Multi-method characterization of synthetic tourmaline: Rossmanite, magnesio-foitite, dravite, and maruyamaite

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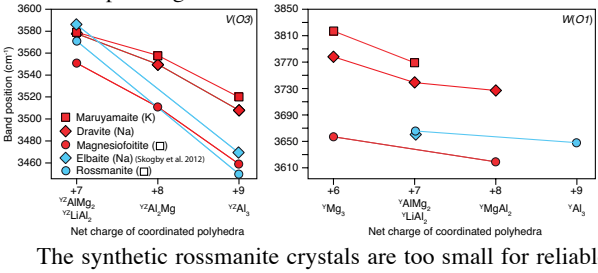
We present EMPA, single crystal (SREF) and powder XRD, polarized Raman and IR spectroscopic data for rossmanite, Mg-foitite, dravite, and maruyamaite, synthesized in the P,T-range 0.4-4.0 GPa, 600–700°C. Highlighted is the first-time synthesis (2.5 GPa, 600°C) of rossmanite $[^{X}\square^{Y}(LiAl_2)^{Z}Al_6(^{T}Si_6O_{18})(BO_3)_3{}^{VW}(OH)_4]$ from starting materials free of tourmaline seeds.

The use of synthetic, compositionally and structurally well-characterized tourmalines facilitates the assignment of their respective spectroscopic bands to specific site compositions. For dravite, maruyamaite and Mg-foitite, with octahedral Al and Mg, we can resolve the effect of the X-site cation and net charge of the octahedral polyhedra on the OH-band positions. Additionally, we are able to calculate the Mg/Al ratios of different octahedral sites from the relative integrated peak intensities and obtain values in good agreement with corresponding EMPA and SREF.



The synthetic rossmanite crystals are too small for reliable EMPA. However, the similarity between their unit cell dimensions (a = 15.759(4) Å, c = 7.053(2) Å, V = 1516.9(7) Å^3) and those of natural rossmanite suggests they have near endmember compositions. Moreover, the IR-spectra of synthetic rossmanite and natural elbaite are very similar and the offsets in their respective band positions are analogous to those observed between the Na-bearing and X-vacant Mg-Al-tourmalines, dravite and Mg-foitite. The effect of net charge on the O3 band position is more pronounced for Li-tourmaline than Mg-Al-tourmalines, as indicated by the steepening of the slope in the attached figure.