Article

On the Chemical Identification and Classification of Minerals

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Abstract: To univocally identify mineral species on the basis of their formula, the IMA-CNMNC recommends the use of the dominant-valency rule and/or the site-total-charge approach, which can be considered two procedures complementary to each other for mineral identification. In this regard, several worked examples are provided in this study along with some simple suggestions for a more consistent terminology and a straightforward use of mineral formulae. IMA-CNMNC guidelines subordinate the mineral structure to the mineral chemistry in the hierarchical scheme adopted for classification. Indeed, a contradiction appears when we first classify mineral species to form classes (based on their chemistry) and subsequently we group together them to form supergroups (based on their structure topology): To date, more than half of recognized mineral supergroups include species with different anions or anionic complexes. This observation is in contrast to the current use of chemical composition as the distinguishing factor at the highest level of mineral classification.

Keywords: nomenclature; classification; IMA-CNMNC; dominant-valency rule; end-member formula; site-total-charge approach; mineral supergroup

1. Introduction: Systematic Mineralogy

In order to have a rational and robust scheme for mineral systematics, a ranking of criteria has to be established. The mineral species is the basic element for any classification scheme we would adopt, and it is defined by a series of rules recommended by the Commission on New Minerals, Nomenclature and Classification (CNMNC) of the International Mineralogical Association (IMA). In accord with Nickel [1], a mineral species can be defined as follows: a solid chemical substance formed as a result of geological processes. Disregarding the geological processes, this definition implies that a mineral can be crystalline, quasi-crystalline, or even non-crystalline (amorphous and metamict). In fact, the minimum requirement for a solid phase to be a mineral is to have a (physico-)chemical homogeneity proving its uniqueness. As most of the mineral species (>99%) have a crystalline structure, and most of them undergo chemical substitution in some structural sites, detailed information on their long-range site populations may also become important. This compositional criterion was formalized by the IMA-CNMNC [2]: *"at least one structural site in the potential new mineral should be predominantly occupied by a different chemical component than that which occurs in the equivalent site in an existing mineral species"*. In minerals with mixed site occupancy, it is also recommended that the mineral formula of any species leads to an end-member formula for its unambiguous identification [3]. As a mineral species is typically characterized by chemical composition and crystallographic properties, its polymorphic forms can be regarded as different species if their structures are topologically different [2] or quite different,

such as forsterite versus ringwoodite, based respectively on a hexagonal and cubic close-packed array of oxygen atoms [4]. At fixed composition and similar topology, symmetry was also adopted as a criterion to identify different mineral species—e.g., in feldspars, monoclinic $K(AlSi_3O_8)$ is sanidine, triclinic $K(AlSi_3O_8)$ is microcline; in the amphibole supergroup, orthorhombic $Mg_2Mg_5Si_8O_{22}(OH)_2$ is anthophyllite, whereas monoclinic $Mg_2Mg_5Si_8O_{22}(OH)_2$ is cummingtonite. However, because of historical reasons and because their names are widely used in the petrological literature, some mineral species may be defined by a range of compositional variability which does not obey strictly the dominance rule, e.g., the join tremolite–actinolite–ferro-actinolite in amphiboles [5].

Mineral nomenclature aims at identifying and naming minerals, whereas mineral classification aims at grouping minerals on the basis of their similar properties and reciprocal relations. At the top of the hierarchical scheme in force, the mineral structure is subordinate to the mineral chemistry [6]. However, a hierarchical contradiction appears if we first classify mineral species at the highest level to form classes (native elements; sulfides and sulfosalts; halides; oxides; carbonates and nitrates; borates; sulfates; phosphates, arsenates and vanadates; silicates; organic compounds; [7]) and if we subsequently group them to form supergroups based essentially on the structural similarities. The latter, by definition, can include different classes [6], e.g., the spinel supergroup includes sulfides such as greigite ($FeFe_2S_4$) and oxides such as magnetite ($FeFe_2O_4$) [4].

The aim of this study is to define the meaning of mineral formulae, and to suggest a coherent procedure to identify mineral species based on their formula, while pointing out a contradiction in the current mineral classification scheme.

2. Mineral Formulae

We report in this section some simple suggestions for a more consistent terminology and a straightforward use of mineral formulae.

Mineral formulae should be written on the basis of crystal-chemical considerations and not as a list of atomic fractions (atoms per formula unit, apfu) calculated from weight percent analysis of elements or oxides. For nomenclature purposes, as well as to assist the geoscience community in identifying mineral species, mineral formulae should also avoid details of atom ordering, either (1) when they require the combination of data obtained by different methods, such as single-crystal X-ray diffraction and electron microprobe analysis, possibly integrated with additional spectroscopic information (e.g., Mössbauer and optical absorption spectroscopy), or (2) when an atom tends to disorder over non-equivalent structural sites, particularly those with the same coordination number.

2.1. Structural Formula

Following Hawthorne et al. [8], a general structural formula is defined as the minimum set of symmetrically distinct sites that constitute the structural arrangement. For any crystalline mineral, a general structural formula can be written.

As examples, consider the *Ia*-3*d* garnet [9] and the *C*2/*m* amphibole [5] structures, respectively:

$$\{X_3\}[Y_2](Z_3)O_{12}$$

$$AM(4)_2[M(1)_2M(2)_2M(3)][T(1)_4T(2)_4]O_{22}O(3)_2$$
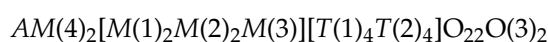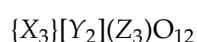
where the italicized letters represent non-equivalent structural sites, and by convention and for convenience, all anion sites occupied solely by O^{2-} are summed and expressed as O_n. Theoretically, the structural formula should be used for mineral identification [2].

2.2. Chemical Formula

The structural formula has been adopted for nomenclature issues for some mineral groups, such as the garnet-supergroup [9]; in other cases, such as for the amphibole-supergroup [5], the simpler general chemical formula $AB_2C_5T_8O_{22}W_2$, where the letter C includes the *M*(1–3) sites, has been kept

as the reference, although all the reasoning on impact of the partitioning of C cations on amphibole nomenclature is based on the structural formula [5]. When their chemical constituents are substituted to the sites in the general structural or to the letters in the general chemical formula, we obtain the structural and chemical formula of the mineral species (respectively). Note that the not-italicized letters should be used to represent constituents in the chemical formula, e.g., $^A\square^BCa_2^CMg_5^TSi_8O_{22}^W(OH)_2$ for the amphibole tremolite. As a further example, consider the spinel magnetite. The general formula of the spinel-supergroup minerals is AB_2X_4, where the letters A and B indicate constituents such as cations and vacancy, which may be disordered over the $^{[IV]}T$ and $^{[VI]}M$ sites, and X represents anions such as O^{2-}, S^{2-}, and Se^{2-} [4], the chemical formula of magnetite is $^A(Fe^{2+})^B(Fe^{3+})_2O_4$, whereas the structural formula is $^T(Fe^{3+})^M(Fe^{2+}Fe^{3+})_2O_4$ and the general structural formula is TM_2O_4.

2.3. End-Member Formula

In accord with Hawthorne [10], an end-member formula can be defined as an algebraic and chemical construct of fixed composition that may have, at most, one site with double occupancy if required for electroneutrality. The end-member formula is important to determine the mineral thermodynamic properties, regardless of whether the end-member exists as a stable phase.

2.4. Simplified Formula

The IMA-CNMNC procedure in force for the approval of a new mineral requires identification of an empirical formula, which should correspond to the above-mentioned structural or chemical formula, and of a simplified formula in which the constituents, joined in parentheses, are separated by commas without any specification of their amounts in terms of apfu, e.g., $(Mg,Fe^{2+})O$. For the sake of simplicity, only major constituents (i.e., with concentrations > 1 wt %) should be reported in the simplified formula.

3. Identification of Mineral Species by the Mineral Formula

3.1. Historical Roots of the Dominant-Valency Rule

The dominant-valency rule became an official rule for mineral classification in 1998, after the paper by Nickel and Grice [2], which was later complemented by that by Hatert and Burke [11]. However, the discussion on its advantages started much earlier, during the work of the second Subcommittee on amphiboles, which started in 1987 (due to a proposal to the then IMA-CNMMN made by D.C. Smith for a different classification scheme which could include new end-members such as sadanagaite and nyböite) [12] and ended with the official report by Leake et al. in 1997 [13]. Since the very beginning, the persons more involved in the crystal-chemical studies of the amphiboles (F.C. Hawthorne, L. Ungaretti, and R. Oberti—the latter contributing without being an official member) proposed a sort of "revolution" from the 1978 report [14], when asking in their so-called Memo 1F for a division in groups that took into account the *total charge* first of the B cations (which should have moved ^BLi amphiboles away from $^B(Mg,Mn,Fe)$ amphiboles and close to ^BNa amphiboles) and then of the A (vacancy included) and C cations (those more relevant to amphibole crystal-chemistry and to their petrological fingerprint), whereas the former report used B and then A and T cations, and *putting the boundaries between groups and end-member at 50%* (the former report used 0.33 and 0.67 for the B cations). The choice of the C-axis in compositional diagrams was suggested because the charge of the C cations is affected also by the heterovalent substitutions involving the W anions (i.e., the oxo component), providing a more informative three-dimensional (3-D) representation of the 4-D (in terms of possible heterovalent group substitutions) amphibole compositional space. Actually, D.C. Smith with his Memo 0 proposed a 4-D system of classification [12] based on the closest end-member composition (i.e., the dominant charge arrangement), defined with a unique four-digit code, such as [0] for tremolite $\square Ca_2Mg_5Si_8O_{22}(OH)_2$ and [1122] for taramite $Na(CaNa)(Mg_3Al_2)Si_8O_{22}(OH)_2$. This system was ready for a further extension to 5-D and/or new compositions, and was computationally reasonable (although not crystal-chemically

well constrained). However, it was graphically awful. In any case, both models were not accepted by the other members of the Subcommittee, who did not rely so much on the crystal-chemical approach and especially on its estimate of the amount and partitioning of high-charged C cations, so that L. Ungaretti and D.C. Smith resigned, respectively, in 1993 and 1994 [13]. A few years later, ion-probe microanalysis combined to structure refinement allowed verifying that Li frequently occurred in sodium amphiboles both as a B and as a C cation [15]. This finding forced the introduction of complex changes to the 1997 scheme [16] which, however, rapidly turned out to be unrealistic [17]. Only the 2012 report on amphibole classification and nomenclature [5] could eventually give the proper credit to the total charge of the W anions (presently used to define the two groups of the amphibole-supergroup), to the dominant valence of the B and C cations (presently used to define the subgroups), and to the dominant component in the dominant valence (to be used for prefixes). However, all the discussion done within the Subcommittee in 1987–1994 brought E.H. Nickel and J.D. Grice (both members of the Subcommittee) to develop their contribution.

3.2. The Site-Total-Charge Approach and the Dominant-Valency Rule

In order to identify mineral species, the IMA-CNMNC recommends the sequential use of the dominant-valency and the dominant-constituent rules [3,11]. These rules are based on the dominance of a chemical constituent (i.e., ions, vacancies, molecular groups, or atom groups with the same valency state) of the dominant-valency state at a given crystallographic site. Along with valency-imposed double site occupancy (i.e., the occurrence of heterovalent pair of ions or ion–vacancy pair at most one site), these two rules should identify a mineral species and its (charge-balanced) end-member formula. Due to the possible occurrence of heterovalent substitution at a single site such as $(B^{2+}_{0.5} + \square_{0.5})^{\Sigma 1+} \leftrightarrow A^+$, the simple application of the dominant-valency rule may fail (i.e., an end-member formula is not identified). In this case, it may be important to apply the site-total-charge approach in which the site total charge (STC) indicates an integer number (charge-constraint) for which possible charge and atomic arrangements can be defined in accord with mineral composition [3]. If (and only if) such arrangements satisfy all the criteria of an end member, the mineral may be identified. Note that *if* the integer number *closest* to the STC is not consistent with an end-member, another integer number in line with the end-member definition must be selected, as shown by the examples below.

Note that, in Section 2, we suggested distinguishing structural and chemical formulae and using italicized and not-italicized symbols, respectively, so that italicized letters identify structural sites and Roman letters identify groups of cations/anions. Admittedly, this rule is not followed in reports on the nomenclature of some mineral groups. Based on our statement, and in order to make the reasoning clearer in this paper, we use the Roman-typed letters for mineral formulae in the examples below.

3.2.1. Mica

Minerals occurring between norrishite, ideally $K^M(LiMn^{3+}_2)Si_4O_{10}{}^A(O)_2$, and polylithionite, ideally $K^M(Li_2Al)Si_4O_{10}{}^A(F)_2$, are related by the substitution:

$$^M(Li + 2Mn^{3+})^{\Sigma 7+} + {}^A(2O^{2-})^{\Sigma 4-} = {}^M(2Li + Al)^{\Sigma 5+} + {}^A(2F^-)^{\Sigma 2-}.$$
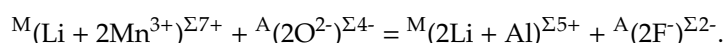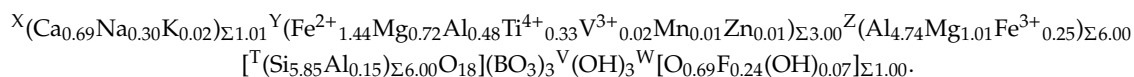
The boundary between these two minerals lies at the composition $K^M(Li_{1.5}Mn^{3+}_{1.0}Al_{0.5})^{\Sigma 6+}Si_4O_{10}{}^A(OF)^{\Sigma 3-}$, corresponding to $^M(STC) = +6$ and $^A(STC) = -3$. Thus, mineral compositions with STC for M cations > +6 and A cations < −3 belong to the norrishite compositional field, whereas those with STC for the M-cations < +6 and A-cations > −3 belong to the polylithionite field. Let us consider the norrishite composition $K^M(Li_{1.49}Mn^{3+}_{1.02}Al_{0.49})Si_4O_{10}{}^A(O_{1.02}F_{0.98})$ having $^M(STC) = +6.02$ and $^A(STC) = -3.02$, very close to the integer numbers +6 and −3 (charge-constraints $M^{\Sigma 6+}$ and $A^{\Sigma 3-}$). These numbers are compatible with the arrangements $^M(Li_{1.50}R^{3+}_{1.50})^{\Sigma 6+}$ and $^A(O_{1.00}F_{1.00})^{\Sigma 3-}$, but such arrangements are inconsistent with the end-member definition (double occupancy of two sites). In order to identify the end-member

formula, we need to consider integer numbers next to +6 and −3, that is, +7 and −4 which are compatible with $^M(Li_{1.00}R^{3+}_{2.00})^{\Sigma 7+}$ and $^A(O_{2.00})^{\Sigma 4-}$, leading to the end-member $K^M(LiMn^{3+}_2)Si_4O_{10}{}^A(O)_2$.

Note that the dominant-valency rule and the valency-imposed double site occupancy can promptly identify the end-member formula: Respectively, O^{2-} predominates for A anions and $(LiMn^{3+}_2)$ prevails for M cations.

3.2.2. Tourmaline

Consider the empirical formula of lucchesiite, ideally $Ca(Fe^{2+}_3)(Al_6)(Si_6O_{18})(BO_3)_3(OH)_3O$, from Ratnapura (Sri Lanka), one of the two co-type localities [18]:

$$^X(Ca_{0.69}Na_{0.30}K_{0.02})_{\Sigma 1.01}{}^Y(Fe^{2+}_{1.44}Mg_{0.72}Al_{0.48}Ti^{4+}_{0.33}V^{3+}_{0.02}Mn_{0.01}Zn_{0.01})_{\Sigma 3.00}{}^Z(Al_{4.74}Mg_{1.01}Fe^{3+}_{0.25})_{\Sigma 6.00}$$
$$[^T(Si_{5.85}Al_{0.15})_{\Sigma 6.00}O_{18}](BO_3)_3{}^V(OH)_3{}^W[O_{0.69}F_{0.24}(OH)_{0.07}]_{\Sigma 1.00}.$$
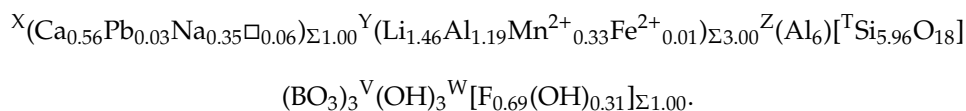
The STC for Y cations (= +7.18, close to +7) and for Z-cations (= +16.99, close to +17) indicate charge-constraints compatible with a double occupancy of two sites, i.e., the arrangement $[^Y(R^{2+}_{2.5}Ti_{0.5})^{\Sigma 7+}]_{0.66}$ = 1.98 apfu (limited by Ti content) and $[^Z(R^{3+}_5R^{2+})^{\Sigma 17+}]_{0.998}$ = 5.998 apfu (limited by the sum of Al and Fe^{3+} contents) leading to a formula $Ca^Y(Fe^{2+}_{2.5}Ti_{0.5})^Z(Al_5Mg)(Si_6O_{18})(BO_3)_3(OH)_3O$ with double occupancy of two sites (*Y* and *Z*). In this case, the unique combination of charge arrangements, consistent with both the chemical composition (R^{2+} and R^{3+} cations prevailing as the Y and Z constituents in the general formula, respectively) and the *overriding* condition of the end-member formula is $^Y(R^{2+}_3)^{\Sigma 6+}$ and $^Z(R^{3+}_6)^{\Sigma 18+}$ that leads to $Ca^Y(Fe^{2+}_3)^Z(Al_6)(Si_6O_{18})(BO_3)_3(OH)_3O$. Also in this example, the simple application of the dominant-valency rule (X = +2, Y = +2, Z = +3, T = +4 and W = −2) can promptly lead to the lucchesiite end-member formula.

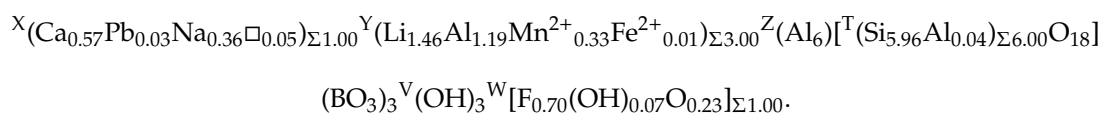### 3.3. Site-Total-Charge Approach Versus Charge-Constraint

The two examples above showed that the dominant-valency rule and the site-total-charge approach can be considered complementary to each other. For the site-total-charge approach, the key point is to find the most appropriate integer number (charge-constraint) consistent with the end-member definition. An incorrect integer number can be recognized from root-charge and atomic arrangements leading to a formula with double occupancy of two sites or charge imbalance. STC may deviate from the correct integer number because of lack of consideration of all the potential end-members involved in the chemical substitution and/or the degree of atom disorder over non-equivalent structural sites.

3.3.1. Understanding the End-Members Involved in the Substitution

Consider the empirical formula of the tourmaline fluor-liddicoatite, ideally $Ca(Li_2Al)Al_6(Si_6O_{18})(BO_3)_3(OH)_3F$, sample L2 [19]:

$$^X(Ca_{0.56}Pb_{0.03}Na_{0.35}\square_{0.06})_{\Sigma 1.00}{}^Y(Li_{1.46}Al_{1.19}Mn^{2+}_{0.33}Fe^{2+}_{0.01})_{\Sigma 3.00}{}^Z(Al_6)[^TSi_{5.96}O_{18}]$$

$$(BO_3)_3{}^V(OH)_3{}^W[F_{0.69}(OH)_{0.31}]_{\Sigma 1.00}.$$

Of particular interest are the STC of the X (=+1.53), and Y cations (= +5.74) and of the W anions (= −1.00) that indicate charge-constraints $X^{\Sigma 2+}$, $Y^{\Sigma 6+}$ and $W^{\Sigma 1-}$, leading to the unbalanced formula $[^X(Ca)^Y(Li_{1.5}Al_{1.5})(Al_6)(Si_6O_{18})(BO_3)_3(OH)_3{}^W(F)]^{\Sigma 1+}$. To better illustrate the chemical substitutions characterizing sample L2, its composition has been recalculated assuming the sum of the (Y + Z + T) cations = 15.00 apfu:

$$^X(Ca_{0.57}Pb_{0.03}Na_{0.36}\square_{0.05})_{\Sigma 1.00}{}^Y(Li_{1.46}Al_{1.19}Mn^{2+}_{0.33}Fe^{2+}_{0.01})_{\Sigma 3.00}{}^Z(Al_6)[^T(Si_{5.96}Al_{0.04})_{\Sigma 6.00}O_{18}]$$

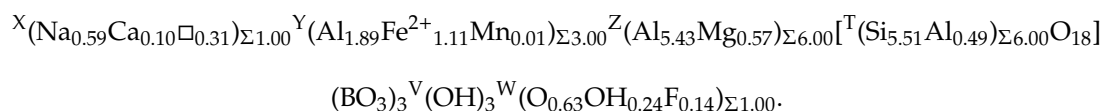$$(BO_3)_3{}^V(OH)_3{}^W[F_{0.70}(OH)_{0.07}O_{0.23}]_{\Sigma 1.00}.$$

Disregarding the minor amounts of Pb, we may arrive at this composition from the fluor-liddicoatite end-member via the following substitution mechanisms:

- $0.23[(^{X}Na + {}^{Y}Al + {}^{W}O) \rightarrow (^{X}Ca + {}^{Y}Li + {}^{W}F)]$, related to darrellhenryite, leads to $^{X}(Ca_{0.77}Na_{0.23})^{Y}(Li_{1.77}Al_{1.23})^{Z}(Al_6)(Si_6O_{18})(BO_3)_3(OH)_3{}^{W}(F_{0.77}O_{0.23})$;
- $0.11[(^{X}Na + 3{}^{Y}Mn) \rightarrow (^{X}Ca + 2{}^{Y}Li + {}^{Y}Al)]$, related to fluor-tsilaisite, leads to $^{X}(Ca_{0.66}Na_{0.34})^{Y}(Li_{1.55}Al_{1.12}Mn_{0.33})^{Z}(Al_6)(Si_6O_{18})(BO_3)_3(OH)_3{}^{W}(F_{0.77}O_{0.23})$;
- $0.05[(^{X}\square + {}^{Y}Al + {}^{W}OH) \rightarrow (^{X}Ca + {}^{Y}Li + {}^{W}F)]$, related to rossmanite, leads to $^{X}(Ca_{0.61}Na_{0.34}\square_{0.05})^{Y}(Li_{1.50}Al_{1.17}Mn_{0.33})^{Z}(Al_6)(Si_6O_{18})(BO_3)_3(OH)_3{}^{W}(F_{0.72}O_{0.23}OH_{0.05})$;
- $0.02[(^{X}Na + 0.5\ {}^{Y}Al + {}^{W}OH) \rightarrow (^{X}Ca + 0.5{}^{Y}Li + {}^{W}F)]$, related to elbaite, leads to $^{X}(Ca_{0.59}Na_{0.36}\square_{0.05})^{Y}(Li_{1.49}Al_{1.18}Mn_{0.33})^{Z}(Al_6)(Si_6O_{18})(BO_3)_3(OH)_3{}^{W}(F_{0.70}O_{0.23}OH_{0.07})$.
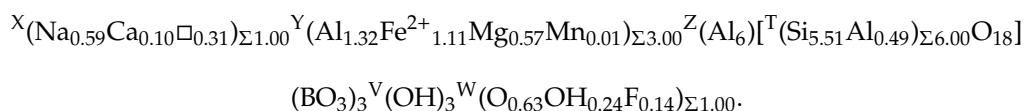
The relative major substitution mechanism for sample L2 is hence related to darrellhenryite (23%), ideally $^{X}(Na)^{Y}(LiAl_2)^{Z}(Al_6)(Si_6O_{18})(BO_3)_3(OH)_3{}^{W}(O)$. Note that the charge constraints for the Y-cations are +5 and +7 for fluor-liddicoatite $^{Y}(Li_{1.5}Al_{1.5})^{\Sigma5+}$ and darrellhenryite $^{Y}(Li_{1.60}Al_{1.40})^{\Sigma7+}$, thus the value +6 indicated by ^{Y}(STC) for sample L2 should be ruled out as inconsistent with the main end-members involved in the chemical substitution. Consequently, we need to consider other charge-constraints: $(X^{\Sigma2+}, Y^{\Sigma5+}$ and $W^{\Sigma1-})$ or $(X^{\Sigma1+}, Y^{\Sigma6+}$ and $W^{\Sigma1-})$ or $(X^{\Sigma2+}, Y^{\Sigma6+}$ and $W^{\Sigma2-})$. Among these, there is no doubt that the most appropriate is $(X^{\Sigma2+}, Y^{\Sigma5+}$ and $W^{\Sigma1-})$: The simple application of the dominant-valency rule shows that Ca^{2+} and F^- prevails among X cations and W anions, respectively, while the arrangement $^{Y}(Li_2Al)^{\Sigma5+}$ is required for the formula electroneutrality.

3.3.2. Atom Disorder

Consider the empirical formula of the tourmaline oxy-schorl, ideally $Na(AlFe^{2+}_2)Al_6(Si_6O_{18})(BO_3)_3(OH)_3O$, from the type locality Zlatá Idka, Slovak Republic [20]:

$$^{X}(Na_{0.59}Ca_{0.10}\square_{0.31})_{\Sigma1.00}{}^{Y}(Al_{1.89}Fe^{2+}_{1.11}Mn_{0.01})_{\Sigma3.00}{}^{Z}(Al_{5.43}Mg_{0.57})_{\Sigma6.00}[^{T}(Si_{5.51}Al_{0.49})_{\Sigma6.00}O_{18}]$$

$$(BO_3)_3{}^{V}(OH)_3{}^{W}(O_{0.63}OH_{0.24}F_{0.14})_{\Sigma1.00}.$$

The dominant-valency rule and the valency-imposed double site occupancy cannot identify an end-member formula. In fact, the dominant-valency criterion (X = +1, Y = +3, Z = +3, T = +4 and W = –2) leads to the unbalanced formula $[^{X}(Na)^{Y}(Al_3)^{Z}(Al_6)^{T}(Si_6O_{18})(BO_3)_3(OH)_3{}^{W}(O)]^{\Sigma2+}$, whereas the double site occupancy criterion leads to a formula with double occupancy of two sites (Y and Z): $^{X}(Na)^{Y}(Al_2Fe^{2+})^{Z}(Al_5Mg)^{T}(Si_6O_{18})(BO_3)_3(OH)_3{}^{W}(O)$. This same formula can also be obtained by considering the STC of the Y cations (= +7.91, close to +8) and that of the Z-cations (= +17.43, close to +17). For classification purposes [21], the oxy-schorl empirical formula can be recast in one with Al ordered at the Z position in the general formula [20]:

$$^{X}(Na_{0.59}Ca_{0.10}\square_{0.31})_{\Sigma1.00}{}^{Y}(Al_{1.32}Fe^{2+}_{1.11}Mg_{0.57}Mn_{0.01})_{\Sigma3.00}{}^{Z}(Al_6)[^{T}(Si_{5.51}Al_{0.49})_{\Sigma6.00}O_{18}]$$

$$(BO_3)_3{}^{V}(OH)_3{}^{W}(O_{0.63}OH_{0.24}F_{0.14})_{\Sigma1.00}.$$

The application of the dominant-valency rule or of the site-total-charge approach to this ordered formula leads to the end-member $Na^{Y}(AlFe^{2+}_2)^{Z}(Al_6)(Si_6O_{18})(BO_3)_3(OH)_3O$. This example shows that disordering over Y and Z group cations results in a deviation of the STC from the most appropriated charge-constraints $Y^{\Sigma7+}$ and $Z^{\Sigma18+}$, which are only compatible with the arrangements $^{Y}(AlFe^{2+}_2)^{\Sigma7+}$ and $^{Z}(Al_6)^{\Sigma18+}$, and is consistent with the end-member definition, towards values as $Y^{\Sigma8+}$ and $Z^{\Sigma17+}$, which are compatible with the arrangements $^{Y}(Al_2Fe^{2+})^{\Sigma8+}$ and $^{Z}(Al_5Mg)^{\Sigma17+}$ but are inconsistent with the end-member definition.

3.4. Site-Total-Charge Approach and Valency-Imposed Double Site Occupancy

The site-total-charge approach is another way to express the dominant-valency rule, where STC is used to identify the dominant root-charge arrangement consistent with the *overriding* condition dictated by the end-member formula.

If the dominant-valency rule fails, we can use the site-total-charge approach, and vice versa. If both are successful but do not identify the same end-member formula, the correct one should be that having the *most abundant atomic arrangement of the dominant (aggregate) root-charge arrangement*. In this regard, the site-total-charge approach may be considered as a *tool* to explore possible charge and atomic arrangements whose quantification, in terms of apfu, identifies the mineral species.

3.4.1. Tourmaline: Schorl or Elbaite?
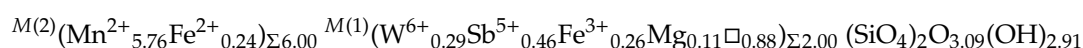
Consider the hypothetical formula:

$$Na^Y(Al^{3+}_{0.8}Fe^{2+}_{1.1}Mg^{2+}_{0.3}Li^+_{0.8})_{\Sigma 3.0}Al_6(Si_6O_{18})(BO_3)_3(OH)_3(OH)$$
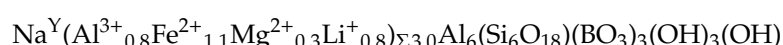
According to the dominant-valency rule, the dominant charge among the Y-cations is +2, which is consistent with the contents of R^{2+} = 1.4 apfu (with $Fe^{2+} >> Mg^{2+}$). Thus, the mineral would be identified as schorl. However, the STC for the Y-cations (= +6) suggests two possible charge and atomic arrangements compatible with +6 and the composition:

- $(R^{3+}_{1.5}R^+_{1.5})^{\Sigma 6+}$, corresponding to $(Al^{3+}_{1.5}Li^+_{1.5})_{0.533}$ = 1.6 apfu
- $(R^{2+}_3)^{\Sigma 6+}$, corresponding to $(Fe^{2+}_3)_{0.467}$ = 1.4 apfu.

As the arrangement $(Al^{3+}_{1.5}Li^+_{1.5})$ is more abundant than (Fe^{2+}_3), the mineral species is identified as elbaite. We can also note that such a mineral species is defined by the most abundant atomic arrangement (in apfu), and that, in this case, the site-total-charge approach prevails over the dominant-valency rule. As a result, a mineral species is identified by the most abundant atomic arrangement, $(Al_{1.5}Li_{1.5})$, of the dominant root-charge arrangement, $(R^{3+}_{1.5}R^+_{1.5})$.

3.4.2. Scorticoite (IMA 2018-159)

Consider the empirical formula (Biagioni et al., work in progress):

$$^{M(2)}(Mn^{2+}_{5.76}Fe^{2+}_{0.24})_{\Sigma 6.00}\ ^{M(1)}(W^{6+}_{0.29}Sb^{5+}_{0.46}Fe^{3+}_{0.26}Mg_{0.11}\square_{0.88})_{\Sigma 2.00}(SiO_4)_2O_{3.09}(OH)_{2.91}$$

The STC of the cations at the $M(1)$ site = +5.04 is consistent with $Mn_6M(1)^{\Sigma 5+}(SiO_4)_2O_3(OH)_3$. The possible charge and atomic arrangements compatible with the $M(1)$-site population are:

- $^{M(1)}(R^{5+}\square)^{\Sigma 5+}$　　　　$\rightarrow (Sb^{5+}\square)_{0.46}$ = 0.92 apfu (limited by Sb contents)
- $^{M(1)}(R^{6+}_{5/6}\square_{7/6})^{\Sigma 5+}$　$\rightarrow (W^{6+}_{5/6}\square_{7/6})_{0.35}$ = 0.70 apfu (limited by W contents)
- $^{M(1)}(R^{6+}_{4/3}R^{3+}_{2/3})^{\Sigma 5+}$　$\rightarrow (W^{6+}_{4/3}Fe^{3+}_{2/3})_{0.22}$ = 0.44 apfu (limited by W contents)
- $^{M(1)}(R^{3+}R^{2+})^{\Sigma 5+}$　　　$\rightarrow (Fe^{3+}Mg^{2+})_{0.11}$ = 0.22 apfu (limited by Mg contents).

As the arrangement $(Sb^{5+}\square)$ is the most abundant one, the end-member composition is $Mn_6(Sb^{5+}\square)(SiO_4)_2O_3(OH)_3$, corresponding to the new mineral species scorticoite [22]. On the basis of this example, one might conclude that this end-member composition can, more straightforwardly, be inferred by considering the two dominant constituents Sb^{5+} (0.46 apfu) and $\square$ (0.88 apfu). However, the following two examples will show that this conclusion cannot be generalized.

3.4.3. Pyrochlore

Consider the hypothetical formula [23]:

$$^A(Na_{1.1}Ca_{0.4}Y_{0.2}U_{0.2}\square_{0.1})_{\Sigma 2.00}{}^B(Nb_{1.7}Ti_{0.3})_{\Sigma 2.00}O_6(OH).$$
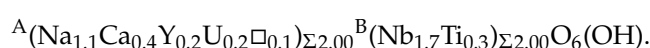
The STC of the B-cations (= +9.7) is consistent with $B^{\Sigma 10+} = Nb^{5+}$.
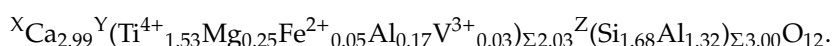
The STC of the A-cations (= +3.3) is consistent with $A^{\Sigma 3+}$. If we consider the most abundant A constituents (Na = 1.1 apfu and Ca = 0.4 apfu), we obtain the atomic arrangement $(Na^+Ca^{2+})^{\Sigma 3+}$ and, hence, the end-member formula $(NaCa)NbO_6(OH)$. However, if we explore all possible charge and atomic arrangements compatible with the A-constituents:

- $^A(R^+{}_{5/3}R^{4+}{}_{1/3})^{\Sigma 3+}$ $\rightarrow (Na^+{}_{5/3}U^{4+}{}_{1/3})_{0.6} = 1.2$ apfu (limited by U contents)
- $^A(R^+R^{2+})^{\Sigma 3+}$ $\rightarrow (Na^+Ca^{2+})_{0.4} = 0.8$ apfu (limited by Ca contents)
- $^A(R^+{}_{1.5}R^{3+}{}_{0.5})^{\Sigma 3+}$ $\rightarrow (Na^+{}_{1.5}Y^{3+}{}_{0.5})_{0.4} = 0.8$ apfu (limited by Y contents)
- $^A(\square R^{3+})^{\Sigma 3+}$ $\rightarrow (\square Y^{3+})_{0.1} = 0.2$ apfu (limited by $\square$ contents)
- $^A(\square_{1.25}R^{4+}{}_{0.75})^{\Sigma 3+}$ $\rightarrow (\square_{1.25}U_{0.75})_{0.08} = 0.16$ apfu (limited by $\square$ contents),

we note that the arrangement $(Na^+{}_{5/3}U^{4+}{}_{1/3})^{\Sigma 3+}$ is the most abundant one. Thus, the correct end-member composition is $(Na_{5/3}U_{1/3})NbO_6(OH)$.

3.4.4. Garnet: Hutcheonite

Consider the empirical formula [24]:

$$^XCa_{2.99}{}^Y(Ti^{4+}{}_{1.53}Mg_{0.25}Fe^{2+}{}_{0.05}Al_{0.17}V^{3+}{}_{0.03})_{\Sigma 2.03}{}^Z(Si_{1.68}Al_{1.32})_{\Sigma 3.00}O_{12}.$$

Applying the dominant-valency rule and considering the *X* site fully occupied by Ca, we would have Ti^{4+} dominant among the Y-cations and Si^{4+} dominant between the Z-cations that lead to unbalanced charge formula $(Ca_3Ti_2Si_3O_{12})^{\Sigma 2+}$. In order to obtain a charge-balanced formula, we may use the valency-imposed double site occupancy principle, which is consistent with two solutions for Y and Z:

- $^Y(Ti^{4+}R^{2+})^{\Sigma 6+} {}^Z(Si^{4+}{}_3)^{\Sigma 12+}$
- $^Y(Ti^{4+}{}_2)^{\Sigma 8+} {}^Z(Si^{4+}Al_2)^{\Sigma 10+}$

Both of these solutions, however, seem to be in contrast with the chemical information, ^YTi is closer to 2.00 apfu than 1.00 apfu and $^ZSi > {}^ZAl$. Moreover, what is the correct solution for the end-member formula? Ma and Krot [24] reported the end-member formula $Ca_3Ti_2(SiAl_2)O_{12}$ by likely using the dominant-end-member approach. The latter sometime converges to the same solution found by the application of the dominant-valency rule and the valency-imposed double site occupancy [3]. In accord with the IMA-CNMNC recommendations [3], to definitively show that $Ca_3Ti_2(SiAl_2)O_{12}$ is correct, we have to demonstrate that the dominant root-charge arrangement is $^Y(R^{4+}{}_2)^Z(R^{4+}R^{3+}{}_2)$ and that the most abundant cation arrangement is $^Y(Ti_2)^Z(SiAl_2)$ in terms of apfu.

In this regard, we can use the site-total charge approach. The STC for the Y (= +7.3) and Z cations (= +10.7) indicate that the integer numbers (charge-constraints) would be $Y^{\Sigma 7+}$ and at $Z^{\Sigma 11+}$, but they can be ruled out because they lead to charge arrangements $^Y(R^{4+}R^{3+})$ and $^Z(R^{4+}{}_2R^{3+})$ inconsistent with the end-member definition. Thus, we have to select other integer numbers such as $Y^{\Sigma 6+}$ and $Z^{\Sigma 12+}$ or $Y^{\Sigma 8+}$ and $Z^{\Sigma 10+}$, where possible charge and atomic arrangements are both consistent with the end-member definition. In detail:

for $Y^{\Sigma 6+}$ and $Z^{\Sigma 12+}$

- $^Y(R^{4+}R^{2+})^{\Sigma 6+} + {}^Z(R^{4+}{}_3)^{\Sigma 12+} \rightarrow {}^Y(Ti^{4+}R^{2+})_{0.30} + {}^Z(Si^{4+}{}_3)_{0.30} = 1.5$ apfu (limited by Mg plus Fe contents)
- $^Y(R^{3+}{}_2)^{\Sigma 6+} + {}^Z(R^{4+}{}_3)^{\Sigma 12+} \rightarrow {}^Y(R^{3+}{}_2)_{0.10} + {}^Z(Si^{4+}{}_3)_{0.10} = 0.5$ apfu (limited by ^YAl plus V contents)

for $Y^{\Sigma 8+}$ and $Z^{\Sigma 10+}$:

- $^Y(R^{4+}{}_2)^{\Sigma 8+} + {}^Z(R^{4+}R^{3+}{}_2)^{\Sigma 10+} \rightarrow {}^Y(Ti^{4+}{}_2)_{0.66} + {}^Z(Si^{4+}Al^{3+}{}_2)_{0.66} = 3.3$ apfu (limited by ^ZAl contents).

From this calculation, it is evident that the dominant root-charge arrangement is $^Y(R^{4+}_2)^Z(R^{4+}R^{3+}_2) = 3.3$ apfu, which is larger than $^Y[(R^{4+}R^{2+}) + (R^{3+}_2)]$ $^Z(R^{4+}_3) = 2.0$ apfu, and that consequently the most abundant atomic arrangement is $^Y(Ti_2)^Z(SiAl_2) = 3.3$ apfu, notwithstanding the misleading chemical information Si > Al at Z. In addition, it is worth noting that the STC for the Y-cations (= +7.3) is closer to +8 than +6, and for the Z-cations (= +10.7) is closer to +10 than +12. The correct end-member formula is, hence, confirmed to be $Ca_3Ti_2(SiAl_2)O_{12}$ [24].

4. One Note on the Mineral Classification Scheme

In accord with the standard IMA-CNMNC guidelines, the mineral species are classified by grouping together minerals of similar structure and chemistry [6]. In order to best express their degree of similarity, a hierarchical scheme is adopted by subdividing them into six levels: (1) mineral class; (2) mineral subclass; (3) mineral family; (4) mineral supergroup; (5) mineral group; and (6) mineral subgroup or mineral series. This scheme is based on the mineral species (mineralogical unit) and therefore on its definition. Note that the possible addition of mineral varieties (particularly used in gemology) is discouraged as it tends to create confusion in the mineralogical literature [2].

Starting from the top of this hierarchical scheme, mineral species are classified primarily into classes based on the nature of the main anion or anionic complex or on the lack of anion (native elements). It is of interest to note that the choice of the mineral supergroup is subordinate to the mineral class in this hierarchical scheme, and that a mineral supergroup consists of two or more groups having essentially the same structure and composed of chemically similar elements. According to Mills et al. [6], a supergroup will generally contain members from the same mineral class, and only *in rare cases* may it also contain groups belonging to different classes.

Although from a didactical and historical viewpoint it is practical to classify mineral species first into classes, this approach seems to be inconsistent with the present list of the supergroups, either approved by the IMA-CNMNC or established following Mills et al. [6]: alluaudite [25], alunite [26], amphibole [5], apatite [27], arctite [28], astrophyllite [29], betpakdalite [30], brackebuschite [31], dumortierite [32], epidote [33], gadolinite [34], garnet [9], gatelite [35], högbomite [36], hollandite [37], hydrotalcite [38], labuntsovite [39], laueite [40], lindackerite [41], lovozerite [42], mayenite [43], perovskite [44], pharmacosiderite [45], pyrochlore [23], sapphirine [46], seidozerite [47], spinel [4], tobermorite [48], and tourmaline [21]. We can note that 15 out of the 29 approved supergroups (hence more than 50%) include mineral species with different anions or anionic complexes: alunite, apatite, arctite, brackebuschite, dumortierite, gadolinite, garnet, hydrotalcite, mayenite, perovskite, pharmacosiderite, sapphirine, seidozerite, spinel, and tourmaline. Therefore, we can conclude that *it is not so rare* that a supergroup can contain species belonging to different classes. As a result, the first hierarchical distinction into classes based on the nature of the anion is in contrast with the current use of chemical composition as the key factor for mineral classification.

The concept of class indeed seems to become a problem for mineral classification. For instance, in addition to the hierarchical contradiction between class and supergroup, we could also wonder whether:

- tourmalines, such as $NaMg_3Al_6(Si_6O_{18})(BO_3)_3(OH)_3(OH)$, and axinites, such as $Ca_6Al_4[B_2Si_8O_{30}](OH)_2$, are to be considered as silicates or borates; or
- minerals such as hanksite, $KN_2Cl(CO_3)_2(SO_4)_9$, thaumasite, $Ca_3Si(OH)_6(CO_3)(SO_4)\cdot 12H_2O$, and jouravskite, $Ca_3Mn^{4+}(OH)_6(CO_3)(SO_4)\cdot 12H_2O$ are to be considered as carbonates or sulfates.

Moreover, quartz (SiO_2) is an oxide or a silicate from a chemical or structural viewpoint, respectively. If we could cancel out the chemical composition as the distinguishing factor at the highest level of mineral classification, the class conflict for minerals such as, for instance, tourmaline, axinite, quartz, hanksite, thaumasite, and jouravskite, would disappear, as they would be classified first based on their structure. Moreover, feldspars could best be identified as a 3-D network of tetrahedra, along with cordierite and osumilite [$(SiO_4) + (AlO_4)$], beryl and bertrandite [$(SiO_4) + (BeO_4)$], tuhualite [$(SiO_4) + (Fe^{3+}O_4)$], hemimorphite [$(SiO_4) + (ZnO_4)$], zektzerite [$(SiO_4) + (LiO_4)$], and so on (e.g., [49]).

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