Contribution ID: **4** Type: **Oral contribution**

A mineral with new loop-branched sechser single chains Khurayyimite Ca7Zn4(Si2O7)2(OH)10 · 4H2O

Monday 15 March 2021 14:45 (20 minutes)

The mineral khurayyimite Caenter code here $Zn_4(Si_2O_7)_2(OH)_{10}\cdot 4H_2O$, (IMA 2018-140) was found in small cavities in altered spurrite marbles, in the northern part of the Siwaqa pyrometamorphic rock area, Central Jordan. It is a low-temperature, hydrothermal mineral and it forms at a temperature of ca. 100 ℃. It builds nearly 50 µm white or colourless, platy crystals arranged in up to 200-300 µm big spherulitic aggregates. Single-crystal X-ray diffraction experiments at ambient conditions were performed at the X06DA beamline at the Swiss Light Source (Paul Scherrer Institute, Villigen, Switzerland). Khurayyimite crystallises in space group P21/*c*, with unit cell parameters (*a*=11.2450(8), *b*=9.0963(5), *c*=14.0679(10)Å, β = 113.237(8)°, V = 1322.25(17)Å^3 and Z = 2. The average structure was solved using direct methods. All H-sites are located by difference Fourier analysis. The resulting structure model was refined up to R1= 0.02. The crystal structure of khurayyimite consists of sheets perpendicular to a. Each sheet is built by very unusual loop-branched sechser single chains $\{\mathrm{lB},1^1_\infty\}[^6Zn_4Si_4O_{21}]$. Voids between chains are filled by blocks of five Ca-octahedra and two CaO_7 polyhedra with additional OH groups and water molecules.

The loop-branched *sechser* single chains $\{\mathrm{lB},1^1_\infty\}[^6Zn_4Si_4O_{21}\ ]$ are made of dimers of Si_2O_7 and two types of $ZnO_2(OH)_2$ tetrahedra connected by corners. Loops of the chain contain three tetrahedra, analogous to *dreier* ring. Strong repulsive forces between the tetrahedra in *dreier* ring are pressing connecting O atoms as far as possible forming equilateral triangle with longer ZnO_4 edge (≈ 3.176 Å) and two shorter two SiO_4 edges (≈ 2.67). These repulsive forces are, according to Libau (1985), a possible reason for why such loops have not been observed more frequent.

Different combinations of chains and frameworks made of ZnO_4 and SiO_4 tetrahedra are known. In $ZnSiO_3$ (Morimoto et al. 1975), with Zn atoms in six and four-fold coordination, two pyroxene-like chains running along the c-direction are branched with two ZnO_4 tetrahedra forming four-membered loops. The crystal structure of the LT and HT forms of $BaZn_2Si_2O_7$ (Lin et al. 1999) exhibit a disilicate group Si_2O_7 linked via corners with ZnO_4 tetrahedra in a three-dimensional framework. In such a manner are created six member rings (2×Si_2O_7, 2×ZnO_4), four member-rings (2×SiO_4, 2×ZnO_4) and three-membered rings (1×SiO_4, 2×ZnO_4). Still, three-membered loops, made of Si_2O_7 and ZnO_4, like in khurayyimite, have not been observed yet.

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Session Classification: Inorganic crystal structures

Track Classification: Inorganic crystal structures