

Classification of the minerals of the tourmaline group

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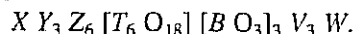
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Abstract: A systematic classification of the tourmaline-group minerals, general formula $X Y_3 Z_6 (T_6 O_{18}) (BO_3)_3 V_3 W$, is proposed, based on chemical composition and ordering at the different crystallographic sites of the tourmaline structure. There are currently thirteen accepted tourmaline species. However, based on the actual chemical compositions of holotype material, several of these species were imprecisely or incorrectly defined. A proper definition of these species is proposed. A crystal-chemical feature that extends the number of possible end-members is the anion occupancy of the *W*-site (dominated by OH^- , F^- or O^{2-}) and the *V*-site (dominated by OH^- or, more rarely, O^{2-}). Thus, based on the *W*-site alone, there can be hydroxy-, fluor-, or oxy-end-members. Furthermore, the presence of dominant O^{2-} at the *W*-site commonly requires local cation-ordering at the *Y*- and *Z*-sites. The tourmaline-group minerals can be divided into three principal groups based on the dominant species at the *X*-site: *alkali tourmalines* (*Na*), *calcic tourmalines* (*Ca*) and *X-site-vacant tourmalines* (\square : vacancy). These groups are further divided, initially based on the *W*-site occupancy, then by the (actual or inferred) *V*-site occupancy, next by the (actual or inferred) *Y*-site occupancy and, finally, by the (actual or inferred) *Z*-site occupancy. A systematic classification procedure is developed that takes into account different levels of knowledge of the chemical composition and site occupancy of the tourmaline. Several examples are used to illustrate the application of this classification procedure.

Key-words: tourmaline, classification, end members, crystal chemistry, chemical composition.

Introduction

The chemical formula of tourmaline may be written as



The advantage of writing the formula in this way is the generality that results; the formula represents the sites within the asymmetric unit of the structure, and makes no assumptions as to the occupancy of sites apart from those occupied by O^{2-} . Thus progress in our knowledge of site occupancy in tourmaline does not require a change in the general formula, but can be encompassed *via* a change in the assignment of chemical species to the letters of the general formula. Ignoring trace

constituents, we can assign the letter symbols of the general formula as follows:

X = Ca, Na, K, \square [vacancy]

Y = Li, Mg, Fe^{2+} , Mn^{2+} , Al, Cr^{3+} , V^{3+} , Fe^{3+} , (Ti^{4+})

Z = Mg, Al, Fe^{3+} , V^{3+} , Cr^{3+}

T = Si, Al, (B)

B = B, (\square)

V = OH, O \equiv [O(3)]

W = OH, F, O \equiv [O(1)]

where the species in parentheses are, as yet, not proven to occur at these sites. Considerable work is currently in progress on the characterization of site occupancies in tourmaline, both directly by crystal-structure refinement and crystal chemistry (Hawthorne *et al.*, 1993; Grice & Ercit, 1993;

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Grice *et al.*, 1993; Burns *et al.*, 1994; MacDonald & Hawthorne, 1995), and indirectly by analysis of light lithophile elements (Foit & Rosenberg, 1977; Povondra, 1981; Povondra & Novak, 1986; Dyar *et al.*, 1994).

Through informal discussions among many people working on tourmaline, it has become apparent that there is considerable confusion in the assignment of names to specific tourmaline compositions. This has arisen for three reasons:

- (1) Some formal descriptions of tourmaline minerals specify the ideal end-member composition but do *not* specify the limits of use of the name;
- (2) Some formal descriptions of tourmaline minerals specify the general composition but do *not* specify the end-member composition;
- (3) promulgation of the idea of the "50 % rule" whereby a specific chemical component in a mineral can only give rise to a new species if it exceeds 50 % occupancy of the site (or group of sites) at which it occurs;
- (4) the use of less-than-optimum graphical representations to show compositional variations in tourmaline.

The purpose of this work is to explicitly address these issues, to develop a series of useful composition diagrams, and to establish procedures whereby a name may be easily assigned to any tourmaline formula.

Status of this proposed classification

This classification scheme has not been submitted to the Commission on New Minerals and Mineral Names of the International Mineralogical Association (IMA). Many of the classification schemes currently in place took ten years or more to be developed by the relevant IMA Committees. This is not intended to be a pejorative comment, just a statement of fact. There is currently a considerable effort directed toward understanding tourmaline, and many people have expressed their desire for a systematic classification scheme *now*; this scheme is in response to this opinion. When more data and a better understanding of the crystal-chemistry of tourmaline are available, perhaps a more 'official' classification scheme can be put in place.

The 50 % rule and ternary solid solutions

In a binary solid-solution, A—B, the 50 % rule results in the assignment of two distinct named species: A for A_xB_{1-x} where $x \geq 0.5$, and B for

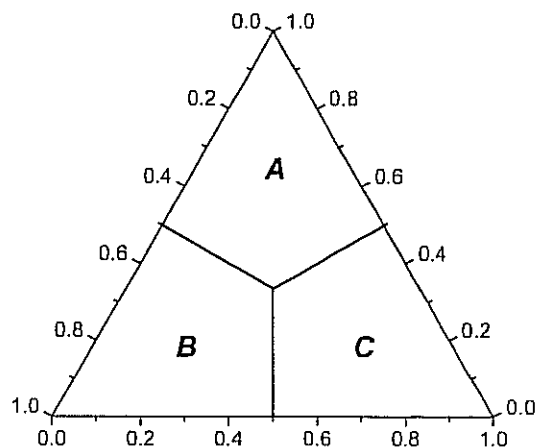


Fig. 1. The nomenclature system for a ternary solid-solution (after Nickel, 1992).

A_xB_{1-x} where $x < 0.5$. What happens if we apply this rule to ternary solid solutions A—B—C? This situation is explicitly dealt with by Nickel (1992) and is illustrated in Fig. 1. *Compositions are named for the dominant chemical species.* The 50 % is still adhered to for binary solid-solutions within the ternary system, but must be seen as a special bounding case within the ternary system itself.

Graphical representation of chemical variations

For several years, it has been fashionable to use vector methods to represent chemical variations in mineralogical and petrological systems, including tourmaline (Burt, 1989). However, such methods have an intrinsic defect that is not generally recognized: they are not "value-free" representations of the data that they show. In a vector representation, one couples two variables together with the assumption that they are completely correlated. This assumption may, or may not, be correct. If the assumption is wrong, this fact may not become apparent from the use of vector representations as it is incorporated as correct into the graphical-representation method. This argument is not meant to negate the use of vector representations for petrological purposes. However, it does indicate that this method is *not* suitable for primary crystal-chemical or mineralogical purposes where one does not necessarily completely understand the coupling between chemical variables in the structure. Thus here, we will use graphs that represent primary compositional data and make no

assumptions (apart from those used to calculate the unit formula) as to the behaviour of specific chemical components.

Definition of an end-member composition

This issue warrants some discussion as several formal descriptions of tourmaline species have defined end-member compositions wrongly. The following points are of significance:

(1) An end-member composition must be fixed. If an end-member is expressed with variable components, it can be factored into (at least) two components that are of fixed composition and can define end-members. For example, MacDonald *et al.* (1993) defined the end-member composition of foitite as $\square [\text{Fe}_2^{2+}(\text{Al}, \text{Fe}^{3+})] \text{Al}_6 \text{Si}_6 \text{O}_{18} (\text{BO}_3)_3 (\text{OH})_4$. This definition of an end-member is wrong, because the composition as written is variable, and can be expressed in terms of the true end-members $\square [\text{Fe}_2^{2+}\text{Al}] \text{Al}_6 \text{Si}_6 \text{O}_{18} (\text{BO}_3)_3 (\text{OH})_4$ and $\square [\text{Fe}_2^{2+}\text{Fe}^{3+}] \text{Al}_6 \text{Si}_6 \text{O}_{18} (\text{BO}_3)_3 (\text{OH})_4$. It should be noted that this structure applies just as much to anion components as to cation components. Thus an end-member *cannot* be specified with $(\text{OH}, \text{F})_4$ or (OH, O) as part of the formula.

(2) An end-member may have more than one species at *one* site. Thus $\square [\text{Mg}_2\text{Al}] \text{Al}_6 \text{Si}_6 \text{O}_{18} (\text{BO}_3)_3 (\text{OH})_4$ is an end-member even though the Y site is occupied by $[\text{Mg}_2\text{Al}]$. The reason for this is that the rest of the structure is completely ordered and the constraint of overall electroneutrality requires a charge of 7+ at the Y site, hence Y = Mg_2Al .

Current tourmaline end-members

Currently valid tourmaline end-members are listed in Table 1 (with some modification as discussed in the rest of this section).

Foitite

As noted above, the end-member composition of foitite was given with a variable cation occupancy at the Y site: $Y_3 = \text{Fe}_2^{2+}(\text{Al}, \text{Fe}^{3+})$ (MacDonald *et al.*, 1993). As Al is dominant over Fe^{3+} in the formula of the holotype material, the Y-site composition of the end-member is $\text{Fe}_2^{2+}\text{Al}$ (Table 1).

Olenite

Sokolov *et al.* (1986) define olenite as

$$\text{Na}_{1-y} (\text{Al}_{3-x}\text{Li}_x) \text{Al}_6 (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3$$

$$[\text{O}_{3-2x-y}(\text{OH})_{1+2x+y}]$$

with $y = 0 - 1$ and $x = 1.5 - 0.75$, and the ideal formula as

$\text{Na}_{1-x} \text{Al}_3 \text{Al}_6 (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{O}, \text{OH})_4$
 with $x = 1 - 0$. The latter composition is unsatisfactory as there are several constituents (Na, O, OH) that are considered variable. The most Al-rich composition listed by Sokolov *et al.* (1986) is

$$(\text{Na}_{0.51} \square_{0.43} \text{K}_{0.01} \text{Ca}_{0.05}) (\text{Al}_{2.91} \text{Mn}_{0.10}) \text{Al}_6$$

$$(\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 [\text{O}_{2.57} \text{OH}_{1.44} \text{F}_{0.03}]$$

Note that H_2O contents were not measured, but were estimated by stoichiometry. The corresponding end-member composition is that listed in Table 1.

Povondraite

Grice *et al.* (1993) give the structural formula of holotype povondraite as

$$(\text{Na}_{0.80} \text{K}_{0.26}) (\text{Fe}_{2.28}^{3+} \text{Fe}_{0.27}^{2+} \text{Mg}_{0.53})$$

$$(\text{Fe}_{4.29}^{3+} \text{Mg}_{1.36} \text{Al}_{0.32}) (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_{3.12} \text{O}_{0.88}$$

and the ideal end-member formula as

$$\text{Na Fe}_3^{3+} \text{Fe}_6^{3+} (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{O}, \text{OH})_4$$

This is not an end-member formula because the content of V and W are written as variable. In fact, they are fixed by the requirement of electroneutrality in the above formula: $(\text{O}, \text{OH})_4 = \text{O}_3(\text{OH})$, with the inference that $W = \text{O}(1) = \text{OH}$ and $V = \text{O}(3) = \text{O}_3$ [rather than $W = \text{O}$, $V = \text{O}_2(\text{OH})$]. The content of these sites in this end-member formula, $\text{O}_3(\text{OH})$, is drastically different from the content of these sites in the structural formula of the holotype: $\text{O}_{0.88}(\text{OH})_{3.12}$. Hence the proposed end-member is wrong; the content of W and V in the correct end-member must be $\text{O}(\text{OH})_3$. In the holotype formula, the dominant trivalent cation is Fe^{3+} and the dominant divalent cation is Mg; therefore, let us write the formula with $\text{Na} \equiv (\text{Na}, \text{K})$, $\text{Fe}^{3+} \equiv (\text{Fe}^{3+}, \text{Al})$ and $\text{Mg} \equiv (\text{Mg}, \text{Fe}^{2+})$:

$$\text{Na} (\text{Fe}_{2.28}^{3+} \text{Mg}_{0.80}) (\text{Fe}_{4.61}^{3+} \text{Mg}_{1.36}) (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3$$

$$(\text{OH})_{3.12} \text{O}_{0.88}$$

The ideal end-member for this composition is

$$\text{Na Fe}_3^{3+} (\text{Fe}_4^{3+} \text{Mg}_2) (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_3 \text{O}$$

All sites except one (the Z site) are completely ordered, in accord with one of the requirements for an end-member composition stated above. A survey of ferrian tourmalines shows compositional trends consistent with this ideal end-member composition (Henry *et al.*, 1999).

Uvite

Kunitz (1929) defined the ideal composition of uvite as $\text{H}_8\text{Ca}_2\text{Mg}_8\text{Al}_{10}\text{Si}_{12}\text{B}_6\text{O}_{62}$, which may be rewritten (after Dunn *et al.*, 1977b) as

$$\text{Ca Mg}_3 (\text{Al}_5\text{Mg}) (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_4$$

Table 1. Current tourmaline end-member species.

Species	(X)	(Y ₃)	(Z ₆)	T ₆ O ₁₈	(BO ₃) ₃	V ₃	W	[Ref.]
Alkali tourmaline								
Elbaite	Na	Li _{1.5} Al _{1.5}	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)	[*]
Dravite	Na	Mg ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)	[*]
Chromdravite	Na	Mg ₃	Cr ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)	[1]
Schorl	Na	Fe ²⁺ ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)	[*]
Olenite**	Na	Al ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	O ₃	(OH)	[2]
Buergerite	Na	Fe ³⁺ ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	O ₃	F	[3]
Povondraite***	Na	Fe ³⁺ ₃	Fe ³⁺ ₄ Mg ₂	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O	[4]
Calcic tourmaline								
Uvite	Ca	Mg ₃	Al ₅ Mg	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F	[5]
"Hydroxy-feruvite" ***	Ca	Fe ²⁺ ₃	Al ₅ Mg	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)	[6]
Liddicoatite**	Ca	Li ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F	[7]
X-site-vacant tourmaline								
Rossmannite		LiAl ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)	[8]
Foilitite**		Fe ²⁺ ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)	[9]
Magnesianfoilitite		Mg ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)	[10]

*The definitions of these end-members are lost in the mists of time.

** These end-members are modified from the original suggested formulae to produce proper end-members. See text for discussion.

***The original end-member "ferridravite" (Valenta & Dunn, 1979) was redefined as povondraite (Grice *et al.*, 1993) because the initially assumed site-populations were incorrect and did not correspond to the Fe³⁺-equivalent of dravite. In turn, in this paper, we suggest that Mg, ordered at the Z-site, should be part of the end-member formula.

* This species was originally defined as feruvite, but it has (OH) at O(1) whereas uvite has F at O(1); hence the name feruvite needs to be modified to "hydroxy-feruvite".

References: [1] Rumiantsseva (1983); [2] Sokolov *et al.* (1986); [3] Donnay *et al.* (1966); [4] Grice *et al.* (1993); [5] Kunitz (1929); Dunn *et al.* (1977b); [6] Grice & Robinson (1989); [7] Dunn *et al.* (1977a); [8] Selway *et al.* (1998); [9] MacDonald *et al.* (1993); [10] Hawthorne *et al.* (in prep.)

Kunitz (1929) examined tourmalines from Uva (Sri Lanka), DeKalb (New York) and Gouverneur (New York); the analyses given by Kunitz (1929) have OH ~ 4 *apfu*. This aspect of the analyses given by Kunitz (1929) is almost certainly wrong, as all other analyses from these localities contain F in the range 0.5–1.0 *apfu*. In particular, Dunn *et al.* (1977b) designate a sample of uvite from Uva, Sri Lanka, as a neotype, and this sample has an anion content of (OH_{2.90}F_{0.76}O_{0.34}). Thus it would seem that uvite should have F dominant at the O(1) site, although it has always been written as (OH)₄.

There are two possibilities here:

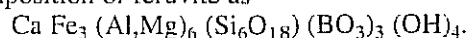
- (1) retaining the current ideal end-member with OH = 4 *apfu* and validating "fluor-uvite";
- (2) defining end-member uvite as having O(1) = F and O(3) = (OH); this has the advantage that all current uvite compositions remain uvite. However,

this provides a problem for feruvite, as type feruvite has (OH) ~ 4 *apfu* and hence would need to be renamed as "hydroxy-feruvite".

As uvite is far more common than feruvite, option (2) produces much less change to current practice than option (1). Hence we will adopt option (2). Note that the mineral corresponding to Ca Fe₃²⁺(Al₅Mg) (Si₆O₁₈) (BO₃)₃ (OH)₃ (OH) is valid, but the name "hydroxy-feruvite" requires validation by the Commission on New Minerals and Mineral Names of the International Mineralogical Association.

Feruvite

Grice & Robinson (1989) define the ideal composition of feruvite as

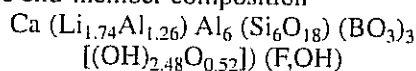


This is not a true end-member and is not adequate as the valence state of Fe is not specified. Refinement of the crystal structure shows that all Fe at the Y site is in the divalent state, and that the Z site is $(\text{Al}_{4.72}\text{Fe}_{0.34}^{3+}\text{Mg}_{0.82}\text{Fe}_{0.12}^{2+})$ which is close to (Al_5Mg) . Thus the end-member formula of "hydroxy-feruvite" can be written as $\text{Ca Fe}_3^{2+} (\text{Al}_5\text{Mg}) \text{Si}_6 \text{O}_{18} (\text{BO}_3)_3 (\text{OH})_3 (\text{OH})$.

Liddicoatite

Dunn *et al.* (1977a) gave the "ideal" composition of liddicoatite as

$\text{Ca} (\text{Li}, \text{Al})_3 \text{Al}_6 (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{O}, \text{OH})_3 (\text{OH}, \text{F})$
and the end-member composition



with the proviso that this is not a "pure end-member". None of these compositions correspond to either the *general* composition or the end-member composition of liddicoatite. The end-member composition of liddicoatite must contain the following features not displayed by the above compositions: the Y cations are fixed, $Y = \text{Li}_2\text{Al}$; as F is dominant at O(1), $\text{O}(1) = \text{F}$; as OH is dominant at O(3), $\text{O}(3) = \text{OH}$. Thus end-member liddicoatite is $\text{Ca} (\text{Li}_2\text{Al}) \text{Al}_6 (\text{Si}_6\text{O}_{18}) (\text{BO}_3)_3 (\text{OH})_3 \text{F}$.

Furthermore, any O at W and V sites should be assigned to W [the O(1) site] (Hawthorne, 1996) in the formula derived from the analysis of Dunn *et al.* (1977a).

Tourmaline classification: crystal-chemical considerations

To establish a framework for classification of the tourmaline-group minerals, it is necessary to consider the crystal-chemical and crystallographic constraints on site-occupancy in tourmaline. To be a useful classification scheme, it must be sufficiently general to be expanded as more information becomes available.

The X-site

The X-site may be occupied by Na (and K), Ca and \square , and hence we may readily represent this compositional variation on a triangular diagram that divides tourmaline into three principal groups (Fig. 2):

- (1) Alkali tourmalines (Na + K dominant at X)
- (2) Calcic tourmalines (Ca dominant at X)
- (3) X-site-vacant tourmalines (\square dominant at X)

This primary grouping follows that in other complex silicates (*e.g.*, amphiboles, pyroxenes) in which the character of the interstitial cation is the primary feature of classification, and chemical variations within the structural unit are secondary characteristics of the classification scheme (Hawthorne, 1994). Each of these primary groups contains a cation (or vacancy) with a different charge such that charge compensation is required at other sites in the tourmaline structure; these group-

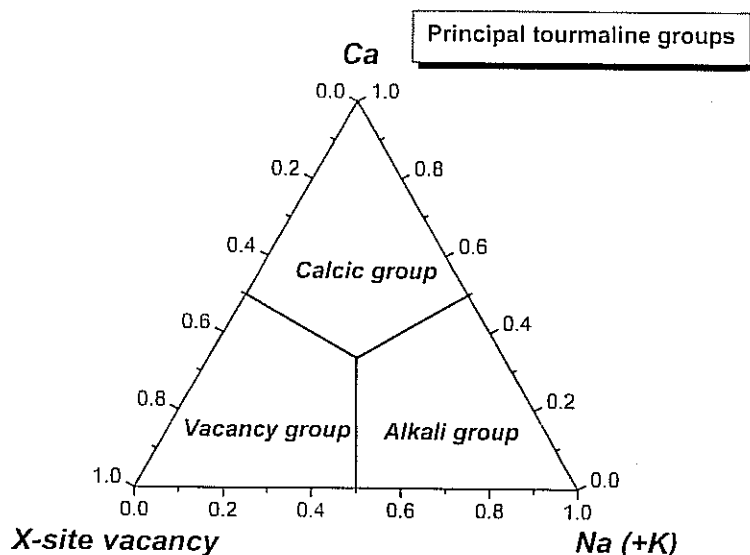


Fig. 2. The major compositional groups of the tourmaline minerals, classified according to the principal constituent at the X-site.

ings commonly reflect significant differences in paragenesis. Table 1 lists end-member compositions of the currently valid tourmaline-group minerals, divided into these three principal classes.

The OH-bearing sites

In the tourmaline structure, there are two sites, $V = O(3)$ and $W = O(1)$, that are occupied by monovalent anions OH^- and F^- , or by the divalent anion O^{2-} . Analytical work has shown that $(OH + F)$ can be less than 4.0 atoms per formula unit (*apfu*), with the deficiency being made up of O^{2-} (e.g., Povondra, 1981; Povondra & Novak, 1986; Dyar *et al.*, 1994; Taylor *et al.*, 1995). The V and W sites are crystallographically distinct and the constituent anions (OH^- , F^- and O^{2-}) order differently over these two sites.

The V site

The V site [$= O(3)$] is generally dominated by OH in tourmaline, but can be occupied by O^{2-} . Based on bond-valence considerations for a variety of tourmalines, Grice & Ercit (1993) argue that tourmalines containing both O^{2-} and OH^- at the V/W sites will preferentially partition OH^- at the V site. They note that buergerite is the exception, with O^{2-} dominantly at the V site. Among the current end-members, the other exception is olenite (Table 1). Consequently, the V site can be considered to be a binary (OH^- – O^{2-}) system with OH^-

more commonly preferred at this site unless the Y and Z sites are completely occupied by trivalent cations (e.g., buergerite and olenite).

The W site

The W site is unique in that F is ordered completely at this site (Grice & Ercit, 1993; MacDonald & Hawthorne, 1995). This site also commonly contains OH^- and O^{2-} (Hawthorne, 1996). As such, the W site can be considered a ternary chemical system that marks a further subdivision of primary tourmalines into secondary hydroxy-, fluor-, and oxy-end-member subgroups (Fig. 3). Where O^{2-} is dominant at the W site, short-range ordering is commonly required at the Y and Z sites in order to satisfy local bond-valence and bond-length requirements (Hawthorne, 1996). The ternary subsystem that is possible at the W site potentially leads to hydroxy-, fluor-, and oxy-members for each root composition, e.g., dravite, fluor-dravite and oxy-dravite. The oxy-end-member requires another substitution within the structure to maintain electroneutrality. Consequently, the potential number of end-members is substantially increased.

In Table 1, there are two root end-members with $W = F$: buergerite and liddicoatite. There are two possibilities for dealing with the end-member names; (1) the holotype samples could be re-defined as "fluor-buergerite" and "fluor-liddicoatite"; (2) the end-member with $W = OH^-$ could be

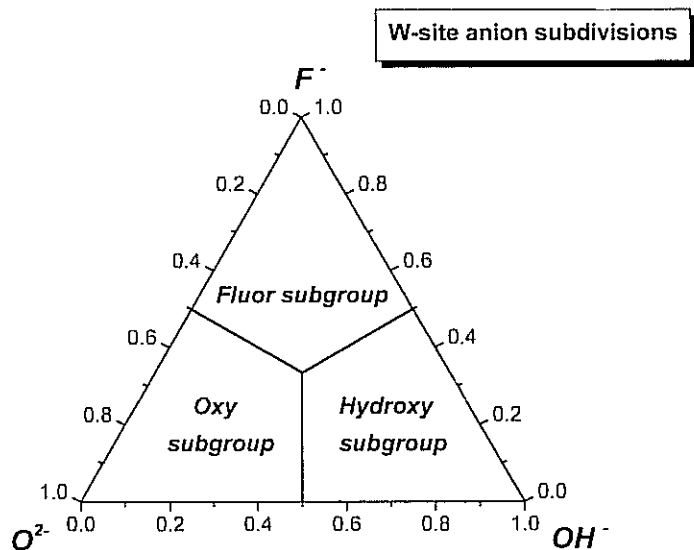


Fig. 3. The major compositional groups of the tourmaline minerals, classified according to the principal constituent at the W -site.

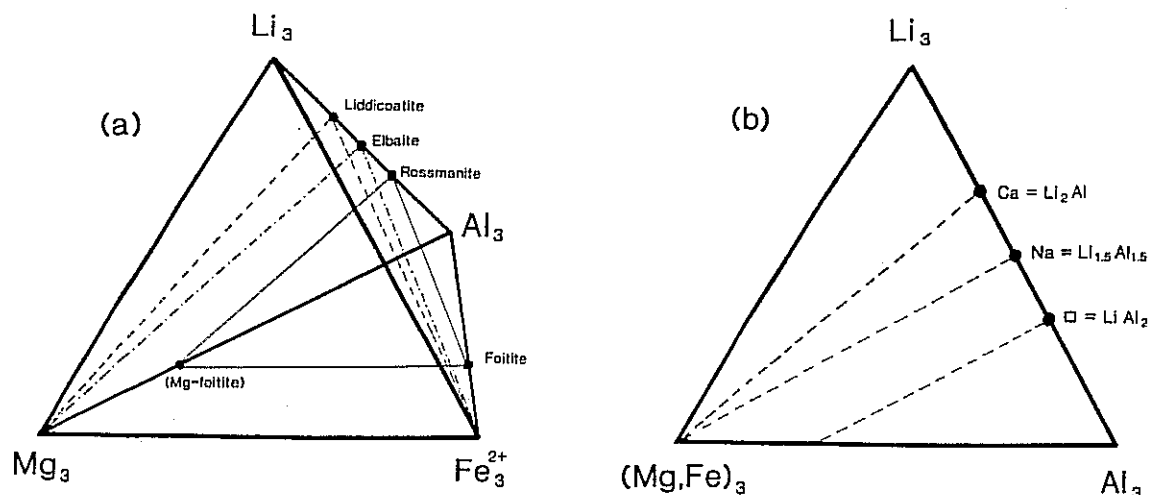


Fig. 4. The compositional planes of the calcic, alkali and X-site-vacant tourmalines in the system (a) $Y = \text{Li, Mg, Fe}^{2+}, \text{Al}$; (b) $Y = [\text{Li, (Mg,Fe}^{2+}), \text{Al}]$.

designated by the prefix hydroxy. We prefer the latter course, as it requires no further action unless the specific compositions are discovered as tourmaline-group minerals.

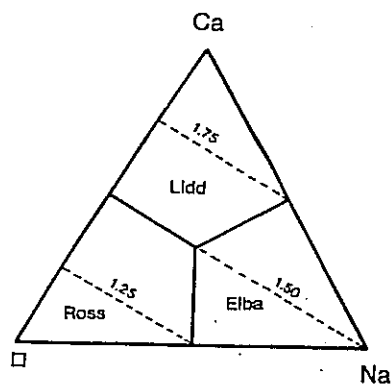
The Y site

The principal constituents at the Y site in tourmaline are Li, Mg, Fe^{2+} , Al and Fe^{3+} . For the more common case in which $V = \text{OH}$, the Y site can be treated as a ternary system with end-members involving Mg, Fe^{2+} , and Li and Al. Each principal group, the calcic, alkali and X-site-vacant tourmalines, needs to be treated separately with regard to the Y site. This is not unusual in complex silicates: the calcic, sodic-calcic, alkali and ferromagnesian amphiboles (Leake *et al.*, 1997) are treated in a similar fashion. Consequently, this ternary division based on the principal Y-site constituents can be used to further subdivide the primary groups (alkali-, calcic- and X-site-vacant) and secondary (hydroxy-, fluor- and oxy-) subgroups.

Li tourmalines

There is often considerable confusion about Li tourmalines because of the mixed occupancy of the Y site. Inspection of Table 1 shows that, for each of the Li tourmalines, only the Y site has mixed occupancy (Fig. 4a,b), and this occupancy is fixed by the requirement of electroneutrality; hence the Li-bearing compositions listed in Table 1 are true end-members. The key difference between these three

tourmaline end-members (rossmanite, elbaite, liddicoatite) occurs at the X site; rossmanite is an X-site-vacant tourmaline, elbaite is an alkali tourmaline, and liddicoatite is a calcic tourmaline (Fig. 5). The differences in composition at the Y site occur to produce electroneutrality.



ROSSMANITE	□ (LiAl_2)	CHARGE = 7+
ELBAITE	Na ($\text{Li}_{1.5}\text{Al}_{1.5}$)	CHARGE = 7+
LIDDICOATITE	Ca (Li_2Al)	CHARGE = 7+

Fig. 5. The Li tourmalines expressed in terms of their X-site composition; the diagram is contoured for Li content.

Table 2. Possible Ca-free end-member compositions of Mn²⁺-bearing tourmalines.

Hypothetical Species	(X)	(Y ₃)	(Z ₆)	T ₆ O ₁₈	(BO ₃) ₃	V ₃	W
"Mn-dravite"	Na	Mn ₃ ²⁺	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Mn-foitite"	□	Mn ₂ ²⁺ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Oxy-Mn-dravite"	Na	Mn ₂ ²⁺ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-Mn-foitite"	□	Mn ²⁺ Al ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O

Y-site ordering

Hawthorne (1996) noted that the presence of O²⁻ at the W site has a profound effect on the occupancy of the Y-site due to local bond-valence and bond-length requirements. In Li-free tourmalines with O²⁻ at the W site, the stable cation configuration at the Y-site is either (M²⁺ + 2M³⁺) or 3M³⁺, where M²⁺ represents divalent cations and M³⁺ represents trivalent cations. For example, for dravite [Na (Mg₃) Al₆ (Si₆O₁₈) (BO₃)₃ (OH)₃ (OH)], the possible oxy-dravite end-members could be Na (Al₃) (Mg₂Al₄) (Si₆O₁₈) (BO₃)₃ (OH)₃ O [Al₃ Y-site configuration] or Na (MgAl₂) (MgAl₅) (Si₆O₁₈) (BO₃)₃ (OH)₃ O [MgAl₂ Y-site configuration]. Note that these short-range-order configurations at the Y site result in disordering such that Mg is displaced to the Z site and Al to the Y site. Interestingly, the Fe³⁺ equivalent of the latter structural formula is the same as that proposed for povondraite (Table 1). For the Li-bearing tourmalines in which there is a monovalent anion at the W-site, the stable cation configuration is (Li + 2Al) or (2Li + Al); the former configuration occurs in rossmanite and the latter configuration occurs in liddicoatite. In end-member elbaite, equal amounts of each of these two cation configurations are likely. In Li-bearing tourmalines, bond-valence and bond-length requirements imply that OH⁻ can only be replaced by O²⁻ to a limited extent, possibly about 25 %.

The Z site

The Z site is occupied dominantly by trivalent cations, most commonly Al. Among the current end-members, chromdravite and povondraite have Cr³⁺ and Fe³⁺, respectively, as the dominant occupant of the Z site. In the currently valid X-site-vacant and alkali-tourmaline end-members, Al is the only trivalent cation to occupy the Z site. In the calcic tourmalines, uvite and "hydroxy"-feruvite, the Z site is occupied by Al₅Mg, whereas liddicoatite has Al₆ at Z (Table 1). If O²⁻ is dominant at

the W site, additional combinations of cations are possible (see below), produced by disordering reactions induced by short-range-ordering requirements of the anions coordinating the Y site (Hawthorne, 1996).

Mn²⁺-bearing tourmaline

The role of Mn²⁺ in tourmaline has been of particular interest (Schmetzer & Bank, 1984; Nuber & Schmetzer, 1984; Burns *et al.*, 1994), specifically with regard to the possible existence of a distinct Mn-bearing species of tourmaline such as the non-valid "tsilaisite" (Schmetzer & Bank, 1984; Shigley *et al.*, 1986). Kunitz (1929) suggested the hypothetical composition Na (Mn₃²⁺) Al₆ (Si₆O₁₈) (BO₃)₃ (OH)₃ (OH), the Mn equivalent of dravite, as an end-member, the name "tsilaisite" originating from the locality Tsilaisina in Madagascar (Duparc *et al.*, 1913). Alternative "tsi-

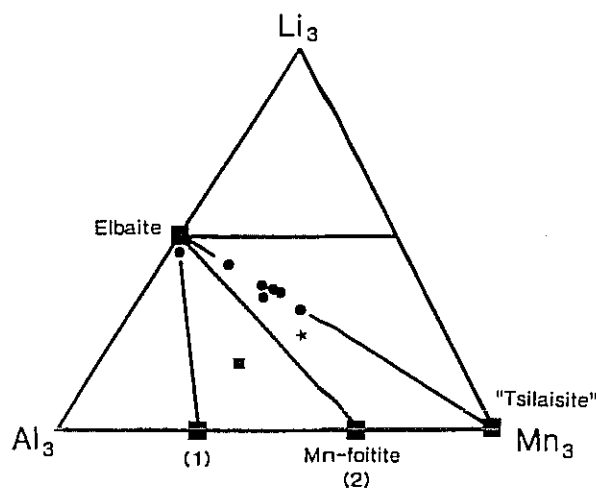


Fig. 6. The compositions of Mn-bearing tourmalines expressed in terms of Li, Al and Mn²⁺ at the Y site (data from Schmetzer & Bank, 1984; Shigley *et al.*, 1986; Burns *et al.*, 1994); possible end-member compositions are shown (cf. Table 2).

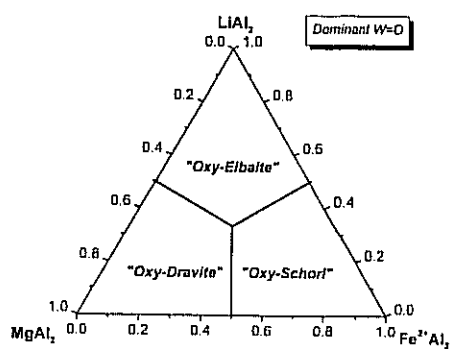
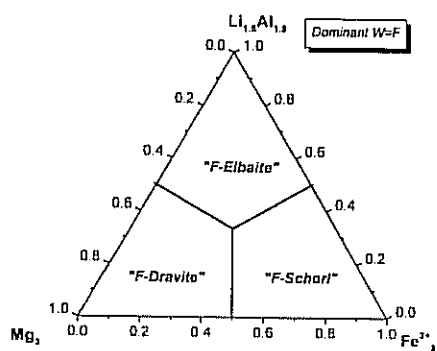
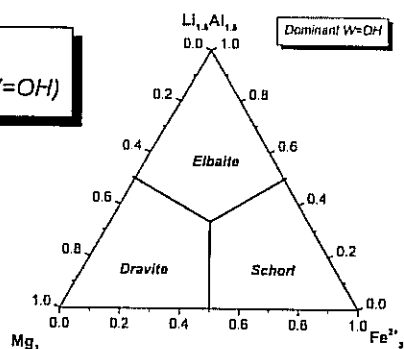
Table 3. Current valid and hypothetical tourmaline end-member species.

Species	(X)	(Y ₃)	(Z ₆)	T ₆ O ₁₈	(BO ₃) ₃	V ₃	W
Alkali tourmaline							
Elbaite	Na	Li _{1.5} Al _{1.5}	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Dravite	Na	Mg ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Chromdravite	Na	Mg ₃	Cr ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Schorl	Na	Fe ²⁺ ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Olenite	Na	Al ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	O ₃	(OH)
"Hydroxy-buergerite"	Na	Fe ³⁺ ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	O ₃	(OH)
"Fluor-elbaite"	Na	Li _{1.5} Al _{1.5}	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Fluor-dravite"	Na	Mg ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Fluor-chromdravite"	Na	Mg ₃	Cr ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Fluor-schorl"	Na	Fe ²⁺ ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Fluor-olenite"	Na	Al ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	O ₃	F
Buergerite	Na	Fe ³⁺ ₃	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	O ₃	F
"Oxy-elbaite"	Na	LiAl ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-dravite"	Na	MgAl ₂	MgAl ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
Povondraite	Na	Fe ³⁺ ₃	Mg ₂ Fe ³⁺ ₄	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-schorl"	Na	Fe ²⁺ Al ₂	Fe ²⁺ Al ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-chromdravite"	Na	MgCr ₂	MgCr ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
Calcic tourmaline							
"Hydroxy-liddicoatite"	Ca	Li ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Hydroxy-uvite"	Ca	Mg ₃	MgAl ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Hydroxy-feruvite"	Ca	Fe ²⁺ ₃	MgAl ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Liddicoatite	Ca	Li ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
Uvite	Ca	Mg ₃	MgAl ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
Feruvite	Ca	Fe ²⁺ ₃	MgAl ₅	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Oxy-liddicoatite"	Ca	Li _{1.5} Al _{1.5}	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-uvite"	Ca	MgAl ₂	Mg ₂ Al ₄	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Ferri-uvite"	Ca	MgFe ³⁺ ₂	Mg ₂ Fe ³⁺ ₄	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-feruvite"	Ca	Fe ²⁺ Al ₂	Mg ₂ Al ₄	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Ferri-feruvite"	Ca	Fe ²⁺ Fe ³⁺ ₂	Mg ₂ Fe ³⁺ ₄	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
X-site-vacant tourmaline							
Rossmannite	□	LiAl ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Mg-foitite"	□	Mg ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
Foitite	□	Fe ²⁺ ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	(OH)
"Fluor-rosmanite"	□	LiAl ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Fluor-Mg-foitite"	□	Mg ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Fluor-foitite"	□	Fe ²⁺ ₂ Al	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	F
"Oxy-rosmanite"	□	Li _{0.5} Al _{2.5}	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-Mg-foitite"	□	MgAl ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-Mg-ferri-foitite"	□	MgFe ³⁺ ₂	Fe ³⁺ ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-foitite"	□	Fe ²⁺ Al ₂	Al ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O
"Oxy-ferri-foitite"	□	Fe ²⁺ Fe ³⁺ ₂	Fe ³⁺ ₆	Si ₆ O ₁₈	(BO ₃) ₃	(OH) ₃	O

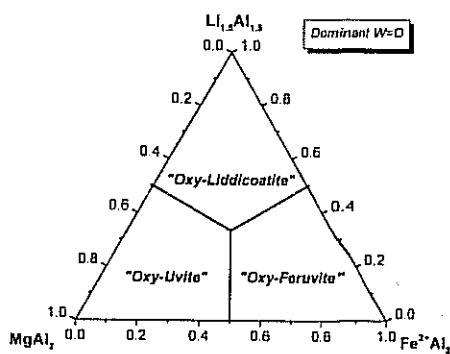
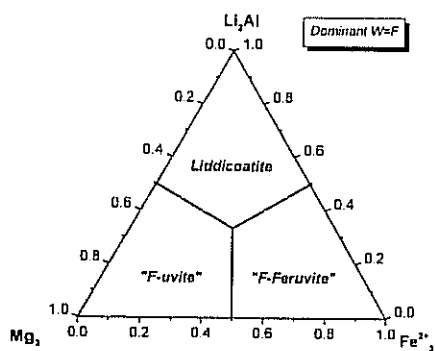
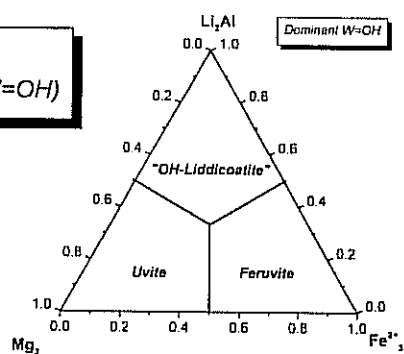
laisite" formulae were suggested by Slivko (1959, 1961) [Na (Mn²⁺Al₂) Al₆ (Si₆O₁₈) (BO₃)₃ [(OH)₂O] (O)] and by Schmetzer & Bank (1984) [Na (Mn²⁺_{1.5}Al_{1.5}) Al₆ (Si₆O₁₈) (BO₃)₃ [(OH)_{2.5}O_{0.5}] (O)]. However, the latter two formulae are not end-members according to the criteria discussed above, and hence are not appropriate compositions for a hypothetical Mn²⁺-dominant tourmaline end-member.

Possible end-member formulae for Mn²⁺-dominant tourmalines of appropriate composition (*i.e.*, Ca-free) are listed in Table 2. Fig. 6 is a Li-Al-Mn ternary diagram that shows the compositions of the Mn-bearing tourmalines from Schmetzer & Bank (1984), Nuber & Schmetzer (1984), Shigley *et al.* (1986) and Burns *et al.* (1994). The tourmalines of Burns *et al.* (1994) extend along the join elbaite — "Mn-dravite". The tourmaline of Shigley

a)

Alkali group*(with dominant Z=Al, V=OH)*

b)

Calcic group*(with dominant Z=Al, V=OH)*

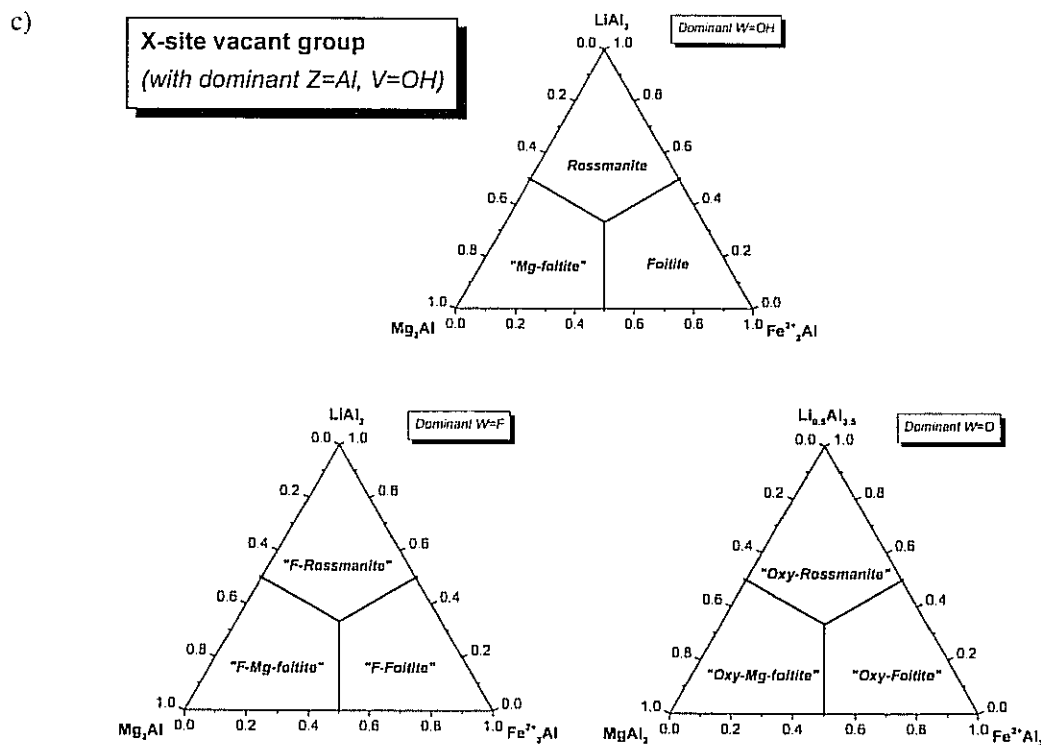


Fig. 7. The compositional ranges of the principal tourmaline minerals in (a) the alkali-tourmaline group; (b) the calcic-tourmaline group; (c) the X-site-vacant tourmaline group.

et al. (1986) shows some solid-solution toward "Mn-foitite", but less than Fig. 6 would suggest, as this tourmaline has only 0.28 □ at the X-site. Hence, these compositions suggest "Mn-dravite" as the appropriate end-member composition. The composition reported by Schmetzer & Bank (1984) is significantly different: $(Na_{0.85}Ca_{0.04}□_{0.11})(Mn_{0.93}^{2+}Al_{1.53}Li_{0.42}Ti_{0.04})Al_6(Si_{5.98}O_{18})(BO_3)_3(OH)_{2.63}O_{0.89}F_{0.48}$. This composition lies almost half-way between the hypothetical oxy-end-members $[Na(LiAl_2)Al_6(Si_6O_{18})(BO_3)_3(OH)_3O]$ and $[Na(Mn^{2+}Al_2)Al_6(Si_6O_{18})(BO_3)_3(OH)_2O_2]$, suggesting that the latter composition is another potential end-member for a Mn^{2+} -dominant tourmaline.

Tourmaline classification procedure

With the previous crystal-chemical considerations, it is apparent that there may be many more end-members than those that are currently considered valid. Table 3 shows the thirteen currently valid tourmaline end-members, together with other hypothetical end-members. The names associated with the hypothetical end-members are gen-

erally modified versions of a root end-member, *e.g.*, schorl, fluor-schorl and oxy-schorl. Possible Mn^{2+} end-members are not currently considered, but could be added if necessary.

With the appropriate analytical data and knowledge of probable site occupancies, the following procedure for systematically naming tourmaline is suggested:

- (1) Consider the dominant X-site species to establish the principal tourmaline group (Fig. 2).
- (2) Establish the dominant anion (OH^- , F^- or O^{2-}) at the W-site (Fig. 3), assuming that F^- occurs exclusively at the W site. The other assumption is that O^{2-} is generally ordered at the W site relative to OH^- for most tourmalines, except those dominated by trivalent cations at the Y-site (Grice & Ercit, 1993). This also requires that OH^- be measured directly (*e.g.*, Povondra, 1981), calculated *via* the electroneutrality constraint, or assumed (Henry & Dutrow, 1996).
- (3) Estimate 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 olenite, and their hypothetical hydroxy- and fluor-equivalents (Table 3).

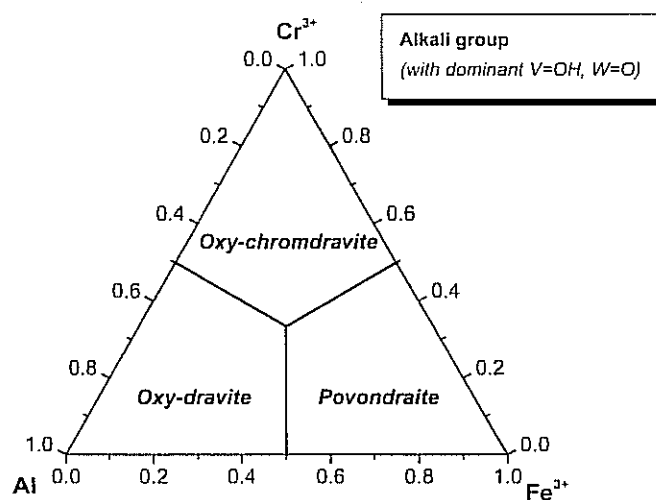


Fig. 8. The compositional range of Z-site cations in the alkali-tourmaline group.

- (4) Determine the dominant Y-cation configuration (Mg, Fe^{2+} or Li). Each of the principal groups has three possible W anions. In turn, there are three possible Y-site cation clusters. For the most common tourmalines, where the V anions are dominated by OH^- and the Z-site cations are dominated by Al, there are 27 possible end-members (Fig. 7a, b, c). To establish the name, it is only necessary to establish the appropriate ternary diagram and plot the Y-site cations.
- (5) Establish the dominant Z-site cation (Al, Cr^{3+} or Fe^{3+}). In the most common Al-dominant case, the 27 possible end-members can be determined by the procedure given in step 4. Equivalent numbers of Cr^{3+} - and Fe^{3+} -end-members could also be written. However, at present, there are only a couple of these that are known (e.g., chromdravite and povondraite). Several other hypothetical Cr^{3+} - and Fe^{3+} -end-members are suggested in Table 3. A potentially significant ternary subsystem involving trivalent cations, chiefly at the Z site, is the following oxy-subsystem: oxy-dravite - povondraite - oxy-chromdravite (Fig. 8).

One of the major problems in using this procedure is that a number of important cations are not always measured (especially Li, H and B), and the oxidation states of Fe and Mn are not always determined. Furthermore, the location of the cations and anions are not necessarily known unless there is an accompanying crystal-structure refinement. Thus the accuracy of the assigned tourmaline name is a function of the level of

knowledge of the tourmaline. We can consider tourmalines in terms of three levels of knowledge as they relate to the actual tourmaline compositions and the locations of the cations and anions in the structure.

Level 1 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. This is the optimum situation, but one which is relatively uncommon.

Level 2 implies direct knowledge of all elements and generally assumes site assignments. This situation is most common where wet-chemical or SIMS analysis is done on the tourmalines.

Level 3 gives basic tourmaline compositional data without direct information about B, H, Li and the oxidation states of transition elements. This is the most common situation, typical of tourmalines analyzed by the electron microprobe. In the examples considered below, the levels of knowledge will also be considered in evaluating the assigned names.

Discussion

An important consideration in expanding a classification system is that there should be evidence that the hypothetical species actually exist, and are appropriately treated by the classification procedure. This aspect may be considered by examining well-characterized (Level 1) tourmalines to see if the hypothetical end-members are appropriate.

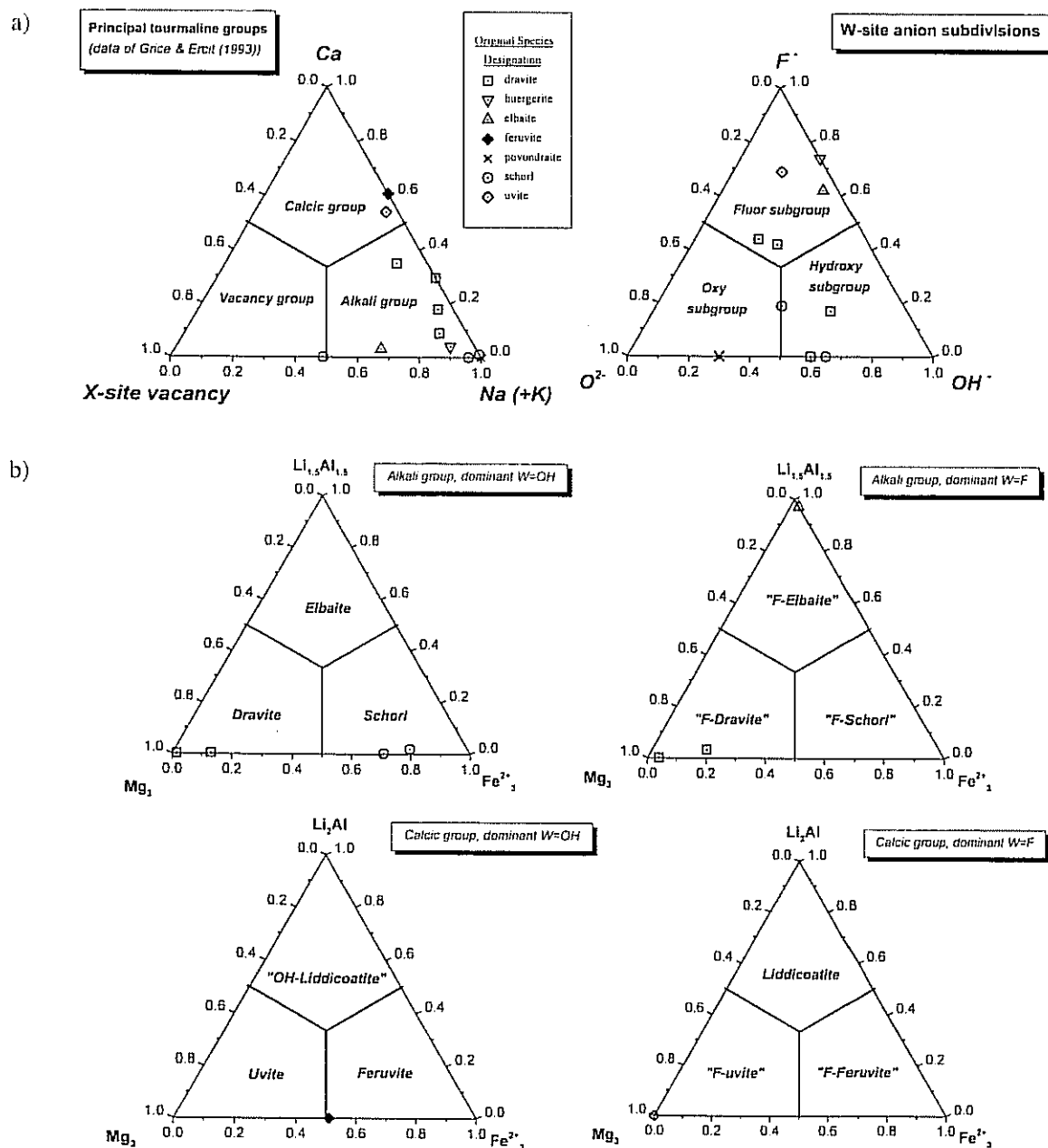


Fig. 9. The data of Grice & Ercit (1993) plotted on the classification diagrams developed here: (a) the X-site and W-site sub-groups; (b) the Y-cation substitution-groups.

In this regard, a useful data set is that of Grice & Ercit (1993) who did nearly complete chemical characterization and crystal-structure refinements on a wide compositional range of tourmalines. The tourmaline species were considered to be povondraite, schorl, buergerite, feruvite, uvite, dravite and elbaite. However, if we take these data and plot them on the appropriate ternary diagrams (Fig. 9), we find that several of the tourmalines

should be renamed. As expected from the original species designation, most of the species are alkali tourmalines (Fig. 9A). Interestingly, the W-anion subgroup is more-or-less equally split between hydroxy- and fluor-species, with povondraite falling in the oxy-subgroup. The dominance of F at the W site results in reclassification of some of the tourmalines to fluor-dravite, uvite and fluor-elbaite (Fig. 9B). The ubiquity of these species

should not be too surprising, as F levels above 0.5 apfu are relatively common in natural dravites, uvites and elbaïtes (MacDonald & Hawthorne, 1995; Henry & Dutrow, 1996). The rest of the tourmalines in this data set accord with the original species designation, with the exception of one "schorl" that just falls into the foitite field.

The "oxy-uvite" end-member corresponds to the Ca-deprotonated tourmaline end-member proposed by Henry & Dutrow (1990), except that Henry & Dutrow (1990) gave an ordered structural formula for Mg and Al at the Y and Z sites rather than the disordered formula suggested in Table 3. Significantly, Henry & Dutrow (1990) synthesized the end-member composition, suggesting that it is a stable phase. Taylor *et al.* (1995) did a detailed chemical analysis and crystal-structure refinement on a "hydroxy-deficient uvite" and the composition and positional disorder of the Mg and Al reported are in accord with that suggested by the oxy-uvite end-member of Table 3.

Tourmaline data such as the wet-chemical analyses of Povondra (1981) often contain formulae in which the OH + F contents are 3–4 apfu. This implies that oxy-end-members are likely to be relatively common. This is somewhat problematic for those tourmalines analyzed solely by electron microprobe because the amount of O²⁻ and OH⁻ cannot be determined directly. Nonetheless, in some cases, it is possible to estimate the amounts of OH⁻ by electroneutrality requirements (e.g., Henry & Dutrow, 1996; Henry *et al.*, 1999). Ultimately, OH⁻ contents, and by inference, the W-site O²⁻, will be critical for a proper understanding not only of the nomenclature, but also of the order-disorder that is likely to be present in many tourmalines.

Naming tourmaline-group minerals

The tourmaline formulae listed in Table 3 all comply with the IMA rules for recognition as distinct mineral species. However, all compositions corresponding to names in quotes are not currently recognized as valid mineral species, and use of any of them to describe a tourmaline does require validation of the mineral and mineral name by the Commission on New Minerals and Mineral Names of the IMA.

In regard to the specific names to be used for future recognized tourmaline species, we recommend that the same principle be used for tourmaline as was used for amphibole (Leake *et al.*, 1997): "The discovery of amphiboles with new or

exotic homovalent substitutions never requires a new species names. They can always be named by use of an appropriate prefix. In future, one root or one trivial name *ONLY* should be approved for each charge arrangement in each amphibole group, and all species defined by homovalent substitutions should be designated by the relevant prefix. New species defined by heterovalent substitutions [including major replacement of (OH,F,Cl) by oxygen.....] result in new root, or new trivial names." Thus names such as "fluor-elbaïte" or "hydroxy-liddicoatite" (or their unhyphenated equivalents) should be retained. All names with the prefix "oxy-" involve a new charge arrangement, and hence require a new root name.

Intention

We recognize that use of this classification scheme is very demanding from a chemical-analytical perspective. The analysis of H, Li, B and Fe³⁺, often required at a microbeam level because of sample heterogeneity, needs sophisticated instrumentation that is not widely available. On the other hand, *Science does not progress by ignoring Nature*; H, Li, B and Fe³⁺ are crucial chemical variables in tourmaline, and must be considered if we are to understand the behaviour of tourmaline in geological processes. It is only by demanding access to the necessary instrumentation that the availability of such instrumentation will improve.

We hope that this new classification scheme will allow a more systematic approach to the study of tourmaline, and, in particular, will promote increased understanding of variations in ordering and chemical composition as a function of paragenesis. In this way, tourmaline may finally take its place with the other groups of complex common silicate minerals as a useful mineral for petrogenetic studies.

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