

The structure of Mn-rich tuperssuatsiaite: A palygorskite-related mineral

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ABSTRACT

The structure of tuperssuatsiaite from the Aris phonolite in central Namibia was refined to an R index of 0.075 for 905 observed reflections [$I > 2\sigma(I)$] obtained with a four-circle X-ray diffractometer. Tuperssuatsiaite is monoclinic, $C2/m$, with $a = 14.034(7)$, $b = 17.841(7)$, $c = 5.265(2)$ Å, and $\beta = 103.67(4)^\circ$. Microprobe analysis gave an average composition of $\text{Na}_{1.87}\text{Fe}_{2.14}\text{Mn}_{0.48}\text{Ti}_{0.14}\text{Al}_{0.03}\text{Mg}_{0.02}[\text{Si}_8\text{O}_{20}](\text{OH})_2 \cdot n(\text{H}_2\text{O})$, with five octahedral sites. The structure is closely related to that of palygorskite $\text{Mg}_5[\text{Si}_8\text{O}_{20}](\text{OH})_2 \cdot \text{H}_2\text{O}$. Tuperssuatsiaite consists of ribbons of SiO_4 tetrahedra linked by bands of octahedra running parallel to c . Channels occur that could be occupied by H_2O as in palygorskite. The octahedral band contains three edge-sharing, six-coordinated sites labeled M1, M2, and M3. This band consists of alternating M3-M1-M3 and M2-M2 octahedra along [001]. The M1 and M2 sites both contain Fe and Mn, and M3 is occupied by Na. Bond-valence calculations indicate a formal charge of 2.48 for M1 and 2.67 for M2, i.e., a charge distribution of $2R^{3+}:1R^{2+}$. Octahedral angle variance and volume are similar for both sites, indicating disorder in the distribution of Fe and Mn atoms between the sites. Charge balance requirements agree with the presence of Fe^{3+} and Mn^{2+} .