

Raman signatures of the distortion and stability of MgCO₃ to 75 GPa

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ABSTRACT

Knowledge of the stability of carbonate minerals at high pressure is essential to better understand the carbon cycle deep inside the Earth. The evolution of Raman modes of carbonates with increasing pressure can straightforwardly illustrate lattice softening and stiffening. Here, we report Raman modes of natural magnesite MgCO₃ up to 75 GPa at room temperature using helium as a pressure-transmitting medium (PTM). Our Raman spectra of MgCO₃ show the splitting of *T* and *v*₄ modes initiated at approximate 30 and 50 GPa, respectively, which may be associated with its lattice distortions. The MgCO₃ structure was referred to as MgCO₃-Ib at 30–50 GPa and as MgCO₃-Ic at 50–75 GPa. Intriguingly, at 75.4 GPa some new vibrational signatures appeared around 250–350 and ~800 cm⁻¹. The emergence of these Raman bands in MgCO₃ under relatively hydrostatic conditions is consistent with the onset pressure of structural transition to MgCO₃-II revealed by theoretical predictions and high-pressure and high-temperature experiments. This study suggests that hydrostatic conditions may significantly affect the structural evolution of MgCO₃ with increasing pressure, which shall be considered for modeling the carbon cycle in the Earth's lower mantle.

Keywords: Carbonate, high pressure, Raman spectroscopy, lattice distortion