MS16-P07 | CRYSTAL STRUCTURE AND DEHYDRATION BEHAVIOR OF Ag^+-EXCHANGED LEVYNE

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The crystal structure and dehydration behavior of a natural zeolite, levyne, exchanged with Ag^+ was investigated by combing *in situ* Single Crystal X-ray Diffraction (SCXRD), X-ray Absorption Spectroscopy (XAS) and Molecular Dynamics (MD) simulations.

At room temperature, structure solution indicated the space group *R*-3*m*. The latter corresponds to the space group of the natural levyne-Ca. However, in contrast to the pristine material, Ag^+-levyne is not twinned by merohedry. The Ag^+ ions are highly disordered on partially occupied sites distributed along the three-fold axis and in the middle of the 8-membered ring window of the *lev* cage. The analysis of pseudo-radial distribution function calculated from XAS data and MD simulations shows that silver is on average coordinated by five oxygen with distances between 2.44 and 2.80 Å.

The thermal stability was investigated by SCXRD from 25 to 400°C. The dehydration starts at 50°C. At 100°C the space group changes from *R*-3*m* to *R*-3. At 250°C new sites, close to the tetrahedral sites T1 and T3, appear, indicating the onset of the rupture of the T1-O2-T3 and T1-O3-T3 connections forming the double six-ring cage. At 300°C the percentage of the broken bridges converge to 13% and the new links T1B-OB1-T3B and T1B-OB2-T3B form. Differently from the natural levyne-Ca no additional T-O-T connection breaks up to 300°C. From 350°C to 400°C the intensity of the reflections significantly dropped and only the cell parameters were extracted. The total unit-cell volume contraction in the investigated temperature range is 4%.