

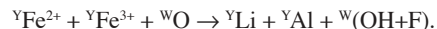
Crystal chemistry of the elbaite-schorl series

**FERDINANDO BOSI,* GIOVANNI B. ANDREOZZI, MARCELLA FEDERICO, GIORGIO GRAZIANI,
AND SERGIO LUCCHESI**

Dipartimento di Scienze della Terra, Università degli Studi di Roma “La Sapienza” Piazzale A. Moro 5, 00185 Roma, Italy

ABSTRACT

The crystal-chemistry of 13 elbaite-schorl tourmaline crystals from the Cruzeiro pegmatite (Minas Gerais, Brazil) was studied with a multi-analytical approach (SREF, EMPA, SIMS, MS). Effective cation radii at the Y and Z sites and site populations were refined by a minimization procedure. The results indicate that the crystals belong to the alkali group. Elbaite crystals are O²⁻-free at the W and V sites and show OH content at the O2 site (up to 0.2 apfu). Conversely, schorl crystals always show O²⁻ at the W site. The main substitutional mechanism is the dehydroxylation type:



The T site is characterized by ^TSi → ^TAl substitution. <X-O> is linearly correlated with vacancy content in crystals with (OH + F) ≤ 4, whereas it is almost constant in crystals with OH at the O2 position. Along the series, <Y-O> is inversely correlated with ^YAl. The Z site is almost fully occupied by R³⁺ (with ^ZAl largely dominant) and the ^ZFe_{tot} ↔ ^ZAl substitution explains the inverse correlation of <Z-O> with ^ZAl.

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, both chemical substitutions and size increase of Y are far larger than those of Z. In spite of this, lattice parameters increase with <Y-O> as much as with <Z-O>. This is due to the role of the [ZO₆] polyhedra, which extend along **a** and **c** to form the skeleton of the tourmaline structure. Therefore, any change in the size of Z leads to a change in the whole structure.