

Nomenclature of the tourmaline-supergroup minerals

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ABSTRACT

A nomenclature for tourmaline-supergroup minerals is based on chemical systematics using the generalized tourmaline structural formula: $XY_3Z_6(T_6O_{18})(BO_3)_3V_3W$, where the most common ions (or vacancy) at each site are $X = Na^{1+}, Ca^{2+}, K^{1+}$, and vacancy; $Y = Fe^{2+}, Mg^{2+}, Mn^{2+}, Al^{3+}, Li^{1+}, Fe^{3+}$, and Cr^{3+} ; $Z = Al^{3+}, Fe^{3+}, Mg^{2+}$, and Cr^{3+} ; $T = Si^{4+}, Al^{3+}$, and B^{3+} ; $B = B^{3+}$; $V = OH^{1-}$ and O^{2-} ; and $W = OH^{1-}, F^{1-}$, and O^{2-} . Most compositional variability occurs at the X, Y, Z, W, and V sites. Tourmaline species are defined in accordance with the dominant-valency rule such that in a relevant site the dominant ion of the dominant valence state is used for the basis of nomenclature. Tourmaline can be divided into several groups and subgroups. The primary groups are based on occupancy of the X site, which yields alkali, calcic, or X-vacant groups. Because each of these groups involves cations (or vacancy) with a different charge, coupled substitutions are required to relate the compositions of the groups. Within each group, there are several subgroups related by heterovalent coupled substitutions. If there is more than one tourmaline species within a subgroup, they are related by homovalent substitutions. Additionally, the following considerations are made. (1) In tourmaline-supergroup minerals dominated by either OH^{1-} or F^{1-} at the W site, the OH^{1-} -dominant species is considered the reference root composition for that root name: e.g., dravite. (2) For a tourmaline composition that has most of the chemical characteristics of a root composition, but is dominated by other cations or anions at one or more sites, the mineral species is designated by the root name plus prefix modifiers, e.g., fluor-dravite. (3) If there are multiple prefixes, they should be arranged in the order occurring in the structural formula, e.g., “potassium-fluor-dravite.”

Keywords: Tourmaline, mineral chemistry, nomenclature, substitutions, order-disorder

INTRODUCTION

The Subcommittee on Tourmaline Nomenclature (STN) of the International Mineralogical Association's Commission on New Minerals, Nomenclature and Classification (IMA-CNMNC) has reconsidered the nomenclature of tourmaline-supergroup¹ minerals. This was prompted by the general ambiguity in the assignment of mineral names to specific tourmaline compositions. There are several reasons for this uncertainty (Hawthorne and Henry 1999). (1) Formal descriptions of tourmaline minerals often specify the ideal end-member compositions, but do

not specify the limits for the use of the name. (2) Some of the formal descriptions of tourmaline minerals specify the general composition, but do not specify the end-member composition. (3) Tourmaline is commonly incompletely chemically characterized, with critical light elements (H, Li, F, and B) and the oxidation states of transition elements (Fe, Mn) often being undetermined. (4) Site assignments can be equivocal in the absence of crystal-structure refinements. (5) Current graphical representations of tourmaline compositional variations are inadequate to express the actual substitutional nature of tourmaline. These considerations motivated Hawthorne and Henry (1999) and the STN to re-examine and, where necessary, redefine end-members and potential new end-members and species, which led to the development of several compositional diagrams that aid in classification of the tourmaline-supergroup minerals. The proposal for systematic classification of the tourmaline-supergroup miner-

¹ Tourmaline is considered to be a supergroup in terms of nomenclature procedures because it “consists of two or more mineral groups, which have essentially the same structure and composed of chemically similar elements” (Mills et al. 2009).

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als submitted by the STN was accepted by the IMA-CNMNC (Novák et al. 2009).

The purpose of this paper is to present the essential elements of tourmaline nomenclature, to define concepts that are central to tourmaline classification, and to provide practical guidelines for application of the nomenclature.

CRYSTALLOGRAPHIC AND CRYSTAL-CHEMICAL ASPECTS OF TOURMALINE-SUPERGROUP MINERALS

Tourmaline is a crystallographically acentric borosilicate mineral with the generalized chemical formula $XY_3Z_6(T_6O_{18})(BO_3)_3V_3W$ (Hawthorne and Henry 1999). This general formula makes no assumptions about site occupancy, besides those sites known to be occupied exclusively by O^{2-} . Consequently, as knowledge of site occupancy in tourmaline progresses, it will be unnecessary to change the general formula. Only the assignment of the cations and anions to the letters of the general formula will be changed. The symmetry of tourmaline is predominantly rhombohedral in the $R\bar{3}m$ space group. However, there are some reports of tourmalines, or sectors within tourmaline crystals, having orthorhombic, monoclinic, or triclinic symmetry (e.g., Akizuki et al. 2001; Shtukenberg et al. 2007; Williams et al. 2010; IMA no. 2009-46).

Table 1 gives the relative abundance of the generalized cations (R^{1+} , R^{2+} , R^{3+} , R^{4+}) and anions (S^{1-} , S^{2-}) at each of these sites, and presents the most common cation and anion substituents for each of the valence states of the ions. Although tourmaline can accommodate a great variety of cations in minor or trace amounts, all current tourmaline species are, and most prospective species will likely be, represented by combinations of the cations, anions, or vacancies listed in Table 1.

In addition to the ionic size and charge of the cations and anions, two related factors influence the content and location of these ions in the tourmaline structure: short-range bond-valence requirements and order-disorder reactions. (1) In the Y site, the incident bond-valence requirements at the W site mandate that only certain short-range configurations are stable (Hawthorne 1996). Table 2 gives the possible stable local cation configurations at the Y site for generalized Li-free and Li-bearing tourmalines. For a given Y-site bulk composition, the tourmaline can have a single local Y-site cation configuration or a mixture of possible local cation configurations. For example, the chemical composition of end-member liddicoatite has the stable Y-site

TABLE 2. Stable local short-range Y-site cation configurations for anions of different charge at the W site

General chemical type of tourmaline	W-site anion	Y-site stable short-range configurations
Li-free tourmaline	$(OH)^{1-}$ or F^{1-}	$3R^{2+}$ or $R^{3+} + 2R^{2+}$
Li-free tourmaline	O^{2-}	$3R^{3+}$ or $2R^{3+} + R^{2+}$
Li-bearing tourmaline	$(OH)^{1-}$ or F^{1-}	$2Al^{3+} + Li^{1+}$ or $Al^{3+} + 2Li^{1+}$
Li-bearing tourmaline	O^{2-}	$3Al^{3+}$ and $Al^{3+} + 2Li^{1+}$

Note: R is a generalized divalent cation (R^{2+}) or trivalent cation (R^{3+}).

configuration of Li_2Al , whereas end-member elbaite, with a Y-site bulk composition of $Al_{1.5}Li_{1.5}$, will have equal proportions of Al_2Li and $AlLi_2$ clusters at the Y site (Hawthorne 1996). These relatively few local cation configurations will constrain the number and type of potential stable end-members possible in tourmaline. (2) Order-disorder reactions control the actual location of ions in the tourmaline structure. When O^{2-} is located at the W site, disordering tends to develop at the Y and Z sites (Hawthorne and Henry 1999). For example, Hawthorne (1996) showed that in Li-free tourmaline the occurrence of Mg at the Z site and Al at the Y site is commonly due to disorder reactions associated with the occurrence of O^{2-} at the W site, and this can be expressed as $2^Y Mg^{2+} + Z Al^{3+} + W(OH)^{1-} \leftrightarrow 2^Y Al^{3+} + Z Mg^{2+} + W O^{2-}$. For the $3R^{3+}$ Y-site configuration in Li-free tourmaline the disorder relation is $3^Y Mg^{2+} + 2^Z Al^{3+} + W(OH)^{1-} \leftrightarrow 3^Y Al^{3+} + 2^Z Mg^{2+} + W O^{2-}$. Effectively, the disordering substitution enhances the amount of Mg that is located at the Z site and Al at the Y site with the maximal amount being 2 Mg atoms per formula unit (apfu) at the Z site (e.g., Bosi and Lucchesi 2007). Similar arguments have been put forward for the disordering of Fe^{2+} to the Z site (Bosi 2008).

In terms of a classification scheme, most of the compositional variability occurs at the X, Y, Z, W and, to a lesser extent, V sites. The T site is typically dominated by Si and the B site exclusively contains B, such that the cationic occupancies at these sites do not serve as primary parameters for classification, except in some unusual tourmaline species. The atomic ordering in the structure will be confidently established only with crystal-structure refinement data and information from allied techniques such as Mössbauer and NMR spectroscopy. The influence of W-site O^{2-} appears to require disordering reactions to occur such that, in this paper, the recognized or prospective W-site O^{2-} -tourmaline species are presented in their disordered form—their most likely actual cation distribution. However, when oxy-tourmalines are considered for classification purposes, they are recast in their

TABLE 1. Relative site abundances of cations and anions in tourmaline-supergroup minerals

Site	Relative abundance of ions with different valence states	Common cations and anions at each site in order of relative abundance
X	$R^{1+} > R^{2+} > \square$ (vacancy)	R^{1+} : Na ¹⁺ >>> K ¹⁺ R^{2+} : Ca ²⁺
Y	$R^{2+} > R^{3+} > R^{1+} > R^{4+}$	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	$R^{3+} >> R^{2+}$	R^{3+} : Al ³⁺ >> Fe ³⁺ > Cr^{3+} > V^{3+} R^{2+} : Mg ²⁺ > Fe^{2+}
T	$R^{4+} >> R^{3+}$	R^{4+} : Si ⁴⁺ R^{3+} : Al ³⁺ > B^{3+}
B	R^{3+}	R^{3+} : B ³⁺
V	$S^{1-} >> S^{2-}$	S^{1-} : OH ¹⁻ S^{2-} : O ²⁻
W	$S^{1-} \sim S^{2-}$	S^{1-} : OH ¹⁻ ~ F ¹⁻ S^{2-} : O ²⁻

Note: The bolded cations and anions represent the most common ions at these sites.

ordered form. Tourmaline species that contain OH¹⁻ and F¹⁻ at the W site are also presented in their ordered form.

DEFINITIONS AND CLASSIFICATION PRINCIPLES

There are several terms associated with mineral classification schemes that should be elucidated. *Mineral species (minerals)* are defined on the basis of their unique chemical and crystallographic properties (Nickel and Grice 1998). In most cases tourmaline-supergroup minerals are isostructural (space group *R3m*), with the exceptions previously noted. Consequently, the primary criterion for classification is such that most tourmaline species are defined in terms of chemical composition, with the dominance of a chemical constituent of the dominant valency state at a given crystallographic site being the primary criterion for classification. A “chemical constituent” designates a specific cation or anion, group of atoms with the same valency state, molecular group, or vacancies. This dominance criterion is a statement of the *dominant-constituent rule* (Hatert and Burke 2008). Tourmaline solid solutions involve both homovalent substitutions at a given site and heterovalent coupled substitutions over single or multiple sites. An extension of the dominant-constituent rule is the *dominant-valency rule* that states that in a relevant site, the dominant ion of the dominant valence state is considered for nomenclature (Hatert and Burke 2008). Additional complexity is encountered where heterovalent coupled substitutions occur on single or multiple sites such that end-members are produced in which two constituent ions occupy a single site: this is termed the *valency-imposed double-site occupancy* (Hatert and Burke 2008). For example, in the case of the chemical substitution that occurs from schorl to elbaite, there is a single-site coupled substitution that involves the incorporation of Li¹⁺ and Al³⁺ in equal amounts for Fe²⁺ to produce an end-member with two cations at the Y site of elbaite, i.e., ^Y(Al_{1.5}Li_{1.5}). In the case of two-site coupled substitution, dravite can be transformed to uvite by the substitution of Ca²⁺ for Na¹⁺ at the X site, coupled with the substitution of Mg²⁺ for Al³⁺ at the Z site, resulting in multiple-cation occupancy of the Z site as ^Z(MgAl₃) for the uvite end-member.

An *end-member* is an algebraic and chemical construct² that is irreducible and is conformable with the crystal structure under consideration (Hawthorne 2002; see also Appendix 1 for more details). For example, the dravite end-member [NaMg₃Al₆(Si₆O₁₈)(BO₃)₃(OH)₃OH] is irreducible in that it cannot be expressed as a combination of other tourmaline end-members. In the case in which a tourmaline is determined to have *dominant* cation and anion occupancies of the crystallographic sites in accordance with this end-member, it is given the *root name* dravite and is, by implication, considered to be the dravite *mineral species*.

In determining the systematics of tourmaline-supergroup mineral species, the STN recommends the following general procedure be considered:

(1) In tourmaline-supergroup minerals that are dominated by S¹⁻ anions (OH¹⁻ and F¹⁻) in the W site, it is recommended that

the OH¹⁻ species be the reference *root composition* for that root name. As such, this OH¹⁻ species becomes the root name without a “hydroxyl-” prefix e.g., dravite.

(2) For a tourmaline composition that has most of the chemical characteristics of a root composition, but is dominated by other cations or anions at one or more sites, the mineral species is designated by the root name *plus* the appropriate prefix modifiers. For example, a tourmaline with a composition that is generally consistent with dravite, but that contains F¹⁻ as the most prevalent S¹⁻ anion where S¹⁻ anions are dominant over S²⁻ anions at the W site, the mineral species is termed fluor-dravite. To take advantage of search capabilities, it is recommended that any modifiers to tourmaline root names be separated by hyphens. Hyphens are considered important to clarify the components of the species name.

(3) If there are multiple prefix modifiers, the modifiers should be arranged in the order in which it occurs in the structural formula i.e., X-site modifier, Y-site modifier, Z-site modifier, T-site modifier, and then W-site modifier. This has the advantage of ordering the modifiers in a consistent and intuitive manner. For example, a composition that is generally consistent with dravite, but with K¹⁺ being the most prevalent R¹⁺ cation for R¹⁺-dominant X-site occupancy and F¹⁻ being the most prevalent S¹⁻ anion for S¹⁻-dominant W-site occupancy, the hypothetical mineral species would be termed “potassium-fluor-dravite.”

(4) Consistent with the IMA-CNMNC and the International Union of Crystallography procedures, any deviation from the reference rhombohedral space group *R3m* symmetry is accommodated in the nomenclature by adding a suffix to the root name that indicates any atypical symmetry i.e., orthorhombic (-O), monoclinic (-M), or triclinic (-T) (Bailey 1977). For example, an elbaite exhibiting triclinic symmetry would be termed “elbaite-T.”

The cationic and anionic occupancy of the X and W sites serve as particularly convenient and petrologically meaningful ways to define the primary tourmaline groups and a subset of general series of tourmaline species.

PRIMARY TOURMALINE GROUPS: X-SITE OCCUPANCY

Tourmaline can be classified into primary groups based on the dominant occupancy of the X site. Tourmalines have been described that contain dominant Na¹⁺, Ca²⁺, ^X□, and, rarely, K¹⁺. However, because of the relatively rare occurrence of K-rich tourmalines, it is practical to combine the cations with like charges, Na¹⁺ and K¹⁺, into an alkali group. This results in primary groups that are termed the alkali-, calcic-, and X-vacant-tourmaline groups. This general grouping makes petrologic sense because X-site occupancy generally reflects the paragenesis of the rock in which these tourmalines crystallize, analogous to similar general groupings in the amphibole- and pyroxene-supergroup minerals. The alkali-, calcic-, X-vacant ternary system for X-site occupancy can be plotted on the simple ternary diagram illustrated in Figure 1. Arithmetically, the primary X-site groups are defined as follows: *alkali* if (Na¹⁺+K¹⁺) ≥ Ca²⁺ and (Na¹⁺+K¹⁺) ≥ ^X□; *calcic* if Ca²⁺ > (Na¹⁺+K¹⁺) and Ca²⁺ > ^X□; and *X-vacant* if ^X□ > (Na¹⁺+K¹⁺) and ^X□ > Ca²⁺. The dominance of Na¹⁺ or K¹⁺ in alkali-group tourmaline is an example of the dominant-valency rule. In the uncommon case,

² End-members are important in a thermodynamic sense because the thermodynamic properties of end-members can be determined, regardless of whether they exist as stable minerals. Thermodynamic properties are essential for modeling the behavior of solid solutions in petrological and geochemical processes.

in which tourmaline is classified as an alkali-group tourmaline and K^{1+} dominates over Na^{1+} , it is considered a “potassium-” tourmaline. In this case, the root name should be prefixed by “potassium-” e.g., “potassium-povondraite.” Arithmetically, to be considered a “potassium-” tourmaline the following conditions must be satisfied: $(Na^{1+}+K^{1+}) \geq Ca^{2+}$, $(Na^{1+}+K^{1+}) \geq X^{\square}$, and $K^{1+} > Na^{1+}$. If there are other cations with relatively large ion ionic radii that are found in significant amounts at the X site (e.g., Pb^{2+}), they should be included with the cations of the same charge to establish the dominance of the valency at the X site

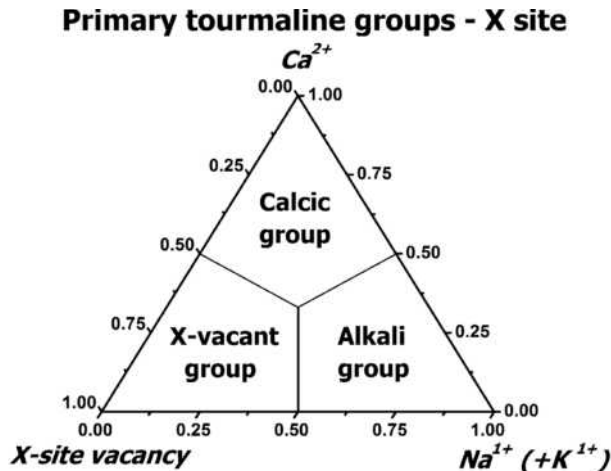


FIGURE 1. Ternary system for the primary tourmaline groups based on the dominant occupancy of the X site.

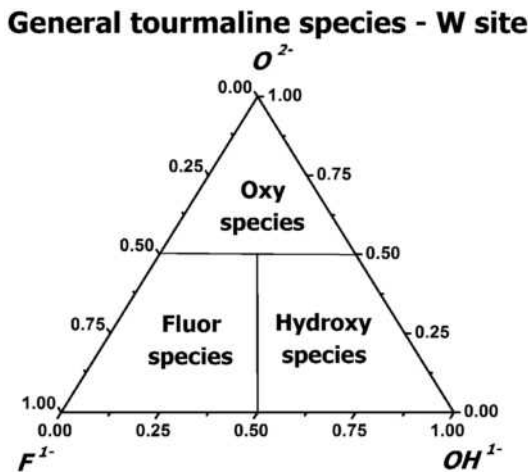


FIGURE 2. Ternary system for a general series of tourmaline species based on the anion occupancy of the W site.

in accordance with the dominant-valency rule. Consequently, X-site occupancy as it relates to tourmaline nomenclature can be extended as needed.

GENERAL SERIES OF TOURMALINE SPECIES: W-SITE OCCUPANCY

Three distinct anions (OH^{1-} , F^{1-} , and O^{2-}) can occur at the W site, and the occupancy of the W site forms the basis for a general series of tourmaline species: hydroxy-, fluor- and oxy-species (Fig. 2). These are defined as follows: *hydroxy* if $OH^{1-} + F^{1-} \geq O^{2-}$ and $OH^{1-} \geq F^{1-}$; *fluor* if $OH^{1-} + F^{1-} \geq O^{2-}$ and $F^{1-} > OH^{1-}$; and *oxy* if $O^{2-} > OH^{1-} + F^{1-}$. The appearance of the general series of tourmaline species based on W-site occupancy differs from the X-site grouping shown in Figure 1 because it involves two anions with a common 1^- charge (OH^{1-} and F^{1-}) and a single anion with a 2^- charge (O^{2-}). Consequently, for O^{2-} to be the dominant anion of the W site, there must be $>50\%$ O^{2-} (cf. Nickel 1992; Chopin 2006). Despite the difficulty of measuring H content in tourmaline, H must be considered in the tourmaline nomenclature because its content does vary, and it can result in oxy-tourmaline species. In the case of an oxy-species, a coupled substitution involving another site is required, and a new root name is typically warranted rather than placing a modifying prefix on the root name.

SPECIFIC TOURMALINE SPECIES

At the time of the revision of this paper, the IMA-CNMNC has recognized 18 tourmaline species with an additional species having a different structure (Appendix 2). Hawthorne and Henry (1999) and the STN re-examined the compositions of the holotype material of these species and, in some cases, redefined the end-member formulas and mineral species in accordance with guidelines suggested by Hawthorne and Henry (1999), Hawthorne (2002), and this paper (Appendix 2). In addition to the IMA-CNMNC-accepted tourmaline species, several varietal names based on the color of tourmaline in hand sample have been used in describing tourmaline, but these were not considered as part of the IMA-CNMNC classification scheme (see Appendix 3). Furthermore, there are a series of names that have been used for tourmaline that are obsolete or have been discredited (Appendix 4).

Tourmaline can be broken into several groups and sub-groups that are useful for classification purposes. The primary tourmaline groups are based on occupancy of the X site, which serves as a convenient division into the alkali-tourmaline group, calcic-tourmaline group or the X-vacant-tourmaline group (Fig. 1). Because each of these groups involves a cation or vacancy with a different charge, coupled substitutions are required to compositionally shift among the groups (Tables 3–6). Within

TABLE 3. Significant tourmaline heterovalent coupled substitutions and associated exchange vectors

	Generalized coupled substitutions	Corresponding exchange vector	Resulting actions
(1)	$X^{R^{1+}} + R^{2+} \leftrightarrow X^{\square} + R^{3+}$	$(X^{\square} R^{3+})(R^{1+} R^{2+})_{-1}$	relates alkali-vacant groups
(2)	$X^{R^{1+}} + R^{3+} \leftrightarrow X^{Ca} + R^{2+}$	$(CaR^{2+})(R^{1+} R^{3+})_{-1}$	relates alkali-calcic groups
(3)	$2^Y R^{2+} \leftrightarrow ^Y Li^{1+} + ^Y Al^{3+}$	$(Li Al)(2R^{2+})_{-1}$	relates incorporation of Li in all groups
(4)	$R^{2+} + OH^{1-} \leftrightarrow R^{3+} + O^{2-}$	$(R^{3+} O^{2-})(R^{2+} (OH^{1-}))_{-1}$	relates deprotonation in all groups
(5)	$0.5Li^{1+} + OH^{1-} \leftrightarrow 0.5^Y Al + O^{2-}$	$(Al_{0.5}O)(Li_{0.5}(OH))_{-1}$	relates deprotonation in Li species
(6)	$R^{2+} + ^T Si^{4+} \leftrightarrow R^{3+} + ^T R^{3+}$	$(R^{3+} R^{3+})(R^{2+} Si^{4+})_{-1}$	relates Tschermak-like tetrahedral-octahedral substitution in all groups

Note: R represents generalized cations such that $^X R^{1+} = Na^{1+}, K^{1+}$; $R^{2+} = Mg^{2+}, Fe^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Zn^{2+}$; $R^{3+} = Al^{3+}, Fe^{3+}, Cr^{3+}, V^{3+}, B^{3+}$ (T site); and no site designation reflects possibilities involving multiple sites.

TABLE 4. Generalized structural formula types for recognized or prospective tourmaline species listed by X-site alkali-group tourmaline

General formula	(X)	(Y ₃)	(Z ₆)	T ₆ O ₁₈	(BO ₃) ₃	V ₃	W
Alkali-subgroup 1	R¹⁺	R₃²⁺	R₆³⁺	R₆⁴⁺O₁₈	(BO₃)₃	S₃¹⁻	S¹⁻
Dravite*	Na	Mg ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Schorl*	Na	Fe ₃ ²⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Chromium-dravite*	Na	Mg ₃	Cr ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Vanadium-dravite*	Na	Mg ₃	V ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Fluor-dravite*	Na	Mg ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
Fluor-schorl*	Na	Fe ₃ ²⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Potassium-dravite"†	K	Mg ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Tsilaisite"‡	Na	Mn ₃ ²⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Alkali-subgroup 2	R¹⁺	R_{1.5}¹⁺ R_{1.5}²⁺	R₆³⁺	R₆⁴⁺O₁₈	(BO₃)₃	S₃¹⁻	S¹⁻
Elbaite*	Na	Li _{1.5} ¹⁺ Al _{1.5} ²⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Fluor-elbaite"†	Na	Li _{1.5} ¹⁺ Al _{1.5} ²⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
Alkali-subgroup 3	R¹⁺	R₃³⁺	R₂³⁺ R₄³⁺§	R₆⁴⁺O₁₈	(BO₃)₃	S₃¹⁻	S²⁻
Povondraite*	Na	Fe ₃ ³⁺	Fe ₄ ³⁺ Mg ₂	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
Chromo-alumino-povondraite*	Na	Cr ₃	Al ₄ Mg ₂	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-dravite"†	Na	Al ₃	Al ₄ Mg ₂	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-schorl"†	Na	Al ₃	Al ₄ Fe ₂ ³⁺	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Na-Cr-O root name"†	Na	Cr ₃	Cr ₄ Mg ₂	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Potassium-povondraite"†	K	Fe ₃ ³⁺	Fe ₄ ³⁺ Mg ₂	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
Alkali-subgroup 4	R¹⁺	R₁¹⁺ R₂²⁺	R₆³⁺	R₆⁴⁺O₁₈	(BO₃)₃	S₃¹⁻	S²⁻
"Na-Li-O root name"†	Na	Li ₁ Al ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
Alkali-subgroup 5	R¹⁺	R₃³⁺	R₆³⁺	R₆⁴⁺O₁₈	(BO₃)₃	S₃²⁻	S¹⁻
Fluor-buergerite*	Na	Fe ₃ ³⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(O) ₃	F
Olenite*	Na	Al ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(O) ₃	(OH)
"Buergerite"‡	Na	Fe ₃ ³⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(O) ₃	(OH)
"Fluor-olenite"‡	Na	Al ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(O) ₃	F
Alkali-subgroup 6	R¹⁺	R₃³⁺	R₆³⁺	R₃³⁺ R₃⁴⁺ O₁₈	(BO₃)₃	S₃¹⁻	S¹⁻
"Na-Al-Al-Al root name"‡	Na	Al ₃	Al ₆	Al ₃ Si ₃ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Na-Al-Al-B root name"‡	Na	Al ₃	Al ₆	B ₃ Si ₃ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Fluor-Na-Al-Al-Al root name"‡	Na	Al ₃	Al ₆	Al ₃ Si ₃ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Fluor-Na-Al-Al-B root name"‡	Na	Al ₃	Al ₆	B ₃ Si ₃ O ₁₈	(BO ₃) ₃	(OH) ₃	F

* Tourmaline species currently recognized by the IMA-CNMNC in the original or modified form (Appendix 2).

† Tourmaline species with compositions found in natural settings, but, as of the time of manuscript revision, not currently recognized by the IMA-CNMNC. Examples of reported compositions consistent with prospective tourmaline species include: "potassium-dravite" (Ota et al. 2008), "fluor-elbaite" (Lussier et al. 2009), "oxy-dravite" (Žáček et al. 2000), "oxy-schorl" (Novák et al. 2004), "Na-Cr-O root name" (Bosi and Lucchesi 2007) and "potassium-povondraite" (Grice et al. 1993), and "Na-Li-O root name" (Quensel and Gabrielson 1939).

‡ Tourmaline species produced experimentally (e.g., Schreyer et al. 2000; Marler et al. 2002) or found in natural settings in which the tourmalines show a tendency for development of these compositions, and not recognized by the IMA CNMNC.

§ For the oxy-tourmaline species the formula is given as the disordered form, consistent with the Y- and Z-site occupancy demonstrated for povondraite, and implied by the short-range disordering effects of O²⁻ at the W site. However, for the verification of each prospective oxy-tourmaline species the disordering on the Z site should be demonstrated for the proper determination of the structural formula.

|| Although a new root name is appropriate, because the species names "oxy-dravite" and "oxy-schorl" have been used relatively commonly in the literature (e.g., Žáček et al. 2000; Novák et al. 2004; Henry et al. 2008), it is recommended that these names be formally accepted as the species names for these end-members.

TABLE 5. Generalized structural formula types for recognized or prospective tourmaline species listed by X-site calcic-group tourmaline

General formula	(X)	(Y ₃)	(Z ₆)	T ₆ O ₁₈	(BO ₃) ₃	V ₃	W
Calcic-subgroup 1	Ca²⁺	R₃²⁺	R₂²⁺ R₄²⁺	R₆⁴⁺O₁₈	(BO₃)₃	S₃¹⁻	S¹⁻
Fluor-uvite*	Ca	Mg ₃	MgAl ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
Feruvite*	Ca	Fe ₃ ²⁺	MgAl ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Uvite*	Ca	Mg ₃	MgAl ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Fluor-feruvite"†	Ca	Fe ₃ ²⁺	MgAl ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
Calcic-subgroup 2	Ca²⁺	R₁²⁺ R₂²⁺	R₆³⁺	R₆⁴⁺O₁₈	(BO₃)₃	S₃¹⁻	S¹⁻
Fluor-liddicoatite*	Ca	Li ₂ ²⁺ Al ³⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Liddicoatite"†	Ca	Li ₂ ²⁺ Al ³⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Calcic-subgroup 3	Ca²⁺	R₃²⁺	R₆³⁺	R₆⁴⁺O₁₈	(BO₃)₃	S₃¹⁻	S²⁻
"Ca-Mg-O root name"‡	Ca	Mg ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Ca-Fe-O root name"‡	Ca	Fe ₃ ²⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
Calcic-subgroup 4	Ca²⁺	R_{1.5}¹⁺ R_{1.5}²⁺	R₆³⁺	R₆⁴⁺O₁₈	(BO₃)₃	S₃¹⁻	S²⁻
"Ca-Li-O root name"‡	Ca	Li _{1.5} Al _{1.5}	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O

* Tourmaline species currently recognized by the IMA-CNMNC in the original or modified form (Appendix 2).

† Tourmaline species with compositions found in natural settings, but, as of the time of manuscript revision, not currently recognized by the IMA-CNMNC. Examples of reported compositions consistent with prospective tourmaline species include: "fluor-feruvite" (Breaks et al. 2008) and "liddicoatite" (Breaks et al. 2008).

‡ Tourmaline species produced experimentally or found in natural settings in which the tourmalines show a tendency for development of these compositions, and not recognized by the IMA-CNMNC.

each group there is a fundamental subgroup, subgroup 1, from which additional subgroups can be generated. Incorporation of Li^{1+} via coupled substitution (3) of Table 3 can result in additional Li-bearing subgroups, which will warrant new root names (e.g., elbaite in alkali-subgroup 2 of Table 4). Likewise, the coupled substitution (4) of Table 3 can result in deprotonated tourmaline species (e.g., alkali-subgroups 3 and 4 of Table 4), and these species should, by analogy, have distinct root names. Coupled substitution (6) of Table 3 could yield species with trivalent cations in up to 50% of the T site. Although such species have not been reported from natural settings, experimental syntheses (e.g., Schreyer et al. 2000; Marler et al. 2002) or compositional tendencies in natural tourmaline warrant their inclusion as prospective species. Within a given tourmaline subgroup there can be several homovalent substitutions that result in extensive or complete solid solution, but it does not change the fundamental character of a tourmaline subgroup (e.g., Fe^{2+} for Mg^{2+} substitution that relates schorl and dravite in alkali-subgroup 1 tourmaline). Within each group, subgroup 1 generally has the most species. For instance, alkali-subgroup 1 contains 8 possible species, mostly variants with dravite or schorl root names. Table 7 presents several additional considerations associated with various substitutions in the tourmaline-supergroup minerals.

This approach of identifying subgroups based on operation of general heterovalent coupled substitutions is similar to that used for the epidote-group nomenclature (Armbruster et al. 2006).

The hypothetical tourmaline species in Tables 4–6 (in quotation marks) are considered to be species likely to be found naturally with many published tourmaline analyses being consistent with these species (see footnotes of Tables 4–6). The hydroxy- and fluor-species are written in the ordered form at the Y and Z sites. The oxy-species are written in the disordered form, with the understanding that disorder over the Y and Z sites is likely (e.g., Hawthorne 1996). Additional end-members that have other cations dominant at one or more sites are likely, and these can be added as new tourmaline species when/if they are discovered and characterized. This proposed scheme is therefore, readily expandable. Whenever possible or reasonable, new tourmaline species should be named using currently recognized root names with appropriate prefix modifiers concatenated to the existing root name. For example, the IMA-CNMNC-accepted Mg-equivalent of foitite is magnesio-foitite (Table 6). Tourmaline compositions generated through heterovalent coupled substitutions of existing root compositions will generally mandate the introduction of new root names. *All proposed mineral species must be submitted to the IMA-CNMNC and fulfill the requirements for new mineral*

TABLE 6. Generalized structural formula types for recognized or prospective tourmaline species listed by X-site vacant-group tourmaline

General formula	(X)	(Y ₃)	(Z ₆)	T ₆ O ₁₈	(BO ₃) ₃	V ₃	W
Vacant-subgroup 1	□	$R_2^{3+} R_2^{3+}$	R_6^{3+}	$R_6^+ O_{18}$	(BO ₃) ₃	S ₃ ⁻	S ⁻
Foitite*	□	Fe ₂ ³⁺ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Magnesio-foitite*	□	Mg ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Vacant-subgroup 2	□	$R_1^{1+} R_2^{3+}$	R_6^{3+}	$R_6^+ O_{18}$	(BO ₃) ₃	S ₃ ⁻	S ⁻
Rossmannite*	□	Li ¹⁺ Al ₂ ³⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Vacant-subgroup 3	□	$R_1^{1+} R_2^{3+}$	R_6^{3+}	$R_6^+ O_{18}$	(BO ₃) ₃	S ₃ ⁻	S ⁻
"□-Mg-O root name"‡	□	MgAl ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"□-Fe-O root name"†	□	Fe ²⁺ Al ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
Vacant-subgroup 4	□	$R_{1.5}^{1+} R_{2.5}^{3+}$	R_6^{3+}	$R_6^+ O_{18}$	(BO ₃) ₃	S ₃ ⁻	S ⁻
"□-Li-O root name"†	□	Li _{0.5} Al _{2.5}	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O

* Tourmaline species currently recognized by the IMA-CNMNC in the original or modified form (Appendix 2).

† Tourmaline species with compositions found in natural settings, but, as of the time of manuscript revision, not currently recognized by the IMA-CNMNC. Examples of reported compositions generally consistent with prospective tourmaline species include: "□-Fe-O root name" (Medaris et al. 2003) and "□-Li-O root name" (Ertl et al. 2005).

‡ Tourmaline species produced experimentally or found in natural settings in which the tourmalines show a tendency for development of these compositions, and not recognized by the IMA-CNMNC.

TABLE 7. Additional considerations associated with homovalent and heterovalent substitutions in tourmaline-supergroup minerals

(a) The most common R^{1+} homovalent substitution in the X-site is $\text{Na}^{1+} \leftrightarrow \text{K}^{1+}$. The tourmaline is considered to be a member of the alkali group if $(\text{Na}^{1+} + \text{K}^{1+}) \geq \text{Ca}^{2+}$ and $(\text{Na}^{1+} + \text{K}^{1+}) \geq \text{X}\square$. In the uncommon case in which tourmaline is classified as an alkali-group tourmaline and $\text{K}^{1+} > \text{Na}^{1+}$, it is considered a "potassium-tourmaline". The tourmaline is considered part of the calcic group if $\text{Ca}^{2+} > (\text{Na}^{1+} + \text{K}^{1+})$ and $\text{Ca}^{2+} > \text{X}\square$. The tourmaline is considered part of the X-site vacancy group if $\text{X}\square > (\text{Na}^{1+} + \text{K}^{1+})$ and $\text{X}\square > \text{Ca}^{2+}$.

(b) R^{2+} homovalent substitutions involve a number of divalent cations such as Mg^{2+} , Fe^{2+} , Mn^{2+} , Co^{2+} , Ni^{2+} , and Zn^{2+} . For example, the most common substitution is probably $\text{Mg}^{2+} \leftrightarrow \text{Fe}^{2+}$. In this case the complicating factor is that Mg^{2+} and possibly Fe^{2+} are generally the primary R^{2+} cations that can be significantly accommodated on the Z site at concentrations up to 2 apfu, most commonly associated with disordering related to incorporation of O^{2-} on the W site. Within a divalent group of elements on a given site, the dominant R^{2+} cations lead to a different modifier/root names. For classification purposes the tourmaline formula should be cast in its ordered form.

(c) R^{3+} homovalent substitutions occur on both the Y and Z sites and include trivalent cations such as Al^{3+} , Fe^{3+} , Cr^{3+} , and V^{3+} . For example, a common substitution is $\text{Fe}^{3+} \leftrightarrow \text{Al}^{3+}$. The R^{3+} cations are most commonly found on the Z site, but the Y site and T site can contain up to 3 apfu R^{3+} cations. If there is O^{2-} on the W site, there is likely to be a disordering resulting in the displacement of the R^{3+} to the Y site with a concomitant substitution of Mg^{2+} on the Z site. For classification purposes the tourmaline formula should be cast in its ordered form.

(d) If there is Li in the tourmaline it is typically introduced via heterovalent substitution (3) ${}^Y 2R^{2+} \leftrightarrow {}^Y \text{Li}^{1+} + {}^Y \text{Al}^{3+}$. Note that for each Li that is introduced there is 2 R^{2+} displaced. That means that plotting parameters in the ternary elbaite-schorl-dravite subsystem are 2Li-Fe²⁺-Mg.

(e) The introduction of O^{2-} in the W or V site can take place via the heterovalent-deprotonation substitution (4) $R^{2+} + \text{OH}^{1-} \leftrightarrow R^{3+} + \text{O}^{2-}$. Note that for each O^{2-} there must be the introduction of an R^{3+} at the expense of R^{2+} .

(f) The introduction of R^{3+} (typically Al or B) into the tetrahedral site can take place via a Tschermak type of heterovalent substitution (5) $R^{2+} + {}^T \text{Si}^{4+} \leftrightarrow R^{3+} + {}^T \text{R}^{3+}$.

species prior to IMA-CNMNC approval as a new mineral species.

For classification, it is recommended that a tourmaline be named for the dominant species in the dominant subgroup, i.e., consistent with the dominant constituent of the dominant-valency state (the last adapted from Hatert and Burke 2008). For example, if there is a mixture of 40% elbaite, 35% schorl, and 25% dravite, the resulting subgroups would be 100% alkali-group tourmaline. However, within this group 60% will be alkali-subgroup 1 tourmaline species and 40% alkali-subgroup 2 species. Alkali-subgroup 1 is the dominant subgroup and schorl is the dominant species within this dominant subgroup such that the tourmaline should be considered a schorl. In this case, these relations for this ternary subsystem can be graphically illustrated (Fig. 3). The addition of other cations beyond the three shown graphically will complicate the application of these subsystem diagrams, but the grouping of common valency components can extend the generality of this approach and allow determination of the proper tourmaline species.

For identification of the wider range of possible natural and synthetic tourmaline species there are general procedures that should be followed. After the primary X-site group is established, the appropriate subgroup should be determined within each of the primary groups. This can be done graphically or by considering the numerical thresholds that serve to separate the subgroups. Identification of the appropriate subgroup 1–4 within each of the primary X-site group tourmalines can be established with a series of diagrams that use the X-site occupancy and $YZR^{2+}/(YZR^{2+} + 2Li^{1+})$ ratio as the primary discriminating factor, with the W-site occupancy as a further discriminator, which will further refine the species within the subgroup (Fig. 4). An alternative diagram of $YZR^{2+}/(YZR^{2+} + 2Li^{1+})$ vs. $WO^{2-}/(WO^{2-} + WOH^{1-} + F^{-})$ results in a comparable discrimination diagram (Fig. 5). Significant variability of T-site and V-site occupancy can result in other relatively uncommon tourmaline species or prospective species. For tourmalines in which the V site contains more than 50% O^{2-} , tourmaline in the alkali group will fall in alkali subgroup 5 and

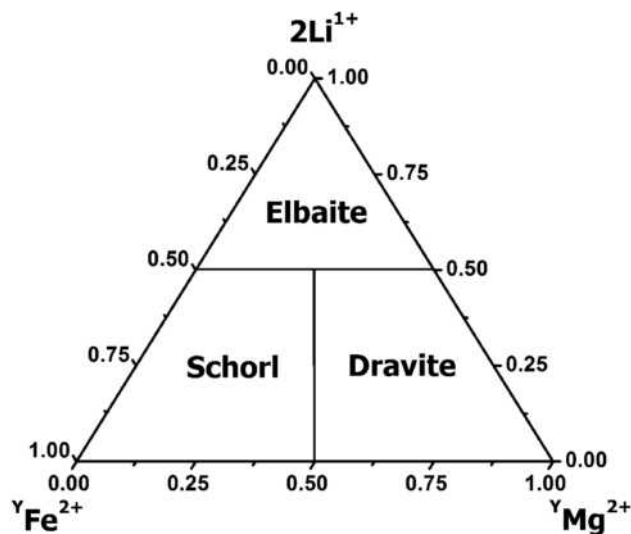


FIGURE 3. Ternary dravite-schorl-elbaite subsystem. Note that dravite and schorl are species within alkali-subgroup 1 and elbaite is a species within alkali-subgroup 2.

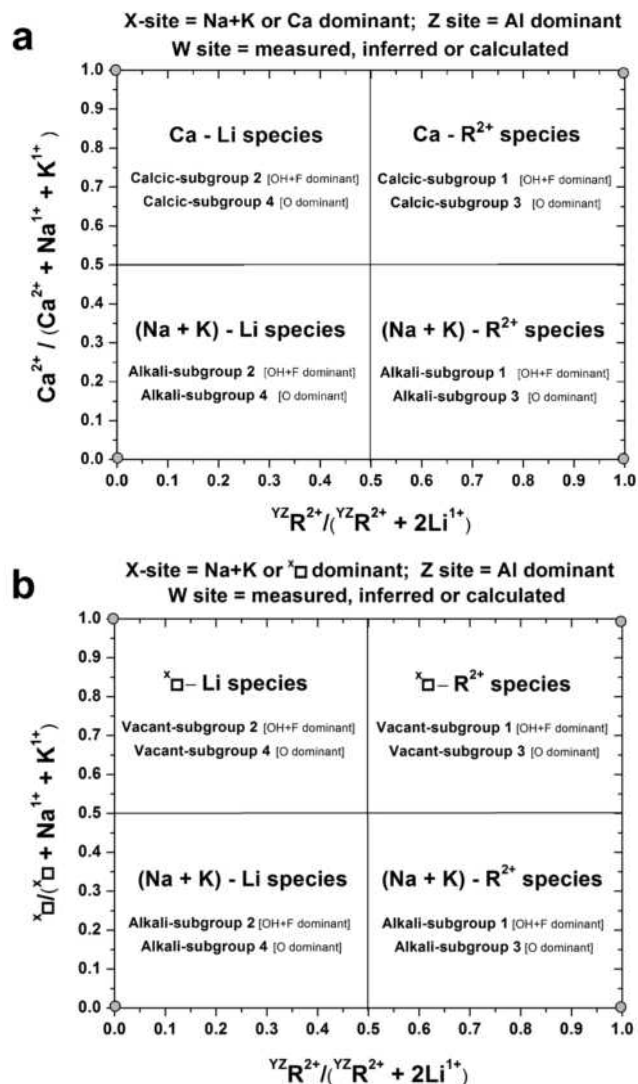


FIGURE 4. Diagrams useful for establishing the appropriate tourmaline subgroups within the alkali, calcic, and vacant groups. (a) Determination of subgroups 1–4 for alkali- and calcic-group tourmalines use parameters $YZR^{2+}/(YZR^{2+} + 2Li^{1+})$ vs. $Ca^{2+}/(Ca^{2+} + Na^{1+} + K^{1+})$ together with the dominant valency anion(s) in the W site i.e., $(OH^{1-} + F^{-})$ vs. O^{2-} . YZR^{2+} represents the total number of divalent cations in the Y and Z site. (b) Determination of subgroups 1–4 for alkali- and X-vacant-group tourmalines use parameters $YZR^{2+}/(YZR^{2+} + 2Li^{1+})$ vs. $X\Box/(X\Box + Na^{1+} + K^{1+})$ together with the dominant valency anion(s) in the W site i.e., $(OH^{1-} + F^{-})$ vs. O^{2-} .

species such as fluor-buergerite and olenite can be recognized. In the alkali-group tourmalines, up to 3 apfu $(Al^{3+} + B^{3+})$ can substitute for Si assuming Y and Z are fully occupied by trivalent cations and W and V sites, by monovalent cations. Thus, the criterion for distinguishing alkali subgroup 6 is $Si^{4+} < 4.5$ apfu. In this case, the dominant tetrahedral trivalent cation (Al^{3+} or B^{3+}) becomes the basis for discriminating the species (Table 4). Once the subgroup is determined, the appropriate species name is given as the dominant species within that subgroup (Tables 4–6). Uncertainties arise when the tourmalines are incompletely analyzed and procedures for dealing with this possibility are addressed in the discussion below.

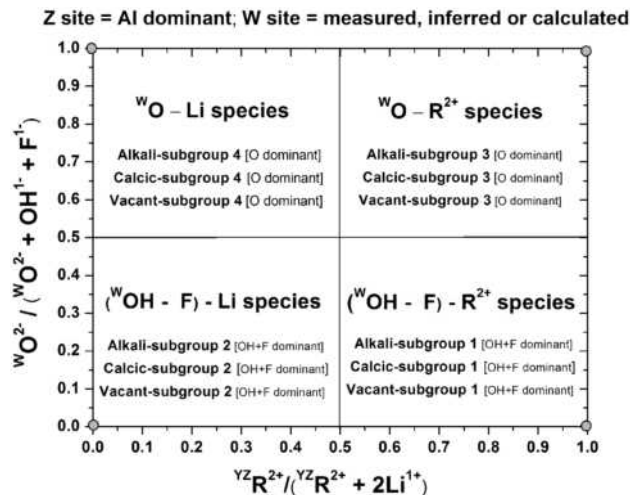


FIGURE 5. Alternative diagram useful for establishing the appropriate tourmaline subgroups within the alkali-, calcic- and vacant groups. The determination of subgroups 1–4 for alkali-, calcic- and vacant-group tourmalines use parameters $YZR^{2+}/(YZR^{2+} + 2Li^{1+})$ vs. $W^{O^{2-}}/(W^{O^{2-}} + OH^{-} + F^{-})$ together with the dominant cation in the X-site and dominant valency anion(s) in the W site, i.e., $(OH^{-} + F^{-})$ vs. O^{2-} .

Additional adjectival modifiers

Although not required, tourmaline species can be further modified with various adjectives that precede the species names (Tables 4–6). In the past, the IMA-CNMNC recommended use of the “Schaller modifiers” in which the valency of the substituent ion is indicated by the suffix “-oan” (for the lower valency cation) and “-ian” (for the higher valency cation). However, this scheme has several shortcomings that have prompted the approval of alternative chemical-element adjectival modifiers in place of the Schaller-type modifiers (Bayliss et al. 2005). In the most general case, it is recommended that adjectival modifier such as “-rich” or “-bearing” be used together with the specific element(s) and, where known, an indication of the oxidation state of the cation and/or the site it occupies, e.g., “Fe²⁺-rich,” “K-bearing,” or “^TAl-rich.” The chemical-element adjectival modifiers are not part of the name of the tourmaline species, and, consequently, authors are free to use chemical-element modifiers that are chemically correct and meet the needs of the author in expressing significant chemical information about the mineral species (Bayliss et al. 2005). However, it is recommended that the authors define the magnitude of the compositional parameters implied by these adjectival modifier terms. Multiple modifiers are possible, and the order of the modifiers should be such that the modifier with the greatest percentage of site occupancy is next to the mineral-species name, the modifier with the second most percentage preceding that one, etc. For example, a hypothetical tourmaline solid solution with 60% dravite-schorl, 40% uvite-feruvite and 2/1 ratio of Mg-Fe²⁺ at the Y site, has a structural formula of $(Na_{0.6}Ca_{0.4})(Mg_2Fe^{2+})(Mg_{0.4}Al_{5.6})(Si_6O_{18})(BO_3)_3(OH)_3(OH)$ and the appropriate name could be expressed as Fe²⁺-,Ca-rich dravite i.e., reflecting 33% Fe²⁺ at the Y site and 40% Ca at the X site.

SITE ALLOCATION OF CATIONS AND ANIONS

Hawthorne (1996) notes that chemical analyses of tourmaline merely establish which elements are present, but do not determine

where they are located in the structure. Structural refinement and site assignment based on crystallographic evidence is required for accurate site allocation. Furthermore, tourmaline site occupancies can be modeled with appropriate optimization procedures (e.g., Wright et al. 2000). In the absence of site assignments directly established by crystal structure refinements, it is possible to make some “reasonable” assumptions concerning site assignments of specific cations and anions (Table 1). With this basic information, it is recommended that cations and anions in tourmaline be allocated with the following procedure:

(1) Based on the type of analytical techniques and data generated, the most appropriate normalization scheme is used and any significant unanalyzed cations or anions are calculated whenever possible (see procedures in Appendix 5).

(2) Only B³⁺ is allocated to the B site. With compelling chemical, crystallographic, or spectroscopic evidence, excess B³⁺ (B³⁺ > 3.0 apfu) may be assumed to be in the T site. Compelling evidence includes NMR spectra indicating tetrahedral B³⁺, structural refinements with tetrahedral bond length determinations and well-constrained analytical evidence that demonstrate B³⁺ > 3.0 apfu (e.g., Tagg et al. 1999; Hughes et al. 2000; Schreyer et al. 2002; Ertl et al. 2006a; Lussier et al. 2009).

(3) Na¹⁺, Ca²⁺, and K¹⁺ are assigned to the X site with any site deficiency assumed to represent X-site vacancy (^X□). Additional large cations, such as Pb²⁺, are likely located in the X site and should be assigned to that site.

(4) Si⁴⁺ is assumed to be exclusively located in the T site with any deficiency made up by Al³⁺ (MacDonald and Hawthorne 1995). If there is compelling chemical, crystallographic, or spectroscopic evidence for tetrahedral B³⁺, this tetrahedral B³⁺ should be assigned to the T site prior to the assignment of the tetrahedral Al³⁺ (e.g., Lussier et al. 2009).

(5) The relative distribution of anions in the V and W sites is reasonably well established. F¹⁻ is exclusively contained in the W site and O²⁻ tends to be preferentially contained in this site (Grice and Ercit 1993). Consequently, it is appropriate that all F¹⁻ be assigned to the W site, and then O²⁻. Any excess O²⁻ is assigned to the V site. To date, evidence from bond angle distortion of the ZO₆ octahedron and Y-O distances and bond-valence sums at the V site indicate that most of the tourmaline species (except buergerite and some olenitic tourmalines) have ~ 3(OH¹⁻) at the V site (Ertl et al. 2002; Cempírek et al. 2006; Bosi and Lucchesi 2007).

(6) The Y and Z site assignments can be more ambiguous. The least problematic assignment is the exclusive allocation of Li¹⁺, Mn²⁺, Zn²⁺, Ni²⁺, Co²⁺, Cu²⁺, and Ti⁴⁺ to the Y site. However, the smaller cation allocation between the Y and Z sites can be more uncertain. Based on crystallographic and mineral chemical information, it is considered that, with the presence of O²⁻ at the W site, Mg²⁺ and possibly Fe²⁺ may be disordered into the Z site and trivalent cations (especially Al³⁺ and Fe³⁺) may be disordered into the Y site (Henry and Dutrow 1990, 2001; Hawthorne et al. 1993; Taylor et al. 1995; Ertl et al. 2003a; Bosi et al. 2004). Consequently, actual tourmaline structures can exhibit a significant amount of disordering.

For the purposes of classification of tourmaline species only, the ordered form of the tourmaline is assumed for all tourmaline species including the oxy-tourmaline. Consequently, the proce-

cedure that is recommended for classification involves allocation of the small cations among the Z and Y sites as follows: Initially assign the most abundant R^{3+} cations to the Z site (not including any Al^{3+} and B^{3+} assigned to the tetrahedral site). Next, the remainder of the R^{3+} cations should be assigned in accordance with their abundance. If there is an excess of R^{3+} cations on the Z site, the excess R^{3+} cations go into the Y site. If there is a deficiency in the Z site after assigning all of the R^{3+} to that site (i.e., <6.0 cations), assign Mg^{2+} and then Fe^{2+} to the Z site up to 2 apfu (Bosi and Lucchesi 2007).

TOURMALINE CLASSIFICATION PROCEDURE: A HIERARCHICAL APPROACH

Tourmaline investigations generally have varying levels of information available. The tourmaline information may range from complete analytical and crystal structural data to incomplete chemical data. However, it is important that a hierarchical classification procedure be used to accommodate the levels of information that are accessible.

Level 1—complete analytical and structural data

This level considers those tourmalines in which all elements are measured, including the oxidation states of transition elements, and the specific cation and anion site occupancies are established by crystal-structure refinement. Note that an ordered structural formula is assumed for classification purposes only, and proper site occupancies should be included in the ultimate tourmaline structural formula, whenever possible (e.g., Ertl et al. 2003a; Bosi and Lucchesi 2004). *This level of complete characterization of tourmaline is the optimal situation, but one which is currently relatively uncommon.*

Level 2—complete analytical data

This level implies direct knowledge of all elements (light elements and oxidation states of transition elements), but generally with assumed site assignments. Because an ordered structural formula is assumed, the site allocation procedure in the previous section can be used and is appropriate for classification purposes.

Recommended classification procedure for tourmaline with Level 1 and Level 2 data. With complete analytical data, the following procedure for systematically naming tourmaline species is suggested:

(1) Cast the structural formula in an ordered form consistent with the site allocation procedures given above.

(2) Determine the dominant X-site cation or vacancy to establish the primary tourmaline group (Fig. 1).

(3) Establish the dominant anion (OH^{-} , F^{-} , or O^{2-}) at the W site (Fig. 2).

(4) Ascertain the dominant anion (OH^{-} or O^{2-}) at the V site. The current state of knowledge is that most tourmalines are dominated by OH^{-} at the V site. The exceptions are buergerite and some olenitic tourmalines (Ertl et al. 2005; Cempirek et al. 2006; Bosi and Lucchesi 2007).

(5) Determine whether $Si^{4+} < 4.5$ apfu with the remainder of the tetrahedral site being occupied by ${}^TAl^{3+}$ and ${}^TB^{3+}$. Although, natural tourmalines with these characteristics have not been identified, tourmalines with these characterizations have been

synthesized (Schreyer et al. 2000; Marler et al. 2002).

(6) Establish the dominant Z-site cation (Al^{3+} , Cr^{3+} , Fe^{3+} , or V^{3+}). This can be done simply by inspection or calculation, or can be illustrated graphically. For example, in tourmaline with low amounts of Fe^{3+} at the Z site of the ordered formula, the Al-V-Cr ternary can be used to graphically display the Z-site dominant cation (Fig. 6). The most common Z-site dominant cation is Al^{3+} , and a procedure for graphically classifying 24 possible ZAl -dominant tourmaline species is given in Figures 7 to 9. There are only a few Cr^{3+} -, Fe^{3+} -, V^{3+} - end-members that have been described at this time (e.g., chromium-dravite, povondraite, and vanadium-dravite) so comparable diagrams were not generated for these chemical systems. The Fe^{3+} -dominant end-member povondraite is commonly in solid solution with the “oxy-dravite” and dravite and the distinction between these species can be evaluated by examining the dominant ${}^ZV^{3+}$ cation i.e., Fe^{3+} or Al^{3+} (Henry et al. 1999, 2008; Žáček et al. 2000).

(7) Determine the Y-site cation occupancy, recalling that an ordered form of the structural formula is used for classification purposes only. The dominant subgroup (subgroup 1–4 of each of the three groups) can be established graphically from Figures 4 and 5.

(8) Once the dominant subgroup is determined, the dominant species in that subgroup defines the species name. In many instances, this can be done simply by comparing the structural formula with the possible species found within the appropriate subgroup (Tables 4–6). If tourmaline compositions fall within the appropriate subsystems, the species can also be generally established through the use of compositional diagrams such as Figures 7–9. A more inclusive approach is to calculate the dominant cation or anion of the dominant valency on given sites to directly establish subgroup and species. An Excel spreadsheet program (TourmalineSpecies-Henry1-1) is available³ for these calculations and species determinations.

³ Deposit item AM-11-036, Excel spreadsheet program. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover) for price information. Online, visit the MSA web site at <http://www.minsocam.org>, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

Z site cation dominance; Al-Cr-V subsystem (low Fe^{3+})

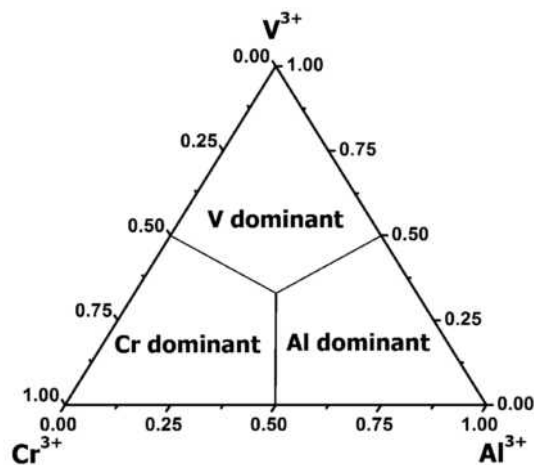


FIGURE 6. Ternary diagram for the Al-V-Cr subsystem of the Al-Fe-V-Cr quaternary system used for illustrating the dominant occupancy of the Z site for tourmaline, assuming minor Fe^{3+} on the Z site.

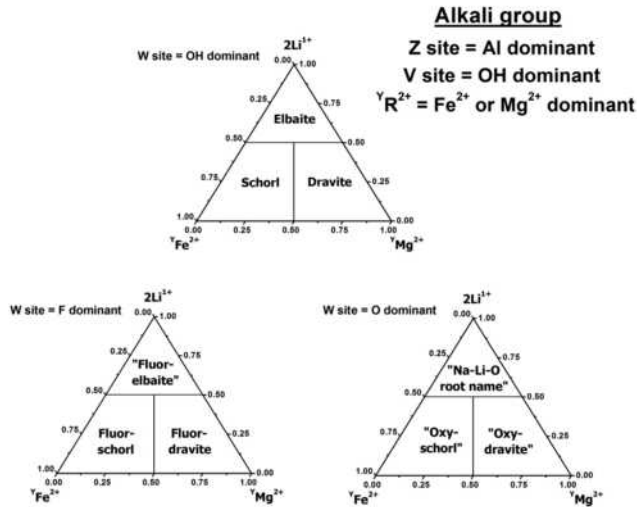


FIGURE 7. Ternary diagrams useful for plotting and classifying alkali-group tourmaline species with Al³⁺ dominance at the Z site and OH⁻ dominance at the V site. The three ternary subsystems represent dominance of OH⁻, F⁻, or O²⁻ at the W site, respectively. Determination of the species is made by plotting Y-site cations on the appropriate ternary. The Y site occupancy is determined by an ordered structural formula. Significant deviation from this chemical subsystem will result in greater uncertainty of species designation.

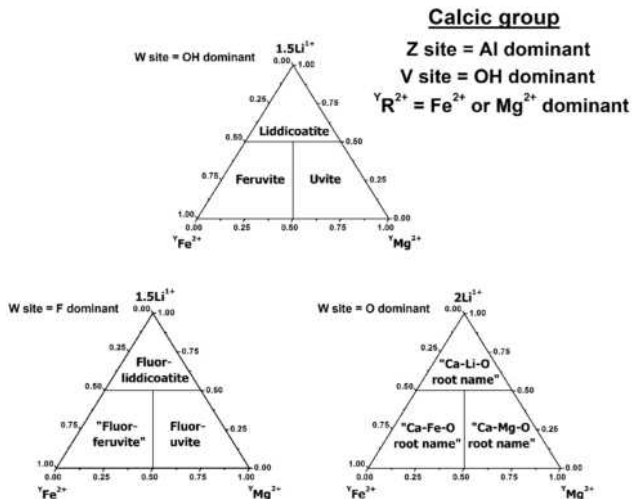


FIGURE 8. Ternary diagrams useful for plotting and classifying calcic-group tourmaline species with Al³⁺ dominance at the Z site and OH⁻ dominance at the V site. The three ternary subsystems represent dominance of OH⁻, F⁻, or O²⁻ at the W site. Determination of the species is made by plotting Y-site cations on the appropriate ternary. The Y site occupancy is determined by an ordered structural formula. Significant deviation from this chemical subsystem will result in greater uncertainty of species designation.

In addition, a table of representative tourmaline analyses with diagnostic parameters for identification of tourmaline species is given in Appendix 6.

Level 3—Partial tourmaline compositional data without direct measurement of B, H, Li, and the oxidation states of transition elements

This is the most common situation, typical of tourmalines analyzed only by the electron microprobe. The procedures out-

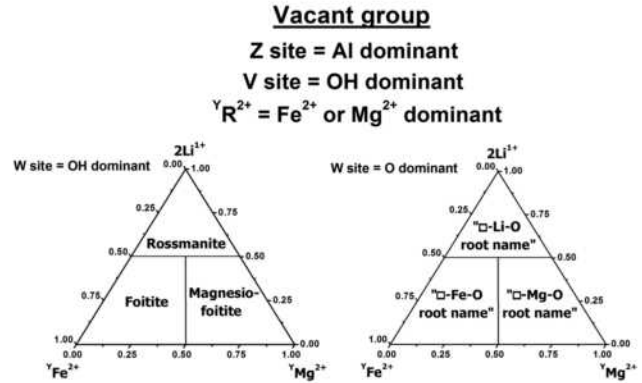


FIGURE 9. Ternary diagrams useful for plotting and classifying vacant-group tourmaline species with Al³⁺ dominance at the Z site and OH⁻ dominance at the V site. The two ternary subsystems represent dominance of OH⁻ or O²⁻ at the W site. F⁻ is likely not a dominant anion at the W site. Determination of the species is made by plotting Y-site cations on the appropriate ternary. The Y-site occupancy is determined by an ordered structural formula. Significant deviation from this chemical subsystem will result in greater uncertainty of species designation.

lined in Appendix 5 allow estimation of some of the unmeasured cations and anions found in tourmaline. However, there can be considerable uncertainty associated with these procedures. As noted earlier, an ordered structural formula is assumed and the cations allocated accordingly.

Recommended classification procedure for tourmaline with Level 3 data. With the appropriate analytical data, estimation of unanalyzed elements and assumed site occupancies, the following procedure for systematically naming tourmaline species is suggested:

(1) Cast the structural formula in an ordered form consistent with the site allocation procedures outlined above.

(2) Determine the dominant X-site cation or vacancy to establish the principal tourmaline subgroup (Fig. 1). This data are readily accessible from a good-quality electron microprobe analysis.

(3) Establish the dominant anion (OH⁻, F⁻, or O²⁻) at the W site (Fig. 2). In the absence of direct measurement of H, the uncertainty associated with estimating H can be large, and the resultant ^WO²⁻ estimate inaccurate. In contrast, F⁻ can be accurately measured with the electron microprobe if proper care is taken in the analytical procedure. If H is undetermined (measured or calculated), it is recommended that the criterion F⁻ > 0.5 apfu, be met for the tourmaline to be considered a fluor-species.

(4) Estimate the dominant anion (OH⁻ or O²⁻) at the V site. The current state of knowledge is that most tourmalines are greatly dominated by OH⁻ at the V site. Consequently, the assumption of ^V(OH)⁻ = 3 is generally correct. The exceptions are buergerite and some olenitic tourmalines (Ertl et al. 2002; Cempírek et al. 2006; Bosi and Lucchesi 2007).

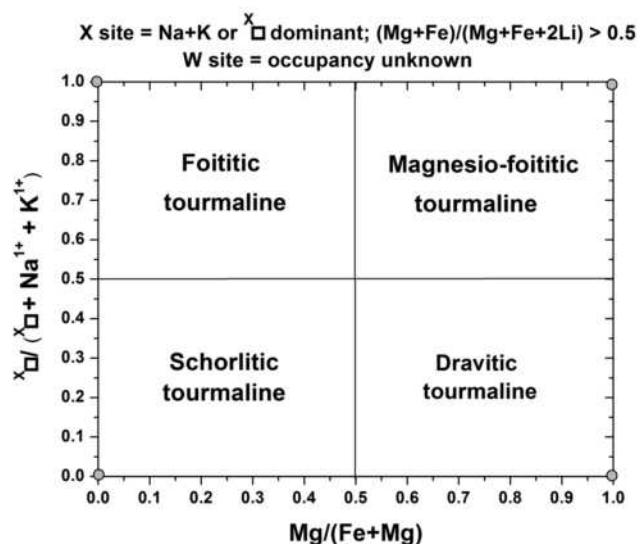
(5) Determine whether Si⁴⁺ < 4.5 apfu with the rest of the tetrahedral site being occupied by ^TAl³⁺ and ^TB³⁺. Although, natural tourmalines with these characteristics have not been identified, tourmalines with these characterizations have been synthesized (Schreyer et al. 2000; Marler et al. 2002).

(6) Establish the dominant Z-site cation (Al³⁺, Cr³⁺, Fe³⁺, or

TABLE 8. Recommended names for incompletely or inadequately determined tourmalines

General formula	(X)	(Y ₃)	(Z ₆)	V ₃ (likely)*	W (unknown)†
Alkali-group tourmaline					
Elbaite tourmaline	Na	Li and Al	Al	(OH ¹⁻)	unknown
Schorlitic tourmaline	Na	Fe ²⁺	Al	(OH ¹⁻)	unknown
Dravitic tourmaline	Na	Mg	Al	(OH ¹⁻)	unknown
Buergeritic tourmaline	Na	Fe ³⁺	Al	(O ²⁻)	unknown
Olenitic tourmaline	Na	Al	Al	(OH ¹⁻)	unknown
Povondraitic tourmaline	Na	Fe ³⁺	Fe ³⁺	(OH ¹⁻)	unknown
Chromium-dravitic tourmaline	Na	Mg	Cr	(OH ¹⁻)	unknown
Vanadium-dravitic tourmaline	Na	Mg	V	(OH ¹⁻)	unknown
Calcic-group tourmaline					
Liddicoatitic tourmaline	Ca	Li and Al	Al	(OH ¹⁻)	unknown
Uvitic tourmaline	Ca	Mg	Al	(OH ¹⁻)	unknown
Feruvitic tourmaline	Ca	Fe ²⁺	Al	(OH ¹⁻)	unknown
Vacant-group tourmaline					
Rossmannitic tourmaline	□	Li and Al	Al	(OH ¹⁻)	unknown
Foitic tourmaline	□	Fe ²⁺	Al	(OH ¹⁻)	unknown
Magnesian-foitic tourmaline	□	Mg	Al	(OH ¹⁻)	unknown

* Anion presumed to occupy the V site.

† Unknown amounts of OH¹⁻ and O²⁻. However, F¹⁻ > 0.5 apfu will signify a fluor-species, and earlier species-designation procedures are warranted.**FIGURE 10.** Example of a diagram that can be used to illustrate the generalized tourmaline species based on $Mg/(Mg + Fe)$ vs. $X\Box/(X\Box + Na^{1+} + K^{1+})$ ratios.

V³⁺). This can be done simply by inspection or calculation, or can be illustrated graphically. For tourmaline with low amounts of Fe³⁺ at the Z site of the ordered formula, the Al-V-Cr ternary can be used to graphically establish this Z-site subgroup (Fig. 6). The most common Z-site dominant cation is Al³⁺, and a graphical approach for classifying 24 possible ^ZAl-dominant tourmaline species is given in Figures 7 to 9. The Fe³⁺-dominant end-member povondraite is commonly in solid solution with the “oxy-dravite” and dravite species (Henry et al. 1999, 2008; Žáček et al. 2000).

(7) Determine the Y-site cation occupancy, recalling that an ordered form of the structural formula is used for classification purposes only. The dominant subgroup (subgroup 1–4 of each of the three subgroups) can be roughly established graphically from Figures 4 and 5.

(8) With the determination of the dominant subgroup, the dominant species in that subgroup can be identified with the

same procedure given in the previous section.

The user must decide whether the results of the assumptions used in calculating unmeasured elements are accurate enough to adequately characterize the tourmaline composition. If the user considers the calculated unanalyzed elements inadequate, it is recommended that a more generalized name be used (Table 8, Fig. 10). However, if F¹⁻ > 0.5 apfu the tourmaline will necessarily be a “fluor-tourmaline” species and the earlier classification procedures can be followed.

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APPENDIX 1. TOURMALINE END-MEMBERS: GENERAL CHARACTERISTICS

There are inconsistencies in the earlier definitions of several of the tourmaline end-member formulas that prompt redefining some of these end-members (Hawthorne and Henry 1999). In defining end-member compositions there are several characteristics that should be considered (Hawthorne 2002).

(1) *An end-member composition must be fixed.* Consequently, formulas expressed with variable cations or anions on a given site, such as $(\text{Al}^{3+}, \text{Fe}^{3+})$ on the Y site or $(\text{F}^-, \text{OH}^-)$ at the W site, can be factored into two or more end-member components of fixed composition. For example, in the case of the original end-member definition of foitite, the composition was expressed as $\square [\text{Fe}_2^{2+} (\text{Al}, \text{Fe}^{3+})] \text{Al}_6 (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_4$ (MacDonald et al. 1993). However, this definition is incorrect because the composition is variable and can be factored into the two fixed compositions: $\square [\text{Fe}_2^{2+} \text{Al}] \text{Al}_6 (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_4$ and $\square [\text{Fe}_2^{2+} \text{Fe}^{3+}] \text{Al}_6 (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_4$.

(2) An end-member may have more than a single cation or anion at a single given site if it is necessary to attain electroneutrality in the crystal structure. Electroneutrality in crystal structures mandate that, in some instances, two cations or anions may be required for charge balance on a single site. One of the best examples is the tourmaline end-member elbaite: $\text{Na} [\text{Li}_{1.5} \text{Al}_{1.5}] \text{Al}_6$

(Si₆O₁₈) (BO₃)₃ (OH)₃ (OH). The X, Z, T, B, V, and W sites are completely ordered (occupied by only one type of cation or anion) such that the aggregate charge is 6⁻. This requires that cations on the Y site have a total charge of 6⁺. In the case of elbaite, with a mix of Li⁺ and Al³⁺, the aggregate charge is only met with the Y-site composition of [Li_{1.5}Al_{1.5}].

(3) Anions are critical in defining end-members, and similar anions can occupy more than one crystallographically distinct site in a crystal structure. Anions such as OH⁻, F⁻, and O²⁻ can define distinct end-members. Anions sites can have crystallographic distinctions that mandate preferences of certain anions for specific anion sites. For example, in the tourmaline structure the V site can be occupied by O²⁻ and OH⁻, but the W site can be occupied by F⁻, O²⁻, and/or OH⁻. In the case of homovalent anion substitution of F⁻ for OH⁻, tourmaline will range from (OH)₃(OH) to (OH)₃(F), thus defining the OH (hydroxy) and F (fluor) end-members. In the case of heterovalent anion substitution of O²⁻ for OH⁻ or F⁻, coupled substitutions must involve other cations in the crystal structure to define an “oxy” end-member.

APPENDIX 2: TOURMALINE SPECIES, END-MEMBER FORMULAS, MODIFICATIONS, ETYMOLOGY, TYPE LOCALITIES, AND REPRESENTATIVE CELL DIMENSIONS

The following tourmaline species have either been previously accepted by the IMA-CNMNC or have been modified by the STN for internal consistency among the tourmaline species. Modifications to the original tourmaline species descriptions are noted.

Chromium-dravite

Structural formula: Na Mg₃ Cr₆ (Si₆O₁₈) (BO₃)₃ (OH)₃ OH
IMA number: IMA 82-055. Original name: chromdravite.
Modifications: Due to its distinction in the tourmaline structure, the structural formula is written to designate two OH-bearing sites (the V and W sites). This contrasts with the earlier formula that combined these two sites into a single “OH” site with four possible OH⁻ anionic groups. The full term “chromium” is used as a prefix for consistency among species.
Etymology: Named for its relationship to dravite and chemical composition.
Type locality: Velikaya Guba uranium occurrence, Zaonezhskiy Peninsula, Karelia, Russia.
Crystal system: Trigonal; *R3m*
Representative cell dimensions (type material): *a* = 16.11 Å, *c* = 7.27 Å, *V* = 1634 Å³
Selected references: Rumyantseva (1983)

Chromo-alumino-povondraite

Structural formula: Na Cr₃ (Al₄Mg₂)(Si₆O₁₈) (BO₃)₃ (OH)₃ O
IMA number: IMA 2009-088
Modifications: none
Etymology: Named for its chemical composition and its relationship to povondraite.
Type locality: Chromite deposits of Nausahi, Keonjhar District, Orissa, India.
Crystal system: Trigonal; *R3m*
Representative cell dimensions (type material): *a* = 16.036 Å, *c* = 7.319 Å, *V* = 1589.9 Å³
Selected references: Williams et al. (2010)

Dravite

Structural formula: Na Mg₃ Al₆ (Si₆O₁₈) (BO₃)₃ (OH)₃ OH
IMA number: First described prior the establishment of IMA in 1958—Grandfathered status.
Modifications: Due to its distinction in the tourmaline structure, the structural formula is written to designate two OH-bearing sites (the V and W sites). This contrasts with the earlier formula that combined these two sites into a single “OH” site with four possible OH⁻ anionic groups.
Etymology: Named in 1884 by Tschermak for the Drava river area, the location of a Mg- and Na-rich tourmaline. The Drava river area, which is the district along the Drava River (in German: Drau; in Latin: Drave) is in Austria and Slovenia (Ertl 2007).
Type locality: Unterdrauburg, Carinthia, Austria (today Dobrava pri Dravogradu, Slovenia); Ertl (2007).

Crystal system: Trigonal; *R3m*
Representative cell dimensions (type material): *a* = 15.96 Å, *c* = 7.21 Å, *V* = 1590 Å³
Selected references: Tschermak (1884), Kunitz (1929), and Dunn (1977)

Elbaite

Structural formula: Na (Li_{1.5}Al_{1.5}) Al₆ (Si₆O₁₈) (BO₃)₃ (OH)₃ OH
IMA number: First described prior the establishment of IMA in 1958—Grandfathered status.
Modifications: Due to its distinction in the tourmaline structure, the structural formula is written to designate two OH-bearing sites (the V and W sites). This contrasts with the earlier formula that combined these two sites into a single “OH” site with four possible OH⁻ anionic groups.
Etymology: Named after the type locality, on the island of Elba, Tuscany, Italy
Type locality: San Piero in Campo, Campo nell’Elba, Elba Island, Livorno Province, Tuscany, Italy.
Crystal system: Trigonal; *R3m*
Representative cell dimensions (type material): *a* = 15.85 Å, *c* = 7.11 Å, *V* = 1546.9 Å³
Selected references: Vernadsky (1913), Donnay and Barton (1972), Novák et al. (1999), and Ertl (2008)

Feruvite

Structural formula: Ca Fe₃²⁺ (Al₃Mg) (Si₆O₁₈) (BO₃)₃ (OH)₃ OH
IMA number: IMA 87-057
Modifications of the end-member definition: The original formula for feruvite is Ca Fe₃ (Al₃Mg)₆ (Si₆O₁₈) (BO₃)₃ (OH)₄ (Grice and Robinson 1989). This is not considered to be an appropriate end-member and it does not specify the valence state of Fe. The Z site was determined to be (Al_{4.72}Fe_{0.34}Mg_{0.82}Fe_{0.12}), which is close to an (Al₃Mg) end-member.
Etymology: Named for its relationship to uvite and chemical composition.
Crystal system: Trigonal; *R3m*
Type locality: Repanga Island (Cuvier Island), Waikato, North Island, New Zealand.
Representative cell dimensions (type material): *a* = 16.01 Å, *c* = 7.25 Å, *V* = 1609 Å³
Selected references: Grice and Robinson (1989) and Selway et al. (1998a)

Fluor-buergerite

Structural formula: Na Fe₃²⁺ Al₆ (Si₆O₁₈) (BO₃)₃ O₃ F
IMA number: IMA 65-005. Original name: buergerite
Etymology: Named for Martin Julian Buerger (1903–1986), a professor of mineralogy at the Massachusetts Institute of Technology and a pioneer of crystal structure analysis.
Modifications: For consistency among tourmaline species, the STN advocates that hydroxy species becomes the root name of a species. For those tourmalines in which the W site exhibits dominance of S¹⁻ relative to S²⁻ anions and dominance F⁻ relative to OH⁻, the species becomes the fluor-species equivalent.
Type locality: Mexquitic, San Luis Potosí, Mexico.
Crystal system: Trigonal; *R3m*
Representative cell dimensions (type material): *a* = 15.87 Å, *c* = 7.19 Å, *V* = 1568 Å³
Selected references: Donnay et al. (1966), Barton (1969), and Tippe and Hamilton (1971)

Fluor-dravite

Structural formula: Na Mg₃ Al₆ (Si₆O₁₈) (BO₃)₃ (OH)₃ F
IMA number: 2009-089
Modifications: For consistency among tourmaline species, the STN advocates that hydroxy species becomes the root name of a species. For those tourmalines in which the W site exhibits dominance of S¹⁻ relative to S²⁻ anions and dominance F⁻ relative to OH⁻, the species becomes the fluor-species equivalent.
Etymology: Named for its relationship to dravite and chemical composition.
Type locality: Crabtree Emerald mine, Mitchell County, North Carolina, U.S.A.
Crystal system: Trigonal; *R3m*
Representative cell dimensions (type material): *a* = 15.955 Å, *c* = 7.153 Å, *V* = 1576.9 Å³
Selected references: Williams et al. (2010)

Fluor-liddicoatite

Structural formula: Ca (Li₂Al) Al₆ (Si₆O₁₈) (BO₃)₃ (OH)₃ F
IMA number: IMA 76-041. Original name: liddicoatite
Modifications of the end-member definition: Dunn et al. (1977b) gave the structural formula for the holotype liddicoatite material as (Ca_{0.72}Na_{0.27}) (Li_{1.59}Al_{1.13}Fe_{0.11}Ti_{0.05}Mn_{0.04}Mg_{0.04}Al_{6.00}Si_{6.00}O₁₈) (BO₃)₃ [(OH)_{2.73}O_{0.27}] [F_{0.87}(OH)_{0.13}]. Based on this composition and the structural analogy with elbaite, they extrapolated the end-member composition of liddicoatite as Ca (Li_{1.74}Al_{1.26}) Al₆ (Si₆O₁₈) (BO₃)₃ [(OH)_{2.48}O_{0.52}] (F,OH), but stipulated that this is not a “pure end-member.” Fur-

therefore, they gave the “ideal” composition of liddicoatite as $\text{Ca}(\text{Li},\text{Al})_3\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{O},\text{OH})_3(\text{OH},\text{F})$. Several aspects of this formula warrant modification of the end-member structural formula to the one given here. (1) Because F partitions exclusively in the W site, the holotype material is an F-dominant species. (2) Any oxygen at the W and V sites should be assigned to the W site in the holotype material structural formula (Hawthorne 1996). (3) The divalent charge of Ca requires an adjustment of the Li:Al ratio so the Y-site is (Li_2Al) .

Etyymology: Named for Richard T. Liddicoat (1918–2002), gemologist and president of the Gemological Institute of America.

Type locality: Pegmatitic area southwest of the towns of Antsirabé and Betafo, Vakinankaratra region, Antananarivo Province, Madagascar.

Crystal system: Trigonal; $R3m$

Representative cell dimensions (type material): $a = 15.87 \text{ \AA}$, $c = 7.14 \text{ \AA}$, $V = 1557 \text{ \AA}^3$

Selected references: Dunn et al. (1977b), Nuber and Schmetzer (1981), and Aurisicchio et al. (1999)

Fluor-schorl

Structural formula: $\text{NaFe}_2^+\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{F}$

IMA number: 2010-067

Modifications: For consistency among tourmaline species, the STN advocates that hydroxy species becomes the root name of a species. For those tourmalines in which the W site exhibits dominance of S^{1-} relative to S^{2-} anions and dominance F^{1-} relative to OH^{1-} , the species becomes the fluor-species equivalent.

Etyymology: Named for its relationship to schorl and chemical composition.

Type locality: Area near Zschorlau, Erzgebirge, Saxony, Germany and area near Grassein, Trentino, South Tyrol, Italy.

Crystal system: Trigonal; $R3m$

Representative cell dimensions (type material): $a = 15.996 \text{ \AA}$, $c = 7.186 \text{ \AA}$, $V = 1576.9 \text{ \AA}^3$

Selected references: Ertl et al. (2006)

Fluor-uvite

Structural formula: $\text{CaMg}_2(\text{Al}_3\text{Mg})(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{F}$

IMA number: First described prior the establishment of IMA in 1958—Grandfathered status. Original name: uvite.

Modifications of the end-member definition: Uvite, originally defined by Kunitz (1929), was considered to have an ideal formula of $\text{CaMg}_3(\text{Al}_3\text{Mg})(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_4$. This formula was based on the examination of tourmalines from Uva (Sri Lanka), De Kalb (New York), and Gouverneur (New York) with OH contents of approximately 4 apfu. However, all other analyses from these localities contain F in the 0.5–1.0 apfu range. Dunn et al. (1977a) designated a sample of uvite from Uva, Sri Lanka as a neotype, and this sample has an anion content of $(\text{OH}_{1.90}\text{F}_{0.76}\text{O}_{0.34})$. This anion content would mandate that the W site would be dominated by F and that uvite should be an F-end-member.

Etyymology: Named for the type locality area, Uva Province, Sri Lanka.

Type locality: Uva Province, Sri Lanka.

Crystal system: Trigonal; $R3m$

Representative cell dimensions (type material): $a = 15.97 \text{ \AA}$, $c = 7.21 \text{ \AA}$, $V = 1592 \text{ \AA}^3$

Selected references: Kunitz (1929), Schmetzer et al. (1979), and Dunn et al. (1977a)

Foiteite

Structural formula: $\square(\text{Fe}_2^+\text{Al})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{OH}$

IMA number: IMA 92-034

Modifications of the end-member definition: The original end-member composition of foiteite was given with a variable cation occupancy at the Y site i.e., $\text{Y}_3 = [\text{Fe}_2^+(\text{Al},\text{Fe}^{3+})]$ (MacDonald et al. 1993). Because Al is dominant relative to Fe^{3+} in the holotype material, the Y-site composition of the end-member is considered Fe_2^+Al .

Etyymology: Named for Franklin F. Foit Jr. (1942–), mineralogist at Washington State University, Pullman, in recognition of his work on tourmaline-supergrupp minerals.

Type locality: Found as museum specimens designated only as from “southern California”, U.S.A., probably from White Queen mine, Pala district, San Diego County, California, U.S.A. (Anthony et al. 1995; Novák and Taylor 2000).

Crystal system: Trigonal; $R3m$

Representative cell dimensions (type material): $a = 15.97 \text{ \AA}$, $c = 7.13 \text{ \AA}$, $V = 1575 \text{ \AA}^3$

Selected references: MacDonald et al. (1993) and Pezzotta et al. (1996)

Magneso-foiteite

Structural formula: $\square(\text{Mg}_2\text{Al})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{OH}$

IMA number: IMA 98-037

Modifications: Due to its distinction in the tourmaline structure, the structural formula is written to designate two OH-bearing sites (the V and W sites). This contrasts with the earlier formula that combined these two sites into a single “OH” site with four possible OH^{1-} anionic groups.

Etyymology: Named for its relationship to foiteite and chemical composition.

Type locality: Kyonosawa, Mitomi-mura, Yamanashi Prefecture, Chubu region, Honshu Island, Japan.

Crystal system: Trigonal; $R3m$

Representative cell dimensions (type material): $a = 15.88 \text{ \AA}$, $c = 7.18 \text{ \AA}$, $V = 1568 \text{ \AA}^3$

Selected references: Hawthorne et al. (1999)

Olenite

Structural formula: $\text{NaAl}_3\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{O}_3)\text{OH}$

IMA number: IMA 85-006

Modifications of the end-member definition: Sokolov et al. (1986) gave the formula for the type olenite as $\text{Na}_{1-x}\text{Al}_3\text{Al}_6\text{B}_3\text{Si}_6\text{O}_{27}(\text{O},\text{OH})_4$. To create an end-member formula with the ideal occupancy of one Na at the X site, three Al at the Y site, and where the T site is completely occupied by Si, the V and W site can only be occupied by $[\text{O}_3(\text{OH})]$. To create an ordered formula, the (OH) is eventually assigned to the W site, while O_3 is assigned to the V site.

Etyymology: Named for the type locality area, Olenek River basin, Russia.

Type locality: Olenek River basin, Olenii (Oleny) Range, Voron'i Tundry, Kola Peninsula, Murmansk Oblast region, Russia.

Crystal system: Trigonal; $R3m$

Representative cell dimensions (type material): $a = 15.80 \text{ \AA}$, $c = 7.09 \text{ \AA}$, $V = 1533 \text{ \AA}^3$

Selected references: Sokolov et al. (1986), Ertl et al. (1997), Hughes et al. (2000), Schreyer et al. (2002), and Cempirek et al. (2006)

Povondraite

Structural formula: $\text{NaFe}_3^+(\text{Fe}_4^+\text{Mg}_2)(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{O}$

IMA number: Renamed/redefined by IMA 90-E

Modifications of the end-member definition: Povondraite was redefined from the original “ferridravite” (Walenta and Dunn 1979) because the initially assumed site assignments were incorrect and did not correspond to the Fe^{3+} -equivalent of dravite (Grice et al. 1993). Hawthorne and Henry (1999) suggested that Mg is ordered at the Z site and should be part of the end-member formula.

Etyymology: Named for Pavel Povondra (1924–), mineralogist and chemist at the Charles University, Prague, Czech Republic, for his extensive work on the tourmaline supergroup.

Type locality: Alto Chapare district, Chapare Province, Cochabamba Department, Bolivia.

Crystal system: Trigonal; $R3m$

Representative cell dimensions (type material): $a = 16.19 \text{ \AA}$, $c = 7.44 \text{ \AA}$, $V = 1689 \text{ \AA}^3$

Selected references: Walenta and Dunn (1979), Grice et al. (1993), and Žáček et al. (2000)

Rossmanite

Structural formula: $\square(\text{LiAl}_2)\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{OH}$

IMA number: IMA 96-018

Modifications: Due to its distinction in the tourmaline structure, the structural formula is written to designate two OH-bearing sites (the V and W sites). This contrasts with the earlier formula that combined these two sites into a single “OH” site with four possible OH^{1-} anionic groups.

Etyymology: Named after George R. Rossmann (1945–), California Institute of Technology, Pasadena, California, U.S.A., in recognition for his work on the spectroscopy of the tourmaline-supergrupp minerals.

Type locality: Hradisko quarry, Rožná, Morava (Moravia), Czech Republic.

Crystal system: Trigonal; $R3m$

Representative cell dimensions (type material): $a = 15.77 \text{ \AA}$, $c = 7.09 \text{ \AA}$, $V = 1527 \text{ \AA}^3$

Selected references: Selway et al. (1998b)

Schorl

Structural formula: $\text{NaFe}_3^+\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{OH}$

IMA number: First described prior the establishment of IMA in 1958—Grandfathered status.

Modifications: Due to its distinction in the tourmaline structure, the structural formula is written to designate two OH-bearing sites (the V and W sites). This contrasts with the earlier formula that combined these two sites into a single “OH” site with four possible OH^{1-} anionic groups.

Etyymology: Name probably derived from the early German mining term “Schor” (mud) or after the name of the former village “Schorl” (today: Zschorlau) in Saxony, Germany. The first relatively detailed description of schorl with the name “schürli” and its occurrence (various tin mines in the Saxony Ore Mountains) was written by Johannes Mathesius (1504–1565) in 1562 under the title “Sarepta oder Bergpostill” (Ertl 2006).

Type locality: Saxony Ore Mountains, Germany.

Crystal system: Trigonal; $R3m$

Representative cell dimensions: $a = 15.98 \text{ \AA}$, $c = 7.16 \text{ \AA}$, $V = 1583 \text{ \AA}^3$.

Selected references: First described in 1562 by Mathesius (Mathesij 1562) as reported in Wallerius (1747), Romé de l'Isle (1772), Werner (1780), Fortier and Donnay (1975), Foit (1989), and Ertl (2006).

Uvite

Structural formula: $\text{Ca Mg}_3 (\text{Al}_3\text{Mg}) (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_3 \text{OH}$

IMA number: IMA 2000-030a

Modifications of the end-member definition: Uvite, originally defined by Kunitz (1929), was considered to have an ideal formula of $\text{Ca Mg}_3 (\text{Al}_3\text{Mg}) (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_4$. This formula was based on the examination of tourmalines from Uva (Sri Lanka), De Kalb (New York) and Gouverneur (New York) with OH contents of approximately 4 apfu. However, all other analyses from these localities contain F in the 0.5–1.0 apfu range. Dunn et al. (1977a) designated a sample of uvite from Uva, Sri Lanka as a neotype, and this sample has an anion content of $(\text{OH}_{2.90}\text{F}_{0.76}\text{O}_{0.34})$. This anion content would mandate that the W site would be dominated by F and that the type uvite should most properly be termed fluor-uvite. More recently, uvitic species with OH dominant on the W site were described by Christine M. Clark, Frank C. Hawthorne and Joel D. Grice from the Brumado mine, Brazil locality.

Etymology: Named for the type locality area of the currently defined fluor-uvite, Uva Province, Sri Lanka. Uvite is redefined as the hydroxy equivalent to fluor-uvite.

Type locality: Brumado mine, Bahia, Brazil.

Type material: deposited in the Royal Ontario Museum (Toronto, Canada), specimen number M55101.

Crystal system: Trigonal; $R\bar{3}m$

Representative cell dimensions (type material): $a = 15.954 \text{ \AA}$, $c = 7.214 \text{ \AA}$, $V = 1590.2 \text{ \AA}^3$

Selected references: Williams et al. (2010)

Vanadium-dravite

Structural formula: $\text{Na Mg}_3 \text{V}_6^{2+} (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_3 \text{OH}$

IMA number: IMA 1999-050

Modifications: Due to its distinction in the tourmaline structure, the structural formula is written to designate two OH-bearing sites (the V and W sites). This contrasts with the earlier formula that combined these two sites into a single "OH" site with four possible OH^- anionic groups.

Etymology: Named for its relationship to dravite and chemical composition.

Type locality: Slyudyanka complex, Lake Baikal region, Siberia, Russia.

Crystal system: Trigonal; $R\bar{3}m$

Representative cell dimensions (type material): $a = 16.12 \text{ \AA}$, $c = 7.39 \text{ \AA}$, $V = 1663 \text{ \AA}^3$

Selected references: Reznitsky et al. (2001)

Additional Potential, but Unnamed, Tourmaline Species

At the time of the manuscript revision the following tourmalines are described either in a proposal to IMA or via the codification for unnamed minerals (Smith and Nickel 2007) and further expanded in the IMA-CNMNC website (<http://pubsites.uws.edu.au/ima-cnmnc/>).

IMA No. 2009-046

Proposed structural formula: $(\text{Na}, \square)(\text{Fe}^{2+}, \text{Mg})_3\text{Al}_6(\text{BO}_3)_3\text{Si}_6\text{O}_{18}(\text{OH})_4$

Localities: Cleveland tin mine, Luina, Waratah, Tasmania, Australia ($41^\circ 28' 57''\text{S}$, $145^\circ 23' 7''\text{E}$; type locality); Mount Bendoc, Victoria, Australia ($37^\circ 7' 60''\text{S}$, $148^\circ 54' 0''\text{E}$); Mount Bischoff, Tasmania, Australia ($41^\circ 25'\text{S}$, $145^\circ 31'\text{E}$); Blue Mountain Saddle (Bald Hornet Claim), North Bend, King County, Washington, U.S.A. ($47^\circ 31'\text{N}$, $121^\circ 43'\text{W}$).

Crystal system: Monoclinic; Cm ; structure determined.

Representative cell dimensions (type material): $a = 10.408(3)$, $b = 15.991(5)$, $c = 7.189(2) \text{ \AA}$, $\beta = 117.44(2)^\circ$, $V = 1061.88 \text{ \AA}^3$

UM2000-//SiO:AIBFLiNa (invalid list)

Proposed structural formula: $\text{Na}(\text{Al}, \text{Li})_3\text{Al}_6(\text{BO}_3)_3\text{Si}_6\text{O}_{18}(\text{F}, \text{OH})_4$

Comment: This is the fluorine-dominant analog of elbaite (e.g., Lussier et al. 2009). The suggested name "fluor-elbaite" has not yet been approved by the IMA-CNMNC.

UM2000-64-SiO:BFeHKMg

Proposed structural formula: $(\text{K}, \text{Na})(\text{Fe}^{3+})_3(\text{Fe}^{3+}, \text{Mg})_6(\text{BO}_3)_3\text{Si}_6\text{O}_{18}(\text{OH}, \text{O})_4$

Comment: This is a K-dominant tourmaline (Žáček et al. 2000).

APPENDIX 3. COLOR-BASED TOURMALINE VARIETAL NAMES

Although mineral varietal names are not under the jurisdiction of the IMA-CNMNC, the STN acknowledges the use of the color-based tourmaline varietal names. Appendix Table 1 is a listing of some of the varietal names that have been used, with possible tourmaline species associations.

APPENDIX 4. OBSOLETE OR DISCREDITED TOURMALINE NAMES

Throughout the history of tourmaline investigations several names have been used for tourmaline or minerals that were considered to be tourmaline. A list of former tourmaline names that are considered obsolete or have been discredited are presented in Appendix Table 2.

APPENDIX 5. ANALYTICAL CONSIDERATIONS AND NORMALIZATION PROCEDURES

The crystal chemistry of tourmaline can be evaluated utilizing various analytical procedures, each with strengths and weaknesses that should be carefully considered when assessing the results and classifying a given tourmaline. Several of the techniques used specifically for tourmaline analysis are briefly mentioned below. Special attention is given to normalization procedures used for the electron microprobe data of tourmaline.

Bulk tourmaline analysis techniques

Several "bulk" sample techniques have been used to analyze tourmaline. The general disadvantage of these techniques is the averaging effect of "bulk" samples in which chemical zonation may be masked, and mineral and fluid inclusions may introduce contamination. (1) Wet chemical analysis was the standard procedure for analysis of materials prior to the widespread use of the electron microprobe (e.g., Peck 1964; Jarosowich 1966; Povondra and Čech 1976). The chief advantages were that light elements could be analyzed and oxidation states of transition elements were determined. (2) Inductively coupled plasma-atomic emission spectroscopy (ICP-AES) has commonly been used to supplement electron microprobe analysis by determining light element concentrations as well as trace element levels in tourmaline (e.g., Shearer and Papike 1986; Kantipuly et al. 1988). Sample amounts as small as 200–300 mg have been analyzed. (3) Induced neutron activation analysis (INAA) has been successfully used to determine REE in tourmaline (e.g., King et al. 1988; Roda et al. 1995).

Tourmaline structural refinement and spectroscopic analysis techniques

Single crystal refinement and spectroscopic techniques provide valuable information about the local environments of specific cations, trace elements and oxidation states of transition elements. (1) Crystal structure refinement is an electron-counting technique that, in combination with chemical analysis, helps determine the site assignments through definition of stereochemical relationships and refined site-scattering values (e.g., Hawthorne and Grice 1990; Hawthorne et al. 1995; Cámara et al. 2002). This technique exhibits spatial resolution that will work on well-constrained analytical problems such as those encountered in elbaite (Burns

APPENDIX TABLE 1. Color-based tourmaline varietal names

Varietal name	Description
Achroite	colorless tourmaline, probably elbaite or rossmanite
Aphrizite	dark gray schorl
Brazilian chrysolite	yellow-green tourmaline resembling chrysolite
Brazilian emerald	green and transparent tourmaline resembling emerald
Brazilian peridot	honey-brown to green tourmaline resembling peridot
Brazilian ruby	transparent red tourmaline resembling ruby
Brazilian sapphire	transparent blue tourmaline resembling sapphire
Canary tourmaline	bright yellow tourmaline
Cat's eye tourmaline	chatoyant tourmaline in a variety of colors
Ceylon chrysolite	yellow-green tourmaline resembling chrysolite
Ceylon peridot	honey yellow tourmaline resembling peridot
Chameleonite	alexandrite-like tourmaline; color changes under different lighting conditions
Cromolite	green tourmaline, originally considered Cr-bearing tourmaline
Deuterolite	alexandrite-like tourmaline, probably a Cr-bearing dravite; color changes under different lighting conditions
Emeralite	emerald-green tourmaline
Indicolite	blue tourmaline, probably elbaite-schorl series
lochroite	violet tourmaline
Moor's Head tourmaline	light-colored tourmaline with black top
Paraibaite	blue-green (neon blue) Cu-bearing elbaite, originally described from the Paraiba State of Brazil
Rubellite	pink or red tourmaline, probably elbaite
Siberian ruby	red tourmaline resembling ruby
Siberite	purple rubellite, probably elbaite
Verdelite	green tourmaline, probably elbaite-schorl series
Watermelon tourmaline	color-zoned tourmaline with pink interiors and green rims, generally elbaite

Note: Source of terms: Dietrich (1985).

APPENDIX TABLE 2. Obsolete, discredited, or misidentified tourmaline species

Name	Additional information
Aluminobuergerite	Term for suggested end-member $\text{Na}_{1-x}\text{Al}_3\text{Al}_6(\text{BO}_3)_3\text{O}_{3-x}(\text{OH})_{1-x}$ or synthetic $\text{NaAl}_3\text{Al}_6(\text{BO}_3)_3\text{O}_3(\text{OH})$
Alumoeibaite	Elbaite
Chrome tourmaline	Green Cr-bearing tourmaline or chromdravite
Cockle	Schorl
Coronite	Dravite
Eicotourmaline	Tourmaline-like mineral without boron
Ferridravite	Povondraite
Ferroelbaite	Schorl
Ferroschorlite	Schorl
Gouverneurite	Dravite
lochroite	Tourmaline
Jochroit	Tourmaline
Lithia tourmaline	Elbaite
Magnesioschorlite	Dravite
Magnodravite	Extremely Mg-rich uvite-like tourmaline
Mineral H	Ti-rich tourmaline from pegmatites
Oxytourmaline	Tourmaline with noteworthy replacement of O for (OH,F)
Pierrepontite	Schorl
Schirl	Schorl
Schorlite	Schorl
Schorlomite	Name mistakenly used for schorl; schorlomite is an accepted garnet group mineral
Taltalite	Mixture of tourmaline with Cu-ore or green tourmaline
Titanschorl (schörl)	Rutile
Titantourmaline	Ti-rich tourmaline
Titantourmaline	Ti-rich tourmaline
Tsilaisite	Mn-rich tourmaline, mostly in solid solution with elbaite
Zeuxite	Acicular tourmaline, Fe^{3+} -rich tourmaline, green tourmaline

Note: Sources of terms: Wang and Hsu (1966); Fleischer (1969); Chukhrov (1981); Dietrich (1985); Bayliss (2000).

et al. 1994). (2) Secondary ion microprobe spectroscopy has provided information on spatial distribution of light elements as well as trace and minor elements in tourmaline (e.g., Wilson and Long 1983; Grew et al. 1990; Harris et al. 1992; Hawthorne et al. 1995). (3) Mössbauer spectroscopy has been used to evaluate

$\text{Fe}^{3+}/\text{Fe}^{2+}$ ratios as well as the locations of Fe^{2+} and Fe^{3+} in the tourmaline structure (e.g., Hermon et al. 1973; Gorelikova et al. 1978; Saegusa et al. 1979; Ferrow et al. 1988; Ferrow 1994; Dyar et al. 1998; Andreozzi et al. 2008), but this approach is also a bulk technique. (4) Proton-induced γ -ray emission has also been used for light-element analysis in tourmaline (e.g., Dyar et al. 1998).

Tourmaline electron microprobe analytical techniques

The electron microprobe is currently the most commonly used analytical tool for tourmaline analysis. However, there are several analytical limitations that must be considered when calculating a structural formula from electron microprobe data. Although it is possible to analyze most of the major elements in tourmaline, Li and H as well as the valence states of transition elements, cannot be directly measured. In addition, a critical constituent of tourmaline is the light element B. Boron has been analyzed with the electron microprobe (e.g., Bastin and Heijligers 2000; McGee and Anovitz 1996; Hawthorne et al. 1995), but the analytical accuracy and precision remain unsatisfactory for confident structural formula calculations. These shortcomings require that the normalization procedure for tourmaline be carefully considered to minimize the limitations of electron microprobe analysis. 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.

Normalization procedures, and light element and ferric Fe estimation

A variety of tourmaline normalization procedures have been used. Each procedure has strengths and weaknesses. However, the most appropriate procedure depends on the completeness of the tourmaline analysis, the quality of the analysis, the assumptions for unanalyzed elements and the petrologic environment in which the tourmalines develop.

Normalization of tourmaline with complete chemical characterization.

Ultimately, the best approach for determination of the structural formula of tourmaline is to analyze tourmaline as completely as possible and by using as many techniques as possible. With a complete analysis, normalization can be properly done on a 31 anion basis (Henry and Dutrow 1996; Clark 2007). The most accurate site assignments are made by means of crystal structure refinements with a combination of site-scattering and mean bond-length information and structural formula optimization procedure (e.g., Hawthorne and Grice 1990; Hawthorne et al. 1993; Taylor et al. 1995; Hawthorne 1996; Ertl et al. 2003a, 2003b; Bosi and Lucchesi 2004).

Normalization of electron microprobe data and estimation of light elements and oxidation states of elements.

Most widespread tourmaline normalization procedures make assumptions concerning the anionic and cationic assignments. In the absence of accurate analyses of B, O, H, Li and the oxidation states of transition elements, several procedures can be used to calculate a structural formula. Each of these procedures, in turn, can provide the basis for estimation of light elements and oxidation states of transition elements.

Normalization procedure 1—fixed number of O atoms.

Assume OH fills the four V+W sites after accounting for F and Cl. In essence, this implies normalization of the cations on the basis of 31 anions (O + F + OH), 29 oxygen atoms (both normalization assuming B is calculated by stoichiometry, $B = 3$ apfu) or 24.5 oxygen atoms (without B calculation). Generally, this approach provides a good first approximation (Clark 2007). However, if there is significant O^{2-} substitution for OH^{-1} , the oxygen normalization factor will be underestimated as will be the number of cations. In fact, significant amounts O^{2-} substitution for OH^{-1} have been demonstrated in uvite (Taylor et al. 1995) and in several other tourmaline compositions (e.g., Povondra 1981; Povondra and Novák 1986; Dyar et al. 1998). Consequently, this approach should be used with those tourmalines in which it is reasonably assured that $OH+F+Cl \sim 4$ (e.g., Burns et al. 1994).

Normalization procedure 2—fixed Y+Z+T cations. Normalize the sum of the T+Z+Y cations to 15. *This is the recommended normalization approach for tourmaline with low Li contents and minor B in the tetrahedral site.* It assumes that there are no vacancies in the Y, Z and T sites, a valid assumption based on a majority of crystal structure refinement data. It also assumes that the amount of tetrahedral B is not significant. However, some recent refinement results indicate small numbers of vacancies in Y and Z sites (<0.22 apfu; Ertl et al. 1997, 2003b; Prowatke et al. 2003). To the extent that all of the significant cations on these sites are accurately analyzed, the structural formula can be calculated without having to rely on estimates of the OH content or valence states of transition elements. Fortunately, those tourmaline containing even a moderate amount of Mg (>0.02 apfu) and that coexist with minerals such as biotite, muscovite and staurolite typically have minor-to-insignificant amounts of Li due to the preferential partitioning of Li into these coexisting minerals (Henry and Dutrow 1996). This normalization procedure will be appropriate for almost all metamorphic and most igneous tourmalines.

Normalization procedure 3—fixed Si. Normalize on the basis of Si = 6. This procedure is useful for normalization of tourmalines with significant amounts of unanalyzed elements, particularly Li. It assumes that there is no significant tetrahedral Al or B. For many Li-rich tourmalines this general assumption is probably reasonable (e.g., Dutrow and Henry 2000). However, many low-Li tourmalines are known to contain significant amounts of tetrahedral Al and B, so that this procedure should be used with care in these instances (e.g., Hawthorne et al. 1993; Lussier et al. 2009).

Estimation of B. Based on the total B found in a series of high-quality wet-chemical analyses of tourmaline from various lithologies, Henry et al. (2002) indicate that the assumption that B fully occupies the triangular B site and can be calculated using stoichiometric constraints (i.e., $B = 3$) is likely to be valid for most petrologic occurrences of tourmaline (see also Clark 2007). Furthermore, crystal structure refinements and bond valence calculations indicate that there are essentially 3 B apfu in those tourmalines that have been determined to date (Hawthorne 1996). However, there are a few uncommon instances involving Al-rich tourmaline (e.g., olenite) in which some B may also be tetrahedral (Ertl et al. 1997, 2006a; Tagg et al. 1999; Hughes et al. 2000). This feature indicates that the assumption of 3 B may not be valid in all cases, but is likely to be reasonable for most tourmalines.

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., Si = 6, see Dutrow and Henry 2000) or that Li be iteratively calculated using a fixed number of oxygens and assuming $OH+F = 4$ (e.g., Burns et al. 1994; Clark 2007). (1) The Si = 6 approach appears to work well for some Li-rich tourmaline (Li >0.7 apfu), but tends to underestimate the Li contents (Henry et al. 2002). The underestimate of Li is likely due to the existence of tetrahedral Al substituting for Si will result in calculated Li being too low. Henry et al. (2002) indicate that this procedure should be within 0.1–0.3 apfu of the correct Li values. (2) The Li by iteration and $OH+F = 4.0$ approach tends to result in high estimates of Li (Henry et al. 2002). For tourmalines with high values of Li (>0.7 apfu) this generally results in an overestimate of 0.1–0.3 Li apfu. This is a more significant problem in low-Li tourmalines, and generally appears to indicate that these tourmalines contain significant amounts of Li. The Li overestimates are a consequence of substantial amounts of substitution of O for OH+F in the W and V sites in many tourmalines or can result because of the occurrence of significant vacancies at the Y site in Al-rich tourmalines. Nonetheless, this procedure is very useful for tourmaline developed in Li-enriched environments (e.g., highly fractionated granitic pegmatites).

Estimation of H. H contents can be determined by charge balance if oxidation states can be measured or inferred, and Li contents can be estimated or inferred. Putative oxidation state evidence can be derived from tourmaline optical properties or by mineral assemblages, particularly graphite-bearing assemblages (Dyar et al. 1998). Minimal Li contents can be generally inferred by presence of significant Mg in tourmaline, which is a function of coexisting mineral assemblages that tend to efficiently partition Li (Henry and Dutrow 1996). Charge-balance estimates of H are subject to significant amounts of uncertainty, and likely result in minimum values of H. Despite the larger amounts of uncertainty, useful information on H contents can be derived using electron microprobe data (e.g., Henry et al. 2002).

Estimation of Fe oxidation states. Fe^{3+} contents can be determined by charge balance if H contents can be measured or inferred, and Li contents can be estimated or inferred. Despite the larger amounts of uncertainty, useful information on Fe^{3+} contents can be derived using electron microprobe data (e.g., Henry et al. 1999). However, all these procedures can have relatively large errors. The best way would be to employ techniques such as Mössbauer spectroscopy to determine the Fe^{2+}/Fe^{3+} ratio (e.g., Dyar et al. 1998). In some instances, the Fe^{2+}/Fe^{3+} ratio can be inferred for tourmalines found in certain mineral assemblages. For example, Dyar et al. (2002) found that tourmaline from graphite-bearing metapelites contained 20–34% of the total Fe as Fe^{3+} .

APPENDIX 6. REPRESENTATIVE TOURMALINE ANALYSES WITH DIAGNOSTIC PARAMETERS FOR CLASSIFICATION

To illustrate the manner in which various parameters are determined for use in the tourmaline nomenclature scheme, several tourmaline analyses from the literature are given in Appendix Table 3. These represent a range of tourmaline species and demonstrate the manner in which an ordered tourmaline is written and presents some of the important chemical parameters used for classification.

APPENDIX TABLE 3. Examples of complete tourmaline analyses with ordered structural formula and important parameters used for classification

Data source	Grice and Ercit (1993)						Povondra et al. (1998)
Sample no.	144478	49356	43293	43167	43873	55224	PAFG - Pr1
Oxides							
B ₂ O ₃	9.17	10.36	10.14	10.83	10.33	11.56	10.18
SiO ₂	30.74	33.58	32.92	34.04	35.27	36.50	34.88
Al ₂ O ₃	1.40	30.62	30.70	27.33	26.69	40.07	32.31
TiO ₂		1.63	0.54	0.39	0.52		0.67
V ₂ O ₃	0.04						
Fe ₂ O ₃	43.89	0.86	12.37	7.63	5.46		1.20
FeO	2.69	12.65	5.98	4.91	2.20	0.22	12.66
MnO		0.06	0.11			3.07	0.21
MgO	6.45	2.69	0.16	7.34	10.77		1.60
Li ₂ O		0.03		0.01	0.00	1.61	0.06
CaO			0.20	0.99	1.67	0.20	0.41
Na ₂ O	2.12	2.84	2.49	2.35	2.15	2.15	2.24
K ₂ O	1.04	0.06	0.07		0.05		0.23
F		0.34	1.32		0.79	1.24	0.61
H ₂ O	2.56	2.96	1.15	3.18	2.92	3.13	2.57
Subtotal	100.10	98.68	98.15	99.00	98.82	99.75	99.83
O=F		0.14	0.56		0.33	0.52	0.26
Total	100.10	98.54	97.59	99.00	98.49	99.22	99.57
31 O atoms normalization							
Total B	3.059	3.089	3.099	3.173	3.001	3.181	3.007
B site: B	3.000	3.000	3.000	3.000	3.000	3.000	3.000
T site: Si	5.941	5.801	5.829	5.778	5.935	5.818	5.969
B	0.059	0.089	0.099	0.173	0.001	0.181	0.007
Al	0.000	0.110	0.072	0.049	0.064	0.001	0.025
T-site Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al (Total)	0.319	6.234	6.407	5.467	5.294	7.528	6.516
Z site: Al	0.319	6.000	6.000	5.418	5.230	6.000	6.000
V ³⁺	0.006						
Fe ³⁺	5.675			0.582	0.691		
Mg ²⁺					0.079		
Z-site Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Y site: Al		0.125	0.335			1.526	0.491
Ti		0.212	0.072	0.050	0.066		0.086
Fe ³⁺	0.707	0.112	1.648	0.392			0.155
Fe ²⁺	0.435	1.828	0.886	0.697	0.310	0.029	1.812
Mn ²⁺		0.009	0.016			0.414	0.030
Mg	1.858	0.693	0.042	1.857	2.623		0.408
Li		0.022		0.003	0.002	1.030	0.041
Y-site Total	3.000	3.000	3.000	3.000	3.001	3.000	3.024
Ca			0.038	0.180	0.301	0.034	0.075
Na	0.794	0.951	0.855	0.773	0.702	0.664	0.743
K	0.256	0.013	0.016		0.011		0.050
X-site vacancy		0.036	0.091	0.047		0.301	0.131
X-site Total	1.051	1.000	1.000	1.000	1.013	1.000	1.000
V+W site: OH	3.300	3.411	1.358	3.600	3.278	3.328	2.933
V site: OH	3.000	3.000	1.358	3.000	3.000	3.000	2.933
V site: O			1.642				0.067
W site OH	0.300	0.411		0.600	0.278	0.328	
W site: F		0.186	0.739		0.420	0.625	0.330
W site O	0.700	0.403	0.261	0.400	0.302	0.047	0.670
V,W-site Total	4.000	4.000	4.000	4.000	4.000	4.000	4.000
X-site primary group:	Alkali	Alkali	Alkali	Alkali	Alkali	Alkali	Alkali
W-site species series:	Oxy-	Hydroxy-	Fluor-	Hydroxy-	Fluor-	Fluor-	Oxy-
V-site dominant anion:	OH	OH	O	OH	OH	OH	OH
Y-site dominant divalent cation:	Mg ²⁺	Fe ²⁺	Fe ²⁺	Mg ²⁺	Mg ²⁺	Mn ²⁺	Fe ²⁺
Y-site dominant trivalent cation:	Fe ³⁺	Al ³⁺	Fe ³⁺	Fe ³⁺	Al ³⁺	Al ³⁺	Al ³⁺
Z-site dominant trivalent cation:	Fe ³⁺	Al ³⁺	Al ³⁺	Al ³⁺	Al ³⁺	Al ³⁺	Al ³⁺
Plotting parameters							
R ²⁺ /(R ²⁺ + 2Li)	1.000	0.983	1.000	0.997	0.999	0.177	0.965
Ca/(Ca+Na+K)			0.042	0.189	0.297	0.049	0.087
Vac/(Na+K+Vac)		0.036	0.095	0.057		0.312	0.142
W site O/(O+OH+F)	0.700	0.403	0.261	0.400	0.302	0.047	0.670
Alkali group							
Subgroup	subgroup 3	subgroup 1	subgroup 5	subgroup 1	subgroup 1	subgroup 2	subgroup 3
Tourmaline species	Povondraite	Schorl	Fluor-buergerite	Dravite	Fluor-dravite	"Fluor-elbaite"	"Oxy-schorl"