

LETTER

High-pressure transition of CaCO₃

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ABSTRACT

Calcite, CaCO₃, is a common carbon-bearing mineral found on the Earth's surface. As carbon dioxide in the atmosphere can be sequestered in carbon-bearing minerals (carbonates), the stability of carbonate minerals is of great interest to earth science. In our study, in-situ X-ray diffraction observations indicate that calcium carbonate (CaCO₃) transforms to an orthopyroxene-type structure that has fourfold coordination of carbon cations, when heated to temperatures >1500 K at pressures >130 GPa, which is in agreement with theoretical predictions from ab initio calculations. The volume reduction of this transition is ~0.5%, and the high-pressure phase did not quench on decompression to ambient pressure. Although the post-aragonite phase, which has threefold coordination of carbon cations, shows strongly anisotropic compressibility of each axis of the unit-cell parameter, no obvious anisotropy in the pyroxene-type phase was observed. The stability of this new calcium carbonate implies that the carbon dioxide could be storable at the base of the lower mantle.

Keywords: Calcium carbonate, phase transition, high pressure, diamond anvil cell