Crystal chemistry of Cu-bearing tourmalines

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ABSTRACT

The crystal structures of two elbaites from the Paraiba deposit with copper contents of 3.51 and 1.61 wt% CuO \([a = 15.881(1), 15.840(3); c = 7.112(1), 7.1028(9)]\), respectively, as well as a synthetic Cu-bearing olenite with a CuO content of 8.39 wt% \([a = 15.840(4), c = 7.091(1)]\) have been refined to R-indices of 2.2, 3.1, and 4.1% using X-ray single-crystal diffraction. On the basis of original and published data (for six structures) the crystal-chemical relationships of copper-bearing tourmalines has been analyzed. It is shown that copper cations and cations of other 3d elements (Mn, Zn, Fe) occupy almost exclusively the Y site. Such an ordered distribution results in a change of the size of the Y-octahedra. There is an inverse correlation between the content of 3d elements (mainly Cu\(^{2+}\) cations) and Al\(^{3+}\) cations in the Y-octahedron and also between the value of \(\langle Y-O \rangle\) and the content of Al\(^{3+}\) cations in the Y site. The direct correlation between values of \(\langle Y-O \rangle\)-distance in the structures of Cu-bearing elbaites and the parameters \((a, c)\) of the unit cell have been found. Distortions of polyhedra in the structures of Cu-bearing elbaites are similar, and significantly higher than those present in the structure of the synthetic Cu-bearing olenite.

Keywords: Cu-rich elbaite, Cu-bearing olenite, Paraiba, crystal chemistry, tourmaline, X-ray structure refinement