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

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Abstract

The new mineral tschörtnerite, ideally $Ca_4(K,Ca,Sr,Ba)_3Cu_3(OH)_8[Si_{12}Al_{12}O_{48}]\cdot xH_2O$, $x \geq 20$, 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 $Ca_{5.60}Sr_{1.04}K_{0.70}Ba_{0.30}Cu_{2.90}Fe_{0.09}Al_{11.85}Si_{12.06}O_{48}(OH)_{8.44}\cdot 14.01H_2O$. Tschörtnerite is cubic, space group $Fm\bar{3}m$ [$a = 31.62(1)$ Å, $V = 31614$ Å^3, $Z = 16$]. The density is $D_{meas} = 2.1$ g/cm^3, $D_{calc} = 2.10$ g/cm^3. 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 $[Cu_{12}(OH)_{24}]Ca_8O_{24}(H_2O)_8$ cluster centered within the truncated cubo-octahedron. The cluster is formed by a rhombdodecahedron-like arrangement of corner connected CuO_4 squares, the eight CaO_7 polyhedra are branched. The sodalite cage houses $Ca_4(OH)_4O_{12}$ 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.