REFINEMENT OF THE CRYSTAL STRUCTURE OF CRONSTEDTITE-\(2H_2\)

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Abstract—The crystal structure of cronstedtite-\(2H_2\) was refined in a hexagonal cell, space group \(P6_3\), \(Z = 2\), using two acicular crystals from Wheal Maudlin, Cornwall, England, and from Příbram, Czech Republic. The Wheal Maudlin sample has the chemical composition \((\text{Fe}^{2+}\text{Fe}^{3+})(\text{Si}_2\text{Al}_0\text{O}_8)(\text{OH})_4\) and the Příbram sample has the composition \((\text{Fe}^{2+}\text{Fe}^{3+})(\text{Al}_2\text{Si}_2\text{O}_8)(\text{OH})_4\). The results of refinements are as follows: \(a = 5.500(1)\) Å, \(c = 14.163(2)\) Å, \(V = 371.08(8)\) Å\(^3\), \(R = 3.83\%\), from 381 independent reflections, and \(a = 5.4927(1)\) Å, \(c = 14.1481(2)\) Å, \(V = 369.70(4)\) Å\(^3\), \(R = 4.77\%\), from 1088 independent reflections for the Wheal Maudlin and Příbram samples, respectively. The best \(F_o\) vs. \(F_c\) agreement was achieved when the structure was interpreted as merohedral twin; several possible twinning laws are discussed. The cronstedtite layer consists of one tetrahedral sheet and one octahedral sheet. There is one octahedral (\(M1\)) position, occupied by Fe only, and two tetrahedral (\(T1, T2\)) positions in the structure. Refinement of occupancy of tetrahedral sites led to values \(\text{Si}:\text{Fe} = 0.45:0.55(1)\) (Wheal Maudlin) and \(0.432:0.568(8)\) (Příbram), space group \(P6_3\) \(\cdots P\) (Wheal Maudlin), \(1.691\) Å \(\text{Fe}^{3+}\) \(0.005\) \(\text{Fe}^{2+}\) 0.004 \(\text{Al}^3\) 0.004 \(\text{Al}^2\)). Because of a deficiency of tetrahedral Fe relative to the ideal formula in most of samples studied, the general formula is often reported as \((\text{Fe}^{2+},\text{Fe}^{3+})(\text{Si}_2\text{Al}_0\text{O}_8)(\text{OH})_4\) (where \(0 < x < 1\)). Presumably, a corresponding proportion of \(\text{Fe}^{3+}\) in the octahedral sites balances the replacement of \(\text{Si}^{4+}\) by \(\text{Fe}^{3+}\) in the tetrahedral sites.

Recently, we refined structures of two polytypes: \(3T\), space group \(P3_1\), \(a = 5.497(2)\) Å, \(c = 21.355(7)\) Å, \(R = 5.0\%\), from Kutná Hora, Czech Republic (Smrčok \textit{et al.}, 1994), and \(1T\), space group \(P31m\), \(a = 5.502(1)\) Å, \(c = 7.106(1)\) Å, \(R = 3.07\%\) from Herja, Romania, and \(a = 5.503(1)\), \(c = 7.104(1)\) Å, \(R = 2.24\%\) from Lostwithiel, England (Hybler \textit{et al.}, 2000). These polytypes represent OD subfamilies, or Bailey’s (1969, 1988) groups A and C, respectively. Earlier studies on cronstedtite of Steadman and Nuttall (1963, 1964), Steadman (1964), Mikloš (1975), Hybler (1997, 1998), Đurovic (1995, 1997), as well as an OD (ordered-disordered) interpretation of the structure presented by Dornberger-Schiff and Đurovic (1975a,b) were more thoroughly referred to in these papers (Smrčok \textit{et al.}, 1994; Hybler \textit{et al.}, 2000).

The first structure refinement of the \(2H_2\) polytype was reported by Geiger \textit{et al.} (1983). They studied a rare crystal of cronstedtite from Příbram, Czech Republic, with an unusually high Mg and Mn substitution for Fe in the octahedral sites. Because of the significant deviations from the hexagonal symmetry of the sample studied, they used a non-standard C-centered triclinic cell (\(a = 5.472(8)\), \(b = 9.467(19)\), \(c = 14.241(39)\) Å, \(\alpha = 90.015(20)\), \(\beta = 90.042(18)\), \(\gamma = 89.952(15)\)) Å, \(V = 737.72(28)\) Å\(^3\), space group symbol \(C1\), corresponding to a slightly deformed orthohexagonal cell. Their crystal contained multiple twins and out-of-step domains, but with a rather complicated structure model, they achieved \(R = 5.4\%\) for 1832 observed reflections.

It is worth mentioning refined structures of related triotahedral 1:1 layer silicates: lizardite-\(1T\) (Mellini, 1982; Mellini and Zanazzi, 1987; Mellini and Viti, 1994; Zhukhlistov and Zvyagin 1998), lizardite-\(2H_4\) (Mellini and Zanazzi, 1987), Al-bearing lizardite-\(2H_2\) (Brigatti \textit{et al.}, 1997), amesite-\(2H_2\), in C-centered triclinic cell (Hall and Bailey, 1979; Anderson and Bailey, 1981), amesite-\(2H_1\) (Zheng and Bailey, 1997), non-standard triclinic polytype of amesite (Wiewiora \textit{et al.}, 1991), lizardite-\(1T\) and \(2H_1\) at high temperatures (Guggenheim and Zhan, 1998). The modulated structure of grena

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