

## STRUCTURAL INVESTIGATION OF A POSSIBLY NEW OH-DOMINANT LIDDICOATITE

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Several Al-rich and Li-bearing tourmalines of pegmatite pockets from different localities were structurally characterised. A colourless tourmaline sample from a pegmatite in Madagascar with lattice parameters  $a = 15.817(1)$ ,  $c = 7.097(1)$  Å was refined by single-crystal X-ray diffraction methods to a  $R1$  value of 1.7%. The obtained formula can be written as  $\sim^X(\text{Ca}_{0.8}\square_{0.2})^Y(\text{Li}_{1.7}\text{Al}_{1.3})^Z\text{Al}_6^T(\text{Si}_{5.8}\text{B}_{0.2})\text{O}_{18}(\text{BO}_3)_3^V(\text{OH})_3^W(\text{OH})$ . Usually samples from this locality are highly enriched in Ca. The  $\langle X\text{-O} \rangle$  distance is 2.627(1) Å, what is in agreement with a dominant Ca occupancy. The  $Y$  site is dominated by Li. The  $Y$ -site occupancy fits very well with the estimated  $\langle Y\text{-O} \rangle$  distance of 2.020(1) Å. The  $Z$  site is only occupied by Al and exhibits a  $\langle Z\text{-O} \rangle$  distance of 1.903(1) Å, that is, within the standard deviation, typically for a  $Z$  site, which is filled by Al. The  $T$  site was refined to  $(\text{Si}_{5.8}\text{B}_{0.2})$ . This is consistent with a reduced  $\langle T\text{-O} \rangle$  distance of 1.616(1) Å. The  $\langle T\text{-O} \rangle$  distance of tourmaline, where the  $T$  site is completely occupied by Si is usually in the range of 1.619-1.620 Å. In a preliminary refinement the  $W$  site was refined with  $\text{O} \leftrightarrow \text{F}$ . However, the resulting F value was insignificant. Based on a charge-balanced formula this site has to be occupied by OH, and not by oxygen alone. Although the microprobe analysis is still in progress, the endmember formula of this investigated tourmaline, only based on the structural refinement, can be written as  $\text{Ca}(\text{Li}_2\text{Al})\text{Al}_6\text{Si}_6\text{O}_{18}(\text{BO}_3)_3(\text{OH})_3(\text{OH})$ . Compared to the F-rich endmember  $\text{Ca}(\text{Li}_2\text{Al})\text{Al}_6\text{Si}_6\text{O}_{18}(\text{BO}_3)_3(\text{OH})_3\text{F}$ , which is called fluor-liddicoatite, this OH-endmember is likely to be a currently non-approved species. Because the "liddicoatite" holotype material from 1977 was found to be F-dominant at the  $W$  site, although the originally suggested formula was OH-dominant, the type material has been recently redefined as fluor-liddicoatite. Because our structurally investigated tourmaline sample has also to be characterised chemically, it can only be proposed on structural data that the investigated tourmaline sample belongs to an OH-dominant liddicoatite, which would have to be submitted as a new mineral of the tourmaline supergroup when a low fluorine content has been proven.

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