

Crystallochemical Formulas and Definition of Species of Tourmaline-Group Minerals

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Abstract—The complex chemical composition of tourmalines, in combination with various mechanisms of isomorphic substitutions, creates difficulties in recalculating the chemical data to the crystallochemical formulas. In each case, the calculated formula is no more than a result of an author's interpretation and hence any formula is a far or close approach to the reality. Different modes of representing the composition of tourmaline-group minerals are discussed in this paper. Special attention is drawn to uncertainties, controversies, and mistakes in writing the crystallochemical formulas and to the problems that emerge in attempts to define species of tourmaline-group minerals from the calculated formulas.

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INTRODUCTION

The correct representation of chemical features of crystals, i.e., calculation of formula coefficients and amount of end members in minerals of variable compositions, as well as a graphic image of chemical variations, are very important for tracing the general evolutionary trends of the mineral-forming process; correlating the chemical composition, properties, and crystal structure of minerals; establishing typochemical features of minerals; defining mineral species and identifying new mineral species on the basis of the study of natural crystal solid solutions; and resolving other mineralogical and geochemical problems.

The aim of this study is to consider and discuss different modes of representing the composition of tourmaline-group minerals. Special attention is paid to uncertainties, controversies, and mistakes in writing the crystallochemical formulas, and the problems arising therewith in defining mineral species belonging to the tourmaline group.

MODES OF CALCULATION OF CRYSTALLOCHEMICAL COEFFICIENTS IN THE TOURMALINE FORMULA

The general chemical formula of tourmaline-group minerals is as follows: $X_{0-1}Y_3Z_6(T_6O_{18})(BO_3)_3V_3W$, where $X = Ca^{2+}, Na^+, K^+$, and \square (vacancy); $Y = Li^+, Mg^{2+}, Fe^{2+}, Mn^{2+}, Al^{3+}, Cr^{3+}, V^{3+}, Fe^{3+}$, and probably Ti^{4+} ; $Z = Mg^{2+}, Al^{3+}, Fe^{3+}, V^{3+}$, and Cr^{3+} ; $T = Si^{4+}, Al^{3+}$, and B^{3+} ; $B = B^{3+}$ (probably \square); $V, W = OH, F$, and O .

Different modes of recalculating chemical data to crystallochemical formulas are known (Borneman-

Starynkevich, 1964; Bulakh, 1964, 1967; Bulakh et al., 1995; Dolivo-Dobrovolsky and Gul'bin, 2002; Krivovichev and Zolotarev, 2003). Calculation on the basis of oxygen or cations is applied most frequently. The major difference in calculation is the basic postulate to define a common factor, which is derived from the theoretical number of oxygen atoms (or portion of them) or theoretical number of cations (or portion of them) in an ideal formula of the mineral. The charge method is also applied frequently. This mode is identical to the oxygen method, but the common factor is determined on the basis of the negative charge number that falls on the portion of oxygen (anion) in an ideal formula of the mineral.

The mode of recalculation of coefficients in a particular mineral formula should be indicated, because the final results of calculations, i.e., the formula coefficients, depend on the calculation methods applied to the same initial chemical composition. Let us illustrate this important statement with the example of dravite (magnesium tourmaline) from the Bazhenovo deposit (Erokhin and Shagalov, 1997). The microprobe analysis of the mineral reported by these authors constrains possible methods of calculation to formula coefficients. Calculation may be performed on the basis of the oxygen portion (24.5 O atoms), 16 cations ($X + Y + Z + T = 16$), 15 cations taking into consideration probable vacancy in the X site ($Y + Z + T = 15$), or 6 Si atoms [$T(Si) = 6$]. Initial chemical data and results of different calculation methods are shown in Table 1.

As can be seen, various modes of recalculation result in different final coefficients. However, Erokhin and Shagalov (1997) did not indicate nor argue the benefits of the recalculation method in their publication.

The observance of charge balance is the first criterion for correct formula calculation. Unfortunately,

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Table 1. Chemical composition of dravite recalculated to formula

Component	Wt %	Cation	Coefficients in different modes of recalculation				Erokhin and Shagalov (1997)
			24.5O	6Si	Y + Z + T = 15	X + Y + Z + T = 16	
SiO ₂	37.92	Si	5.99	6.00	6.11	6.17	6.19
Al ₂ O ₃	36.04	Al	6.71	6.72	6.83	6.91	6.94
FeO	2.51	Fe	0.33	0.33	0.34	0.34	0.34
MgO	7.16	Mg	1.69	1.69	1.72	1.74	1.76
CaO	0.07	Ca	0.01	0.01	0.01	0.01	0.01
Na ₂ O	2.61	Na	0.80	0.80	0.82	0.82	0.82

Note: 0.02 wt % NiO and 0.03 wt % Cr₂O₃ were detected in the mineral composition.

Table 2. Chemical composition of uvite and coefficients in its formula

Composition	SiO ₂	TiO ₂	Al ₂ O ₃	Cr ₂ O ₃	MgO	CaO	Na ₂ O	F
Weight %	36.95	0.42	29.53	0.05	13.47	3.81	1.09	0.86
Element	Si	Ti	Al	Cr	Mg	Ca	Na	F
Coefficient in formula	6.01	0.05	5.66	0.01	3.27	0.66	0.34	0.44

Note: 0.02 wt % FeO, 0.01 wt % MnO, and 0.01 wt % K₂O were detected in the mineral composition.

mineral formulas are often published with a violation of the total electroneutrality (especially by calculation on the basis of cations). The dravite formula (Na_{0.82}Ca_{0.01})_{0.83}(Mg_{1.76}Al_{0.94}Fe_{0.34})_{3.04}[Al_{6.00}Si_{6.19}O₂₇](BO₃)₃(OH)₂ from (Erokhin and Shagalov, 1997) is an example. If obvious misprints, for example, in the general formula of tourmaline-group minerals are excluded, then the imbalance of charge is +1.62. Substitution of a part of OH⁻ with O²⁻ compensates the charges, and the formula can be rewritten as (Na_{0.82}Ca_{0.01})_{0.83}(Mg_{1.76}Al_{0.94}Fe_{0.34})_{3.04}Al_{6.00}(Si_{6.19}O₁₈)(BO₃)₃(OH_{2.38}O_{1.62})_{4.00}. The recalculation of this analysis on the basis of 15 or 16 cations also requires substitution of a part of OH⁻ with O²⁻, and resulting formulas look like (Na_{0.82}Ca_{0.01})_{0.83}(Mg_{1.72}Al_{0.83}Fe_{0.34})_{2.89}Al_{6.00}(Si_{6.11}O₁₈)(BO₃)₃(OH_{3.11}O_{0.89})_{4.00} and (Na_{0.82}Ca_{0.01})_{0.83}(Mg_{1.74}Al_{0.91}Fe_{0.34})_{2.99}Al_{6.00}(Si_{6.17}O₁₈)(BO₃)₃(OH_{2.59}O_{1.41})_{4.00}, respectively. The recalculated results of initial data on the basis of the 24.5 O atoms and 6 Si atoms are practically identical and the crystallochemical formula of dravite looks like (Na_{0.80}Ca_{0.01})_{0.81}(Mg_{1.69}Al_{0.72}Fe_{0.33})_{2.74}Al_{6.00}(Si_{6.00}O₁₈)(BO₃)₃(OH)_{4.00}. A small charge imbalance (+0.02) resulting from rounding off can be neglected in this case. In our view, this variant is the most acceptable as a resulting crystallochemical formula of dravite from the Bazhenovo deposit due to the least number of assumptions and adjustments.

As follows from the general formula of the tourmaline-group minerals, the same cation (for example Al) can occupy different sites in the mineral structure. Therefore, the substantiation of cation distribution by

different sites is very important. However, based on chemical analysis only, authors, as a rule, act as follows: the Z octahedral site is occupied first (if the Al coefficient is more than 6) and remaining Al is added to the Y site. Results of spectroscopic studies and determination of unit cell parameters allow more reasonable distribution of cations by different structural sites. The chemical analysis of uvite from magnesian skarn at the Kukhi-lal deposit and result of recalculation on the basis of 15 cations (Zolotarev, 1996) may be considered as an example (Table 2).

Stemming from the chemical analysis, various modes of Mg and Al distributions by Y and Z sites may be suggested. If the known technique (Gorskaya et al., 1991) based on comparison of the dimensions of Y and Z octahedrons calculated from the unit cell parameters and computed for various cation distributions at these sites is used, then the resulting formula of uvite can be written in the following form (Zolotarev, 1996): (Ca_{0.66}Na_{0.34})_{1.00}(Mg_{2.31}Al_{0.62}Ti_{0.05}Cr_{0.01})_{2.99}(Al_{5.04}Mg_{0.96})_{6.00}(Si_{6.01}O₁₈)(BO₃)₃(OH_{3.09}O_{0.47}F_{0.44})_{4.00}.

As follows from this formula, tourmaline from the Kukhi-lal deposit is Fe-free and distinguished by a high Al in Y-octahedron. The incorporation of Al into the structure is compensated by substitution of a part of Ca and OH groups with Na and O, respectively. It should be noted that a partial disorder of cation distributions at Y and Z octahedral sites is characteristic of tourmaline-group minerals and the technique elaborated by Gorskaya et al. (1991) allows this disorder to be taken into account and demonstrates that Al and Mg in this uvite are distributed by two octahedral sites.

Table 3. Chemical composition of blue tourmaline (sample T-14) and coefficients in its formula

Composition	SiO ₂	TiO ₂	Al ₂ O ₃	FeO	MnO	CaO	Na ₂ O	K ₂ O	F
Weight, %	35.68	0.04	36.16	6.93	0.07	0.17	2.75	0.03	1.16
Element	Si	Ti	Al	Fe	Mn	Ca	Na	K	F
Coefficient in formula	6.00	0.01	7.17	0.97	0.01	0.03	0.90	0.01	0.62

Note: Li content in formula was calculated by additional occupancy of Y site up to 3.

In the literature, the crystallochemical formulas of tourmalines are usually published without consideration of these general features. Chromdravite described by Rumyantseva (1983) from Karelia is an indicative example. The empirical crystallochemical formula of this tourmaline calculated from chemical analysis on the basis of a theoretical number of 19 cations after subtraction of chromium phengite impurity can be written as follows: $(\text{Na}_{0.97}\text{Ca}_{0.03})_{1.00}(\text{Mg}_{2.57}\text{Mn}_{0.03}\text{V}_{0.22}\text{Al}_{0.16}\text{Ti}_{0.02})_{3.00}(\text{Cr}_{4.71}\text{Fe}_{1.08}\text{Al}_{0.21})_{6.00}(\text{B}_{2.91}\text{Al}_{0.09})_{3.00}(\text{Si}_{5.81}\text{Al}_{0.19})_{6.00}\text{O}_{27}(\text{O}_{0.23}\text{OH}_{3.77})_{4.00}$.

All of the Cr was placed into the Z octahedral site and the ideal formula of chromdravite mineral species is $\text{NaMg}_3\text{Cr}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_4$.

However, the subsequent structural examination of this Cr-rich tourmaline from Karelia (Gorskaya et al., 1987) led to a somewhat different writing of its formula with allowance for Cr distribution by different octahedral sites: $(\text{Na}_{0.88}\text{K}_{0.07}\text{Ca}_{0.01})_{0.96}(\text{Cr}_{1.62}\text{Fe}_{0.75}\text{Mg}_{0.63})_{3.00}(\text{Cr}_{3.36}\text{Mg}_{2.34}\text{Fe}_{0.30})_{6.00}(\text{Si}_{6.00}\text{O}_{18})(\text{BO}_3)_3(\text{OH})_{4.00}$.

Gorskaya et al. (1987) established that if the Cr content in tourmaline is sufficiently high, this element occupies both Y and Z sites. Hence, the ideal formula $\text{NaCr}_6\text{Cr}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3\text{O}_3(\text{OH})$ distinct from chromdravite can be ascribed to such tourmaline. According to the modern nomenclature rules, this situation permits either existence of a novel natural mineral species of Cr-rich tourmalines in addition to chromdravite or suggests that this variant is a theoretical formula of chromdravite.

In the case of microprobe analyses of Fe-bearing tourmalines, maximum difficulties in writing formulas emerge from iron distribution by different sites and its division by the valence. The crystallochemical formula of blue tourmaline (sample T-14) from the Mika pegmatite vein, eastern Pamirs, recalculated from microprobe data (Table 3) on the basis of Si = 6 looks as follows (Zolotarev et al., 1996):

$(\text{Na}_{0.90}\text{Ca}_{0.03}\text{K}_{0.01})_{0.94}(\text{Al}_{1.17}\text{Fe}_{0.97}\text{Li}_{0.85}\text{Mn}_{0.01})_{3.00}\text{Al}_{6.00}(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH}_{3.08}\text{F}_{0.62}\text{O}_{0.30})_{4.00}$.

Further, using Mössbauer spectroscopy, iron was divided by structural sites and the valence (Ovchinnikov and Zolotarev, 1997). The resulting formula of this sample was rewritten as $(\text{Na}_{0.90}\text{Ca}_{0.03}\text{K}_{0.01})_{0.94}(\text{Al}_{1.23}\text{Fe}_{0.86}^{2+}$

$\text{Li}_{0.85}\text{Fe}_{0.05}^{3+}\text{Mn}_{0.01})_3(\text{Al}_{5.94}\text{Fe}_{0.06}^{2+})_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH}_{3.04}\text{F}_{0.62}\text{O}_{0.34})_4$.

Thus, at present, while microprobe analyses are prevalent, especially as concerns zonal tourmaline crystals, the crystallochemical coefficients depend on the mode of recalculation and validity of distribution of cations and anions by different structural sites. In some cases, different modes of recalculation of the same data may result in the attribution of one tourmaline sample to different mineral species. Therefore, structurally grounded crystallochemical formulas are the most reliable. The X-ray structural examination of blue tourmaline (sample T-14) revealed a split of the W site into two subsites—the triple W1 and ninefold W2, which is occupied by fluorine anions—and confirmed iron distribution by octahedral sites (Rozhdestvenskaya et al., 2005). The resulting crystallochemical formula is

$(\text{Na}_{0.90}\text{Ca}_{0.03}\text{K}_{0.01})_{0.94}(\text{Al}_{1.11}\text{Fe}_{0.99}\text{Li}_{0.84}\text{Fe}_{0.06}^{3+})_3(\text{Al}_{5.94}\text{Fe}_{0.06}^{2+})_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3(\text{F}_{0.60}\text{O}_{0.5}\text{OH}_{0.15})_{1.0}$.

As follows from the above formula, fluorine that is predominant in the W site allows us formally to speak of a new mineral species, F-rich elbaite. Thus, on the basis of the fifty-percent rule, elbaite, like apatite, may be considered a supraspecies term. At the same time, on the simple recalculation of chemical data to formula, additional anions are, as a rule, detected without partition by V and W sites, although these sites are separated in the general formula of tourmaline (see the first page of this paper).

Thus, the complexity of the chemical composition of tourmaline and variable mechanisms of isomorphic substitutions create notable difficulties in the recalculation of chemical data to crystallochemical formulas. The resulting crystallochemical formula is controlled by the following factors.

1. *The mode and accuracy of determination of mineral chemistry.* Microprobe analysis does not allow precise estimation of the light elements and H₂O in tourmaline and gives only the total iron, making possible only an indirect estimation of the coefficients for these components in the formula.

2. *Compositional features of the studied tourmaline sample and choice of mod for calculating the coefficients of the formula.* The presence or absence of lithium in a composition; the probable lack of cations in the X site; and the low accuracy of quantitative estima-

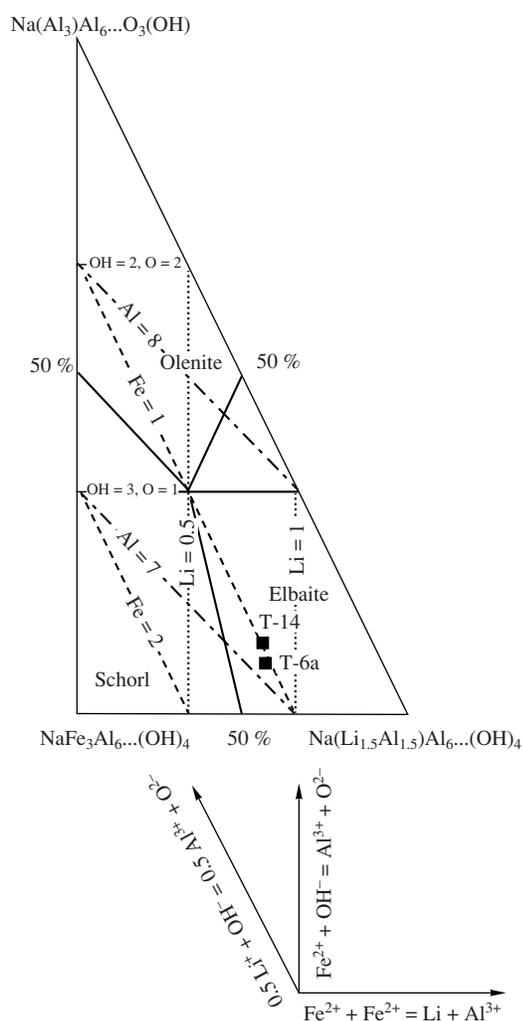


Fig. 1. Compositions of blue tourmaline from the Mika pegmatite vein, eastern Pamirs, plotted in a vector diagram. Data points are results of microprobe analysis (Zolotarev, 1996) recalculated to formula coefficients.

tion of B, Li, and H₂O determine the mode of recalculation of chemical data to the crystallochemical formula. The recalculation schemes based on O + F + OH = 31, 29 O atoms; 24.5 O atoms; 19, 18, 16 and 15 cations; and 6 Si atoms may be applied to tourmaline. Each mode has its own constraints, because it is not feasible to take into account all possible isomorphous substitutions in tourmaline-group minerals.

3. Validity of the applied mode of cation distribution by structural sites and isomorphous substitutions. The modes of cation distribution by structural sites may be different and exert influence on the resulting crystallochemical formula of tourmaline. Spectroscopic methods, determination of unit cell parameters, and structural examination make it possible to substantially change the general appearance of the tourmaline crystallochemical formula.

Different estimations of these factors lead to alternative versions of the published crystallochemical formulas and hamper comparison of tourmaline compositions. Full knowledge of the mode of calculation is necessary for correct comparison, as well as close conditions and quality of analyses.

GRAPHIC REPRESENTATION OF TOURMALINE COMPOSITION

Ternary plots of mineral compositions are commonly used in analyzing the paragenetic assemblages and spatiotemporal evolution of mineral chemistry, as well as in classifying minerals and identifying new mineral species. Such triangles are simple in plotting and reading.

Triangular diagrams display concentrations of isomorphous cations (or anions) occupying the same site in the crystal structure of a mineral. Such plots are recommended for classification of tourmaline species (Hawthorne and Henry, 1999). However, application of ternary plots to the end-member composition of minerals with complex chemistry encounters certain difficulties. The point is that graphic representation of the mineral composition as a percentage of end-member contents depends on the choice of end members and the succession of calculations.

To avoid this dependence, one adverts to vector methods of graphic representation of mineral chemistry. The principles of constructing vector diagrams are not complicated, and such a method was used, for example, by Burt (1989), Zolotarev et al. (2003), and Krivovichev and Zolotarev (2003). Vector diagrams depict the chemical composition of minerals according to formula coefficients plotted in diagrams where end members serve as coordinates. Such an imaging mode is especially helpful for tourmalines and other minerals with heterovalent isomorphous substitutions in several structural sites.

The crystallochemical formula of tourmaline from sample T-14 illustrates the capability of vector plots. As can be inferred from the formula, the composition of this mineral may be represented as a mixture of three major end members: elbaite, schorl, and olenite. In other words, chemical variations of this sample are determined by three mechanisms of isomorphous substitutions: $\text{Fe}^{2+} + \text{OH}^- \rightleftharpoons \text{Al}^{3+} + \text{O}^{2-}$; $\text{Fe}^{2+} + \text{Fe}^{3+} \rightleftharpoons \text{Li}^+ + \text{Al}^{3+}$; and $0.5\text{Li}^+ + \text{OH}^- \rightleftharpoons 0.5\text{Al}^{3+} + \text{O}^{2-}$. The composition of this tourmaline may be plotted easily in a vector diagram using coefficients at Al, Li, and Fe (Fig. 1). According to the position of this point, tourmaline species may be identified (elbaite in our case) and the simplest variant of isomorphous substitutions may be suggested for a series of samples. As follows from Fig. 1, the chemical variations of two plotted tourmaline samples may be described by a common mechanism of isomorphous substitutions: $0.5\text{Li}^+ + \text{OH}^- \rightleftharpoons 0.5\text{Al}^{3+} + \text{O}^{2-}$.

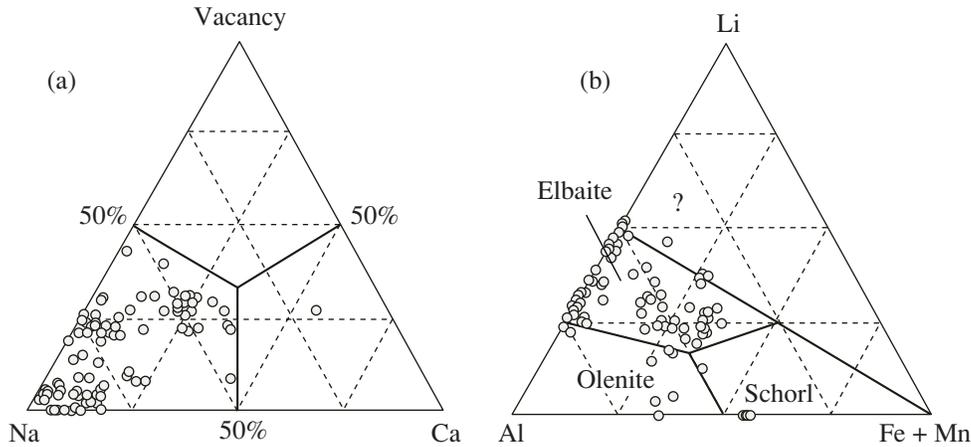


Fig. 2. Compositions of tourmalines from miarolitic pegmatites of the eastern Pamirs plotted in triangular diagrams displaying occupancies of (a) X and (b) Y sites. Data points are results of an original microprobe analysis recalculated to formula coefficients.

DEFINITION OF SPECIES OF TOURMALINE-GROUP MINERALS FROM THEIR FORMULAS

Fourteen mineral species are known to date in tourmaline-group minerals. Proposals for the classification of minerals from this group on the basis of the fifty-percent rule (Hawthorne and Henry, 1999) are now being discussed by the subcommittee on tourmalines of the Commission on New Minerals and Mineral Names, International Mineralogical Association.

Application of the fifty-percent rule to nomenclature gives us an opportunity to describe separate mineral species by the predominant ion (or vacancy) and serves as a reason for the recognition of new minerals in the tourmaline group. The complex chemical composition of tourmaline-group minerals and numerous structural sites, which are occupied by isomorphically connected elements, create an extensive background for increasing the number of mineral species in the tourmaline group as is illustrated by recent “discoveries” (olenite, rossmanite, magnesiofuite, etc.).

The uncertainties and problems in describing new species in the tourmaline group were considered earlier by the example of rossmanite (Zolotarev and Bulakh, 1999). We repeat our major conclusion: while identifying new mineral species in the tourmaline group, one ought not to limit himself by considering the atoms that occupy only one structural site, but should involve all interrelated atomic substitutions in different sites. The fifty-percent rule is easily applicable to isovalent substitutions in one structural site. In the case of heterovalent substitutions, the replacement of heterovalent atoms in one structural site must be accompanied by modifications in a particular site to maintain electroneutrality.

Furthermore, application of the fifty-percent rule seems to be efficient only for minerals with similar crystallochemical formulas. The ideal formula of

elbaite $\text{Na}(\text{Li}_{1.5}\text{Al}_{1.5})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_4$ suggests equal amounts of Li and Al in the Y site, whereas in the case of schorl $\text{NaFe}_3^{2+}\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_4$, this site is occupied entirely by Fe^{2+} and by Al in the case of olenite $\text{NaAl}_3\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3\text{O}_3(\text{OH})$. The Mn-dominant tourmalines are discussed frequently in publications. Hawthorne and Henry (1999) suggested two formulas for the end members of Mn-dominant tourmalines with the prevalence of Na in the X site. These are Mn-dravite $\text{NaMn}_3\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_4$ and Mn-oxhydravite $\text{Na}(\text{Mn}_2\text{Al})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{O}$. These authors do not discuss as acceptable the formula suggested for tsalaisite $\text{Na}(\text{Mn}_{1.5}\text{Al}_{1.5})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3[(\text{OH})_{2.5}\text{O}_{1.5}]$ by analogy with elbaite (Schmetzer and Bank, 1984) and formula $\text{Na}(\text{MnAl}_2)\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3[(\text{OH})_2\text{O}_2]$ (Slivko, 1961). $\text{Na}(\text{MnLiAl})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_4$ is another possible hypothetical version of the ideal formula of this mineral. What decision should be taken and what should be the argument for it?

In the context of arising controversies in application of the fifty-percent rule to defining mineral species belonging to tourmaline-group minerals, we consider the compositions of these minerals from miarolitic pegmatites in the eastern Pamirs and Transbaikalia.

The compositions of tourmalines from the miarolitic pegmatites of the eastern Pamirs are plotted in triangular diagrams (Fig. 2). As is seen from Fig. 2a, Na dominates in the X site of almost all tourmalines. Following the recommendations given by Hawthorne and Henry (1999), by occupancy of the Y site, this mineral species may be defined as elbaite, schorl, or olenite. At the same time, four data points fall into the field of uncertainty. Hawthorne and Henry (1999) do not stipulate how to define mineral species in this case.

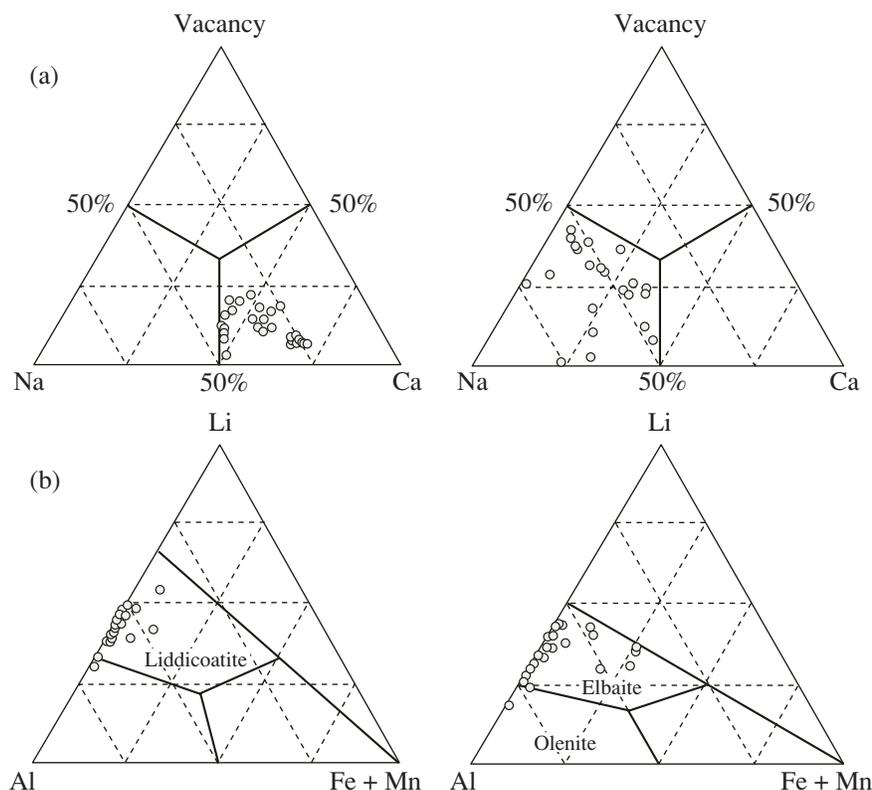


Fig. 3. Compositions of tourmalines from miarolitic pegmatites of central Transbaikalia plotted in triangular diagrams displaying occupancies of (a) X and (b) Y sites. Data points are results of microprobe analysis (Zagorsky and Peretyazhko, 1992 and our data) recalculated to formula coefficients.

Tourmalines from the Malkhan pegmatite field in Transbaikalia (Fig. 3) may be attributed to alkali and calcic groups, after Hawthorne and Henry (1999). Handling of calcic tourmalines is the most intriguing. According to occupancy of the Y site, they should be referred to as liddicoatite. One data point falls into the field with predominance of Al in this site (Fig. 3b); i.e., this tourmaline should be regarded in formal terms as a new mineral species not envisaged by Hawthorne and Henry (1999).

In addition, calcic tourmalines are noteworthy in terms of their symmetry. Zones with anomalous $2V_{\text{meas}} = 26^\circ$ (Shtukenberg et al., 2005) were identified in the sample from Transbaikalia. According to the unit cell parameters, the symmetry of this tourmaline is no higher than monoclinic, in accordance with the data obtained by Akizuki et al. (2001), who showed that liddicoatite–elbaite tourmaline is triclinic. Thus, the likely existence of natural tourmalines with symmetry lower than trigonal gives rise to much more diverse mineral species in the mineral group.

The interesting problem of incorporation of Cu, Zn, Ni, and other elements in the structure of tourmaline has not been studied outright. Detailed structural examinations of such tourmalines may lead to recognition of sites or subsites with predominant occupancies by these

elements and to further complication in naming tourmaline-group minerals.

CONCLUSIONS

The subtle differences in composition and structure of tourmalines, e.g., recognition of fluor- and hydroxyl-elbaite, the calcic analog of olenite, and other varieties, may be established only from very detailed structural examinations. In geological practice, we commonly deal with microprobe analyses of tourmaline composition and their recalculation to formulas. In each case, the calculated formula of tourmaline is a result of an author's interpretation of chemical data and should be regarded as a certain approximation. Therefore, in the context of currently existing rules of recognition of mineral species, the problem of identifying structural and chemical mineral varieties becomes extremely topical (Bulakh, 2004). In our opinion, the development and application of criteria for establishing structural and chemical mineral varieties should contribute to the elaboration of more rational naming rules, which would reduce the number of new mineral species that differ either at the level of detailed and comprehensive studies or in the formal or insignificant predominance of specific cations or anions at a particular structural site on the basis of the fifty-percent rule.

To eliminate the existing errors and alternative versions, a unified approach to the naming of crystal solid solutions with such a high isomorphic capacity as that in tourmaline-group minerals should be elaborated. Only structural studies, feasible now in any modern scientific mineralogical center, may serve as a theoretical and practical basis for such an approach. Vector analysis of mineral compositions with obligatory differentiation in applying the fifty-percent rule to the cases of isovalent and heterovalent isomorphic substitutions might be very helpful. Progress in this line of research and its refinement by specific examples will facilitate efficient modes of formal mineral speciation.

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