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Pyroxmangite: A high-pressure single-crystal study

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Abstract

We present the results of a single-crystal X-ray diffraction structural study on pyroxmangite in a diamond-anvil cell up to 5.6 GPa. The sample comes from Yokone-Yama, Awano Town, Tochigi Prefecture, Japan. Crystals are triclinic, centrosymmetric, with composition $[Mn_{0.576(2)}Fe_{0.284(5)}Ca_{0.044(3)}Mg_{0.089(2)}]Si_{1.003(4)}O_3$. Structure refinements were performed with intensity data collected at 1.24 and 3.57 GPa on a CCD-equipped diffractometer. Lattice parameters were accurately measured with the point-detector mounted on the same instrument.

The bulk modulus of pyroxmangite fitting data to a second-order Birch-Murnaghan equation of state is $K_0 = 109.6(7)$ GPa. Axial compressibility values were $\beta_a = 2.2(1)$, $\beta_b = 3.3(1)$, and $\beta_c = 2.6(1)$ 10^{-3} GPa^{-1} showing slightly anisotropic behavior, with the most compressible direction along the *b* axis, as commonly found in the related family of pyroxene.

Silicon tetrahedra are almost incompressible in the pressure range investigated. M polyhedra are more compressible: the volume change is smaller in the more regular octahedra M1–M4 (–3.3%) and greater in the more irregular polyhedra M5–M7 (–5.2%). Owing to the different contraction of Si tetrahedra and cation polyhedra, the sevenfold tetrahedral chains in pyroxmangite must kink to avoid misfit between chains and octahedral bands. This results in shortening of 1.2% of the *c* axis and a decrease in both O_{br} -O_{br}-O_{br} and Si-O_{br}-Si angles.

The behavior of pyroxmangite at high *P* is approximately inverse to that observed at high *T*. Compressibility data may be combined with those on thermal expansion to formulate the approximate equation of state: $V = V_0 (1 - 9.12 \times 10^{-3} \Delta P + 3.26 \times 10^{-5} \Delta T)$, where *P* is in GPa and *T* in degrees Celsius.

Keywords: Pyroxmangite, pyroxenoid, equation of state, compressibility