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Elastic behavior and high pressure-induced phase transition in chabazite: new data from a sample from Nova Scotia

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Recently, the high pressure (HP) behavior of a natural chabazite from Vallerano [1] (VALL), and on the synthetic phases SAPO-34 [1] and ALPO-34 [2], was investigated in the frame of a wider project aimed at understanding the role of the framework/extraframework content on the compressibility of CHA-type porous materials.

In this work, further structural information is obtained studying the response to HP of another natural chabazite sample from Nova Scotia (Canada) (NS) (s.g. R-3*mR* [3]), characterized by a different chemical composition with respect to VALL. The study was performed by means of *in situ* synchrotron X-ray powder diffraction (XRPD) and silicone oil as non-penetrating P-transmitting medium. XRPD experiments were performed in DAC at the BM01 beamline at ESRF (Grenoble, France) with a fixed λ=0.7355 Å. Powder patterns were collected from P_{amb}up to 8.6 GPa and upon decompression. All the features of the P_{amb} pattern and the unit cell parameters are well recovered upon P release. Below 2.1 GPa, a and α cell parameters slightly decrease and increase respectively with a resulting volume reduction of 3.6 %. Above 2.1 GPa, a transition to a triclinic P-1 pseudo-rhombohedral phase is observed. The rhombohedral to triclinic phase transition is accompanied by an abrupt decrease in the unit cell parameters and in the unit cell volume (ΔV=-4.0%). Between 2.5 and 5.9 GPa, the triclinic/pseudo-rhombohedral cell parameters decrease regularly and the unit cell volume variation (ΔV=-3.0%) indicates a lower compressibility with respect to that observed before the transition. In the highest P regime (5.9-7.2 GPa), a further slope change, with an increase in compressibility, is observed. As a whole, ΔV between P_{amb} and 7.2 GPa is -12.6%. The elastic parameters, calculated with a second order BM-EoS, are V_0 = 826 (1) Å^3, K_0 = 54(3) GPa and V_0 = 784(2) Å^3, K_0 = 91(5) GPa, for the rhombohedral and triclinic phase, respectively.

Preliminary results from Rietveld refinements up to about 1 GPa, suggest that the deformation mechanism acting in the low-P regime is a cooperative tilting of the tetrahedra belonging to the double 6-ring – resulting in a decrease of its thickness – accompanied by a simultaneous di-trigonalization of the two 6-rings. A similar mechanism was previously observed during compression of levyne [4].

The HP-induced cell volume contraction of NS (12.6 %) is higher than that of VALL (10.3%) in the same P range. This is congruent with the lower content in large extraframework potassium cations of NS, which contribute to sustain the porous structure in VALL.

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