

Crystal chemistry of Cu-bearing tourmalines

OLGA S. VERESHCHAGIN,^{1,*} IRA V. ROZHDESTVENSKAYA,¹ OLEG V. FRANK-KAMENETSKAYA,¹
ANATOLY A. ZOLOTAREV,¹ AND RUDOLF I. MASHKOVTSSEV²

¹Saint-Petersburg State University, Universitetskaya nab. 7/9, Saint Petersburg, 199034, Russia

²VS Sobolev Institute of Geology and Mineralogy SB RAS, Koptyuga Avenue 3, Novosibirsk, 630090, Russia

ABSTRACT

The crystal structures of two elbaïtes 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 Cu²⁺ cations) and Al³⁺ cations in the Y-octahedron and also between the value of <Y-O> and the content of Al³⁺ cations in the Y site. The direct correlation between values of <Y-O>-distance in the structures of Cu-bearing elbaïtes and the parameters (a, c) of the unit cell have been found. Distortions of polyhedra in the structures of Cu-bearing elbaïtes are similar, and significantly higher than those present in the structure of the synthetic Cu-bearing olenite.

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