

## The MnCO<sub>3</sub>-II high-pressure polymorph of rhodocrosite

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### ABSTRACT

We investigated the behavior of MnCO<sub>3</sub> in the pressure range 0–50 GPa and ambient temperature by synchrotron X-ray single-crystal diffraction technique. MnCO<sub>3</sub> maintains the calcite-type structure ( $R\bar{3}c$  symmetry) up to 44 GPa. Above this pressure we observed a phase transition. The high-pressure phase, MnCO<sub>3</sub>-II, is triclinic, with cell parameters  $a = 2.928(2)$ ,  $b = 4.816(4)$ ,  $c = 5.545(4)$  Å,  $\alpha = 101.71(6)^\circ$ ,  $\beta = 94.99(6)^\circ$ ,  $\gamma = 89.90(6)^\circ$ , and  $V = 76.28(10)$  Å<sup>3</sup> at 46.8 GPa. The structure is solved with the charge flipping algorithm. MnCO<sub>3</sub>-II is isostructural with CaCO<sub>3</sub>-VI. The density increase on phase transition is 4.4%. The occurrence of CaCO<sub>3</sub>-VI structure in MnCO<sub>3</sub> composition indicates that CaCO<sub>3</sub>-VI structure is also adopted by carbonates with cations smaller than calcium.

**Keywords:** Carbonates, high-pressure crystal structure, rhodocrosite, single crystal