American Mineralogist, Volume 105, pages 1631–1638, 2020

Crystal structure of Ag-exchanged levyne intergrown with erionite: Single-crystal X-ray diffraction and Molecular Dynamics simulations

GEORGIA CAMETTI[1,*,†] AND SERGEY V. CHURAKOV[1,2]

[1]Institute of Geological Sciences, Mineralogical Crystallography, Baltzerstrasse 1+3, 3012 Bern, Switzerland
[2]Paul Scherrer Institut, Forschungstrasse 111, 5232 Villingen PSI, Switzerland

ABSTRACT

The modification of natural zeolites via ion exchange is an efficient technique used to improve their performances and tune their properties for specific applications. In this study, a natural levyne-Ca intergrown with erionite was fully exchanged by Ag^+ and its structure [with idealized chemical composition $Ag_6(Si,Al)_{18}O_{36}\cdot 18H_2O$] was investigated by combining a theoretical and experimental approach. Single-crystal X-ray diffraction data demonstrated that Ag-levyne maintained the $R\overline{3}m$ space group, characteristic of the natural levyne. Ag ions distribute over partially occupied sites along the threefold axis and, differently from the pristine material, at the wall of the 8-membered ring window of the *lev* cavity. The lack of ~30% of Ag ions that could not be located by the structural refinement is ascribed to the strong disorder of the extraframework occupants. The structural results obtained by Molecular Dynamics simulations are in overall agreement with the experimental data and showed that, on average, Ag^+ is surrounded by ~2 H_2O and 1 framework oxygen at distances between 2.43 and 2.6 Å. Molecular Dynamics trajectories indicate that the occurrence of silver inside the D6R cage depends on the water content: silver occupancy of D6R cages is estimated to be 83, 30, and 0% when the structure contains 3, 2.5, and 2 H_2O per Ag ion, respectively.

The cation-exchange process, as demonstrated by scanning electron microscopy and energy-dispersive spectroscopy (SEM-EDS) spectrometry, affects the intergrown erionite as well. A structural characterization of the Ag-erionite phase (with dimension <100 μm) was possible by means of a Cu*K*α micro-focus source: structure solution pointed to $P6_3/mmc$ space group, indicating no change with respect to natural erionite. In agreement with previous studies, K ions in the cancrinite cage could not be exchanged, whereas Ag^+ is found in the *eri* cavity.

Keywords: Zeolites, Ag-levyne, LEV, Ag-erionite, X-ray diffraction, Molecular Dynamics; Microporous Materials: Crystal-Chemistry, Properties, and Utilizations