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High-pressure study of a natural cancrinite

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Abstract

The high-pressure elastic behavior and the *P*-induced structure evolution of a natural cancrinite from Cameroun $\{Na_{6.59}Ca_{0.93}[Si_6Al_6O_{24}](CO_3)_{1.04}F_{0.41}\cdot 2H_2O$, a = 12.5976(6) Å, c = 5 .1168(2) Å, space group: $P6_3\}$ were investigated by in situ single-crystal X-ray diffraction under hydrostatic conditions up to 6.63(2) GPa with a diamond-anvil cell. The *P*-*V* data were fitted with an isothermal Birch-Murnaghan type equation of state (BM EoS) truncated to the third order. Weighted fit (by the uncertainty in *P* and *V*) gave the following elastic parameters: V_0 = 702.0(7) Å^3, K_{V0} = 51(2) GPa, and K_V' = 2.9(4). A linearized BM EoS was used to fit the *a*-*P* and *c*-*P* data, giving the following refined parameters: a_0 = 12.593(5) Å, K_{a0} = 64(4) GPa, K_a' = 4.5(9), for the *a*-axis, and c_0 = 5.112(3) Å, K_{c0} = 36(1) GPa, K_c' = 1.9(3) for the *c*-axis (elastic anisotropy: K_{a0}:K_{c0} = 1.78:1). A subtle change of the elastic behavior appears to occur at P > 4.62 GPa, and so the elastic behavior was also described on the basis of BM EOS valid between 0.0001–4.62 and 5.00–6.63 GPa, respectively. The high-pressure structure refinements allowed the description of the main deformation mechanisms responsible for the anisotropic compression of cancrinite on (0001) and along [0001]. A comparative analysis of the structure evolution in response of the applied pressure and temperature of isotypic materials with cancrinite-like topology is carried out.

Keywords: Cancrinite, zeolites, high pressure, compressibility, structure evolution