

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 $^X(\text{Na}_{0.90}\text{Ca}_{0.05}\text{K}_{0.01}\square_{0.04})^Y(\text{Mg}_{1.78}\text{Al}_{0.99}\text{Fe}_{0.12}^{2+}\text{Ti}_{0.03}^{4+}\square_{0.08})^Z(\text{Al}_{5.10}\text{Mg}_{0.90})(\text{BO}_3)_3^T\text{Si}_{6.00}\text{O}_{18}^V(\text{OH})_3^W[(\text{OH})_{0.72}\text{F}_{0.28}]$. Dravite from Lago di Cignana, Western Alps, Italy (~2.7–2.9 GPa, 600–630 °C), has a formula of $^X(\text{Na}_{0.84}\text{Ca}_{0.09}\text{K}_{0.01}\square_{0.06})^Y(\text{Mg}_{1.64}\text{Al}_{0.79}\text{Fe}_{0.48}^{2+}\text{Mn}_{0.06}^{2+}\text{Ti}_{0.02}^{4+}\text{Ni}_{0.02}\text{Zn}_{0.01})^Z(\text{Al}_{5.00}\text{Mg}_{1.00})(\text{BO}_3)_3^T(\text{Si}_{5.98}\text{Al}_{0.02})\text{O}_{18}^V(\text{OH})_3^W[(\text{OH})_{0.65}\text{F}_{0.35}]$. “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 $^X(\text{Na}_{0.86}\text{Ca}_{0.02}\text{K}_{0.02}\square_{0.10})^Y(\text{Al}_{1.63}\text{Fe}_{1.23}^{2+}\text{Ti}_{0.11}^{4+}\text{Mg}_{0.03}\text{Zn}_{0.01})^Z(\text{Al}_{5.05}\text{Mg}_{0.95})(\text{BO}_3)_3^T(\text{Si}_{5.96}\text{Al}_{0.04})\text{O}_{18}^V(\text{OH})_3^W[\text{O}_{0.81}\text{F}_{0.10}(\text{OH})_{0.09}]$. There is no structural evidence for significant substitution of ^{14}Si by ^{14}Al or ^{14}B in the UHP tourmaline ($<\text{T-O}>$ 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 ^{14}Al . There is an excellent positive correlation ($r^2 = 1.00$) between total ^{16}Al (i.e., $^Y\text{Al} + ^Z\text{Al}$) 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 ^YAl content ($r^2 = 1.00$) that is best explained by the exchange vector $^Y\text{AlO}(\text{R}^{2+}\text{F})_{-1}$. 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