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Crystal chemistry of three tourmalines by SREF, EMPA, and SIMS

FERNANDO CÁMARA,[1] LUISA OTTOLINI,[1,*] AND FRANK C. HAWTHORNE[2]

[1]CNR-Instituto di Geoscienze e Georisorse (IGG), Sezione di Pavia, Via Ferrata 1, I-27100 Pavia, Italy
[2]Department of Geological Sciences, University of Manitoba, Winnipeg, MB R3T 2N2, Canada

ABSTRACT

The crystal structures of three tourmaline crystals: $(Na_{0.49}\,K_{0.01}\,Ca_{0.48})\,(Mg_{1.35}\,Fe^{2+}_{0.94}\,Fe^{3+}_{0.49}\,Ti_{0.20})\,(Al_{4.58}\,Fe^{3+}_{0.62}\,Mg_{0.80})\,(Si_{5.99}\,Al_{0.01})\,O_{18}\,(BO_3)_{3.03}\,(OH)_{3.18}\,F_{0.18}\,O_{0.64}$, $a = 16.017(2)$, $c = 7.256(2)$ Å, $V = 1612.2(4)$ Å^3, $R3m$, $Z = 3$; $(Na_{0.64}\,K_{0.01}\,Ca_{0.03})\,(Mn_{0.18}\,Fe^{2+}_{1.71}\,Al_{0.88}\,Li_{0.11}\,Zn_{0.03}\,Ti_{0.07})\,(Al_{5.67}\,Fe^{3+}_{0.28}\,Mg_{0.05})\,(Si_{5.76}\,Al_{0.24})\,O_{18}\,(BO_3)_{2.99}\,(OH)_{3.96}\,F_{0.17}$, $a = 15.983(2)$, $c = 7.152(2)$ Å, $V = 1582.1(4)$ Å^3; $(Na_{0.81}\,K_{0.01}\,Ca_{0.01})\,(Mn_{0.02}\,Mg_{0.61}\,Fe^{2+}_{0.90}\,Al_{0.80}\,Li_{0.70}\,Zn_{0.01}\,Ti_{0.06})\,Al_{6.00}\,(Si_{5.97}\,Al_{0.03})\,O_{18}\,(BO_3)_{2.93}\,(OH)_{3.42}\,F_{0.55}\,O_{0..03}$, $a = 15.921(3)$, $c = 7.137(2)$ Å, $V = 1566.7(6)$ Å^3, have been refined to **R-**indices of 1.3–2.2% using X-ray intensity data collected with a four-circle diffractometer using Mo$K\alpha$ X-radiation. The crystals were analyzed by electron- and ion-microprobe techniques for all major and minor elements in the crystals. Unit formulae were calculated on the basis of 31 anions (O, OH, F) and the $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ ratio was calculated for electroneutrality. The refined site-scattering values and the observed <Y-O> and <Z-O> distances were used to assign site populations that are in accord with the unit formulae calculated from the electron- and ion-microprobe compositions. The B contents are equal to 3.0 apfu (atoms per formula unit) within experimental error. In two of the crystals, (OH + F) = 4.0 apfu. However, the third crystal has (OH + F) = 3.36 apfu and O^{2-} is dominant at the W(O1) site, and is an "oxy" tourmaline as defined by Hawthorne and Henry (1999). Non-spherical electron-density was observed at the X site, suggesting that there is some positional disorder at this site associated with occupancy of X by Ca and Na, possibly coupled with variable anion occupancy of the O1 site.