

The MnCO₃-II high-pressure polymorph of rhodocrosite

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ABSTRACT

We investigated the behavior of MnCO₃ in the pressure range 0–50 GPa and ambient temperature by synchrotron X-ray single-crystal diffraction technique. MnCO₃ 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, MnCO₃-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 $V = 76.28(10)$ Å³ at 46.8 GPa. The structure is solved with the charge flipping algorithm. MnCO₃-II is isostructural with CaCO₃-VI. The density increase on phase transition is 4.4%. The occurrence of CaCO₃-VI structure in MnCO₃ composition indicates that CaCO₃-VI structure is also adopted by carbonates with cations smaller than calcium.

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