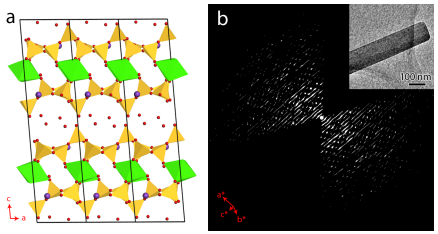

Figure 1. (a) Crystal structure of shlykovite viewed along the *b*-axis. Si: yellow tetrahedral; Ca: green octahedral; K: purple sphere; O: red sphere. (b) 3D reciprocal lattice of the synthetic shlykovite reconstructed from the RED data. Insert is the crystal from which the RED data was collected.

Keywords: electron crystallography, cryo-electron microscopy, electron diffraction, crystal structure, phyllosilicates, shlykovite.

MS15-P11 Cronstedtite-6T_2, a non-MDO polytype

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The new 6T_2 polytype of cronstedtite was identified, together with known 2H_1, 2H_2, 3T, 1M and probably 2M_1 polytypes in the mineral assemblage of an ore veinlet in the active quarry near Pohled, Czech Republic. The GPS co-ordinates of the locality are 49°35'50.326"N, 15°39'49.730"E [1].

Lattice parameters are a=5.4976(3), c=42.601(1) Å, Z=6, space group $P3_1$, composition $(Fe^{2+}_{2.515}\ Fe^{3+}_{0.485})(Si_{1.515}\ Fe^{3+}_{0.485})\ O_5\ (OH)_4$. The refinement converged to R_{obs} = 4.13% for 3244 independent reflections [2]. The polytype belongs to the subfamily (Bailey's group) A.

The structure is built of edge-sharing octahedral (*Oc*), and corner-sharing tetrahedral (*Tet*) sheets forming the 1:1 layers (corresponding to OD packets) by sharing apical corners of *Tet* sheet. There are two independent 1:1 layers, where the odd one is shifted with respect of the even one by $-(\mathbf{a}_1+\mathbf{a}_2)/3$ and raised by **c**/6 of the hexagonal cell. The sextuple multiplicity is achieved by mapping this pair of layers by 3_1 axis repeatedly to two other equivalent positions raised by **c**/3, 2**c**/3 There are two tetrahedral and three octahedral sites per each 1:1 layer (*T*1, *T*2, *M*1, *M*2, *M*3 in even layers, *T*11, *T*12, *M*11, *M*12, *M*13 in odd layers), all in general positions. The *M*3, *M*13 octahedra are smaller than *M*1, *M*2, *M*11, *M*12, thus *Oc* sheets in both layers are *meso-octahedral*. In even layers, however, the *M*2 octahedron is somewhat smaller than *M*1, so the *Oc* sheet is "transitional" to a *hetero-octahedral* character. The occupancies of Si:Fe in *T* positions were refined to: *T*1: 0.96:0.04(1), *T*2: 0.63:0.37(1), *T*11: 0.55:0.45(1), *T*12: 0.89:0.11(1). Ditrigonalization angles α are +11.4(5)°, and +10.9(5)°, in even and odd layers, respectively. Hydrogen positions were localized and geometries of hydrogen bonds linking the 1:1 layers were described. The structure is an example of OD structure of more than one kind of layers with a very low degree of desymmetrization. Cronstedtite-6T_2 is a non-MDO polytype, because more than one kind of packet triplets can be distinguished in the stacking sequence.

Another, quite different sextuple non-MDO polytype 6T_1 of the isostructural mineral lizardite [3] belongs to the group D.

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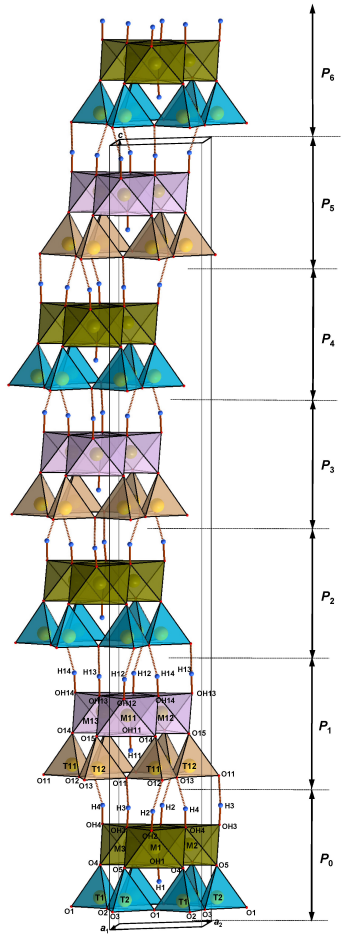

Figure 1. Structure of cronstedtite-6T_2, side view, projection close to a$_1$. For sake of clarity, only a small part of every OD packet (1:1 layer) is displayed: one ring of tetrahedra and three adjacent octahedra. Delimitations of packets (P_0, P_1, P_2 ….) are indicated on the right side.

Keywords: Cronstedtite, 1:1 layer silicate, polytypism, non-MDO polytype 6T2, crystal structure

MS15-P12 Chemical preparation, crystallographic characterization and vibrational study of condensed phosphates associated to Barium-Cesium $BaCs(P_3O_9)_2.2H_2O$

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Methods of chemical preparation and XRD data are reported for the new condensed phosphates associated to Barium-Cesium $BaCs(P_3O_9)_2.2H_2O$. $BaCs(P_3O_9)_2.2H_2O$ was prepared by the method of ion-exchange resin. This salt crystallizes in the monoclinic system, space group P21/n a = 7.6992(2) Å b = 12.3237(3) Å c = 11.8023(3) Å, β=101.181°(3)., M(20) = 1313,35; F (20) = 1004,53 and V = 333,95(2) (Å3), the vibrational study by IR absorption spectroscopy of the title compound reveals the presence of three bands and confirm the existence of non-equivalent positions of water molecules in the structure.

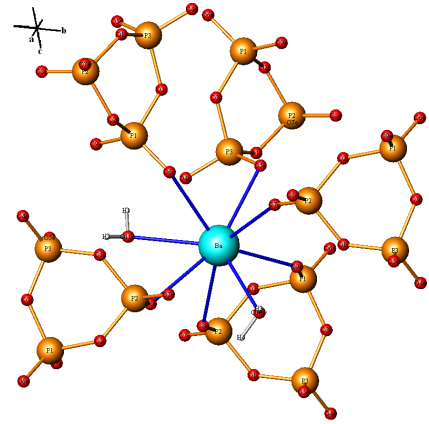

Figure 1. Projection of the structure Barium-Cesium $BaCs(P_3O_9)_2.2H_2O$

Keywords: condensed phosphates, ion-exchange resin, vibrational study