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Structural effects of pressure on monoclinic chlorite: A single-crystal study

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Abstract

A single-crystal X-ray diffraction study in a diamond anvil cell up to 5.41 GPa was carried out on a clinochlore [monoclinic polytype II*b*-2, S.G. *C*2/*m*, $(Mg_{9.09}Fe^{2+}_{1.01}Mn_{0.02}Ti_{0.01}Cr_{0.02}Al_{1.80})_{\Sigma=11.95}(Si_{6.35}Al_{1.65})_{\Sigma=8}O_{20}(OH)_{16}$] from Val Malenco, Italy.

The bulk modulus of monoclinic clinochlore calculated by fitting unit-cell volumes and pressures to a third-order Birch-Murnaghan Equation of State (EoS), is $K_0 = 71(9)$ GPa with $K' = 8(5)$. Axial compressibility values were $\beta_{0a}^{EoS} = 3.8(1)$, $\beta_{0b}^{EoS} = 3.6(1)$, and $\beta_{0c}^{EoS} = 5.4(5)\ 10^{-3}$ GPa^{-1}, showing that axial anisotropy is much less than that found for other phyllosilicates. Compressibility data are in fair agreement with literature data, which are based on powder neutron and synchrotron diffraction methods. Results were compared with the behavior of the triclinic polytype of similar composition and coexisting in the same rock. Symmetry has little overall influence on compressibility, but compared with the triclinic polytype of similar composition and coexisting in the same hand specimen, the monoclinic polytype is slightly less rigid.

Comparison of structural refinements at different pressures showed that structural deformations mainly affect the interlayer region, where hydrogen bonds are important for the structural properties of the phase. The mean decrease in OH-O distances was about 9% in the pressure range 0–5 GPa. Structural behavior was very similar to that found for the triclinic polytype.

Although energy differences between polytypes are relatively small, their compressional behavior may have implications in terms of relative stability. A computation of molar volume applying an isothermal EoS shows that the triclinic polytype is lower in volume up to 0.9 GPa, above which the volume of the monoclinic phase is smaller. This fact gives information on the relative stability of the two polytypes and a possible explanation for the greater abundance of the triclinic polytype in low to medium-*P* environments, as is commonly observed in nature.

Keywords: Chlorite, high pressure, polytypism, equation of state