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The stability and Raman spectra of ikaite, $CaCO_3 \cdot 6H_2O$, at high pressure and temperature

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Abstract

Raman analyses of single crystals of ikaite, $CaCO_3 \cdot 6H_2O$, synthesized in a diamond-anvil cell at ambient temperature yield spectra from 0.14 to 4.08 GPa; the most intense peaks are at 228 and 1081 cm^{-1} corresponding to E_g (external) and A_{1g} (internal) modes of vibrations in CO_3^{2-} ions, respectively. These are in good agreement with Raman spectra previously published for ikaite in powder form at ambient temperature and pressure. Visual observations of a sample consisting initially of a mixture of calcite + water in a hydrothermal diamond-anvil cell yielded a *P-T* phase diagram up to 2 GPa and 120 °C; the boundary for the reaction ikaite ↔ aragonite + water has a positive slope and is curved convexly toward the aragonite + water field similar to typical melt curves. This curvature can be explained in terms of the Clapeyron equation for a boundary between a solid phase and a more compressible liquid phase or largely liquid phase assemblage.