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# Jahnsite-(NaFeMg), a new mineral from the Tip Top mine, Custer County, South Dakota: Description and crystal structure

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## Abstract

Jahnsite-(NaFeMg), $NaFe^{3+}Mg_2Fe^{3+}_2(PO_4)_4(OH)_2 \cdot 8H_2O$, space group $P2/a$, $a$ = 15.0811(16), $b$ = 7.1403(8), $c$ = 9.8299(11) Å, β = 110.445(1)°, $V$ = 991.8(2) Å$^3$, and $Z$ = 2, is a new mineral from the Tip Top mine, Custer County, South Dakota. It occurs as the dominant chemical zone in transparent pseudo-orthorhombic twinned prisms up to 1 mm long with shallow wedge-like terminations, both as isolated twinned crystals and in subparallel to divergent intergrowths. The crystals are yellow with orange-red bands just below the terminations. The mineral has a white streak, vitreous luster, Mohs hardness of 4, and good {001} cleavage. The measured density is 2.58(2) g/cm$^3$, and the calculated density is 2.608 g/cm$^3$. It is optically biaxial (–), with α = 1.632(1), β = 1.669(1), γ = 1.671(1) (589 nm); $2V$ (meas.) = 25(5)°, $2V$ (calc.) = 26°; dispersion: $r > v$, very strong; orientation: $Y = b$, $Z \wedge a = +28°$ (in β obtuse); pleochroism: $X$ = colorless, $Y$ and $Z$ = beige; $Y = Z > X$. Electron microprobe analyses provided: $Na_2O$ 2.82, CaO 0.34, MnO 0.32, MgO 10.27, $Fe_2O_3$ 27.35, $P_2O_5$ 35.93, $H_2O$ 21.58 (calc.), total 98.61, which in terms of the general formula for the whiteite-jahnsite group $XM1M2_2M3_2(PO_4)_4(OH)_2 \cdot 8H_2O$, yields the empirical formula: $(Na_{0.72}Ca_{0.05}Mn^{2+}_{0.04})(Fe^{3+}_{0.72}Mg_{0.01})Mg_{2.00}Fe^{3+}_{2.00}(PO_{3.77}OH_{0.23})_4(OH)_2 \cdot 8H_2O$. Crystal structure refinement ($R_1$ = 0.041) supports these cation site assignments. Typical crystals have as many as five chemical zones from base to termination corresponding to the following jahnsite species: jahnsite-(NaMnMg), jahnsite-(NaFeMg), jahnsite-(CaMnMg), jahnsite-(NaFeMg), jahnsite-(CaMgMg). The characterization of the new mineral jahnsite-(NaFeMg) is based upon the second zone listed, which corresponds to roughly 80% of the crystal volume. Jahnsite-(NaMnMg) and jahnsite-(CaMgMg) also represent new species; however, the very small volume of these zones is insufficient to permit complete characterization of these species. Jahnsite-(NaFeMg) is the first member of the whiteite-jahnsite group in which a monovalent cation ($Na^+$) predominantly occupies the X site and a trivalent cation ($Fe^{3+}$) the M1 site. The structure differs from that determined for jahnsite-(CaMnMg) in that the X site is [8]-coordinated and the M1 and P1 polyhedra exhibit greater distortions caused by cation-cation repulsion across their shared edges. The determination of H positions allows the elucidation of a definitive H-bonding scheme.

**Keywords:** Jahnsite, Tip Top mine, new mineral, crystal structure, whiteite-jahnsite group, crystal chemistry, pegmatite phosphate