

Crystal structure analyses of four tourmaline specimens from the Cleopatra's Mines (Egypt) and Jabal Zalm (Saudi Arabia), and the role of Al in the tourmaline group

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ABSTRACT

Fe-rich “oxydravite” and dravite from the Late Proterozoic ophiolitic mélangé of the Arabo-Nubian Shield, located in Egypt and Saudi Arabia, were structurally and chemically characterized by using crystal structure refinement based on single-crystal X-ray diffraction data, electron microprobe analysis, and Mössbauer spectroscopy. Structural formulae obtained by optimization procedures indicate disordering of Al, Mg, and Fe²⁺ over the Y and Z sites, and an ordering of Fe³⁺ at Y. The disordering can be explained by the substitution mechanisms $2^Y\text{Mg}+^Z\text{Al}+^W\text{OH} = 2^Y\text{Al}+^Z\text{Mg}+^W\text{O}^{2-}$ and $2^Y\text{Fe}^{2+}+^Z\text{Fe}^{3+}+^W\text{OH} = 2^Y\text{Fe}^{3+}+^Z\text{Fe}^{2+}+^W\text{O}^{2-}$, which are consistent with reducing the mismatch in dimensions between YO₆ and ZO₆ octahedra.

To explain the Mg-Al disordering process, as well as the occurrence of B at the T site in tourmaline, analogies have been drawn between the crystal structure of tourmaline and that of lizardite. A critical constraint in both structures is the geometrical fit of the six-membered tetrahedral ring with the attached group of three YO₆ octahedra. In tourmaline, the disordering of Mg and Al over Y and Z relieves the strain due to the misfit in dimensions of the larger triads of edge-sharing MgO₆ octahedra and the smaller Si₆O₁₈ tetrahedral rings. In Al-rich tourmaline, where the octahedral cluster is smaller, the strain can be relieved by incorporating B in the tetrahedra. An opposite effect is observed by substitution of Al for Si at the tetrahedral site in Mg-rich tourmaline. Because the Al radius is intermediate between those of Mg and Si, Al plays an important structural role in accommodating the potential misfit between YO₆, ZO₆, and TO₄ polyhedra. The amount of Al and its distribution in the structure strongly affects the values of the unit-cell parameters of tourmaline and yields volume variations according to a quadratic model. This results from the effect of ^ZAl combined with the occurrence of B at T in Al-rich tourmaline. ^ZAl has a greater effect than ^YAl as long as Al does not fully occupy the Z site.

Keywords: Chemical analysis, tourmaline, crystal structure, Mössbauer spectroscopy, order-disorder, XRD data