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Crystal structure-crystal chemistry relationships in the zeolites erionite and offretite

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ABSTRACT

This study clarifies the crystal structure variations and relationships in the zeolites erionite and offretite. The crystal structure analyses used Rietveld analysis of X-ray powder diffraction data, obtained both by synchrotron radiation and conventional X-ray sources, and on diffraction patterns obtained by transmission electron microscopy. The framework Al atoms in erionite are preferentially located in the single six-membered ring of tetrahedra (T2 site), whereas the Si-Al distribution is essentially disordered on the tetrahedral framework sites in offretite. In both zeolites, the center of the cancrinite cage is always occupied by K cations in similar amounts in both minerals. The erionite cage in erionite is occupied by Ca and Na atoms distributed on four distinct cation sites. Mg ions can be present up to 0.8 atoms per cell and are located between the Ca1 and Ca3 sites and very close to the Ca2 site on the symmetry axis. In offretite, the Mg site is located on the trigonal axis of the gmelinite cage and the Mg atoms are bonded to a variable number (five or six) of H_2O molecules, depending on the site population. The structural data and TEM analysis clearly show that the crystal chemistry of the extraframework cations, Mg in particular, is a major factor controlling whether erionite or offretite crystallizes, the Si-Al distribution in the framework, and the possible stacking intergrowths of the two minerals.