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The crystal structure of lahnsteinite $Zn_4(SO_4)(OH)_6 \cdot 3H_2O$, a new mineral from Friedrichssegen, Germany

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A new mineral lahnsteinite was found on the dump of the Friedrichssegen mine, Lahn valley, Bad Ems district, Rhineland-Palatinate (Rheinland-Pfalz), Germany. It occurs in the supergene association including goethite, hydrozincite, pyromorphite and native copper. The new mineral forms soft colourless tabular crystals with perfect mica-like cleavage in one direction. A very pure grain with size 0.4 x 0.25 x 0.1 mm was selected for the X-ray investigation.

The empirical formula based on 13 oxygen atoms (Z=8) is: $(Zn_{3.53}Fe_{0.27}Cu_{0.11})(SO_4)_{0.98}(OH)_{5.86} \cdot 3.22H_2O$.

The triclinic unit-cell parameters are: a = 8.312(1) Å, b = 14.545(1) Å, c = 18.504(2) Å, α = 89.71(1)°, β = 90.08(1)°, γ = 90.13(1)°, V = 2237.3(3) Å^3. Diffraction experiment was carried out using Xcalibur S CCD diffractometer and contained 16314 $I > 2\sigma I$. The analysis of the diffraction reflections showed that the crystal symmetry could be described by monoclinic space group $P2_1$. However, searching for a structural model and its refinement remained problematic. Only the transition to the triclinic symmetry with space group $P1$ made it possible to determine the mineral structure. All calculations were performed with the AREN program [1]. The structure was solved by direct methods with an automatic iteration procedure. The refinement of the model converged to R = 10.7% [2].

The basic features of the composition and the structure of lahnsteinite are reflected in its crystal-chemical formula (Z=8): $[(Zn_{2.6}Fe_{0.3}Cu_{0.1})^{VI}(OH)_3][Zn^{IV}(OH)_3(H_2O)][SO_4]\ 2H_2O$, where Roman numerals denote the coordination of atoms, and square brackets separate the layer of edge-shared Zn-octahedra and isolated Zn- and S-tetrahedra. The OH groups and water molecules in vertex of Zn tetrahedra were determined by the bond-valence method according to Brese [3].

The basis of the structure is represented by brucite-like layers of Zn-octahedra which are characterized by six-membered rings with vacant central octahedra. Vacant octahedra are capped by Zn-tetrahedra above and below the plane of the sheet. Such type of octahedral-tetrahedral layers is present in namuwite, schulenbergite, ktenasite and some other minerals and synthetic compounds, where they are decorated by attached S-tetrahedra above and below the plane of the sheet as well.

There are two chemical and topology identical electro-neutral layers in the structure of lahnsteinite. The linkage between them is provided by hydrogen bonding via interlayer H_2O groups. Unlike namuwite [4], in lahnsteinite neighbouring layers are shifted relative to each other on 1/2 a. The period c/2 = 9.52 Å corresponds to the distance between the layers. The distribution of water molecules in the interlayer space does not fit to the center of symmetry and this is the main reason of the symmetry lowering.

Lahnsteinite fully corresponds to its synthetic analogue [5].

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