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

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ABSTRACT

We present the results of a single-crystal X-ray diffraction structural study of chlorite in a diamond anvil cell up to 5.47 GPa. The sample is a clinochlore from Val Malenco, Italy, triclinic polytype II*b*-4, S.G. $C\bar{1}$, with pseudomonoclinic metric and composition $(Mg_{9.14}Fe^{2+}_{1.02}Fe^{3+}_{0.01}\ Mn_{0.01}Ti_{0.01}Al_{1.76})_{\Sigma=11.95}(Si_{6.32}\ Al_{1.68})_{\Sigma=8}O_{20}(OH)_{16}$. Structural refinements were performed at several pressures with intensity data collected on a CCD diffractometer. Unit-cell parameters were accurately measured with the point-detector mounted on the same instrument.

The bulk modulus of chlorite fitting data to a third-order Birch-Murnaghan equation of state is K_0. = 88(5) GPa with K' = 5(3). Results are in fair agreement with data based on powder neutron and synchrotron diffraction methods. The axial compressibility values were β_{0a}^{EoS} = 3.4(2), β_{0b}^{EoS} = 3.4(1), and β_{0c}^{EoS} = 5.4(2) 10^{-3} GPa^{-1}. The metric of the lattice remains triclinic in the investigated pressure range. Axial anisotropy is strongly reduced with respect to the axial compressibilities observed in other phyllosilicates. Comparison of structural refinements at different pressures shows that the main structural deformations affect the interlayer region, where the hydrogen bonds are relevant to the structural properties of the phase. The mean decrease of the OH-O distances is about 10% from ambient pressure to ~5 GPa.

Compressibility data may be combined with those on thermal expansion to formulate an equation of state for clinochlore. Taking into account the thermal expansion coefficient reported in literature for a chlorite with a composition quite similar to that of our sample, we can write the equation: $V = V_0\ (1 - 1.14\ 10^{-2}\ \Delta P + 2.316\ 10^{-5}\ \Delta T)$, where P is in GPa and T in Celsius. Assuming an average rock density of 2.7 g/cm^3, this corresponds to an isochoric P-T geothermal gradient of 18 °C/km.

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