Oxy-dravite, Na(Al$_2$Mg)(Al$_5$Mg)(Si$_6$O$_{18}$)(BO$_3$)$_3$(OH)$_5$O, a new mineral species of the tourmaline supergroup

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ABSTRACT

Oxy-dravite, Na(Al$_2$Mg)(Al$_5$Mg)(Si$_6$O$_{18}$)(BO$_3$)$_3$(OH)$_5$O, is a new mineral of the tourmaline supergroup. The holotype specimen originates from the locality of Osarara (Narok district, Kenya) and occurs in quartz-muscovite schist. Crystals of oxy-dravite are dark red, partially translucent with a vitreous luster, a pink streak, and conchoidal fracture. It has a Mohs hardness of approximately 7, and a calculated density of 3.073 g/cm$^3$. In plane-polarized light, oxy-dravite is pleochroic (O = orange and E = pink) and uniaxial negative: $\omega = 1.650(5)$, $\epsilon = 1.620(5)$. Oxy-dravite is rhombohedral, space group $R3m$, with the unit-cell parameters $a = 15.9273(2)$ Å, $c = 7.2001(1)$ Å, $V = 1581.81(4)$ Å$^3$, $Z = 3$. Chemical characterization based on electron microprobe analysis, single-crystal structure refinement, Mössbauer, and optical spectroscopy, resulted in the empirical structural formula:

$$X(Na_{0.83}K_{0.15}O_{0.02})_{1.00}Y(Al_{1.34}Fe^{3+}_{0.58}Mg_{1.03}Fe^{2+}_{0.03}Ti_{0.02})_{3.00}Z(Al_{4.95}Mg_{1.03}Fe^{3+}_{0.02})_{6.00}T(Si_{5.98}Al_{0.02}O_{18})_{6.00}B(BO_3)_3V(OH)W(OH,F)_{1.00}.$$ 

While the end-member formula of oxy-dravite may be formalized as Na$^+(Al)_{2}(Al,Mg)\cdot SiO_{18}(BO_3)_{3}(OH)_5 O$, the most representative structural formula is Na$^+(Al,Mg)_{2} SiO_{18}(BO_3)_{3}(OH)_5 O$. The difference between these two formulas is solely in Al-Mg order-disorder, i.e., there is no difference in chemical composition. Although the Mg-Al disorder over the Y and Z sites is controlled by the short-range bond-valence requirements of O$^2-$ at the O1 (= W) site, the amount of Mg at the Z site is a function of the degree of cation size mismatch at Z.

The crystal structure of oxy-dravite was refined to statistical index $R1$ of 1.17% using 1586 equivalent reflections collected with MoK$_\alpha$ X-radiation. Oxy-dravite is chemically related to dravite (and fluor-dravite), NaMg$_{1.5}$Si$_{0.5}$O$_{18}(BO_3)_{3}(OH)_5(OH,F)$, by the heterovalent substitution Al$^{3+} + O^{2-} \rightarrow Mg^{2+} + (OH,F)^{3-}$.

**Keywords:** Oxy-dravite, tourmaline, new mineral species, crystal-structure refinement, electron microprobe, Mössbauer spectroscopy, order-disorder