

## **Structural study and cation distribution of elbaite-schorl tourmaline**

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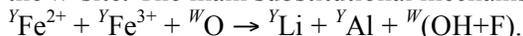
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### **Abstract**

The crystal-chemistry of 13 elbaite–schorl tourmaline crystals from the Cruzeiro pegmatite (Minas Gerais, Brazil) was studied by a multi-analytical approach (SREF, EMPA, SIMS, MS). Effective cation radii in *Y*, *Z* and *T* sites and site populations were refined by a minimization procedure (Bosi and Lucchesi 2004). Specific cation radii were refined from 44 tourmaline samples accurately characterized. These cation radii were successfully tested on 90% of the published tourmaline data. Results reveal that the ionic radii of Al and Fe<sup>3+</sup> in *Z* site are larger in samples with <sup>Z</sup>R<sup>2+</sup> < 0.4 apfu than in samples with <sup>Z</sup>R<sup>2+</sup> > 0.4 apfu.

The studied crystals belong to the alkali group. Elbaite crystals are O<sup>2-</sup>-free in the *W* and *V* sites and show OH<sup>-</sup> content in O2 site (up to 0.2 apfu). Conversely, schorl crystals always show O<sup>2-</sup> in the *W* site. The main substitutional mechanism is the dehydroxylation type:



Along the elbaite–schorl series, the *T* site is characterized by <sup>T</sup>Si → <sup>T</sup>Al substitution. Mean bond distance <*X*-O> is linearly correlated with vacancy content in crystals with (OH+F) ≤ 4 apfu, whereas it is almost constant in crystals with (OH+F) > 4, that is with OH on O2 position. The *Y* site is populated by Al, Li, Fe<sup>3+</sup>, Fe<sup>2+</sup>, Mg and Mn<sup>2+</sup>, with <sup>Y</sup>Al never lower than 0.87 apfu and (Al+Fe<sup>3+</sup>) never lower than 1.17 apfu. Moreover, the most important substitution is <sup>Y</sup>Fe<sup>2+</sup> ↔ <sup>Y</sup>Li, which shows about a 1:1 slope. The *Z* site is almost fully occupied by R<sup>3+</sup> (with <sup>Z</sup>Al largely dominant). The substitution <sup>Z</sup>Fe<sub>tot</sub> ↔ <sup>Z</sup>Al explains the inverse correlation shown by <*Z*-O> versus <sup>Z</sup>Al.

In the elbaite compositional range, lattice parameters are functions of <*Y*-O>, whereas in the schorl range they are essentially functions of <*Z*-O>. Along the whole elbaite–schorl series, chemical substitutions in the *Y* site are more extensive than those in the *Z* site, and these variations are paralleled by size increase of *Y* which is far larger than that of *Z*. In spite of this, lattice parameters increase as a function of <*Y*-O> as much as <*Z*-O>. Such a surprising behavior is due to the role of the [ZO<sub>6</sub>] polyhedra, which extend along *a* and *c* axes to form the skeleton of the tourmaline. Therefore, any change in *Z* size is a change in the whole structure.

### **References**

Bosi, F. and Lucchesi, S. (2004) Crystal chemistry of the schorl–dravite series. *European Journal of Mineralogy*, 16, 335-344.