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## High-pressure compressibility and vibrational properties of (Ca,Mn)CO<sub>3</sub>

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## ABSTRACT

Knowledge of potential carbon carriers such as carbonates is critical for our understanding of the deepcarbon cycle and related geological processes within the planet. Here we investigated the high-pressure behavior of (Ca,Mn)CO<sub>3</sub> up to 75 GPa by synchrotron single-crystal X-ray diffraction, laser Raman spectroscopy, and theoretical calculations. MnCO<sub>3</sub>-rich carbonate underwent a structural phase transition from the CaCO<sub>3</sub>-I structure into the CaCO<sub>3</sub>-VI structure at 45–48 GPa, while CaCO<sub>3</sub>-rich carbonate transformed into CaCO<sub>3</sub>-III and CaCO<sub>3</sub>-VI at approximately 2 and 15 GPa, respectively. The equation of state and vibrational properties of MnCO<sub>3</sub>-rich and CaCO<sub>3</sub>-rich carbonates changed dramatically across the phase transition. The CaCO<sub>3</sub>-VI-structured CaCO<sub>3</sub>-rich and MnCO<sub>3</sub>-rich carbonates were stable at room temperature up to at least 53 and 75 GPa, respectively. The addition of smaller cations (e.g.,  $Mn^{2+}$ ,  $Mg^{2+}$ , and Fe<sup>2+</sup>) can enlarge the stability field of the CaCO<sub>3</sub>-I phase as well as increase the pressure of the structural transition into the CaCO<sub>3</sub>-VI phase.

Keywords: Carbonate, X-ray diffraction, raman spectroscopy, high pressure