

Equation of state and structural evolution of manganese dolomite (kutnohorite) under high pressures

LIANGXU XU¹, WEIBIN GUI¹, KEWEI SHEN^{1,*}, DONGZHOU ZHANG^{2,†}, JINGUI XU³, AND JIN LIU^{4,*}‡

¹Center for High Pressure Science and Technology Advanced Research, Beijing 100193, China

²Center for Advanced Radiation Sources, University of Chicago, Chicago, Illinois 60439, U.S.A.

³Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, Guizhou 550002, China

⁴Center for High Pressure Science, State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, China

ABSTRACT

Understanding the structural evolution of carbonate minerals with increasing pressure is essential to decoding the role of Earth's mantle in the global carbon cycle and long-term climate change. Here, we carried out synchrotron single-crystal X-ray diffraction measurements on a natural sample of manganese dolomite [kutnohorite, $\text{Ca}_{1.11}\text{Mn}_{0.89}(\text{CO}_3)_2$] in a diamond-anvil cell up to 51.2 GPa at room temperature with neon as the pressure-transmitting medium. The manganese dolomite sample remains stable in the rhombohedral structure from 1 bar to ~13.3 GPa. The equation of state of $\text{Ca}_{1.11}\text{Mn}_{0.89}(\text{CO}_3)_2$ was determined: $V_0 = 334.06 \pm 0.29 \text{ \AA}^3$, $K_0 = 99.9 \pm 4.7 \text{ GPa}$, and $K'_0 = 4.3 \pm 0.9$; when K'_0 is fixed at 4.0, $V_0 = 334.04 \pm 0.24 \text{ \AA}^3$, and $K_0 = 101.4 \pm 1.5 \text{ GPa}$. Upon further compression at room temperature, the split and disappearance of diffraction spots were observed. That is, the rhombohedral structure of manganese dolomite becomes highly distorted to lose its long-range order at 13.3–51.2 GPa at room temperature. Moreover, our single-crystal X-ray diffraction results reveal the mechanisms of the reported lattice and internal Raman mode splits of the same manganese dolomite sample approximately at 13 and 24 GPa, respectively. These results suggest manganese-bearing carbonates may play a distinct role in the deep carbon cycle.

Keywords: High pressure, manganese dolomite, X-ray diffraction, deep carbon cycle; Physics and Chemistry of Earth's Deep Mantle and Core