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Isothermal equation of state and compressional behavior of tetragonal edingtonite

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ABSTRACT

The high-pressure (H*P*) structural evolution of a natural tetragonal edingtonite from Ice River, Canada, was investigated up to 5.1 GPa using in situ single-crystal X-ray diffraction and a diamond-anvil cell. The isothermal equation of state was determined. The values of V_0, K_{T0}, and K' refined with a third-order Birch-Murnaghan equation of state (BM-EoS) are $V_0 = 601.6(3)$ Å^3, $K_{T0} = 59(2)$ GPa, and $K' = 3.4(8)$. Under high-pressure conditions the main deformation mechanisms can be described by rotation/kinking of "rigid units," represented by the 4 = 1 secondary building unit (SBU), due to the tetrahedra tilting. The angle between the SBUs (ϕ) increased from 17.15(8)° at 0.0001 GPa to 20.03(9)° at 4.61 GPa.

The bulk structural compression results from the combination of the "soft" behavior of the not fully occupied channels [$K_{T0} = 19(1)$ GPa for [100]-channels; $K_{T0} = 21(1)$ GPa for [110]-channels] and of the rigid behavior of the tetrahedral framework.

The extra-framework cations do not increase in coordination number within the pressure range investigated. The barium occupancy factors for the Ba1 and Ba2 sites change with increasing pressure. For $P > 2.3$ GPa the Ba2 site is completely empty, and only the position Ba1 is occupied.