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Elastic behavior, phase transition, and pressure induced structural evolution of analcime

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Abstract

Elastic and structural behavior of a natural cubic analcime (space group: $Ia\bar{3}d$) from Sardinia (Italy) was investigated at high pressure by in situ single-crystal X-ray diffraction. A first-order phase transition is observed in the pressure range between 0.91(5) and 1.08(5) GPa. Unit-cell constants and reflection conditions confirm that the space group of the HP-polymorph is $P\bar{1}$. No further phase-transition has been observed at least up to 7.14 GPa. Fitting the volume data of the cubic polymorph with a second-order BM-EoS we obtain: V_0 = 2571.2(4) Å^3, K_{T0} = 56(3) GPa, and K' = 4 (fixed). For the triclinic polymorph, a third-order EoS gives: V_0 = 2607(9) Å^3, K_{T0} = 19(2) GPa, and K' = 6.8(7). Axial bulk moduli of the triclinic polymorph, calculated with a linearized BM-EoS, are: $K_{T0}(a)$ = 29(2) GPa, with $K'(a)$ = 4.9(6) and a_0 = 13.727(10) Å; $K_{T0}(b)$ = 20(1) GPa, with $K'(b)$ = 5.2(5), and b_0 = 13.751(15) Å; $K_{T0}(c)$ = 11(1) GPa, with $K'(c)$ = 12.6(6) and c_0 = 13.822(31) Å. The elastic behavior of the HP-polymorph appears to be strongly anisotropic, being $K_{T0}(a)$:$K_{T0}(b)$:$K_{T0}(c)$ = 2.64:1.82:1.00. The relevant structural variations in response to the cubic → triclinic phase transition are due to tetrahedral tilting. The tetrahedral framework distortion gives rise to a change of the eight- and six-ring channels ellipticity and of the extra-framework topological configuration: it appears in fact that for the high-pressure triclinic polymorph the coordination number of some of the Na atoms is seven ($2H_2O$ + five framework O atoms) instead of six ($2H_2O$ + four framework O atoms).

Key words: Analcime, zeolite, high-pressure, compressibility, phase transition