

Comparative compressional behavior of chabazite with Li⁺, Na⁺, Ag⁺, K⁺, Rb⁺, and Cs⁺ as extra-framework cations

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ABSTRACT

The high-pressure behavior of monovalent-cation-exchanged chabazites was investigated by means of in situ synchrotron X-ray powder diffraction with a diamond-anvil cell, and using water as penetrating pressure-transmitting medium, up to 5.5 GPa at room temperature. In all cases, except for Na-containing chabazites, a phase transition from the original rhombohedral ($R\bar{3}m$) to triclinic symmetry (likely $P\bar{1}$) was observed in the range between 3.0 GPa and 5.0 GPa. The phase transition is accompanied by an abrupt decrease of the unit-cell volume by up to 10%. Evidence of pressure-induced hydration (PIH), i.e., P -induced penetration of H₂O molecules through the zeolitic cavities, was observed, as reflected by the incompressibility of the cation-exchanged chabazites, which is governed by the distribution of the extra-framework cations. The reversibility of the PIH and P -induced phase transitions in the high-pressure behavior of the cation-exchanged chabazites are discussed in the context of the role played by the chemical nature and bonding configuration of the extra-framework cations, along with that of the H₂O content at room conditions.

Keywords: Chabazite, compressibility, high pressure, pressure-induced hydration, synchrotron diffraction; Microporous Materials: Crystal-Chemistry, Properties, and Utilizations