

Estimation of light element concentrations in tourmaline: How accurate can it be?

Darrell J. Henry¹, David Viator¹ and Barbara L. Dutrow¹

¹Louisiana St. Univ., Dept. of Geology and Geophysics, Baton Rouge LA 70803 USA, dhenry@geol.lsu.edu

Electron microprobe analysis of tourmaline can be a somewhat daunting process, particularly with light elements (B, Li and H) comprising up to 18% of the total oxide wt%, and with the possibility of transition elements having multiple oxidation states. Because of a greatly improved understanding of tourmaline's crystal structure and chemistry as well as the constraints imposed by geochemical settings of tourmaline, estimation techniques for unanalyzed light elements and oxidation states are possible. The general chemical formula of tourmaline is $\text{XY}_3\text{Z}_6(\text{T}_6\text{O}_{18})(\text{BO}_3)_3\text{V}_3\text{W}$; with the most common site occupancies being $\text{X} = \text{Ca, Na, K, }^{\text{X}}\square$ [vacancy]; $\text{Y} = \text{Li, Mg, Fe}^{2+}, \text{Mn}^{2+}, \text{Al, Cr}^{3+}, \text{Fe}^{3+}$; $\text{Z} = \text{Al, Mg, Fe}^{3+}, \text{Cr}^{3+}$; $\text{T} = \text{Si, Al (B)}$; $\text{B} = \text{B}$; $\text{V} = \text{OH, O}$; $\text{W} = \text{OH, F, O}$. Apparent lack of vacancies in the Y, Z and T sites enable several viable normalization and light element estimation procedures.

Light element and oxidation states estimation procedures are tested against high-quality, completely-characterized tourmaline analyses that were carried out with a variety of techniques (wet chemical, SIMS, Mössbauer spectroscopy, U-extraction line, SREF, ICP-AES). The results indicate that light element estimation can be reasonably accurate with the appropriate assumptions. [1] Estimation of B. The assumption that B fully occupies the triangular B site and can be calculated using stoichiometric constraints (i.e. $\text{B} = 3$) is generally valid. However, there are a few unusual instances involving high-pressure, Al-rich tourmaline in which some B may also be tetrahedral. [2] Estimation of Li. Li can be approximated by assuming that Li fills any cation deficiency in the Y site. However, this requires that the formula be calculated either on a fixed cation basis (e.g. $\text{Si} = 6$) or that Li be iteratively calculated using a fixed number of oxygens. The $\text{Si} = 6$ approach appears to work well for Li-rich tourmaline ($\text{Li} > 0.7$ apfu). A lack of significant amounts of Li can also be inferred for those tourmalines that coexist with other mafic silicates due to preferential partitioning of Li into coexisting silicates relative to tourmaline. [3] Estimation of H. H contents can be determined by charge balance if oxidation states can be measured or inferred. Putative oxidation state evidence can be derived from tourmaline optical properties or by mineral assemblages, particularly graphite-bearing assemblages. Charge balance estimates of H likely result in minimum values. Variations in H contents can be further examined by exchange vector limitations.

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Submitting author: **Darrell J Henry, Louisiana St. Univ., Dept. of Geology and Geophysics, Baton Rouge LA 70803 USA; Tel: 225-578-2693; Fax: 225-578-2302; E-mail: dhenry@geol.lsu.edu**