Crystal chemistry of tourmalines from Minas Gerais, Brazil

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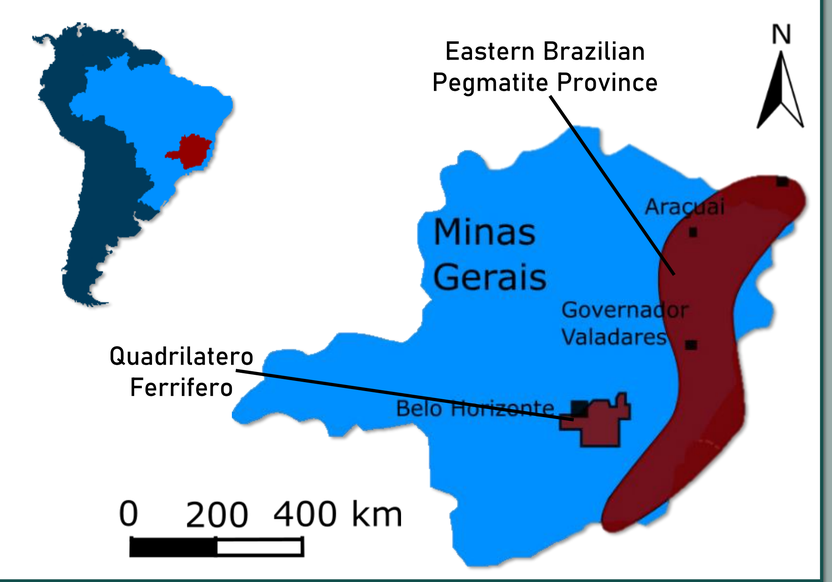
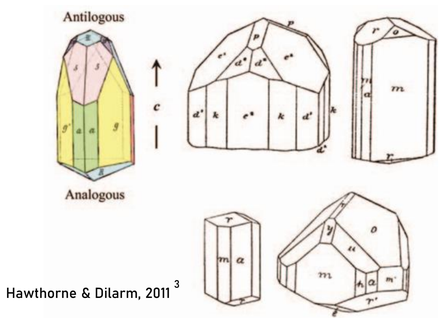
Introduction

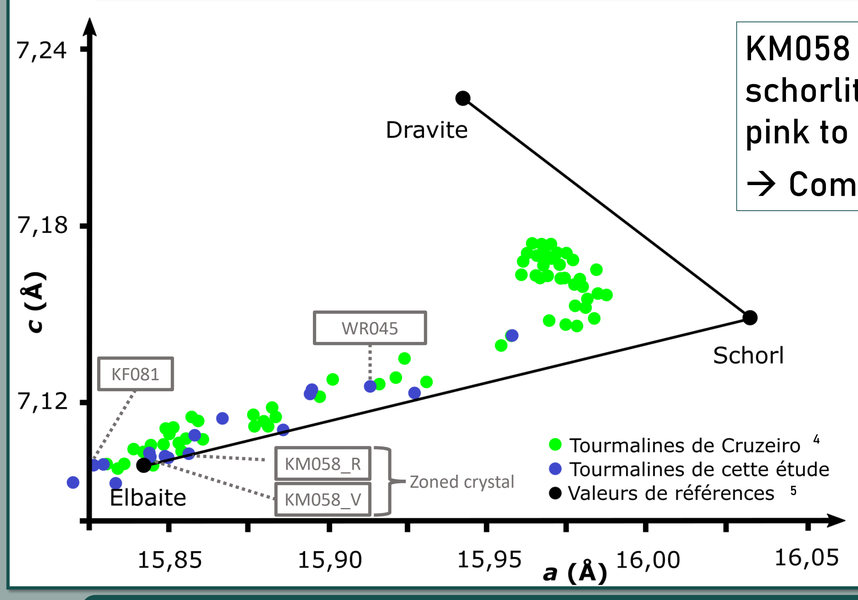
- Tourmalines were found in Minas Gerais at the dawn of the 17th century but stayed misunderstood until the beginning of the 20th century.
- Supergroup of complex rhombohedral borosilicates with a *R*3*m* space group.
- General formula : $XY_3Z_6[T_6O_{18}](BO_3)_3V_3W$.
- Main occurrences in granitic pegmatites, lithium-poor granitoids and hydrothermal environments (gold deposits).

Occurrences of tourmalines in Minas Gerais





Unit-cell parameters



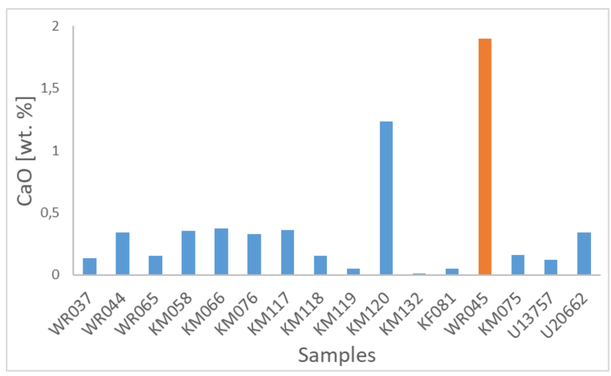
KM058 shows an increasing schorlitic component from pink to green elbaite

→ Compositional zonation

15.82 Å ≤ *a* ≤ 15.93 Å

7.09 Å ≤ *c* ≤ 7.13 Å

Particular cases from the Lavra do Urucum Pegmatite

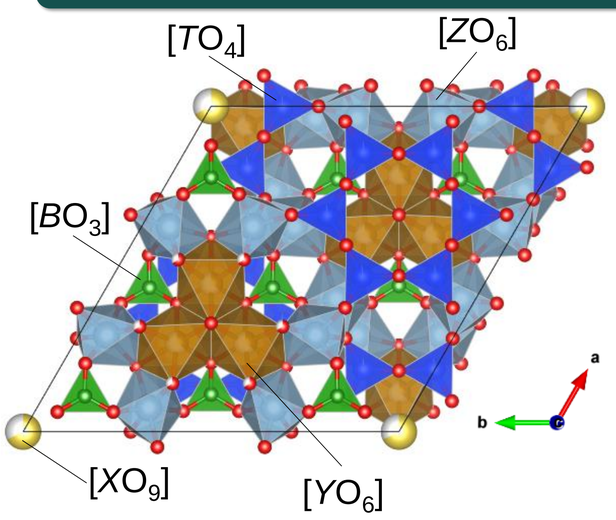


WR045 is deeply enriched in calcium and tends toward a liddicoatite composition

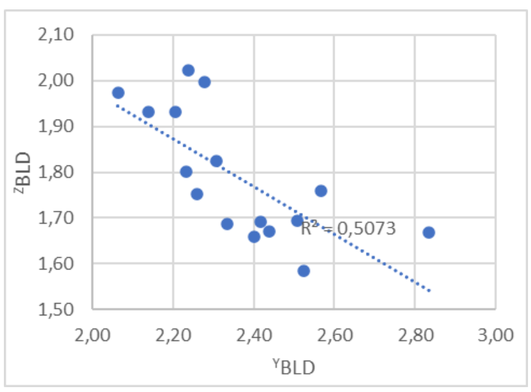
KF081 contains 2 ^{Y}Al + ^{Y}Li and a low amount of Na compared to the other samples

KF081 shows a typical rossmanite composition

Single crystal X-ray diffraction to refine the structure

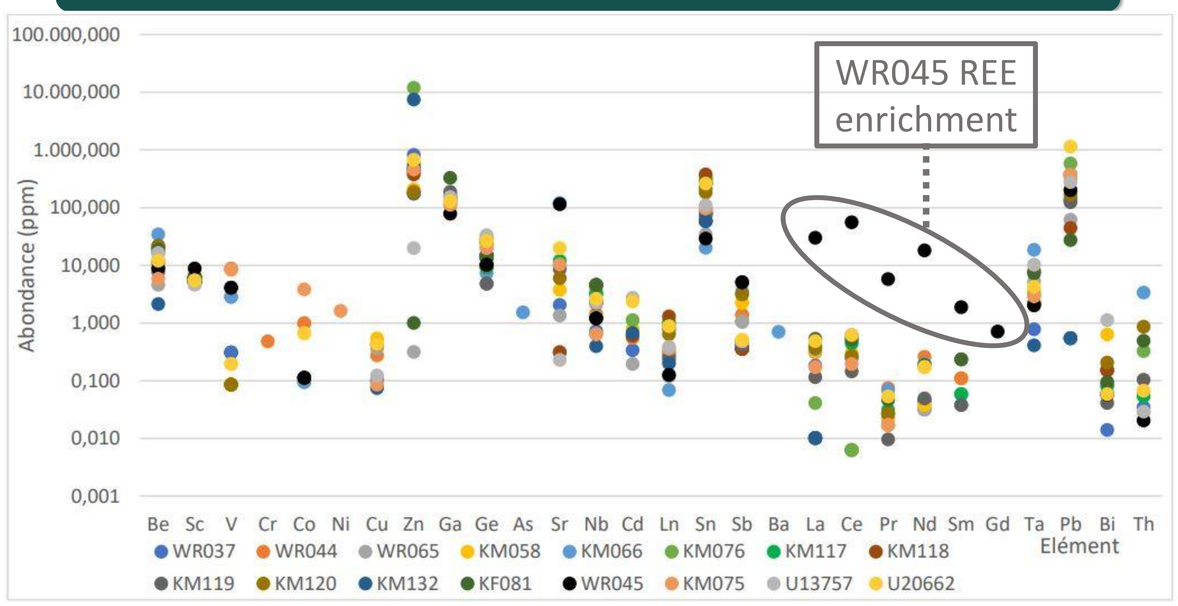


Site	Common cations and anions at each site
X	R^{1+}: **Na^{1+}**>>K^{1+} R^{2+}: **Ca^{2+}**
Y	R^{2+}: **Fe^{2+}** ~ **Mg^{2+}** > **Mn^{2+}** >>> Zn^{2+} , Ni^{2+} , Co^{2+}, Cu^{2+} R^{3+}: **Al^{3+}** >> **Fe^{3+}** > Cr^{3+} >> V^{3+} R^{1+}: **Li^{1+}** R^{4+}: **Ti^{4+}**
Z	R^{3+}: **Al^{3+}** >> **Fe^{3+}** > Cr^{3+} > V^{3+} R^{2+}: **Mg^{2+}** > Fe^{2+}
T	R^{4+}: **Si^{4+}** R^{3+}: **Al^{3+}** > B^{3+}
B	R^{3+}: **B^{3+}**
V	S^{1-}: **OH^{1-}** S^{2-}: **O^{2-}**
W	S^{1-}: **OH^{1-}** ~ **F^{1-}** S^{2-}: **O^{2-}**



Inverse correlation between distortions of the Y and Z sites

Minor and trace elements



Conclusions

- Main substitutions take place on the *Y* crystallographic site between the major elements (Al+Li) (elbaite) and Fe (schorl).
- Optical and compositional zonations reflect the evolving set-up conditions of granitic pegmatites.
- Atypical compositions have been identified in the Lavra do Urucum Pegmatite samples : A rossmanite and a liddicoatite component
- The liddicoatite component is linked to an REE enrichment
- An inverse correlation has been highlighted between the distortions of Y and Z sites. Highest distortions values are observed for schorl-rich compositions

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