

## MS14-P13 Cronstedtite-1M, occurrence and structure

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Cronstedtite is trioctahedral 1:1 phyllosilicate of general formula  $(\text{Fe}^{2+}_{3-x}\text{Fe}^{3+}_x)(\text{Si}_{2-x}\text{Fe}^{3+}_x)\text{O}_5(\text{OH})_4$ , where  $0 < x < 0.8$ . Polytypes refined to date are: 3T, (Šmrček *et al.*, 1994); 1T, (Hybler *et al.*, 2000); 2H<sub>2</sub>, (Hybler *et al.*, 2002). Other polytypes including 1M are rare.

Pignatelli *et al.* (2013) prepared small (1-5 μm) cronstedtite crystals by reacting a claystone with iron at 60-90 °C. The TEM studies and SAED images revealed prevailing 1M polytype accompanied by less abundant 3T, and 2M<sub>1</sub>.

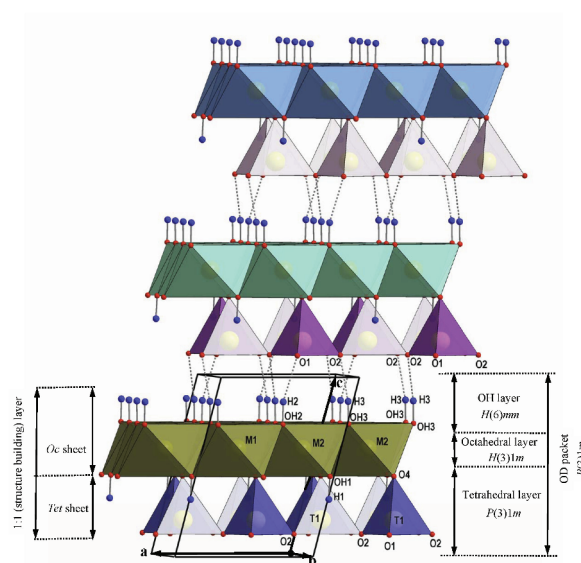
A rare crystal of cronstedtite-1M from Eisleben (Saxony-Anhalt, Germany) was identified by Mikloš (1975). This crystal was long time regarded as inappropriate for data collection because it provided diffusely streaked characteristic reflections due to the partial stacking disorder. Nevertheless, its recent re-investigation allowed data collection and structure refinement (Hybler, 2014).

Lattice parameters are:  $a = 5.5033(3)$ ,  $b = 9.5289(6)$ ,  $c = 7.3328(5)$  Å,  $\beta = 104.493(7)^\circ$ , space group *Cm*, formula  $(\text{Fe}^{2+}_{2.461}\text{Fe}^{3+}_{0.539})(\text{Si}_{1.461}\text{Fe}^{3+}_{0.539})\text{O}_5(\text{OH})_4$ ,  $Z = 2$ ,  $R_{\text{obs}} = 2.42\%$ . The structure is built of octahedral (*Oc*), and tetrahedral (*Tet*) sheets forming the 1:1 layer by sharing apical corners of *Tet* sheet. The polytype is generated by a monotonous repetition of  $-(\mathbf{a}_1 + \mathbf{a}_2)/3$  layer shifts ( $\mathbf{a}_1, \mathbf{a}_2$  are vectors of the hexagonal proto-cell), and it belongs to the Bailey's group A. There are two octahedral Fe sites M1 (at *m*), M2 (in a general position). The M2 octahedron is larger than M1, the *Oc* sheet is thus *meso-octahedral*. Only one tetrahedral position, T1, is occupied by Si/Fe in the ratio 0.731:0.269(9). The *Tet* sheet is ditrigonalized,  $\alpha = +12.7^\circ$ . Hydrogen atoms were localised, two of them are involved in hydrogen bonds, linking OH groups of the *Oc* sheet with basal oxygen atoms of the *Tet* sheet.

The study was partially supported by the grant 15-0204S of the Czech Science Foundation.

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**Figure 1.** Structure of cronstedtite-1M, model of coordination polyhedra, side view (close to monoclinic b). Delimitation of structure building and OD layers, as well as atom labels and hydrogen bonds are indicated. Note shifts of consecutive layers due to the stacking mode of the polytype.

**Keywords:** Cronstedtite, polytypism, OD structure