**Poster Presentation**

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## *Bond valence constraints on the composition of 3d-elements bearing tourmalines*

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F.C. Hawthorne (2002) and F. Bosi (2011) showed that bond valence approach is to be applied to stability prediction of tourmaline structure with different chemical composition. Using this approach we considered bond valence constraints on occupation of Y, Z, V and W sites of Cu-, Ni-bearing tourmalines. From the standpoint of the bond valence approach, [3YW] unit is unstable if W site is fully occupied by O2-. The stability of [3YW] unit decreases along a row: 3 divalent cations → 2 divalent cations + 1 trivalent cation → 2 trivalent cation + 1 divalent cations → 3 trivalent cations if W site is fully occupied by OH- or F-. There is no limitation on 3d elements and aluminum content in [2ZYV] if V site is fully occupied by OH-. The [2ZYV] unit is unstable if V site is fully occupied by O2-. The data, obtained from calculation of bond valences are in a good agreement with results of single crystal structure refinements of synthetic Cu- (Ertl et al., 2013) and Ni-tourmalines: Cu-bearing olenite with a CuO content of 8.39 wt.% [a = 15.849(1), c =7.087(1) Å, R = 2.5%] and Ni-bearing olenite with a NiO content of 18.96 wt.% [a = 15.890(2), c = 7.1815(8), R = 3.1%]. In all cases W and V sites are predominantly occupied by OH- anions. The composition of [3YW] units are [(Cu1.80Al1.20)(OH)0.60F0.40] and [(Ni1.80Al1.20)(OH)1.00]. Breaking of charge balance with increasing of bivalent cations is maintained by increasing of portion of vacancies at X site and increasing of content of trivalent cations (Al, B) at T site.

***[1]*** *F.C. Hawthorne, 2002, Canadian Mineralalogist, 40, 789-797,* ***[2]*** *F. Bosi, 2011, Canadian Mineralalogist, 49, 17-27,* ***[3]*** *A. Ertl, 2013, MITT.ÖSTERR.MINER.GES., 159*

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