Cronstedtite-6$T_2$, a non-MDO polytype

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The new 6$T_2$ polytype of cronstedtite was identified, together with known 2$H_1$, 2$H_2$, 3$T$, 1$M$ and probably 2$M$ 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 $P\overline{3}$, composition (Fe$^{2+}0.515$ Fe$^{3+}0.485$) (Si$1.515$ Fe$^{3+0.485}$) O$_5$(OH)$_4$. The refinement converged to $R_{\text{obs}}=4.13\%$ 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 $-(a+a_1)/3$ and raised by $c/6$ of the hexagonal cell. The sextuple multiplicity is achieved by mapping this pair of layers by 31 axis repeatedly to two other equivalent positions raised by $c/3$, $2c/3$. 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 $\alpha$ are +11.4(5)º, and +10.9(5)º, 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-6$T_2$ 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 6$T_1$ of the isostructural mineral lizardite [3] belongs to the group D.

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References:
**MS15-P12 Chemical preparation, crystallographic characterization and vibrational study of condensed phosphates associated to Barium-Cesium**

BaCs\(\left(P_3O_9\right)_2\cdot2\text{H}_2\text{O}\)

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Methods of chemical preparation and XRD data are reported for the new condensed phosphates associated to Barium-Cesium BaCs\((P_3O_9)_2\cdot2\text{H}_2\text{O}\). BaCs\((P_3O_9)_2\cdot2\text{H}_2\text{O}\) was prepared by the method of ion-exchange resin. This salt crystallizes in the monoclinic system, space group P2\(_1\)/n a = 7.6992(2) Å b = 12.3237(3) Å c = 11.8023(3) Å, \(\beta=101.181\degree\)) M(20) = 1313.35, F(20) = 1004.53 and \(V = 333.95(2)\) (Å\(^3\)), 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](attachment:image.png)

**Figure 1.** Projection of the structure Barium-Cesium BaCs\((P_3O_9)_2\cdot2\text{H}_2\text{O}\)

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

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**Figure 1.** Structure of cronstedtite-6\(_T\), side view, projection close to \(a\). 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 \((P_0, P_1, P_2,\ldots)\) are indicated on the right side.

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