**Crystal chemistry of tourmalines from Minas Gerais, Brazil**

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Keywords: tourmalines, Minas Gerais, Brazil, crystal structure

The State of Minas Gerais, located in the south-eastern part of Brazil, is one of the main producers of high-quality tourmalines in the world. Officially discovered in this region at the dawn of the 17th century, these minerals have remained misunderstood for a long time because of their complexity. They are now considered as a supergroup of rhombohedral borosilicates with a *R*3*m* space group and a general formula that may be written as *XY*3*Z*6[*T*6O18](BO3)3*V*3*W*, in which *X*, *Y*, *Z* and *T* represent cation groups present on the [9]*X*, [6]*Y*, [6]*Z*, and [4]*T* crystallographic sites. Anions in groups *V* and *W* occupy the [3]O3 and [3]O1 sites in the structure, respectively (1-2).

Most of the tourmalines from Minas Gerais occur in the granitic pegmatites of the Eastern Brazilian Pegmatite Province (EBPP) and in the magmatic and hydrothermal environments of the Quadrilatero Ferrifero (QF). Therefore, several samples from these different regions have been submitted to single crystal X-ray diffraction experiments in order to refine their structure (Rigaku Xcalibur diffractometer, EOS detector, MoKα radiation). The samples were also analysed by X-ray fluorescence spectroscopy to get a first idea of their chemical composition (Thermo Fischer Niton XL3t spectrometer, GOLDD detector).

Tourmalines from Minas Gerais, despite their diverse origins, often show similar compositions varying between the elbaite-schorl and schorl-dravite series. Elbaite is by far the most represented species, then comes schorl and finally dravite. The main substitutions take therefore place between the major elements (Al+Li) (elbaite), Fe (schorl) and Mg (dravite) on the *Y* crystallographic site.

These compositional data are confirmed by the structure refinements, which show unit-cell parameters in the ranges 15.83 Å ≤ *a* ≤ 15.89 Å and 7.09 Å ≤ *c* ≤ 7.12 Å, consistent with an elbaite-to-schorl composition according to previous studies. The tourmaline structure is characterized by tetrahedral *T*-sites mainly occupied by Si, and linked by their corners to form [*T*6O18] rings located in planes perpendicular to the *c* axis. Three *Y* octahedral sites share their edges to form trimers, and [*Z*O6] octahedra are linked by their edges to the periphery of these trimers. B sites form triangular polyhedra, sharing their corners with the two types of octahedra. The 9-coordinated *X* sites are located along the *c* axis, outside the plane containing the rings. Finally, the *W* anions occupy the O1 sites located along the *c* axis, in a central position of the unit-cell, and each *V* anion, located at the O3 position, is shared by an [*Y*O6] octahedron and by a [*Z*O6] octahedron.

1. Hawthorne, F.C. & Henry, D.J. (1999). *European Journal of Mineralogy*, 11(2), 201-215.
2. Hawthorne, F.C. & Dirlam, D.M. (2011). *Elements*, 7(5), 307-312.