Oxy-dravite, Na(Al₂Mg)(Al₅Mg)(Si₆O₁₈)(BO₃)₃(OH)₃O, a new mineral species of the tourmaline supergroup

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ABSTRACT

Oxy-dravite, Na(Al₂Mg)(Al₅Mg)(Si₆O₁₈)(BO₃)₃(OH)₃O, 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/cm³. In plane-polarized light, oxy-dravite is pleochroic (O = orange and E = pink) and uniaxial negative: $\omega = 1.650(5)$, $\varepsilon = 1.620(5)$. Oxy-dravite is rhombohedral, space group *R*3*m*, with the unit-cell parameters *a* = 15.9273(2) and *c* = 7.2001(1) Å, *V* = 1581.81(4) Å³, *Z* = 3. Chemical characterization based on electron microprobe analysis, single-crystal structure refinement, Mössbauer, and optical spectroscopy, resulted in the empirical structural formula:

 ${}^{X}(Na_{0.83}\Box_{0.15}K_{0.02})_{\Sigma1.00} \,\, {}^{Y}(Al_{1.34}Fe_{0.58}^{3+}Mg_{1.03}Fe_{0.03}^{2+}Ti_{0.02})_{\Sigma3.00} \,\, {}^{Z}(Al_{4.95}Mg_{1.03}Fe_{0.02}^{3+})_{\Sigma6.00} \,\, {}^{T}(Si_{5.98}Al_{0.02}O_{18})_{\Sigma6.00} \,\, {}^{B}(BO_{3})_{3} \,\, {}^{V}(OH)_{3} \,\, {}^{V}(O_{0.76}OH_{0.24})_{\Sigma1.00}.$

While the end-member formula of oxy-dravite may be formalized as $Na^{Y}(Al_{3})^{Z}(Al_{4}Mg_{2})$ Si₆O₁₈(BO₃)₃(OH)₃O, the most representative structural formula is $Na^{Y}(Al_{2}Mg)^{Z}(Al_{5}Mg)$ Si₆O₁₈(BO₃)₃(OH)₃O. 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 O²⁻ at the O1 (\equiv 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 *R*1 of 1.17% using 1586 equivalent reflections collected with MoK α X-radiation. Oxy-dravite is chemically related to dravite (and fluor-dravite), NaMg₃Al₆Si₆O₁₈(BO₃)₃(OH)₃(OH,F), by the heterovalent substitution Al³⁺ + O²⁻ \rightarrow Mg²⁺ + (OH,F)¹⁻.

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