

# Poster Presentations

## [MS18-P06] Crystal Chemical Features of Cr, Cu and Ni-Bearing Tourmalines.

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Crystal-chemical features of 3d elements (Cr, Cu and Ni) bearing tourmalines are analyzed on the basis of 11 original and 14 published [1-3] single crystal X-ray diffraction studies. The incorporation of 3d elements into the tourmaline structure starts from Y octahedron. As their content increase up to 5-8 wt. %, these elements begin to occupy Z octahedron. In most cases the distribution of Cr, Cu and Ni atoms between the octahedral sites and their maximum concentrations (Table) is explained by the ratio of sizes of substitution cations (Goldschmidt rule). In the dravite - chromdravite series Cr<sup>3+</sup> cations readily enter into both octahedral sites so that chromdravite mineral (Na(Cr<sub>2</sub>Mg)(Cr<sub>4</sub>Mg<sub>2</sub>)(BO<sub>3</sub>)<sub>3</sub>(Si<sub>6</sub>O<sub>18</sub>)(OH)<sub>4</sub>, with statistic distribution of Cr cations at octahedral sites is formed [4]. In elbaite - Cu-elbaite series the incorporation of Cu cations into Z octahedron is difficult and Cu content does not exceed 0.19 atoms per formula unit. In Ni-bearing tourmaline Ni content in Z octahedron is significantly higher and does not exceed 1.14 apfu. Table. Concentration of 3d elements in tourmalines

Characteristic	Admixture		
	Cr	Cu	Ni
$C_{max}$ wt. %	35.56 Cr <sub>2</sub> O <sub>3</sub>	8.39 CuO	18.96 NiO
$C_{max}$ apfu	Y	1.71	1.80
	Z	3.60	0.19

The content and distribution of Cr, Cu and Ni cations significantly effect the geometry of the structure. As content of 3d elements increases, the charge distribution between the octahedral

sites changes and sizes of the octahedra approach each other. In general, the structure becomes less deformed, <Y-O>/<Z-O> ratio tends to 1. For all considered tourmalines the direct correlation between *a* and *c* unit cell parameters as well as between unit cell parameters and dimensions of the Z octahedron was found. The inverse correlation between unit cell parameters and the total content of Al atoms was revealed.

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