditions using ID28 at ESRF.

From the present results we infer that the structural compression is due mainly to the pressure-induced shortening of the hydrogen bond, which becomes significantly more symmetric with pressure up to 50 GPa (Friedrich et al. 2007a, 2007b). Our results show a significant LO/TO splitting of the O-H stretching frequencies and a significant dispersion along some directions in the Brillouin zone. The Γ -point stretching frequencies of the O-H bond of diaspore decrease approximately linearly with increasing pressure, and therefore also with increasing O-H bond length and decreasing hydrogen bond length. The dispersion is predicted to increase drastically at high pressure. These results will be discussed with respect to existing correlation diagrams.

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