Crystal chemistry of tourmalines from Minas Gerais, Brazil

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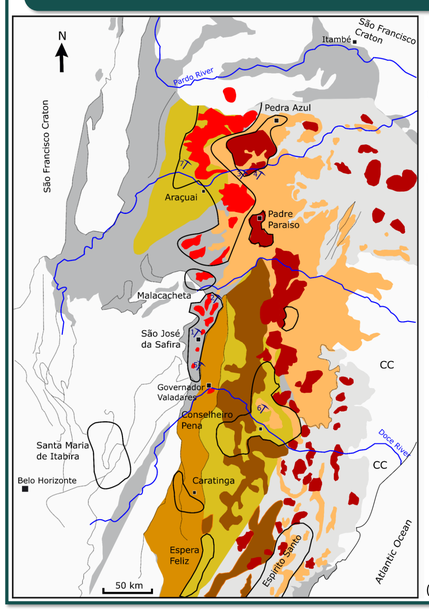
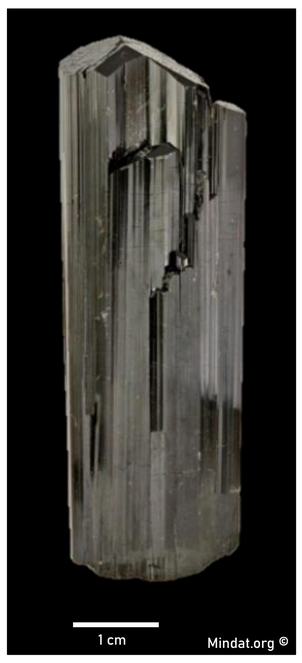
Introduction

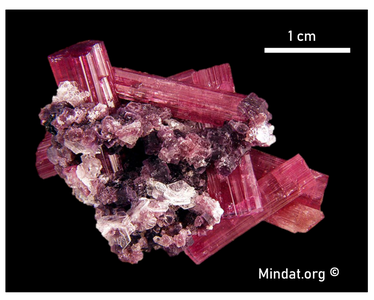
- Tourmalines were found in Minas Gerais at the dawn of the 17th century but remained misunderstood until the beginning of the 20th century.
- Main occurrences in granitic pegmatites of the Eastern Brazilian Pegmatite Province (EBPP).
- Supergroup of complex trigonal borosilicates with a *R*3*m* space group.
- General formula : $XY_3Z_6[T_6O_{18}](BO_3)_3V_3W$.

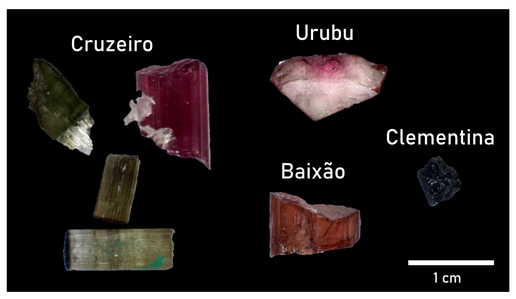
Occurrences of tourmalines in Minas Gerais



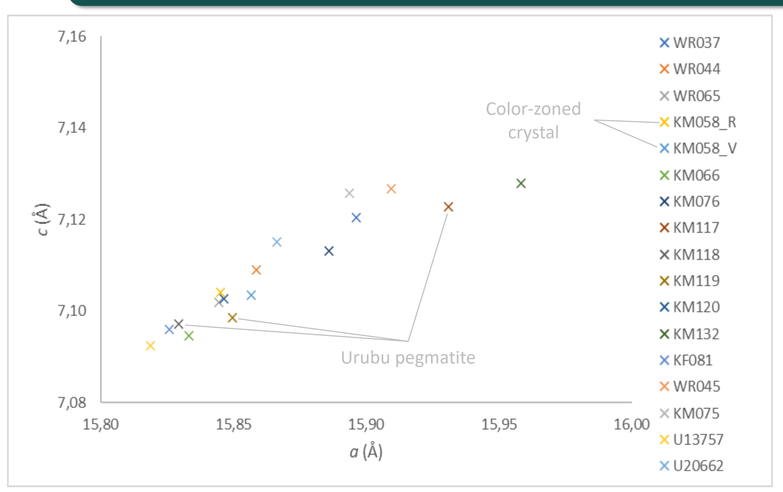
(Pedrosa-Soares *et al.*, 2009[4], modified)







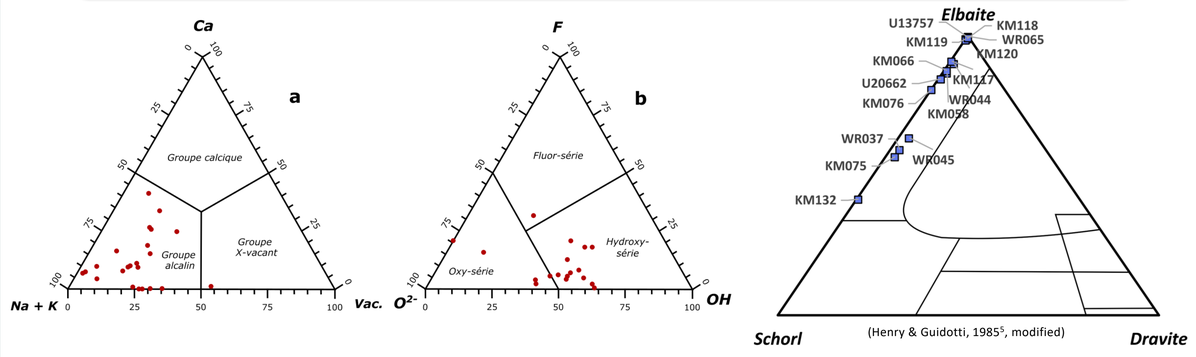
Unit-cell parameters



- *a* and *c* parameters linearly increasing with ^{Y}(Li+Al) → ^{Y}(Fe)
- Heterogeneous cell sizes amongst the same deposits
- Increasing schorlitic component in pink to green zoned elbaite

  → Compositional zonations in the parent deposit

Major elements



(Henry & Guidotti, 1985[5], modified)

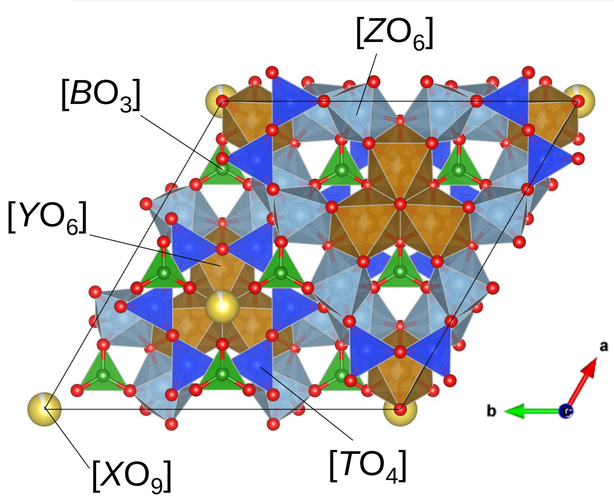
KF081 :
- 2 ^{Y}Al + ^{Y}Li
- low amount of ^{X}Na

→ Typical rossmanite composition

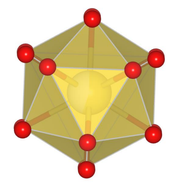
WR045 :
- 0.329 ^{X}Ca
- High amount of F

→ Elbaite tends towards fluor-liddicoatite

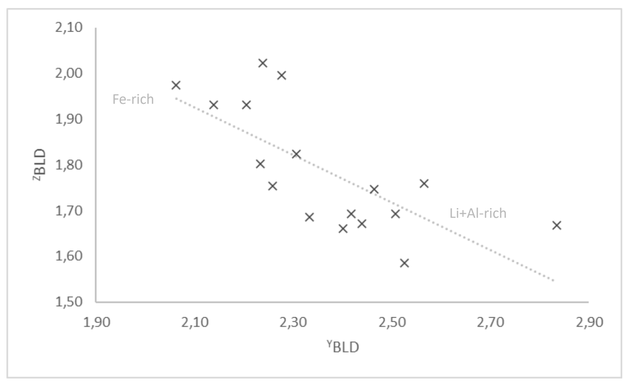
Single crystal X-ray diffraction



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-}**

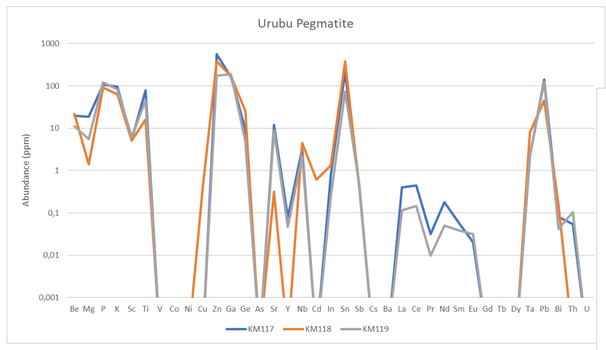


X-site coordination



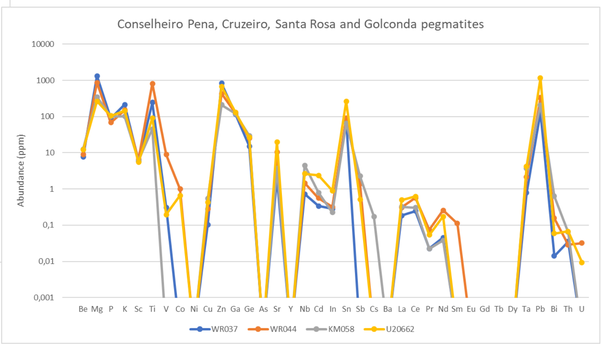
Inverse correlation between distortions of the *Y* and *Z* sites

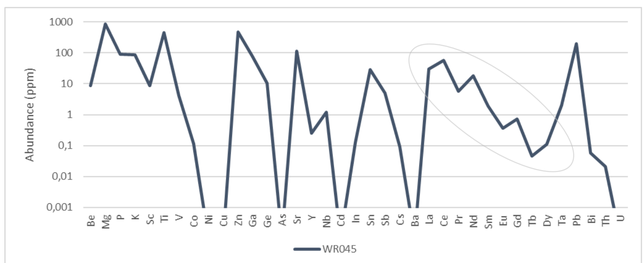
Minor and trace elements



… but are sometimes similar between different pegmatites

Concentrations may vary amongst samples from the same occurrence …





Atypical REE enrichment in WR045 crystal

→ Origin ?

Conclusions

- An inverse correlation has been highlighted between the distortions of Y and Z sites. Highest distortion values are observed for schorl-rich compositions.
- Main substitutions take place on the *Y* crystallographic site between the major elements (Al+Li) (elbaite) and Fe (schorl).
- Optical, compositional and structural zonations reflect the evolving set-up conditions of granitic pegmatites.
- Atypical compositions have been identified in the Urubu (rossmanite) and Urucum (liddicoatite + REE) pegmatites.
- Trace elements concentrations seem to be independent from the occurrence → position in the pegmatite and/or external factors

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5. Henry, D.J. & Guidotti, C.V., 1985. Tourmaline as a petrogenetic indicator mineral: an example from the staurolite-grade metapelites of NW Maine. *American Mineralogist,* 70(1-2), 1-15.