**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$^{3+}$ in Z site are larger in samples with $Z_{R}^{2+} < 0.4$ apfu than in samples with $Z_{R}^{2+} > 0.4$ apfu.

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

$$^{Y}Fe^{2+} + ^{Y}Fe^{3+} + ^{W}O \rightarrow ^{Y}Li + ^{Y}Al + ^{W}(OH+F).$$

Along the elbaite–schorl series, the T site is characterized by $^{T}Si \rightarrow ^{T}Al$ substitution. Mean bond distance $<X-O>$ is linearly correlated with vacancy content in crystals with $(OH+F) \leq 4$ 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$^{3+}$,Fe$^{2+}$, Mg and Mn$^{2+}$, with $^{Y}Al$ never lower than 0.87 apfu and $(Al+Fe^{3+})$ never lower than 1.17 apfu. Moreover, the most important substitution is $^{Y}Fe^{2+} \leftrightarrow ^{Y}Li$, which shows about a 1:1 slope. The Z site is almost fully occupied by $^{Z}R^{3+}$ (with $^{Z}Al$ largely dominant). The substitution $^{Z}Fe_{tot.} \leftrightarrow ^{Z}Al$ explains the inverse correlation shown by $<Y-O>$ versus $^{Z}Al$.

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$_6$] 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**