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A new trigonal (3*T*) polytype of chloritoid, $Fe^{2+}Al_2(SiO_4)O(OH)_2$, from the Kosoy Brod deposit, Middle Urals, Russia: Chemical composition, crystal structure, and complexity analysis

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Abstract

A new trigonal (3*T*) polytype of chloritoid, $Fe^{2+}Al_2(SiO_4)O(OH)_2$, a rock-forming schist mineral, has been found in samples from the chloritoid type locality, Kosoy Brod deposit, Middle Urals, Russia. Single-crystal X-ray diffraction indicated that the mineral crystallizes in the space group $P3_2$, $a = 5.4890(2)$, $c = 26.7612(14)$ Å, $V = 698.27(6)$ Å^3. The structure was solved and refined to $R_1 = 0.0564$ ($wR_2 = 0.1545$) for 2534 unique reflections with $I > 2\sigma(I)$. After known triclinic (1*A*) and monoclinic (2M_2) modifications, chloritoid-3*T* is the third chloritoid polytype. The crystal structures of all three polytypes are based upon the same types of octahedral and tetrahedral layers. The main difference between the polytypes is in the stacking of dioctahedral layers L2 and trioctahedral layers L1 interconnected with a tetrahedral net. The new polytype (3*T*) can be detected by its powder X-ray diffraction pattern. The complexity analysis indicates that the crystal structure of chloritoid-3*T* is the most complex among known polytypes. The discovery of a new chloritoid polytype is essential for the potential development of chloritoid-based geothermometers and has implications for the general conception of polytypism.

Keywords: Chloritoid, crystal structure, polytype, structure topology, layered mineral, X-ray diffraction