A STRUCTURAL INVESTIGATION OF TOURMALINES FROM MOZAMBIQUE

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Minerals of the tourmaline supergroup are constituted by rhombohedral borosilicates with a *R*3*m* space group, and with the general formula $XY_3Z_6[T_6O_{18}](BO_3)_3V_3W$. Over the last decade, Mozambique has established itself as one of the most important producers of high-quality tourmalines in the world; those samples mainly occur in pegmatites of the Alto Ligonha region. A set of 68 tourmalines from that region were investigated with various techniques, including single-crystal X-ray structure refinements, electron-microprobe analyses, and Laser Ablation Inductively Coupled Plasma Time-Of-Flight Mass Spectrometry (LA-ICP-TOF-MS). Most of the samples were collected on the field, in 15 pegmatites ranging from well-known to new deposits. A detailed mapping of those pegmatites has been realized whenever possible, and the position of each sample in its respective pegmatite is accurately known.

Chemically, the first analysed tourmaline samples are Na-dominant on the X site, and therefore, belong to the alkali group. They correspond to fluor-elbaites, where similar proportions of Al and Li are sharing the Y positions, while the W site is dominated by F. These fluor-elbaites tend to align along the fluor-elbaite to fluor-schorl solid solution, with a noticeable replacement of Al and Li by Fe^{2+}, observed in zoned samples. Three samples from the Marinia and Mavuco deposits also display strong Mn enrichments, while being completely Fe-free.

For most samples, single-crystal data indicate *a* unit-cell parameters varying between 15.8647 and 15.9503 Å, and *c* parameters ranging from 7.107 to 7.1545 Å. These values are similar to those obtained for Brazilian tourmalines of the fluor-elbaite to fluor-schorl solid solution. However, two crystals from the Marinia pegmatite display very high unit-cell parameters values ($16.008 < a < 16.0474$ Å; $7.2193 < c < 7.2338$ Å), which could be explained by the presence of Mn^{3+} in the structure. A detailed cation distribution has also been established, showing that the B site is fully occupied by boron, and that the T site is mainly occupied by Si and sometimes by minor amounts of B. The X site contains vacancies, Na, K, and Ca, and the Y site is occupied by Li, Al, Fe^{2+}, and minor amounts of Mn^{2+} and Mg.

Finally, the trace element contents, including REE, are discussed and appear to be influenced by both the geochemical pegmatitic context, and by crystal-chemical constraints.