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Metamorphic ultrahigh-pressure tourmaline: Structure, chemistry, and correlations to *P-T* conditions

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Abstract

Tourmaline grains extracted from rocks within three ultrahigh-pressure (UHP) metamorphic localities have been subjected to a structurally and chemically detailed analysis to test for any systematic behavior related to temperature and pressure. Dravite from Parigi, Dora Maira, Western Alps (peak *P-T* conditions ~3.7 GPa, 750 °C), has a structural formula of $^{X}(Na_{0.90}Ca_{0.05}K_{0.01}\square_{0.04})$ $^{Y}(Mg_{1.78}Al_{0.99}Fe^{2+}_{0.12}Ti^{4+}_{0.03}\square_{0.08})^{Z}(Al_{5.10}Mg_{0.90})(BO_3)_3{}^{T}Si_{6.00}O_{18}{}^{V}(OH)_3{}^{W}[(OH)_{0.72}F_{0.28}]$. Dravite from Lago di Cignana, Western Alps, Italy (~2.7–2.9 GPa, 600–630 °C), has a formula of $^{X}(Na_{0.84}Ca_{0.09}K_{0.01}\square_{0.06})$ $^{Y}(Mg_{1.64}Al_{0.79}Fe^{2+}_{0.48}Mn^{2+}_{0.06}Ti^{4+}_{0.02}Ni_{0.02}Zn_{0.01})^{Z}(Al_{5.00}Mg_{1.00})(BO_3)_3{}^{T}(Si_{5.98}Al_{0.02})O_{18}{}^{V}(OH)_3{}^{W}[(OH)_{0.65}F_{0.35}]$. "Oxy-schorl" from the Saxonian Erzgebirge, Germany (≥4.5 GPa, 1000 °C), most likely formed during exhumation at >2.9 GPa, 870 °C, has a formula of $^{X}(Na_{0.86}Ca_{0.02}K_{0.02}\square_{0.10})^{Y}(Al_{1.63}Fe^{2+}_{1.23}Ti^{4+}_{0.11}Mg_{0.03}Zn_{0.01})$ $^{Z}(Al_{5.05}Mg_{0.95})(BO_3)_3{}^{T}(Si_{5.96}Al_{0.04})O_{18}{}^{V}(OH)_3{}^{W}[O_{0.81}F_{0.10}(OH)_{0.09}]$. There is no structural evidence for significant substitution of $^{[4]}$Si by $^{[4]}$Al or $^{[4]}$B in the UHP tourmaline (<T-O> distances ~1.620 Å), even in high-temperature tourmaline from the Erzgebirge. This is in contrast to high-*T*–low-*P* tourmaline, which typically has significant amounts of $^{[4]}$Al. There is an excellent positive correlation ($r^2 = 1.00$) between total $^{[6]}$Al (i.e., ^{Y}Al + ^{Z}Al) and the determined temperature conditions of tourmaline formation from the different localities. Additionally, there is a negative correlation ($r^2 = 0.97$) between F content and the temperature conditions of UHP tourmaline formation and between F and ^{Y}Al content ($r^2 = 1.00$) that is best explained by the exchange vector $^{Y}AlO(R^{2+}F)_{-1}$. This is consistent with the W site (occupied either by F, O, or OH), being part of the YO_6-polyhedron. Hence, the observed Al-Mg disorder between the Y and Z sites is possibly indirectly dependent on the crystallization temperature.

Keywords: Tourmaline, ultrahigh pressure, Saxonian Erzgebirge, Western Alps, Dora Maira, Lago di Cignana