

Tschörtnerite, a copper-bearing zeolite from the Bellberg volcano, Eifel, Germany

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ABSTRACT

The new mineral tschörtnerite, ideally $\text{Ca}_4(\text{K,Ca,Sr,Ba})_3\text{Cu}_3(\text{OH})_8[\text{Si}_{12}\text{Al}_{12}\text{O}_{48}] \cdot x\text{H}_2\text{O}$, $x \geq 20$, occurs as well-formed cubes up to a maximum size of 0.15 mm in a Ca-rich xenolith at the Bellberg volcano near Mayen, Eifel, Germany. The light blue, transparent crystals are optically isotropic, $n = 1.504(2)$. Microprobe analysis (in weight percent) gave CaO 13.10, CuO 9.64, SrO 4.49, BaO 1.93, K_2O 1.37, Fe_2O_3 0.30, Al_2O_3 25.21, SiO_2 30.25, H_2O (calc. by difference) 13.71. The empirical formula based on 48 O atoms within the tetrahedral net is $\text{Ca}_{5.60}\text{Sr}_{1.04}\text{K}_{0.70}\text{Ba}_{0.30}\text{Cu}_{2.90}\text{Fe}_{0.09}\text{Al}_{11.85}\text{Si}_{12.06}\text{O}_{48}(\text{OH})_{8.44} \cdot 14.01\text{H}_2\text{O}$. Tschörtnerite is cubic, space group $Fm\bar{3}m$ [$a = 31.62(1)$ Å, $V = 31614$ Å³, $Z = 16$]. The density is $D_{\text{meas}} = 2.1$ g/cm³, $D_{\text{calc}} = 2.10$ g/cm³. Single-crystal X-ray investigations showed that tschörtnerite is a zeolite; the structure contains interconnection of double six-rings, double eight-rings, sodalite cages, truncated cubo-octahedra, and previously unknown 96-membered cages (tschörtnerite cage). A new structural unit is the $[\text{Cu}_{12}(\text{OH})_{24}]\text{Ca}_8\text{O}_{24}(\text{H}_2\text{O})_8$ cluster centered within the truncated cubo-octahedron. The cluster is formed by a rhombododecahedron-like arrangement of corner connected CuO_4 squares, the eight CaO_7 polyhedra are branched. The sodalite cage houses $\text{Ca}_4(\text{OH})_4\text{O}_{12}$ clusters of edge-sharing CaO_6 octahedra. Half-occupied (K,Ca,Sr,Ba) positions were located in the basal and top face of the double eight-rings, i.e., the border to the tschörtnerite cage. Within the large tschörtnerite cage only H_2O molecules were localized.