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Phase relations of $CaCO_3$ at high pressure and high temperature

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ABSTRACT

Phase transitions in calcite, a naturally occurring crystalline form of $CaCO_3$, have been investigated by three different experimental techniques: (1) in-situ X-ray diffraction (XRD) using synchrotron radiation to 6 GPa and 1750 °C in a cubic anvil press; (2) Raman scattering to 10 GPa at room temperature using a diamond-anvil cell; and (3) post-compression XRD on samples retrieved after heat treatment at temperatures to 2000 °C and pressures to 9 GPa in an octahedral anvil press. At room temperature, calcite I transformed into calcite II at 1.7 GPa and then to calcite III at ~2 GPa. Calcite III persisted to at least 10 GPa. Elevation of temperature at 3, 4, and 6 GPa caused a sequence of transitions: calcite III → aragonite → disordered calcite → liquid, and aragonite was retained upon rapid cooling of the liquid. The melting curve of disordered calcite increased with pressure following a relation: T_m (°C) = 1338 + 82 P – 2.9 P^2 where P is in units of GPa.