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A new framework topology in the dehydrated form of zeolite levyne

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ABSTRACT

The thermoelastic behavior and structural evolution of a natural levyne-Ca [$(\mathrm{Ca}_{7.8}\ \mathrm{Na}_{2.2}\mathrm{K}_{1.1})_{\Sigma 11.1}\mathrm{Al}_{20.0}\mathrm{Si}_{34.2}\mathrm{O}_{108}\cdot 51.5\mathrm{H}_2\mathrm{O}$; $R3m$; a = 13.377(4) Å, c = 22.870(1) Å, V = 3544.1(3) Å^3] were studied by both *T*-resolved synchrotron X-ray powder diffraction (SR-XRPD) between room temperature and 800 °C, and by conventional-source high-temperature single-crystal X-ray diffraction (SC-XRD). Above 230 °C, water loss and reallocation of extraframework cations induce the straining and consequent breaking of T-O-T bridges in the D6R, with resulting migration of tetrahedral cations to new tetrahedral sites. The new tetrahedra share an edge with the previously occupied tetrahedra. This phenomenon gives rise to a new topology, which coexists to about 40%, with the original one. The new framework consists of a sequence of a novel zeolitic cage (described as a 20-hedron formed by fourteen 6mR and six 4mR) and two consecutive cancrinite cages along [0001]. This topology, which is reported in the database of the hypothetical zeolite structures as 166_2_293, belongs to the ABC-6 family and can be described by the following sequence of 6-rings: **ABCBCACAB**, to be compared with that of levyne AABCCABBC. In the new topology the extraframework cations are distributed over 3 new sites: one at the center of the 6mR ⊥ [0001] shared by the two cancrinite cages, one near the center of the 6mR ⊥ [0001] at the base of the new cage, and a last one in a 6mR window of the new cage. The 8mR bidimensional channel system originally present in levyne is therefore absent in the new topology and hence molecular diffusion is likely to be partially hindered in the dehydrated form. The phase transition is not completely reversible, at least in the short term, as only partial rehydration was demonstrated.

Keywords: Zeolites, diffraction, high temperature, phase transition