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Anomalous elastic behavior and high-pressure structural evolution of zeolite levyne

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ABSTRACT

Elastic behavior and high-pressure (HP) structural evolution of a natural zeolite levyne, $(Ca_{0.5},Na,K)_6(Al_6Si_{12}O_{36})\cdot 18H_2O$, has been investigated up to 5 GPa by means of in situ single-crystal X-ray diffraction with a diamond-anvil cell using a non-penetrating pressure-transmitting medium. Peculiar elastic behavior has been observed in the range 0–1 GPa: the *c* parameter decreases between 0 and 0.2 GPa, then increases up to 0.5–0.6 GPa. Above this *P*-value, the parameter decreases as expected. Anomalous behavior is also shown by the *a*-parameter, which first increases up to 0.2 GPa, then decreases as expected. However, these anomalous lattice variations are only slightly reflected in the cell volume behavior. The low-*P* trend ($P < 1$ GPa) is also followed by the lattice parameters in decompression. The isothermal Equation-of-State (EoS) at $P > 1$ GPa, refined with a second-order Birch-Murnaghan EoS, yields the following parameters: $V_0 = 3539(3)$ Å^3 and $K_{T0} = 48(1)$ GPa. Comparison of structural refinements performed at 0.0001, 0.79(5), and 3.00(5) GPa highlights two distinct deformation mechanisms of the Si/Al-framework, one predominant at low pressures (0–1 GPa) and the other at high pressures (1–5 GPa).

The extra-framework content does not show any evident modification within the pressure range investigated.