A spreadsheet for calculating normative mole fractions of end-member species for Na-Ca-Li-Fe\(^{2+}\)-Mg-Al tourmalines from electron microprobe data

**George B. Morgan VI**

Electron Microprobe Laboratory, University of Oklahoma, 100 East Boyd Street, SEC 710, Norman, Oklahoma 73019, U.S.A.

**ABSTRACT**

This work presents a spreadsheet that calculates the mole fractions of end-member components for simple Na-Ca-Li-Mg-Fe\(^{2+}\)-Al tourmalines from electron microprobe data. The input includes the B\(_2\)O\(_3\) concentration obtained either from direct analysis or by estimation on the basis of stoichiometry. The concentration of Li\(_2\)O can either be input from other analysis or estimated by the spreadsheet. The spreadsheet does not address the mole fractions of Cr, V, oxidized or deprotonated tourmaline species, nor account for species involving tetrahedral boron or aluminum. Therefore, the spreadsheet is not a comprehensive tool that includes all IMA approved tourmaline species, and so is not intended for naming tourmalines according to IMA convention. The present method includes a useful subset of end-member species that can be described simply from electron microprobe data and so, akin to a normative mineralogical analysis for rock composition, the calculations are intended to provide a normative result that serves as simple basis for comparing tourmalines that is more direct than names derived from the most abundant species present.

**Keywords:** Tourmaline, formula, mole fractions, end-members, electron microprobe analysis

**INTRODUCTION**

Tourmaline is by far the most important mineral phase in the Earth’s crust that contains boron as an essential structural component. A complex borosilicate, the general formula for tourmaline can be expressed as XY\(_3\)Z\(_6\)(BO\(_3\))\(_3\)(T\(_6\)O\(_{18}\))V\(_3\)W, where most commonly X = (Na, Ca, K, or vacancy), Y = (Mg, Fe\(^{2+}\), Al, Li, Mn, Ti, Cr\(^{3+}\), V\(^{3+}\), Z = Al, Fe\(^{3+}\), Cr\(^{3+}\), V\(^{3+}\), Fe\(^{2+}\), Mg, or vacancy), T = (Si, Al, or B), B = (B or vacancy), V = (OH, O), and W = (OH, O, F, Cl) (Hawthorne and Henry 1999; Filip et al. 2012; Henry et al. 2011; Bosi et al. 2012). Simple, yet informative, description of tourmaline composition is hindered by naming the mineral for the most abundant end-member species present—with or without other compositional modifiers. A more direct approach for tourmaline description would result from presentation of the mole fractions of end-member species, similar to methods used for other mineral groups such as the feldspars and pyroxenes. Despite considerable previous efforts toward calculating tourmaline chemical formula, a mole fraction approach has been hindered by the complexity of tourmaline crystal chemistry and resultant lack of a simple tool for calculation.

Calculating a chemical formula for tourmaline from an electron microprobe analysis (EMPA) is complicated by the incorporation of up to three elements (B, H, and Li) that are difficult or impossible to analyze using fluorescent X-rays. Moreover, the stoichiometric abundance of hydrogen can vary due to several coupled substitutions and, thus, change the total charge basis that provides the normalizing factor for calculating the chemical formula. Several methods and spreadsheets for recalculating composition and formula from EMPA previously have been discussed and distributed (e.g., Henry and Dutrow 2002; Selway and Xiong 2002; Yavuz et al. 2006; Clark 2007), and these are useful for naming a tourmaline species and/or classifying composition using a series of ternary and quaternary diagrams (e.g., Selway and Xiong 2002; Hawthorne and Henry 1999; Henry et al. 2011). The program of Yavuz et al. (2006) calculates the structural formula, including estimation of oxidized species, and provides the relative percentages (mole fractions) of tourmaline types based on X-site speciation (sodic, calcic, and vacancy series), but the program does not estimate mole fractions of any tourmaline end-member species. The TOURCOMP program of Pesquera et al. (2008) calculates mole fractions of tourmaline species, albeit using a somewhat outdated list of species, but does so from a tourmaline formula as input rather than from compositional (oxide weight percent) data. Hence, to date none of these approaches easily furnish mole fractions of end-member components from an oxide weight fraction analysis, which is unfortunate because component mole fractions would be more instructive for conveyance of tourmaline composition in text than a simple name, and so would be more useful for comparing tourmaline compositions and relating those compositions to chemical environment of formation. For example, consider the hypothetical tourmaline composition shown in Table 1. This composition was calculated from a formula corresponding to 40% schorl, 25% dravite, 20% foitite, and 15% olenite on a molar basis. Use of spreadsheets like that of Selway and Xiong (2002) does a fine job of calculating the atomic formula and assigns the name “schorl” to the phase. Although “schorl” is the correct name for this mineral according to the present rules (e.g., Henry et al. 2011), the name does not convey a compositional difference relative to a mineral that is pure schorl. The use of other descriptive or Schaller modifiers along with species...