

Symmetry and crystal structure of biaxial elbaite-liddicoatite tourmaline from the Transbaikalia region, Russia

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ABSTRACT

Optical anomalies and crystal structures have been studied for an elbaite-liddicoatite tourmaline specimen from the Malkhan pegmatite field (Transbaikalia region, Russia). The specimen is characterized by a complicated zoning and sector zoning distribution of anomalous biaxiality, with the axial angle $2V$ increasing from 3 up to 23° going from the first to the last growth zones of the most developed growth sector, $o\{02\bar{2}1\}$. The crystal structures of three samples cut out from different growth zones of that sector and characterized by the axial angles 11, 16, and 23° were refined in the trigonal space group $R3m$ as well as in its monoclinic and triclinic subgroups Cm , $R1$, and $P1$, respectively ($R = 0.019$ – 0.039). The final choice of the low symmetry space group $R1$ is based on the analysis of the diffraction patterns and on the results of crystal structures refinements, which revealed ordered Al/Li distributions over the Y octahedral sites. The degree of order at Y sites correlates with the axial angle $2V$, which implies a causal relationship. The Al/Li ordering reflects the geometrical differences of the octahedral sites with respect to the growth front orientation. The results obtained suggest that a growth dissymmetrization mechanism is the main reason for the observed cation ordering and optical anomalies.

Keywords: Optical anomalies, tourmaline crystal structure, elbaite, liddicoatite, growth ordering of atoms, dissymmetrization