CORRELATIONS IN Cu- AND Mn-BEARING TOURMALINES FROM BRAZIL AND MOZAMBIQUE

ERTL, A.[1]*, GIESTER, G.[1], TILLMANNS, E.[1], OKRUSCH, M.[2], SCHÜSSLER, U.[2] & BRÄTZ, H.[3]
[1] Institut für Mineralogie und Kristallographie, Universität Wien, Althanstrasse 14, Wien, Austria
[2] Lehrstuhl für Geodynamik und Geomaterialforschung, Institut für Geographie und Geologie, Universität Würzburg, Am Hubland, Würzburg, Germany
[3] GeoZentrum Nordbayern, Universität Erlangen-Nürnberg, Schloßgarten 5a, Erlangen, Germany
* E-mail: andreas.ertl@a1.net

Cu- and Mn-bearing tourmalines from Brazil and Mozambique were characterised chemically (EMPA and LA-ICP-MS) and by single-crystal structure refinement. All these samples are rich in Al, Li and F (fluor-elbaite) and contain significant amounts of CuO (up to ~1.8 wt%) and MnO (up to ~3.5 wt%). MgO and FeO contents are relatively low in the 15 investigated samples (≤0.2 wt%). Single-crystal structure refinements were done on 8 samples.

Tourmaline is a silicate mineral group with a highly complex crystal structure and a large variety of chemical compositions. The general chemical formula of the tourmaline-group minerals is $XY_3Z_6[T_6O_{18}](BO_3)_3V_3W$ (HENRY *et al.,* 2011). Our investigated samples, which were also characterised structurally, show a pronounced positive correlation between the <*Y*-O> distances and the (MnO + CuO) content in this site with $r^2 = 0.84$. There is no significant correlation between the Li content in the *Y* site and the <*Y*-O> distances. The valence states of Mn have not been determined, but we consider it mainly as Mn^{2+}. Another correlation, which is even better, shows a negative correlation between the <*Y*-O> distances and the Al_2O_3 content ($r^2 = 0.94$). In the structurally characterised samples the *T* site is only occupied by Si (<*T*-O> distances of ~1.618 Å). The samples at each locality generally show a strong negative correlation between the *X*-site vacancies and the MnO content ($r^2 \approx 0.9$ for all samples with F<0.9 apfu). The Mn content in these tourmalines is dependent on the availability of Mn, at the formation temperature, as well as on stereochemical constraints. Based on various data ERTL *et al*. (2012) suggest that increasing formation temperatures exist for tourmalines with increasing (Fe^{2+} + Mn^{2+}) contents. Our investigated samples also show evidence for a positive correlation between the Mn content (Fe content is only very low) and the formation temperature, because *X*-site vacancies decrease when the formation temperature increases (HENRY & DUTROW, 1996).

The very weak correlation between MnO and CuO ($r^2 = 0.01$) demonstrates that there is no evidence for a temperature dependent incorporation of Cu into the tourmaline structure. Hence, the Cu content in tourmaline is essentially dependent on the availability of Cu and on stereochemical constraints.

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