

## **Comparative compressional behavior of chabazite with Li<sup>+</sup>, Na<sup>+</sup>, Ag<sup>+</sup>, K<sup>+</sup>, Rb<sup>+</sup>, and Cs<sup>+</sup> 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 H<sub>2</sub>O 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 H<sub>2</sub>O content at room conditions.

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