# Nomenclature of the amphibole supergroup

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## Abstract

A new classification and nomenclature scheme for the amphibole-supergroup minerals is described, based on the general formula $AB_2C_5T_8O_{22}W_2$, where A = □, Na, K, Ca, Pb, Li; B = Na, Ca, $Mn^{2+}$, $Fe^{2+}$, Mg, Li; C = Mg, $Fe^{2+}$, $Mn^{2+}$, Al, $Fe^{3+}$, $Mn^{3+}$, $Ti^{4+}$, Li; T = Si, Al, $Ti^{4+}$, Be; W = (OH), F, Cl, $O^{2-}$. Distinct arrangements of formal charges at the sites (or groups of sites) in the amphibole structure warrant distinct *root names*, and are, by implication, distinct species; for a specific root name, different homovalent cations (e.g., Mg vs. $Fe^{2+}$) or anions (e.g., OH vs. F) are indicated by prefixes (e.g., ferro-, fluoro-). The classification is based on the A, B, and C groups of cations and the W group of anions, as these groups show the maximum compositional variability in the amphibole structure. The amphibole supergroup is divided into two groups according to the dominant W species: *$^{W}$(OH,F,Cl)-dominant amphiboles* and *$^{W}$O-dominant amphiboles (oxo-amphiboles)*. Amphiboles with (OH, F, Cl) dominant at W are divided into eight subgroups according to the dominant charge-arrangements and type of B-group cations: magnesium-iron-manganese amphiboles, calcium amphiboles, sodium-calcium amphiboles, sodium amphiboles, lithium amphiboles, sodium-(magnesium-iron-manganese) amphiboles, lithium-(magnesium-iron-manganese) amphiboles and lithium-calcium amphiboles. Within each of these subgroups, the A- and C-group cations are used to assign specific names to specific compositional ranges and root compositions. Root names are assigned to distinct arrangements of formal charges at the sites, and prefixes are assigned to describe homovalent variation in the dominant ion of the root composition. For amphiboles with O dominant at W, distinct root-compositions are currently known for four (calcium and sodium) amphiboles, and homovalent variation in the dominant cation is handled as for the $^{W}$(OH,F,Cl)-dominant amphiboles. With this classification, we attempt to recognize the concerns of each constituent community interested in amphiboles and incorporate these into this classification scheme. Where such concerns conflict, we have attempted to act in accord with the more important concerns of each community.

**Keywords:** Amphibole, nomenclature, classification, chemical composition, crystal chemistry

## Introduction

Leake (1968) presented a classification for calcic amphiboles, and this was expanded into the International Mineralogical Association (IMA) classification of Leake (1978), henceforth referred to as IMA1978. An IMA Subcommittee on Amphibole Classification was formed, and Leake et al. (1997), henceforth referred to as IMA1997, presented the current classification, as modified by Leake et al. (2003), henceforth referred to as IMA2003, to incorporate new discoveries in amphibole compositions in the intervening years. However, these schemes of classification do not adequately address subsequent discoveries of new compositional types of amphibole (e.g., Oberti et al. 2000, 2003, 2004, 2006; Caballero et al. 2002). Moreover, increasing appreciation of the crystal-chemical and petrological importance of compositional variables not incorporated into the previous schemes [e.g., $Fe^{3+}$, $Fe^{2+}$, Li, and $^{W}O^{2-}$ contents] forced reconsideration of the basis of amphibole classification. To focus on the classification and nomenclature, any extensive discussion of specific points is given in a series of Appendices.

## General statement

Any classification scheme, particularly one involving a supergroup of minerals as complicated as the amphiboles, is of necessity a compromise: simplicity commonly conflicts with

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convenience of use. Moreover, crystallographers, mineralogists, and petrologists will generally have different expectations of a classification. Crystallographers will want a classification that encompasses all aspects of the crystal chemistry of the amphiboles in as concise a way as possible, whereas petrologists will be more concerned with utility and convenience of use from a petrological perspective. We have attempted to recognize the concerns of each constituent community interested in amphiboles and incorporate these into this new classification scheme. Where such concerns conflict, we have attempted to act in accord with the more important concerns of each community.

## THE NEW CLASSIFICATION

The new classification presented here is based on the chemical formula of an amphibole measured by electron microprobe or wet-chemical techniques, possibly augmented by additional analytical, structural and spectroscopic data. It does *not* address classification or nomenclature of amphiboles characterized solely in hand specimen or in thin section; these issues need to be addressed in separate classifications.

This new classification scheme is based on the concept of dominance, and hence:

(1) All distinct arrangements of integral charges over the amphibole formula are considered as *root charge arrangements*.

(2) Specific ions [$Na^+$, $Mg^{2+}$, $Al^{3+}$, $Si^{4+}$, $(OH)^-$] of appropriate charge are associated with sites in the structure, and each distinct chemical composition is a *root composition*. These compositions are assigned trivial[1] names.

(3) Where another homovalent ion is dominant at a site (or group of sites) in the structure, a prefix (see Table 1) is used in conjunction with the root name to indicate the composition (except where well-established names of common species, e.g., grunerite, riebeckite, are involved).

(4) The approach described in 1–3 was applied to the amphiboles by Hawthorne and Oberti (2006), and has since been adopted by the IMA as being broadly applicable (Hatert and Burke 2008).

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[1] The word *trivial* is defined by the International Union of Pure and Applied Chemistry to denote a non-scientific name that does not follow directly from the systematics of composition, and it is used thus in this report.

## AMPHIBOLE CLASSIFICATION BY CHEMICAL FORMULA

The general chemical formula of the minerals of the amphibole supergroup can be written as $A\,B_2\,C_5\,T_8\,O_{22}\,W_2$, where

A = □, Na, K, Ca, Pb, Li;
B = Na, Ca, $Mn^{2+}$, $Fe^{2+}$, Mg, Li;
C = Mg, $Fe^{2+}$, $Mn^{2+}$, Al, $Fe^{3+}$, $Mn^{3+}$, $Cr^{3+}$, $Ti^{4+}$, Li;
T = Si, Al, $Ti^{4+}$, Be;
W = (OH), F, Cl, $O^{2-}$.

In addition, minor elements such as Zn, $Ni^{2+}$, $Co^{2+}$, $V^{3+}$, Sc, and Zr are also observed as C cations. Note that we use non-italicized letters to represent groups of cations in the general formula, thus distinguishing between groups of cations and crystallographic sites (which are denoted by italicized letters). The monoclinic $C2/m$ amphibole structure is illustrated in Appendix I. In minerals as chemically complicated as the amphiboles, particularly where not all constituents are determined (e.g., H, Li, $Fe^{3+}$), there is the significant problem of how to calculate the chemical formula from the chemical composition; this issue has been addressed by Hawthorne (1983) and Schumacher (1991, 1997, 2007), and is also discussed in Appendices II and III.

## SIGNIFICANT ISSUES INVOLVED IN THE CLASSIFICATION OF AMPHIBOLES

### Root names

Compositional variation may involve cations of the same valence [homovalent variation] or cations of different valence [heterovalent variation]. Previous classifications are based on the premise that distinct arrangements of formal charges at the sites (or groups of sites) in the amphibole structure warrant distinct *root names*, and are, by implication, distinct species; for a specific root name, different homovalent cations (e.g., Mg vs. $Fe^{2+}$) or anions (e.g., OH vs. F) are indicated by prefixes. The definition that only distinct arrangements of formal charges for each amphibole group warrant distinct root names implicitly applied only to the A, B, and T cations in IMA1978 and IMA1997, and it explicitly applies only to the A, B, and C cations in the present classification.

**TABLE 1.** Prefixes to be used in naming amphiboles

| Prefix | Meaning (apfu) | Not applicable to |
|---|---|---|
| Chloro | Cl > OH, F | Oxo-amphiboles |
| Chromio | $^C$Cr > $^C$Al, $^C$Fe$^{3+}$, $^C$Mn$^{3+}$ | Amphiboles which do not contain trivalent cations in their root formulae* |
| Ferri † | $^C$Fe$^{3+}$ > $^C$Al, $^C$Cr, $^C$Mn$^{3+}$ | Amphiboles which do not contain trivalent cations in their root formulae*, plus riebeckite, arfvedsonite, hastingsite |
| Ferro | $^C$Fe$^{2+}$ > $^C$Mg, $^C$Mn$^{2+}$ | Any amphibole whose ferro-end-member has a trivial name: tremolite, cummingtonite, grunerite, hastingsite, riebeckite, arfvedsonite, rootname 16 |
| Fluoro | F > OH, Cl | Oxo-amphiboles |
| Magnesio | $^C$Mg > $^C$Fe$^{2+}$, $^C$Mn$^{2+}$ | All amphiboles except riebeckite, arfvedsonite, hastingsite, hornblende |
| Mangano | $^C$Mn$^{2+}$ > $^C$Mg, $^C$Fe$^{2+}$ | |
| Mangani | $^C$Mn$^{3+}$ > $^C$Al, $^C$Cr, $^C$Fe$^{3+}$ | Amphiboles that do not contain trivalent cations in their root formulae* |
| Oxo | $^W$O$^{2-}$ > OH + F + Cl | Oxo-amphiboles where Ti = 1 *apfu* in the root formula‡, plus ungarettiite |
| Potassic | $^A$K > $^A$Na, $^A$Ca, $^A$□ | Amphiboles that do not contain A-site cations in their root formulae§ |
| Zinco | $^C$Zn > $^C$Mg, $^C$Fe$^{2+}$ | |

* Tremolite, actinolite, edenite, richterite, anthophyllite, rootnames 1 and 3, cummingtonite, grunerite.
† Where it is known that Fe$^{3+}$ is involved in dehydrogenation via the oxo-component ($^W$O$^{2-}$), the prefix ferri- is assigned on the basis of [$^C$Fe$^{3+}$ $-$ $^{M(1,3)}$Fe$^{3+}$] if $^{M(1,3)}$Fe$^{3+}$ is known. If the oxo-component is not known, *ferri*- is assigned on the basis of $^C$Fe$^{3+}$.
‡ Obertiite, dellaventuraite, kaersutite.
§ Tremolite, actinolite, magnesio-hornblende, tschermakite, winchite, barroisite, glaucophane, riebeckite, clino-holmquistite, cummingtonite, grunerite, rootname 3, anthophyllite, gedrite, holmquistite.

It would be good to have consistent use of prefixes in amphibole names. Most root names apply to the Mg-Al-dominant species, e.g., tremolite, pargasite, glaucophane. However, (1) some amphiboles were originally described as the ferro- and/or ferri- equivalent of the Mg-Al-containing species, and (2) some amphiboles are presently defined without specifying the dominant trivalent cation [e.g., winchite = $\square$(NaCa) $Mg_4(AlFe^{3+})Si_8O_{22}(OH)_2$]. We could define all root names as referring to the Mg-Al-dominant compositions; thus, for example, leakeite, currently $NaNa_2(Mg_2Fe_2^{3+}Li)Si_8O_{22}(OH)_2$, becomes $NaNa_2(Mg_2Al_2Li)Si_8O_{22}(OH)_2$, and winchite becomes $\square$(NaCa)$(Mg_4Al)Si_8O_{22}(OH)_2$. If this were done, we could dispense with the prefixes *magnesio* and *alumino*. However, such a course of action would result in the loss of some common and petrologically important names (e.g., riebeckite would become "ferro-ferri-glaucophane" and arfvedsonite would become "ferro-ferri-eckermannite", and a riebeckite-arfvedsonite granite would become…). On the other hand, uncommon amphiboles may be redefined without hardship (e.g., alumino-leakeite becomes leakeite, and sodic-kornite becomes mangani-leakeite). Thus except for some common amphiboles of major petrological significance (e.g., riebeckite, arfvedsonite, actinolite, hastingsite), we define all root names as the equivalent Mg-Al-dominant species.

## Prefixes

The topic of prefixes and adjectival modifiers has generated much discussion since IMA1978 formalized their use for amphiboles. First, it must be noted that *the use of prefixes has nothing to do with the number of species*; the number of species is dictated (1) by the details of the classification criteria, and (2) by Nature herself. The issue here is what kind of names are preferable. There are two strategies that we may use: (1) each distinct species is a trivial name; (2) we may identify root names corresponding to distinct charge arrangements, and indicate homovalent variants by prefixes. In the amphibole classifications of IMA1978 and IMA1997, the authors chose the second option and discredited 220 trivial names for amphiboles. Few would wish to return to a situation where there are several hundred trivial names for amphiboles. Here, we use root names plus indicators of homovalent variants.

Prefixes are listed in Table 1; note that we have attempted to make the use of prefixes more homogeneous among the groups and subgroups. Burke and Leake (2004) specified in which order prefixes (where more than one is used) must be attached to the root name. We use a different sequence, which follows the order of the amphibole formula itself: A $B_2$ $C_5$ $T_8$ $O_{22}$ $W_2$; hence, *potassic-ferro-ferri-fluoro-* followed by the root name. The one exception is the prefix *oxo-*, which is put first because this involves the primary division between the two amphibole groups: amphiboles with (OH, F, Cl) dominant at W and amphiboles with $O^{2-}$ dominant at W. The prefix *proto-* is used to denote orthorhombic amphiboles with $a \sim 9.8$ Å and the space group *Pnmn*, and should precede all chemical adjectival modifiers. All prefixes must be followed by a hyphen (thus root names are easily identified in the complete name and can be found by computer search).

## Adjectival modifiers

Although their suggested ranges were specified by adjectival modifiers, these modifiers were *not* part of previous classifications of amphiboles (IMA1978, IMA1997, IMA2003); their use was optional, and they are used to provide more information about an amphibole composition than is present in its formal name. For example, the presence of 0.54 Cl apfu (atoms per formula unit) in an amphibole is obviously of considerable crystal-chemical and petrological interest, but is not represented in the name of the amphibole; in the interest of propagating this information (particularly in this age of databases and keywords), the use of the adjectival modifier is a useful option both for an author and for a reader interested in Cl in amphiboles. However, a recent International Mineralogical Association Commission on New Minerals and Mineral Names (IMA-CNMMN) decision (voting proposal 03A; Bayliss et al. 2005) discredited the use of Schaller modifiers, and recommended using expressions of the type Cl-rich or Cl-bearing preceding the amphibole name (including the valence state of the species where appropriate and where known, e.g., $Fe^{3+}$-rich). Use of such descriptors is at an author's discretion.

## Named amphiboles

The IMA-CNMMN introduced a new category of amphibole: *named amphiboles* (Burke and Leake 2004). These are names that are in accord with the current IMA-approved nomenclature scheme (i.e., involve no new root names) but have not been formally approved as accredited mineral species by the IMA-CNMMN or its successor, International Mineralogical Association Commission on New Minerals Nomenclature and Classification (IMA-CNMNC). The use of these names is thus allowed, but formal description for official recognition is desirable.

## Synthetic amphiboles

There are many recent studies focusing on the synthesis and characterization of amphibole compositions, which are important in understanding such issues as (1) stability, (2) symmetry, (3) thermodynamics, and (4) short-range order. Some of these studies have produced compositions that have not (as yet) been observed in nature, either because the chemical systems in which they occur are enriched in geochemically rare elements or because the synthetic system is chemically simpler than is usual in geological systems. As a result, there is need for a way to name synthetic amphiboles. Bayliss et al. (2005) stated that any synthetic species that is still unknown in Nature should be named with the mineral name followed by a suffix indicating the exotic substitution, and that the whole name must be given within quotation marks, e.g., "topaz-(OH)". In the case of the amphiboles, the situation is more complicated, as new root compositions may occur only in synthesis experiments. Obviously, it is inappropriate to designate a new name for such compositions (until or unless they are discovered as minerals). It seems appropriate to designate such compositions by their chemical formula, possibly preceded by the word *synthetic* to distinguish it from hypothetical compositions (such as end-members) or suggested formulas. Where the natural analogue of the root composition of a synthetic amphibole does exist, the approach of Bayliss et al. (2005) seems appropriate.

However, the use of suffixes is not compatible with the use of prefixes in the current classification, and we recommend the use of chemical symbols denoting the substitution [e.g., Na(NaCa) $Ni_5Si_8O_{22}(OH)_2$ = synthetic Ni-richterite]. Note that the use of element symbols as a prefix to the name is not allowed for minerals (as distinct from synthetic materials).

### Other issues

Issues such as the role of Li, justification for the existence of the sodium-calcium subgroup, and the role of the oxo-component [$^WO$], are discussed at length in Appendix II; recommendations for the calculation of the chemical formula, OH content and $Fe^{3+}$/($Fe^{2+}+Fe^{3+}$) values are given in Appendix III.

### THE PRINCIPAL VARIABLES USED IN THE CLASSIFICATION PROCEDURE

The total variation in amphibole composition can be described by the quinary system A–B–C–T–W. However, authors of previous IMA classifications of amphiboles did not explicitly define the meanings of A, B, C, T, and W. Inspection of the general formula given above shows that each of these symbols represents several compositional variables, and we must be clear which of these variables we use to represent A, B, C, T, and W. The authors of IMA1997 used Si apfu to represent T, but used (Na + K) to represent A and (Ca + Na) to represent B. The latter two examples make it clear that in IMA1997, the *aggregate charges* at A, B, C, T, and W are used as classification variables (as T contains only Si and Al, plus very rarely $Ti^{4+}$, the Si content proxies as the aggregate charge). Here, we follow the same practice, and use aggregate charges as classification parameters. The variation of these parameters is constrained by the electroneutrality principle, and hence only four parameters are needed to formally represent this variation. In IMA1978 and IMA1997, variations in A, B, T, and W are the primary classification parameters. Here, we use variations in A, B, C, and W as our primary classification parameters; the reasons for this are discussed in Appendix IV, and the major differences between this classification and IMA1997 and IMA2003 are outlined in Appendix V. The classification diagrams introduced below involve the A and C cations, and we write the aggregate charges in the following way:

$$A^+ = {}^A(Na + K + 2Ca)$$
$$C^+ = {}^C(Al + Fe^{3+} + 2Ti^{4+})†$$

where the cations are expressed in apfu. Thus the axes of the diagrams involve amounts of cations in apfu and are convenient for plotting amphibole formulas. *Note that in all diagrams, amphibole names are for Na as the dominant monovalent A-cation and Al as the dominant trivalent C-cation. These diagrams provide the root name, and homovalent analogues are named by addition of the appropriate prefixes* (except where trivial names of petrological significance have been retained, e.g., riebeckite, hastingsite, see Appendix VI[2] for details).

### A NEW SCHEME FOR THE CLASSIFICATION OF AMPHIBOLES[3]

First, the amphibole supergroup is divided into two groups according to the dominant W species. This scheme is consistent with the CNMNC guidelines (Mills et al. 2009) for mineral groups. The groups are:

(1) $^W$(OH, F, Cl)-dominant amphiboles;
(2) $^W$O-dominant amphiboles (oxo-amphiboles).

### AMPHIBOLES WITH (OH, F, Cl) DOMINANT AT W

We use the symbols of Kretz (1983) for the amphiboles, and introduce new symbols for amphiboles not included in the original list of symbols. The full list of symbols used here for amphiboles is given as Appendix VII.

Amphiboles with (OH, F, Cl) dominant at W are divided into subgroups according to the dominant charge-arrangements and type of B-group cations. To make the notation simpler, let us write the sum of the small divalent cations at B as $^B\Sigma M^{2+} = {}^BMg + {}^BFe^{2+} + {}^BMn^{2+}$, and the sum of the B cations as $\Sigma B = {}^BLi + {}^BNa + {}^B\Sigma M^{2+} + {}^BCa$ (which generally is equal to 2.00 apfu). End-member (root) compositions may involve monovalent cations (Na, Li), divalent cations (Ca, $\Sigma M^{2+}$), and both monovalent and divalent cations in 1:1 proportion (e.g., Na + Ca, Li + $^B\Sigma M^{2+}$). The necessity for end-member compositions involving cations of different charge at one site is discussed in Appendix IV. There are eight subgroups, the first four of which comprise the most common rock-forming amphiboles:

Magnesium-iron-manganese amphiboles
Calcium amphiboles
Sodium-calcium amphiboles
Sodium amphiboles
Lithium amphiboles
Sodium-(magnesium-iron-manganese) amphiboles
Lithium-(magnesium-iron-manganese) amphiboles
Lithium-calcium amphiboles.

The dominant B constituents may be represented as follows:

Magnesium-iron-manganese $^B\Sigma M^{2+}$
Calcium $^B$(Ca + Na)
Sodium-calcium $^B$(Ca + Na)
Sodium $^B$(Ca + Na)
Lithium $^B$Li
Sodium-(magnesium-iron-manganese) $^BNa + {}^B\Sigma M^{2+}$
Lithium-(magnesium-iron-manganese) $^BLi + {}^B\Sigma M^{2+}$
Lithium-calcium $^BLi + {}^BCa$.

The dominant constituent (or group of constituents) defines the subgroup. For example, $^B$(Ca + Na) defines only the dominance of the calcium, sodium-calcium, and sodium subgroups

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† This expression for C is somewhat simplified here; a more detailed discussion of its definition is given in Appendix IV.

[2] Deposit item AM-12-091, Appendix VI. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at http://www.minsocam.org, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

[3] A program for assigning amphibole names, using the content of the formula as input, is available at http://www_crystal.unipv.it/labcris/AMPH2012.zip.

collectively. Once the dominance of a collective group of constituents is established, which amphibole subgroup occurs is defined by the ratio of the constituents as indicated below for $^B$Ca/$^B$(Ca + Na):

Calcium $^B$Ca/$^B$(Ca + Na) $\geq$ 0.75
Sodium-calcium 0.75 > $^B$Ca/$^B$(Ca + Na) > 0.25
Sodium 0.25 $\geq$ $^B$Ca/$^B$(Ca + Na).

Boundaries at 0.25 and 0.75 apfu separate root compositions at 0.0, 0.5, and 1.0 according to the dominant cation or group of cations.

## The magnesium-iron-manganese amphiboles

Defined by

$$^B(Ca + \Sigma M^{2+})/\Sigma B \geq 0.75, \ ^B\Sigma M^{2+}/\Sigma B > ^BCa/\Sigma B$$

Amphiboles of this subgroup may be orthorhombic (space groups $Pnma$ or $Pnmn$) or monoclinic (space groups $C2/m$ or $P2_1/m$). Although we distinguish between the B and C cations in amphiboles in general, we cannot identify accurately the relative amounts of Mg and Fe$^{2+}$ in the B- and C-cation groups in the magnesium-iron-manganese amphiboles without crystal-structure refinement or Mössbauer spectroscopy. Hence for this subgroup, we treat the divisions between Mg-Fe$^{2+}$ homovalent analogues in terms of the sum of the B and C cations. However, Mn$^{2+}$ has a significant preference for the $M(4)$ site, and hence distinct species are recognized with Mn$^{2+}$ assigned as the dominant B-cation (where direct experimental data are available, they take precedence over such an assignment).

**Orthorhombic magnesium-iron-manganese amphiboles.** The space group $Pnma$ is assumed, and the space group $Pnmn$ (where determined) is indicated by the prefix $proto$. There are four root compositions with Mg dominant at C (Table 2). The composition NaMg$_2$Mg$_5$(Si$_7$Al)O$_{22}$(OH)$_2$ was named sodicanthophyllite in IMA1997. However, this composition has a different charge arrangement from other root compositions for orthorhombic amphiboles and hence warrants a new root name, rootname 1. The composition Na Mg$_2$ (Mg$_3$ Al$_2$) (Si$_5$ Al$_3$) O$_{22}$ (OH)$_2$ is introduced as a new root composition, rootname 2, replacing sodicgedrite, NaMg$_2$(Mg$_4$Al)(Si$_6$Al$_2$)O$_{22}$(OH)$_2$ in IMA1997. There are four homovalent analogues involving Fe$^{2+}$ dominant at (B + C). The compositional ranges of the orthorhombic magnesium-iron-manganese amphiboles are shown in Figure 1.

**Monoclinic magnesium-iron-manganese amphiboles.** The space group $C2/m$ is assumed, the space group $P2_1/m$ (where determined) is indicated by the hyphenated suffix $P2_1/m$. There is one root composition with Mg dominant at (B + C), one analogue involving Fe$^{2+}$ instead of Mg dominant at (B + C), and two additional analogues with Mn$^{2+}$ dominant at (B + C) and at B only. IMA1997 designated the Mn$^{2+}$ analogues by the prefix $mangano$. However, it is not consistent to apply the prefix $mangano$ to the composition □Mn$_2^{2+}$Mg$_5$Si$_8$O$_{22}$(OH)$_2$ as all other prefixes are used to indicate compositions of the A and C cations. Thus the composition □Mn$_2^{2+}$Mg$_5$Si$_8$O$_{22}$(OH)$_2$ warrants a new root name: rootname 3, □Mn$_2^{2+}$Fe$_5^{2+}$Si$_8$O$_{22}$(OH)$_2$ is ferro-rootname 3, and □Mn$_2^{2+}$Mn$_5^{2+}$Si$_8$O$_{22}$(OH)$_2$ is mangano-rootname 3; note that the

**TABLE 2.** End-member compositions in magnesium-iron-manganese amphiboles

| End-member formula | Name |
|---|---|
| **Orthorhombic** | |
| □Mg$_2$Mg$_5$Si$_8$O$_{22}$(OH)$_2$ | Anthophyllite |
| NaMg$_2$Mg$_5$(Si$_7$Al)O$_{22}$(OH)$_2$ | Rootname 1 |
| □Mg$_2$(Mg$_3$Al$_2$)(Si$_6$Al$_2$)O$_{22}$(OH)$_2$ | Gedrite |
| NaMg$_2$(Mg$_3$Al$_2$)(Si$_5$Al$_3$)O$_{22}$(OH)$_2$ | Rootname 2 |
| □Fe$_2^{2+}$Fe$_5^{2+}$Si$_8$O$_{22}$(OH)$_2$ | Ferro-anthophyllite |
| NaFe$_2^{2+}$Fe$_5^{2+}$(Si$_7$Al)O$_{22}$(OH)$_2$ | Ferro-rootname 1 |
| □Fe$_2^{2+}$(Fe$_3^{2+}$Al$_2$)(Si$_6$Al$_2$)O$_{22}$(OH)$_2$ | Ferro-gedrite |
| NaFe$_2^{2+}$(Fe$_3^{2+}$Al$_2$)(Si$_5$Al$_3$)O$_{22}$(OH)$_2$ | Ferro-rootname 2 |
| **Monoclinic** | |
| □Mg$_2$Mg$_5$Si$_8$O$_{22}$(OH)$_2$ | Cummingtonite |
| □Fe$_2^{2+}$Fe$_5^{2+}$Si$_8$O$_{22}$(OH)$_2$ | Grunerite |
| □Mn$_2^{2+}$Mg$_5$Si$_8$O$_{22}$(OH)$_2$ | Rootname 3 |
| □Mn$_2^{2+}$Fe$_5^{2+}$Si$_8$O$_{22}$(OH)$_2$ | Ferro-rootname 3 |
| □Mn$_2^{2+}$Mn$_5^{2+}$Si$_8$O$_{22}$(OH)$_2$ | Mangano-rootname 3 |

prefix $mangano$ is used only where $^C$Mn$^{2+}$ is dominant.

The compositional ranges of the monoclinic magnesium-iron-manganese amphiboles are shown in Figure 2, and end-member compositions are given in Table 2.

## The calcium amphiboles

Defined by

$$^B(Ca + \Sigma M^{2+})/\Sigma B \geq 0.75, \ ^BCa/\Sigma B \geq ^B\Sigma M^{2+}/\Sigma B$$

The eight root compositions are given in Table 3, and six of them are shown in Figure 3. Rootname 4, Na Ca$_2$ (Mg$_4$ Ti) (Si$_5$ Al$_3$) O$_{22}$ (OH)$_2$, is discussed in Appendix IV in the section on amphiboles with Ti >0.50 apfu. Note that the name $hornblende$ is never used without a prefix, as was the case in IMA1997, as hornblende is routinely used as a term when working in the field. Also, kaersutite is no longer considered as an $^W$(OH, F, Cl)-dominant calcium amphibole; it is classified as an $^W$O$^{2-}$-dominant amphibole. Ferrous-iron and ferric-iron analogues are generally named by the prefixes $ferro$- and $ferri$- (Table 1), although some compositions retain their traditional name (e.g., hastingsite, magnesio-hastingsite) because of the petrological
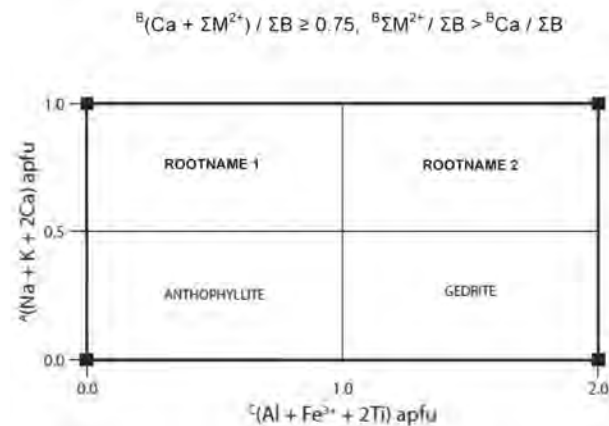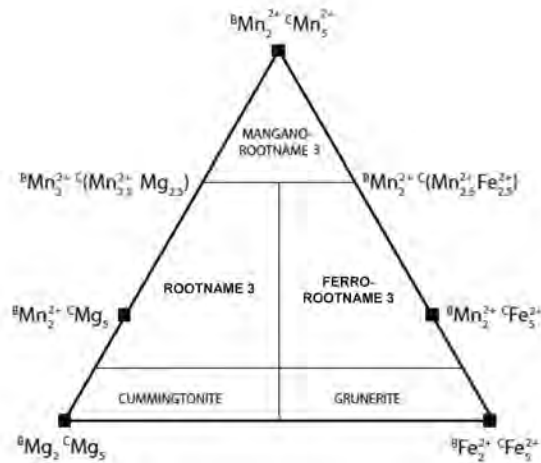


**FIGURE 1.** Orthorhombic magnesium-iron-manganese amphiboles and their compositional boundaries. Filled black squares are the locations of named and unnamed Mg end-members.

importance of these names.

Note that the IMA1997 definition of actinolite is retained for petrological reasons. In the tremolite–ferro-actinolite series, $\square Ca_2Mg_5Si_8O_{22}(OH)_2 - \square Ca_2Fe_5^{2+}Si_8O_{22}(OH)_2$, the compositional range of tremolite extends from $\square Ca_2Mg_5Si_8O_{22}(OH)_2$ to $\square Ca_2Mg_{4.5}Fe_{0.5}^{2+}Si_8O_{22}(OH)_2$, actinolite extends from $\square Ca_2Mg_{<4.5}Fe_{>0.5}^{2+}Si_8O_{22}(OH)_2$ to $\square Ca_2 Mg_{2.5}Fe_{2.5}^{2+}Si_8O_{22}(OH)_2$, and ferro-actinolite extends from $\square Ca_2Mg_{<2.5}Fe_{2.5}^{2+}Si_8 O_{22}(OH)_2$ to $\square Ca_2Fe_5^{2+}Si_8O_{22} (OH)_2$.



**FIGURE 2.** Monoclinic magnesium-iron-manganese amphiboles and their compositional boundaries. Filled black squares are the locations of named and unnamed Mg-$Fe^{2+}$-Mn end-member compositions.

**TABLE 3.** End-member compositions in calcium amphiboles

| End-member formula | Name |
|---|---|
| $\square Ca_2Mg_5Si_8O_{22}(OH)_2$ | Tremolite |
| $\square Ca_2(Mg_4Al)(Si_7Al)O_{22}(OH)_2$ | Magnesio-hornblende |
| $\square Ca_2(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$ | Tschermakite |
| $NaCa_2Mg_5(Si_7Al)O_{22}(OH)_2$ | Edenite |
| $NaCa_2(Mg_4Al)(Si_6Al_2)O_{22}(OH)_2$ | Pargasite |
| $NaCa_2(Mg_3Al_2)(Si_5Al_3)O_{22}(OH)_2$ | Sadanagaite |
| $CaCa_2(Mg_4Al)(Si_5Al_3)O_{22}(OH)_2$ | Cannilloite |
| $NaCa_2(Mg_4Ti)(Si_5Al_3)O_{22}(OH)_2$ | Rootname 4 |
| $Pb^{2+}Ca_2(Mg_3Fe_2^{3+})(Si_6Be_2)O_{22}(OH)_2$ | Joesmithite |
| $\square Ca_2Fe_5^{2+}Si_8O_{22}(OH)_2$ | Ferro-actinolite |
| $\square Ca_2(Fe_4^{2+}Al)(Si_7Al)O_{22}(OH)_2$ | Ferro-hornblende |
| $\square Ca_2(Fe_3^{2+}Al_2)(Si_6Al_2)O_{22}(OH)_2$ | Ferro-tschermakite |
| $NaCa_2Fe_5^{2+}(Si_7Al)O_{22}(OH)_2$ | Ferro-edenite |
| $NaCa_2(Fe_4^{2+}Al)(Si_6Al_2)O_{22}(OH)_2$ | Ferro-pargasite |
| $NaCa_2(Fe_3^{2+}Al_2)(Si_5Al_3)O_{22}(OH)_2$ | Ferro-sadanagaite |
| $CaCa_2(Fe_4^{2+}Al)(Si_5Al_3)O_{22}(OH)_2$ | Ferro-cannilloite |
| $NaCa_2(Fe_4^{2+}Ti)(Si_5Al_3)O_{22}(OH)_2$ | Ferro-rootname 4 |
| $\square Ca_2(Mg_4Fe^{3+})(Si_7Al)O_{22}(OH)_2$ | Magnesio-ferri-hornblende |
| $\square Ca_2(Mg_3Fe_2^{3+})(Si_6Al_2)O_{22}(OH)_2$ | Ferri-tschermakite |
| $NaCa_2(Mg_4Fe^{3+})(Si_6Al_2)O_{22}(OH)_2$ | Magnesio-hastingsite |
| $NaCa_2(Mg_3Fe_2^{3+})(Si_5Al_3)O_{22}(OH)_2$ | Ferri-sadanagaite |
| $CaCa_2(Mg_4Fe^{3+})(Si_5Al_3)O_{22}(OH)_2$ | Ferri-cannilloite |
| $\square Ca_2(Fe_4^{2+}Fe^{3+})(Si_7Al)O_{22}(OH)_2$ | Ferro-ferri-hornblende |
| $\square Ca_2(Fe_3^{2+}Fe_2^{3+})(Si_6Al_2)O_{22}(OH)_2$ | Ferro-ferri-tschermakite |
| $NaCa_2(Fe_4^{2+}Fe^{3+})(Si_6Al_2)O_{22}(OH)_2$ | Hastingsite |
| $NaCa_2(Fe_3^{2+}Fe_2^{3+})(Si_5Al_3)O_{22}(OH)_2$ | Ferro-ferri-sadanagaite |
| $CaCa_2(Fe_4^{2+}Fe^{3+})(Si_5Al_3)O_{22}(OH)_2$ | Ferro-ferri-cannilloite |

Joesmithite is an amphibole of unusual composition, ideally $Pb^{2+}Ca_2(Mg_3Fe_2^{3+})(Si_6 Be_2)O_{22}(OH)_2$, and space group $P2/a$ (Moore et al. 1993). It is a calcium amphibole but, because of the presence of Be as a T-group cation, it does not fit the compositional diagrams used here for calcium-amphibole classification; however, it is included in Table 3. It has been found only at one locality (Långban, Värmland, Sweden), and there is no information as to the extent of any solid solution.

Cannilloite, ideally $CaCa_2(Mg_4Al)(Si_5Al_3)O_{22}(OH)_2$ (Hawthorne et al. 1996), is also an unusual composition with Ca as the A cation and hence with 3 Al apfu as T cations. It does not fit the compositional diagrams used here for amphibole classification; however, it is included in Table 3. Its fluoro- counterpart has been found only at one locality (Pargas, Finland).

**The sodium-calcium amphiboles**

Defined by

$$0.75 > {}^B(Ca + \Sigma M^{2+})/\Sigma B > 0.25, \quad {}^BCa/\Sigma B \geq {}^B\Sigma M^{2+}/\Sigma B$$

and

$$0.75 > {}^B(Na + Li)/\Sigma B > 0.25, \quad {}^BNa/\Sigma B \geq {}^BLi/\Sigma B.$$

There are five root compositions with Mg and Al dominant at C, together with their ferrous-iron, ferric-iron, and ferrous-ferric-iron analogues (Table 4). The compositional ranges of the root sodium-calcium amphiboles are shown in Figure 4.

**The sodium amphiboles**

Defined by

$${}^B(Na + Li)/\Sigma B \geq 0.75, \quad {}^BNa/\Sigma B \geq {}^BLi/\Sigma B.$$

Three root compositions are shown in Figure 5, and all end-member compositions are listed in Table 5. Leakeite, ideally,
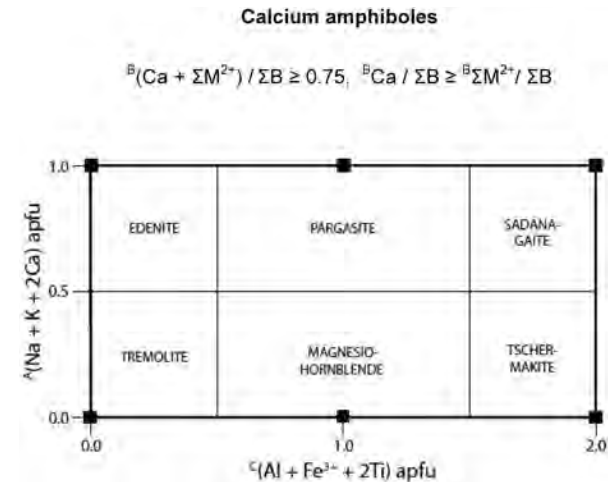


**FIGURE 3.** Calcium amphiboles and their compositional boundaries. The heavy solid black line is a two-dimensional section of amphibole compositional space (see Appendix Fig. 3) at ${}^BCa/{}^B(Ca + Na) = 1.0$ that contains the calcium end-member compositions.

$NaNa_2(Mg_2Al_2Li)Si_8O_{22}(OH)_2$, occupies the same compositional space as eckermanite, ideally $NaNa_2(Mg_4Al)Si_8O_{22}(OH)_2$, in the compositional diagrams used here for amphibole classification [after subtracting from $^C(Al,Fe)^{3+}$ the same amount as $^CLi$; cf. Appendix IV for more detail]. Riebeckite and arfvedsonite retain their traditional names because of their petrological importance.

### The lithium amphiboles

Defined by

$$^B(Na + Li)/\Sigma B \geq 0.75, \quad ^BLi/\Sigma B > ^BNa/\Sigma B$$

Amphiboles of this subgroup may be orthorhombic (space group $Pnma$) or monoclinic (space group $C2/m$).

**Orthorhombic lithium amphiboles.** There is one root composition plus its ferro-, ferri-, and ferro-ferri- analogues (Table 6).

**Monoclinic lithium amphiboles.** There are two root compositions plus their ferro-, ferri- and ferro-ferri- analogues (Table 6, Fig. 6). Note that "clinoholmquistite" has recently been discredited (Oberti et al. 2005); also, current knowledge and comparison with cummingtonite suggest that compositions close to that of the end-member clinoholmquistite formula (if stable) should have the space group $P2_1/m$. The composition $NaLi_2(Mg_4Al)Si_8O_{22}(OH)_2$ has not yet been described as a mineral; it is a root composition and warrants a new rootname: rootname 5.

### The sodium-(magnesium-iron-manganese) amphiboles

Defined by

$$0.75 > {}^B(Ca + \Sigma M^{2+})/\Sigma B > 0.25, \quad ^B\Sigma M^{2+}/\Sigma B > ^BCa/\Sigma B$$

and

$$0.75 > {}^B(Na + Li)/\Sigma B > 0.25, \quad ^BNa/\Sigma B \geq ^BLi/\Sigma B.$$

**TABLE 4.** End-member compositions in sodium-calcium amphiboles

| End-member formula | Name |
|---|---|
| $\square(NaCa)(Mg_4Al)Si_8O_{22}(OH)_2$ | Winchite |
| $\square(NaCa)(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$ | Barroisite |
| $Na(NaCa)Mg_5Si_8O_{22}(OH)_2$ | Richterite |
| $Na(NaCa)(Mg_4Al)(Si_7Al)O_{22}(OH)_2$ | Katophorite |
| $Na(NaCa)(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$ | Taramite |
| $\square(NaCa)(Fe_4^{2+}Al)Si_8O_{22}(OH)_2$ | Ferro-winchite |
| $\square(NaCa)(Fe_3^{2+}Al_2)(Si_7Al)O_{22}(OH)_2$ | Ferro-barroisite |
| $Na(NaCa)Fe_5^{2+}Si_8O_{22}(OH)_2$ | Ferro-richterite |
| $Na(NaCa)(Fe_4^{2+}Al)(Si_7Al)O_{22}(OH)_2$ | Ferro-katophorite |
| $Na(NaCa)(Fe_3^{2+}Al_2)(Si_6Al_2)O_{22}(OH)_2$ | Ferro-taramite |
| $\square(NaCa)(Mg_4Fe^{3+})Si_8O_{22}(OH)_2$ | Ferri-winchite |
| $\square(NaCa)(Mg_3Fe_2^{3+})(Si_7Al)O_{22}(OH)_2$ | Ferri-barroisite |
| $Na(NaCa)(Mg_4Fe^{3+})(Si_7Al)O_{22}(OH)_2$ | Ferri-katophorite |
| $Na(NaCa)(Mg_3Fe_2^{3+})(Si_6Al_2)O_{22}(OH)_2$ | Ferri-taramite |
| $\square(NaCa)(Fe_4^{2+}Fe^{3+})Si_8O_{22}(OH)_2$ | Ferro-ferri-winchite |
| $\square(NaCa)(Fe_3^{2+}Fe_2^{3+})(Si_7Al)O_{22}(OH)_2$ | Ferro-ferri-barroisite |
| $Na(NaCa)(Fe_4^{2+}Fe^{3+})(Si_7Al)O_{22}(OH)_2$ | Ferro-ferri-katophorite |
| $Na(NaCa)(Fe_3^{2+}Fe_2^{3+})(Si_6Al_2)O_{22}(OH)_2$ | Ferro-ferri-taramite |

**TABLE 5.** End-member compositions in sodium amphiboles

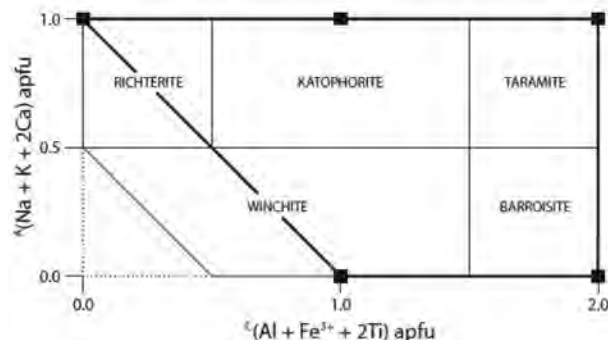| End-member formula | Name |
|---|---|
| $\square Na_2(Mg_3Al_2)Si_8O_{22}(OH)_2$ | Glaucophane |
| $NaNa_2(Mg_4Al)Si_8O_{22}(OH)_2$ | Eckermannite |
| $NaNa_2(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$ | Nybøite |
| $NaNa_2(Mg_2Al_2Li)Si_8O_{22}(OH)_2$ | Leakeite |
| $\square Na_2(Fe_3^{2+}Al_2)Si_8O_{22}(OH)_2$ | Ferro-glaucophane |
| $NaNa_2(Fe_4^{2+}Al)Si_8O_{22}(OH)_2$ | Ferro-eckermannite |
| $NaNa_2(Fe_3^{2+}Al_2)(Si_7Al)O_{22}(OH)_2$ | Ferro-nybøite |
| $NaNa_2(Fe_2^{2+}Al_2Li)Si_8O_{22}(OH)_2$ | Ferro-leakeite |
| $\square Na_2(Mg_3Fe_2^{3+})Si_8O_{22}(OH)_2$ | Magnesio-riebeckite |
| $NaNa_2(Mg_4Fe^{3+})Si_8O_{22}(OH)_2$ | Magnesio-arfvedsonite |
| $NaNa_2(Mg_3Fe_2^{3+})(Si_7Al)O_{22}(OH)_2$ | Ferri-nybøite |
| $NaNa_2(Mg_2Fe_2^{3+}Li)Si_8O_{22}(OH)_2$ | Ferri-leakeite |
| $\square Na_2(Fe_3^{2+}Fe_2^{3+})Si_8O_{22}(OH)_2$ | Riebeckite |
| $NaNa_2(Fe_4^{2+}Fe^{3+})Si_8O_{22}(OH)_2$ | Arfvedsonite |
| $NaNa_2(Fe_3^{2+}Fe_2^{3+})(Si_7Al)O_{22}(OH)_2$ | Ferro-ferri-nybøite |
| $NaNa_2(Fe_2^{2+}Fe_2^{3+}Li)Si_8O_{22}(OH)_2$ | Ferro-ferri-leakeite |



**FIGURE 4.** Sodium-calcium amphiboles and their compositional boundaries. The heavy solid black line is a two-dimensional section of amphibole composition space (see Appendix Fig. 3) at $^BCa/^B(Ca + Na)$ = 0.5 that contains the sodium-calcium end-member compositions. The thick solid lines show the possible range of amphibole compositions at $^BCa/^B(Ca + Na)$ = 0.5 and the solid lines to the left of the diagonal heavy solid black line show the possible range of amphibole compositions at $^BCa/^B(Ca + Na)$ = 0.75, the boundary between the sodium-calcium amphiboles and the calcium amphiboles.
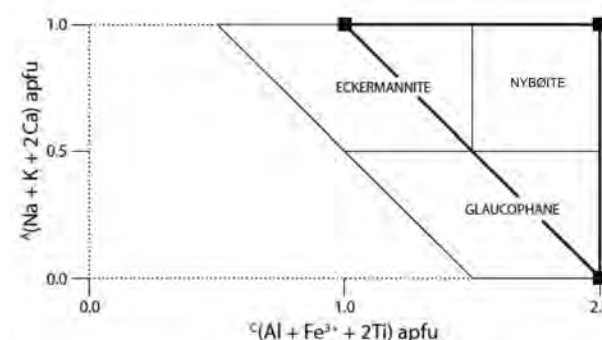


**FIGURE 5.** Sodium amphiboles and their compositional boundaries. The heavy solid black line is a two-dimensional section of amphibole compositional space (Appendix Fig. 3) at $^BCa/^B(Ca + Na)$ = 0.0 that contains sodium end-member compositions. The thick solid lines show the possible range of amphibole compositions at $^BCa/^B(Ca + Na)$ = 0.0 and the solid lines to the left of the diagonal heavy solid black line show the possible range of amphibole compositions at $^BCa/^B(Ca + Na)$ = 0.25, the boundary between the sodium amphiboles and the sodium-calcium amphiboles.

**TABLE 6.** End-member compositions in lithium amphiboles

| End-member formula | Name |
|---|---|
| **Orthorhombic** | |
| $\square Li_2(Mg_3Al_2)Si_8O_{22}(OH)_2$ | Holmquistite |
| $\square Li_2(Fe_3^{2+}Al_2)Si_8O_{22}(OH)_2$ | Ferro-holmquistite |
| $\square Li_2(Mg_3Fe_2^{3+})Si_8O_{22}(OH)_2$ | Ferri-holmquistite |
| $\square Li_2(Fe_3^{2+}Fe_2^{3+})Si_8O_{22}(OH)_2$ | Ferro-ferri-holmquistite |
| **Monoclinic** | |
| $\square Li_2(Mg_3Al_2)Si_8O_{22}(OH)_2$ | Clino-holmquistite |
| $NaLi_2(Mg_2Al_2Li)Si_8O_{22}(OH)_2$ | Pedrizite |
| $NaLi_2(Mg_4Al)Si_8O_{22}(OH)_2$ | Rootname 5 |
| $\square Li_2(Fe_3^{2+}Al_2)Si_8O_{22}(OH)_2$ | Clino-ferro-holmquistite |
| $NaLi_2(Fe_2^{2+}Al_2Li)Si_8O_{22}(OH)_2$ | Ferro-pedrizite |
| $\square Li_2(Mg_3Fe_2^{3+})Si_8O_{22}(OH)_2$ | Clino-ferri-holmquistite |
| $NaLi_2(Mg_2Fe_2^{3+}Li)Si_8O_{22}(OH)_2$ | Ferri-pedrizite |
| $\square Li_2(Fe_3^{2+}Fe_2^{3+})Si_8O_{22}(OH)_2$ | Clino-ferro-ferri-holmquistite |
| $NaLi_2(Fe_2^{2+}Fe_2^{3+}Li)Si_8O_{22}(OH)_2$ | Ferro-ferri-pedrizite |

**TABLE 7.** End-member compositions in the sodium-(magnesium-iron-manganese) amphiboles

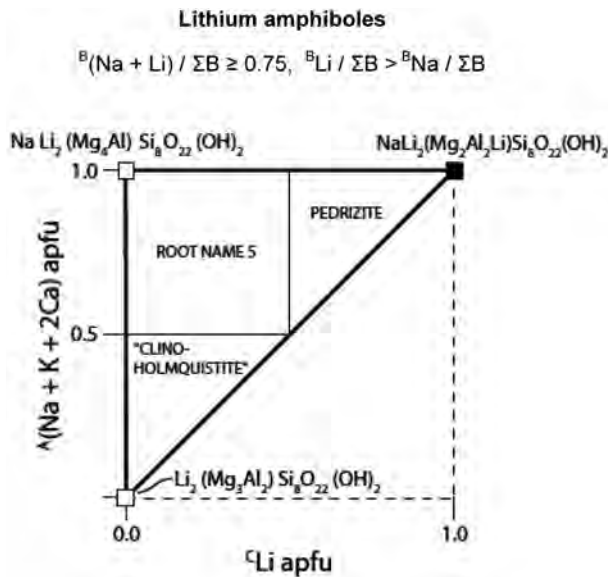| End-member formula | Name |
|---|---|
| $\square(NaMg)(Mg_4Al)Si_8O_{22}(OH)_2$ | Rootname 6 |
| $\square(NaMg)(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$ | Rootname 7 |
| $Na(NaMg)Mg_5Si_8O_{22}(OH)_2$ | Rootname 8 |
| $Na(NaMg)(Mg_4Al)(Si_7Al)O_{22}(OH)_2$ | Rootname 9 |
| $Na(NaMg)(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$ | Rootname 10 |
| $\square(NaMn^{2+})(Mg_4Al)Si_8O_{22}(OH)_2$ | Rootname 11 |
| $\square(NaMn^{2+})(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$ | Rootname 12 |
| $Na(NaMn^{2+})Mg_5Si_8O_{22}(OH)_2$ | Rootname 13 |
| $Na(NaMn^{2+})(Mg_4Al)(Si_7Al)O_{22}(OH)_2$ | Rootname 14 |
| $Na(NaMn^{2+})(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$ | Rootname 15 |
| $\square(NaFe^{2+})(Fe_4^{2+}Al)Si_8O_{22}(OH)_2$ | Rootname 16 |



**FIGURE 6.** Monoclinic lithium amphiboles and their compositional boundaries. The filled black square is the location of a named end-member composition, white squares are as-yet un-named end-member compositions, and the solid black lines show the ranges of possible amphibole compositions. Note that "clino-holmquistite" is currently not an accredited species.
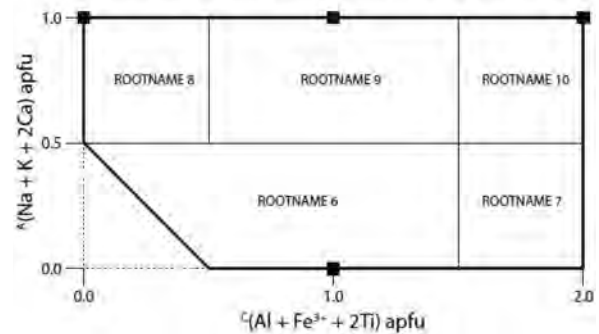


**FIGURE 7.** Sodium-(magnesium-iron-manganese) amphiboles and their compositional boundaries. Filled black squares are the locations of presently unnamed end-member compositions. The thick solid line refers to end-member compositions at $^BNa/^B(Na + \Sigma M^{2+}) = 0.5$. The solid lines to the left of the diagonal thick solid line show the possible range of amphibole compositions at $^BNa/^B(Na + \Sigma M^{2+}) = 0.25$, the boundary between the sodium-(magnesium-iron-manganese) amphiboles and the magnesium-iron-manganese amphiboles.

These amphiboles are the (Mg-Fe-Mn) analogues of the sodium-calcium amphiboles, where Ca is replaced by (Mg, Fe, Mn). The root compositions and compositional ranges are given in Table 7. Where possible, we recognize the dominant divalent B-cation: Mg, $Fe^{2+}$, or $Mn^{2+}$. The $^B(Na\ Mg)$ root compositions (Table 7) are labeled rootnames 6–10 and are shown in Figure 7; note that rootname 8 is the $^BMg$ analogue of richterite (Table 4); note that its synthetic analogue has $P2_1/m$ symmetry (Cámara et al. 2003). $^BMn$ analogues of the $^BMg$ root compositions may be recognized from electron-microprobe data as $Mn^{2+}$ orders very strongly at $M(4)$ (where the B cations reside) relative to Mg or $Fe^{2+}$. Note that this requires another set of root names as the prefix *mangano-* refers to the $^CMn$ analogue of a $^CMg$ root composition (rootnames 11–15, Table 7). However, we cannot recognize $^BFe^{2+}$ analogues of $^BMg$ root compositions from a chemical analysis as we are unable to assign $Fe^{2+}$ as a B or C cation; crystal-structure refinement or Mössbauer spectroscopy

is necessary. Should $^B(Na\ Fe^{2+})$ compositions be detected, they would deserve new rootnames. Moreover, intermediate compositions can be named only using crystal-structure refinement or Mössbauer spectroscopy. The one exception is the root composition $\square(NaFe^{2+})(Fe_4^{2+}Al)Si_8O_{22}(OH)_2$ as $Fe^{2+}$ is the only divalent B- and C-cation present (rootname 16, Table 7).

At the moment, there is only one known amphibole in this group, and that is close to the root composition, $\square(NaMn^{2+})$ $(Mg_4Fe^{3+})Si_8O_{22}(OH)_2$ (Oberti and Ghose 1993). A new name for this amphibole must be assigned via submission to IMA: rootname 11. The analogues with $Fe^{2+}$ at C will be named by the prefix *ferro-*, and the sample of Oberti and Ghose (1993) with $Fe^{3+}$ dominant at C should be named with the prefix *ferri-*.

### The lithium-(magnesium-iron-manganese) amphiboles

Defined by

$$0.75 > \ ^B(Ca + \Sigma M^{2+})/\Sigma B > 0.25, \ ^B\Sigma M^{2+}/\Sigma B > \ ^BCa/\Sigma B$$

and

$$0.75 > \ ^B(Na + Li)/\Sigma B > 0.25, \ ^BLi/\Sigma B > \ ^BNa/\Sigma B.$$

These amphiboles are the lithium analogues of the sodium-(magnesium-iron-manganese) amphiboles, where Na is replaced by Li. The root compositions and compositional ranges are given in Table 8 and Figure 8. As these amphiboles are only known as synthetic phases (Iezzi et al. 2006), only the $^B$(Li Mg) root compositions are listed and are labeled rootnames 17–21; note that rootname 19 is the $^B$(Li Mg) analogue of richterite (Table 4).

### The lithium-calcium amphiboles

Defined by

$$0.75 > {}^B(Ca + \Sigma M^{2+})/\Sigma B > 0.25, \, {}^BCa/\Sigma B \geq {}^B\Sigma M^{2+}/\Sigma B$$

and

$$0.75 > {}^B(Na + Li)/\Sigma B > 0.25, \, {}^BLi/\Sigma B > {}^BNa/\Sigma B.$$

These amphiboles are the lithium analogues of the sodium-calcium amphiboles, where Na is replaced by Li. The root compositions and compositional ranges are given in Table 9 and Figure 9. The $^B$(Li Ca) root compositions (Table 9) are labeled rootnames 22–26; note that rootname 24 is the $^B$(Li Ca) analogue of richterite (Table 4).

## AMPHIBOLES WITH $O^{2-}$ DOMINANT AT W

Dominance of W by $O^{2-}$ is accompanied by the occurrence of additional high-charge ($\geq 3^+$) C-cations ordered at the $M(1)$ and/or $M(3)$ sites; the aggregate charge at C may thus exceed $12^+$. There are four distinct root-compositions currently known for calcium and sodium amphiboles (Table 10), and $Fe^{2+}$ and $Fe^{3+}$ analogues can be indicated by the prefixes *ferro-* and *ferri-*.

Three of these amphiboles (root names obertiite, ungarettiite, and dellaventuraite) are rare, and analysis for H to characterize these species should not be regarded as unduly onerous. However, this is not the case for kaersutite, which is a reasonably common and petrologically important amphibole. Thus a different criterion would be convenient for the classification of kaersutite; this can be done on the basis of the Ti content. Although Ti is not completely related to the oxo component in amphibole, it is a useful indicator. Consequently, we use Ti content as a proxy for the oxo component in pargasite, and define kaersutite as having $^CTi > 0.50$ apfu ($\approx O^{2-} > 1.00$ apfu). However, if the $O^{2-}$ content is known from chemical or crystal-chemical analysis, it takes precedence over use of the Ti content as a proxy (see Appendix II).

**TABLE 8.** End-member compositions in the lithium-(magnesium-iron-manganese) amphiboles

| End-member formula | Name |
|---|---|
| $\square$(LiMg)(Mg$_4$Al)Si$_8$O$_{22}$(OH)$_2$ | Rootname 17 |
| $\square$(LiMg)(Mg$_3$Al$_2$)(Si$_7$Al)O$_{22}$(OH)$_2$ | Rootname 18 |
| Na(LiMg)Mg$_5$Si$_8$O$_{22}$(OH)$_2$ | Rootname 19 |
| Na(LiMg)(Mg$_4$Al)(Si$_7$Al)O$_{22}$(OH)$_2$ | Rootname 20 |
| Na(LiMg)(Mg$_3$Al$_2$)(Si$_6$Al$_2$)O$_{22}$(OH)$_2$ | Rootname 21 |

**TABLE 9.** End-member compositions in the lithium-calcium amphiboles

| End-member formula | Name |
|---|---|
| $\square$(LiCa)(Mg$_4$Al)Si$_8$O$_{22}$(OH)$_2$ | Rootname 22 |
| $\square$(LiCa)(Mg$_3$Al$_2$)(Si$_7$Al)O$_{22}$(OH)$_2$ | Rootname 23 |
| Na(LiCa)Mg$_5$Si$_8$O$_{22}$(OH)$_2$ | Rootname 24 |
| Na(LiCa)(Mg$_4$Al)(Si$_7$Al)O$_{22}$(OH)$_2$ | Rootname 25 |
| Na(LiCa)(Mg$_3$Al$_2$)(Si$_6$Al$_2$)O$_{22}$(OH)$_2$ | Rootname 26 |

Amphiboles with $O^{2-}$ dominant at W are commonly characterized by Ti as the dominant high-charge C-cation. However, $Fe^{3+}$ may also be the principal high-charge C-cation related to the presence of $^WO^{2-}$, and we need to recognize such amphiboles. In oxo-amphiboles, $Fe^{3+}$ balancing $^WO^{2-}$ is ordered at the $M(1)$ [and less commonly at the $M(3)$] site, so that the sum of high-charge cations does exceed 2.0 apfu and may reach 4.0 apfu. The
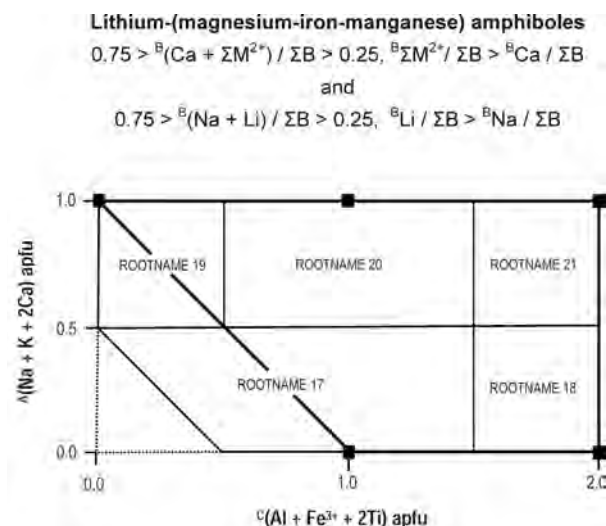


**FIGURE 8.** Lithium-(magnesium-iron-manganese) amphiboles and their compositional boundaries. Filled black squares are the locations of presently unnamed end-member compositions. The thick solid line refers to end-member compositions at $^BLi/^B(Li + \Sigma M^{2+}) = 0.5$. The solid lines to the left of the diagonal thick solid line show the possible range of amphibole compositions at $^BLi/^B(Li + \Sigma M^{2+}) = 0.75$, the boundary between the lithium-(magnesium-iron-manganese) amphiboles and the magnesium-iron-manganese amphiboles.
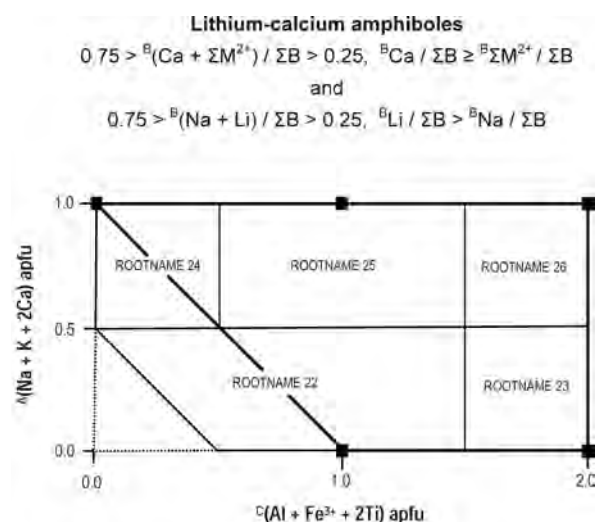


**FIGURE 9.** Lithium-calcium amphiboles and their compositional boundaries. Filled black squares are the locations of presently unnamed end-member compositions. The thick solid line refers to end-member compositions at $^BLi/^B(Li + Ca) = 0.5$. The solid lines to the left of the diagonal thick solid line show the possible range of amphibole compositions at $^BLi/^B(Li + Ca) = 0.75$, the boundary between the lithium-calcium amphiboles and the calcium amphiboles

**TABLE 10.** End-member compositions in oxo amphiboles

| End-member formula | Name |
|---|---|
| $NaNa_2(Mg_3Fe^{3+}Ti^{4+})Si_8O_{22}O_2$ | Ferri-obertiite |
| $NaNa_2(MgMn_3^{2+}Ti^{4+}Li)Si_8O_{22}O_2$ | Mangani-dellaventuraite |
| $NaNa_2(Mn_3^{2+}Mn_3^{3+})Si_8O_{22}O_2$ | Mangano-mangani-ungarettiite |
| $NaCa_2(Mg_3Ti^{4+}Al)(Si_6Al_2)O_{22}O_2$ | Kaersutite |
| $NaCa_2(Fe_3^{2+}Ti^{4+}Al)(Si_6Al_2)O_{22}O_2$ | Ferro-kaersutite |
| $NaCa_2(Fe_3^{2+}Ti^{4+}Fe^{3+})(Si_6Al_2)O_{22}O_2$ | Ferro-ferri-kaersutite |
| $NaCa_2(Mg_3Ti^{4+}Fe^{3+})(Si_6Al_2)O_{22}O_2$ | Ferri-kaersutite |

site preference of the C cations is not relevant for classification purposes. However, the prefix *ferri-* cannot be used to deal with $Fe^{3+}$ related to the presence of $^WO^{2-}$. This is done by using the prefix *oxo-* with the appropriate rootname, e.g., $Na(NaCa)(Fe_3^{2+}Fe_2^{3+})Si_8O_{22}O_2$: oxo-ferro-richterite; $\Box Ca_2(Mg_2Fe_3^{3+})(Si_7Al)O_{22}O_2$: oxo-magnesio-ferri-hornblende; $Na(NaCa)(Mg_2Fe_2^{3+}Al)(Si_7Al)O_{22}O_2$: oxo-katophorite; $NaNa_2(Fe^{2+}Fe_2^{3+}Al)(Si_7Al)O_{22}O_2$: oxo-ferro-nybøite.

## Coda

The amphiboles are chemically and structurally complicated, petrologically important, and they are the subject of extensive ongoing scientific attention. The classification and nomenclature of the amphiboles are obviously influenced considerably by this work: as we discover more about them, there is a need to incorporate this knowledge into their classification and nomenclature. Of particular importance in this respect is the extensive amphibole synthesis that has been done in the past 10–15 yr. This work has indicated major new chemical fields in which the amphibole structure is stable. Although from the point of view of the formal definition of a mineral, such synthetic compounds are not minerals, it is our view that the classification of the amphiboles should be able to incorporate such information, as it will deepen our understanding of this group. Thus we have expanded the number of subgroups from four (IMA1997) to eight. Minerals from one of the new subgroups, the lithium amphiboles, have since been found to be reasonably common rock-forming minerals (e.g., Oberti et al. 2000, 2003, 2004, 2006; Caballero et al. 2002), and synthesis work (e.g., Iezzi et al. 2004, 2005a, 2005b, 2006; Maresch et al. 2009) has resulted in new compositions (Oberti et al. 2007). There have been several amphibole classifications produced in the last 50 yr, and the introduction of these new schemes has caused some irritation in the mineralogical and petrological communities. Here, we have tried to minimize such problems by introducing a scheme that can accommodate future compositional and structural discoveries in the amphiboles.

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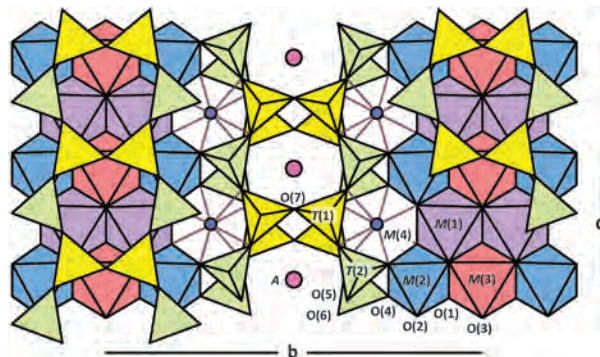
## APPENDIX I: THE *C*2/*m* AMPHIBOLE STRUCTURE

A schematic representation of the $C2/m$ structure type is shown in Appendix Figure 1 (below). There are two distinct $T$ sites that are occupied by the T cations, $T(1)$ and $T(2)$, that are tetrahedrally coordinated and link to form one distinct type of double chain of tetrahedra. The $T(1)$ and $T(2)$ tetrahedra alternate along the length of the double chain, and the $T(1)$ tetrahedra bridge across the double chain. There are three distinct octahedrally coordinated $M$ sites that are occupied by the C cations. The $M(1)$ site is coordinated by two O(1) and two O(2) O-atoms, and by two O(3) W anions (OH, F, Cl, O) in a *cis* arrangement,

and the $M(3)$ site is coordinated by four O(1) oxygen atoms and two O(3) W anions in a *trans* arrangement. The double chain of tetrahedra links to the strip of octahedra in the **b** direction through $T(2)$–$M(2)$ linkage via common O(4) O-atoms, and in the **a** direction through $T(1)$ and $T(2)$ linkage to the strip via common O(1) and O(2) O-atoms. The $M(4)$ site is situated at the periphery of the strip of octahedra and is occupied by B cations. Note that the cation occupancy of this site (1) is the primary feature on which the major subgroups of amphiboles are classified, and (2) correlates strongly with the space-group variations in amphiboles. The $A$ site occurs at the center of a large cavity between the back-to-back double-chains of the structure. The center of the cavity has point symmetry 2/$m$, but the A cations actually occupy off-centered sites of point symmetry 2 or $m$, $A(2)$, and $A(m)$, respectively.

## APPENDIX II: THE ROLE OF FE, H, AND LI

Prior to the development of the electron microprobe, all major and minor constituents in amphiboles were analyzed as a matter of course, and compilations such as that of Leake (1968) are invaluable sources of complete results of chemical analysis. The advent of the electron microprobe completely changed the situation with regard to mineral analysis. It became relatively easy to make numerous chemical analyses at a very fine scale, making available chemical data on finely zoned materials. However, this step forward came at a cost: the concentration of some elements (e.g., H, Li) cannot be so established, and valence state is not accessible. For many minerals, these limitations are not relevant; for amphiboles, they are major disadvantages. Recent work has shown that (1) Li is a much more common constituent in amphiboles than had hitherto been realized (Hawthorne et al. 1994; Oberti et al. 2003), and (2) H, as (OH), can be a variable component in amphiboles unassociated with the process of oxidation-dehydrogenation (Hawthorne et al. 1998). Moreover, the role of Fe in amphiboles is very strongly a function of its valence state and site occupancy. Lack of knowledge of these constituents results in formulas that generally must be regarded as only semiquantitative. Of course, if Li and $Fe^{3+}$ are not present and (OH + F) = 2 apfu, the resulting formula can be accurate. However, such a situation is uncommon [few amphiboles have Li = $Fe^{3+}$ = 0 and (OH + F) = 2 apfu], resulting in formulas with significant systematic error.

All previous classifications have obscured this issue by not



**APPENDIX FIGURE 1.** The crystal structure of a monoclinic $C2/m$ amphibole projected onto (100). (Color online.)

incorporating C cations into the classification procedure, and thus the problem is not visually apparent in the classification diagrams. However, the problem is still present in that the formulas are still inaccurate, and the lack of H, Li, and $Fe^{3+}$ seriously distorts the amounts of other constituents, particularly those that are distributed over two different groups of sites (e.g., $^TAl$ and $^CAl$, $^BNa$, and $^ANa$). There are methods available to determine these components, and amphibole analysts should be acquiring or using these on a routine basis. For "small-laboratory" instrumentation, secondary-ion mass spectrometry (SIMS) can microbeam-analyze amphiboles for H and Li (using the appropriate methodology and standards); laser-ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) can microbeam-analyze amphiboles for Li; single-crystal-structure refinement (SREF) can characterize the levels of Li, $Fe^{2+}$ and $Fe^{3+}$ at a scale of $\geq 30$ μm, and with structure-based equations, one can estimate the amount of $^WO^{2-}$; electron energy-loss spectroscopy (EELS) can measure $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ at a scale of $\geq 1$ μm; electron microprobe (the Flank method, Höfer et al. 1994; the peak-shift method, Fialin et al. 2004) can measure $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ at a scale of $\geq 1$ μm where $FeO_{tot} > \sim6–8$ wt% with reasonable accuracy in amphiboles (Enders et al. 2000; Lamb et al. 2012); milli-Mössbauer spectroscopy can measure $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ at a scale of $\geq 50$ μm. For "big-laboratory" instrumentation, usually involving a synchrotron light-source, single-crystal refinement of the structure can characterize Li, $Fe^{2+}$ and $Fe^{3+}$ at a scale of $\geq 2$ μm, and milli-X-ray photoelectron spectroscopy (XPS) can measure $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ at a scale of $\geq 40$ μm. Where only small amounts of separate are available (a few milligrams), hydrogen-line extraction and Karl-Fischer titration can give accurate values for H (as $H_2O$) content. Values for $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ can also be calculated using assumed site-occupancy limitations and the electroneutrality principle (Appendix III), and although the values obtained are not very accurate (Hawthorne 1983), they are in general better than assuming $Fe^{3+}/(Fe^{2+} + Fe^{3+}) = 0.0$ (Schumacher 1991, 1997). Values for $^WO^{2-}$ can be calculated also using $Ti^{4+}$ as a proxy (Appendix III), although it is probable that the proxy relation does not always hold. As noted in the main text, if the $^WO^{2-}$ content is known from chemical or crystal-chemical analysis, it replaces use of the Ti content as a proxy. To give an example, analyses done by EMP, SIMS, SREF, and Mössbauer spectroscopy on a sample from Kaersut, Greenland (rather ironically, the type locality of kaersutite) gave $^CTi$ 0.62–0.69 and $^WO^{2-}$ 0.88–0.95 apfu with half of the Ti ordered at $M(2)$ (Oberti et al., in prep). In terms of attributing a name, the $^WO^{2-}$ content dominates over the Ti content, and this is an (OH, F, Cl)-dominant amphibole, despite the fact that Ti >0.50 apfu.

Hydrogen in excess of 2 apfu was long suspected in amphiboles, but was never considered as confirmed because of the difficulty in obtaining reliable and accurate analytical data for H in solids. Maresch et al. (2009) reviewed the synthesis and spectroscopic evidence for H > 2 apfu in synthetic amphibole in the system $Na_2O–MgO–SiO_2–H_2O$, and Cámara et al. (2004) solved the structure of a triclinic synthetic amphibole of composition $Na_3Mg_5Si_8O_{21}(OH)_3$. Thus the evidence is now incontrovertible that H > 2 apfu can occur in amphiboles. However, it is likely that the additional H is itinerant (i.e., not associated with a specific anion longer than a few picoseconds); if this is the case,

then such an amphibole would have a high ionic conductivity relative to other amphiboles, and the formula should then be written as $Na_3Mg_5Si_8O_{22}(OH)_2H$. According to our principles of nomenclature, $Na_3Mg_5Si_8O_{22}(OH)_2H$ is a $^W(OH, F, Cl)$-dominant amphibole and would require a new root name if found in Nature. Homovalent variants and new root compositions can be named according to our general rules.

Here, we make the case for basing amphibole classification on the contents of the A, B, and C cations, and hence the $Fe^{3+}$ content of an amphibole plays a major role in the classification scheme. Thus use of some of the techniques outlined above, in addition to electron-microprobe analysis, is required to characterize the chemical formulas of amphiboles accurately. To make an analoguey with 40 yr ago, wet-chemical analysis was in widespread use and the electron microprobe was a novel instrument of limited availability. However, the ability of the electron microprobe to deal with heterogeneous material and obviate problems of sample contamination led to its current extensive use. We are in a similar situation today. The electron microprobe is in widespread use, but the techniques for the analysis of $Fe^{3+}/Fe^{2+}$ and light lithophile elements outlined above are far less widespread. However, these techniques considerably increase our ability to analyze minerals accurately. To increase our knowledge of the chemistry of minerals in general (and amphiboles in particular), as a community we need to acquire this instrumentation so that in the near future, these other analytical techniques become as routine as electron-microprobe analysis.

## APPENDIX III: CALCULATION OF $Fe^{3+}$ AND (OH) IN AMPHIBOLES

As discussed in Appendix II, $Fe^{3+}$ and (OH) are significant and variable constituents in amphiboles but are generally not determined in most analytical work. This generally has the result of distorting the stoichiometry, e.g., indicating unusual site-occupancies: $Ti^{4+}$ as a T-group cation, Na or Ca as a C-group cation, greater than 16 total cations, which in turn may affect the assignment of a name. This situation may be resolved by measuring one or more of these constituents, or somewhat alleviated by numerical modeling: calculating the $Fe^{3+}$ content and/or calculating the formula using expressions for the (OH) content other than (OH + F + Cl) = 2.0 apfu. Although not a substitute for direct measurement, these different methods of normalization are a way of addressing missing constituents and the ensuing problems with stoichiometry.

### Calculation of amphibole formulas and (OH) content

There are many papers on the calculation of amphibole formulas (Hawthorne and Oberti 2007, and references therein). It is usually recommended that amphibole formulas be normalized on the basis of 24(O, OH, F, Cl) with (OH, F, Cl) = 2 apfu where $H_2O$ is not known. Although this is equivalent to the 23O calculation, it has the advantage of generating a calculated $H_2O$ content and hence a more appropriate sum of constituent oxides.

One of the principal problems in the chemical characterization of amphiboles is the lack of determination of $H_2O$, and the general assumption that (OH, F, Cl) = 2 apfu is probably not correct in the majority of cases. It is well known (Leake 1968; Saxena and Ekström 1970; Hawthorne et al. 1998; Tiepolo et

al. 1999) that a deficiency of monovalent anions correlates with an increase in Ti in amphiboles. Although $^C$Ti may occur at all three $M$ sites, $^{M(3)}$Ti is very rare (Tiepolo et al. 1999), whereas Ti partition between $M(1)$ and $M(2)$ is common and depends on conditions of formation. Titanium is incorporated at the $M(1)$ site according to the following local mechanism (Oberti et al. 1992):

$$^{M(1)}Ti^{4+} + 2^WO^{2-} \rightarrow {}^{M(1)}(Mg, Fe^{2+}) + 2^W(OH)^-.$$
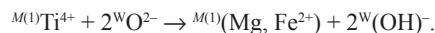
This substitution will reduce the amount of (OH) at O(3) by twice the amount of Ti at $M(1)$. In principle, one may use the Ti content of $M(1)$ as a proxy for OH. We do not commonly know $^{M(1)}$Ti; however, Ti generally preferentially orders at $M(1)$, and we may use the approximation $^{M(1)}$Ti = Ti. The correlations presented by Leake (1968) and Saxena and Ekström (1970) support the general applicability of the relations $^{M(1)}$Ti = Ti and Ti$^{4+}$ = 2 – 2(OH). Thus in the absence of a direct estimate of the (OH, F, Cl) content, we recommend that amphibole formulas be calculated on the basis of 24(O, OH, F, Cl) with (OH, F, Cl) = (2 – 2Ti) apfu (being aware that this choice will produce the maximum value of O$^{2-}$). However, the reader should also be aware that, in some cases, a significant fraction of Ti may occur at $M(2)$ (Hawthorne et al. 1998; Tiepolo et al. 1999).

## Calculation of amphibole formulas and Fe³⁺ content

The Fe$^{3+}$/(Fe$^{2+}$ + Fe$^{3+}$) value in an amphibole can be calculated by constraining the sum of a set of cations to a particular value and adjusting Fe$^{3+}$/(Fe$^{2+}$ + Fe$^{3+}$) for electroneutrality. The particular cation sums may be strictly adhered to (or may be "usually" adhered to) except for particular compositions or parageneses. Below, we note where there are exceptions to the criteria listed.

Above, we discuss the use of two different schemes of calculation for amphiboles: (1) 24(O, OH, F, Cl) with (OH, F, Cl) = 2 apfu and (2) 24(O, OH, F, Cl) with (OH, F, Cl) = (2 – 2Ti) apfu. The calculation of Fe$^{3+}$ content described below is done on the basis of 24(O, OH, F, Cl) with (OH, F, Cl) = 2 apfu. The methods are the same if one uses the basis 24(O, OH, F, Cl) with (OH, F, Cl) = (2 – 2Ti) apfu (although the numbers are somewhat different).

## General points

(1) Where not adjusting the Fe$^{3+}$/(Fe$^{2+}$ + Fe$^{3+}$) value, the formula is normalized to 24(O, OH, F, Cl) with (OH, F, Cl) = 2 apfu [except where O$^{2-}$ enters the O(3) site through the presence of Ti$^{4+}$ at the $M(1)$ site; in this case, the formula should be normalized to 24(O, OH, F, Cl) with (OH, F, Cl) = (2 – 2Ti) apfu, see above]. The advantage over the 23O calculation is that H$_2$O is also calculated and the total oxide sum is derived, giving another criterion for evaluation of the analytical results.

(2) Some constituents of amphiboles are not routinely measured, and their presence in the amphibole considered will invalidate the calculations that are done here. Thus major and variable Li occurs in certain types of amphiboles, and will invalidate the procedures discussed here if present and not quantified.

(3) In some (rare) cases, Fe$^{3+}$ plays a similar role to Ti, i.e., is involved in (usually) post crystallization dehydrogenation, $^{M(1,3)}$Fe$^{3+}$ + $^{O(3)}$O$^{2-}$ → $^{M(1,3)}$Fe$^{2+}$ + $^{O(3)}$(OH)$^-$, and orders at the $M(1)$

and $M(3)$ sites. In those cases, calculations should be done based on (OH, F, Cl) = (2 – 2Ti – xFe$^{3+}$) apfu, where x is the amount of Fe$^{3+}$ involved in dehydrogenation.

## Calculation procedures

For the calculations shown here, we use a composition from Deer et al. (1992, page 678). The chemical composition and unit formula are given in Appendix Table 1 (below), analyses (1) [the original analysis calculated on the basis of 24(O,OH)] and (2) [the original analysis omitting H$_2$O and calculated on the basis of 24(O,OH) with (OH) = 2 apfu].

*(1) Calculate formula with Fe$_2$O$_3$ set to zero (all-ferrous calculation) and FeO set to zero (all-ferric calculation), both with (OH + F + Cl) = 2 apfu and normalizing on 24 (O + OH + F + Cl) (analyses 3 and 4, Appendix Table 1).*

(i) The all-ferrous calculation gives the maximum amount of cations in the amphibole formula. Conversion of FeO into Fe$_2$O$_3$ in the analysis increases the amount of O and hence decreases the resulting amounts of normalized cations (compare analyses 3 and 4).

(ii) Because of (i), the sums of the A, B, C and T cations are at their maximum for the all-ferrous formula. If they exceed their maximum possible stoichiometric value(s), the sums may be reduced by conversion of FeO into Fe$_2$O$_3$.

(2) *Assign the cations in the all-ferrous formula to the T-, C-, B-, and A-cation groups as described in the main report.*

(3) *If the following criteria are violated, Fe$^{3+}$ may be present in the formula:*

(i) Si ≤8 apfu.

(ii) Sum [Si + Al + Ti + Fe$^{3+}$ + Fe$^{2+}$ + Mn$^{2+}$ + Mg + Ca + Na + K] ≤ 16 apfu.

(iii) Sum [Si + Al + Ti + Fe$^{3+}$ + Fe$^{2+}$ + Mn$^{2+}$ + Mg + Ca] ≤ 15 apfu.

**APPENDIX TABLE 1.** Calculation of Fe$^{3+}$ for an amphibole

| | (1) | (2) | (3) | (4) | (5) | (6) | (7) |
|---|---|---|---|---|---|---|---|
| SiO$_2$ wt% | 51.63 | 51.63 | 51.63 | 51.63 | 51.63 | 51.63 | 51.63 |
| Al$_2$O$_3$ | 7.39 | 7.39 | 7.39 | 7.39 | 7.39 | 7.39 | 7.39 |
| Fe$_2$O$_3$ | 2.50 | 2.50 | 0.00 | 8.30 | 1.26 | 6.25 | 6.07 |
| FeO | 5.30 | 5.30 | 7.55 | 0.00 | 6.42 | 1.93 | 2.08 |
| MnO | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 |
| MgO | 18.09 | 18.09 | 18.09 | 18.09 | 18.09 | 18.09 | 18.09 |
| CaO | 12.32 | 12.32 | 12.32 | 12.32 | 12.32 | 12.32 | 12.32 |
| Na$_2$O | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 |
| H$_2$O | 2.31 | 2.14 | 2.13 | 2.17 | 2.14 | 2.16 | 2.16 |
| Total | 100.32 | 100.15 | 99.89 | 100.68 | 100.02 | 100.55 | 100.53 |
| Si apfu | 7.196 | 7.220 | 7.261 | 7.128 | 7.240 | 7.158 | 7.161 |
| Al | 0.804 | 0.780 | 0.739 | 0.872 | 0.760 | 0.842 | 0.839 |
| ΣT | 8.000 | 8.000 | 8.000 | 8.000 | 8.000 | 8.000 | 8.000 |
| Al | 0.410 | 0.438 | 0.486 | 0.330 | 0.461 | 0.366 | 0.369 |
| Fe$^{3+}$ | 0.262 | 0.263 | – | 0.862 | 0.132 | 0.652 | 0.634 |
| Fe$^{2+}$ | 0.618 | 0.620 | 0.888 | – | 0.753 | 0.223 | 0.242 |
| Mn | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 |
| Mg | 3.759 | 3.771 | 3.793 | 3.723 | 3.782 | 3.739 | 3.740 |
| ΣC | 5.069 | 5.112 | 5.187 | 4.935 | 5.148 | 5.000 | 5.005 |
| Δ | 0.069 | 0.112 | 0.187 | – | 0.148 | – | 0.005 |
| Ca | 1.840 | 1.846 | 1.856 | 1.822 | 1.851 | 1.830 | 1.831 |
| Na | 0.091 | 0.039 | 0.163 | 0.178 | – | 0.164 | 0.164 |
| ΣB | 2.000 | 2.000 | 2.043 | 1.985 | 1.999 | 1.994 | 2.000 |
| Na | 0.074 | 0.126 | – | – | 0.166 | – | – |
| OH | 2.148 | 2.000 | 2.000 | 2.000 | 2.000 | 2.000 | 2.000 |
| Fe$^{3+}$/(Fe$^{2+}$+ Fe$^{3+}$) | 0.298 | 0.298 | 0 | 1 | 0.149 | 0.745 | 0.724 |

(1) Original analysis; (2) original FeO and Fe$_2$O$_3$, H$_2$O set to OH = 2 apfu; (3) all FeO, OH = 2 apfu; (4) all Fe$_2$O$_3$, OH = 2 apfu; (5) sum (cations to Ca) = 15 apfu, Fe$^{3+}$ calc, OH = 2 apfu; (6) sum (cations to Mg) = 13 apfu, Fe$^{3+}$ calc, OH = 2 apfu; (7) sum (cations to Na) = 15 apfu, Fe$^{3+}$ calc, OH = 2 apfu.

Criterion (i): This is rigorously fixed by the structure, i.e., Si cannot exceed 8 apfu as there are no other tetrahedrally coordinated sites in the amphibole structure for Si to occupy.

Criterion (ii): This is rigorously fixed by the structure, i.e., all cation sites are fully occupied at 16 apfu.

Criterion (iii): With this criterion, one assumes that Ca is not an A cation. This is not constrained by the structure and is not always correct; in amphiboles from marbles, Ca may be an A cation. However, in most rocks, this is not the case, and criterion iii may be applied (with caution).

(*4*) *The all-ferrous formula (analysis 3, Appendix Table 1) is inspected with regard to each of the above criteria:*

(i) Si = 7.261 < 8 apfu.

(ii) Sum [Si + Al + Ti + $Fe^{3+}$ + $Fe^{2+}$ + $Mn^{2+}$ + Mg + Ca + Na] = 15.209 < 16 apfu.

(iii) Sum [Si + Al + Ti + $Fe^{3+}$ + $Fe^{2+}$ + $Mn^{2+}$ + Mg + Ca] = 15.043 > 15 apfu.

(*5*) *Criterion (iii) is violated; this indicates the possible occurrence of $Fe^{3+}$; the formula is normalized on [Si + Al + Ti + $Fe^{3+}$ + $Fe^{2+}$ + $Mn^{2+}$ + Mg + Ca] = 15 apfu and $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ is adjusted for electroneutrality (analysis 5, Appendix Table 1).*

(i) This normalization gives the minimum estimate for the $Fe^{3+}$ content.

(ii) If more than one of the three criteria does not hold in analysis (3), then the calculation scheme used is that which gives a formula that accords with all of these criteria.

(*6*) *The following criteria limit the maximum possible amount of $Fe^{3+}$ in the formula:*

(i) Si + Al = 8 apfu.

(ii) [Si + Al + Ti + $Fe^{3+}$ + $Fe^{2+}$ + $Mn^{2+}$ + Mg + Ca + Na] = 15 apfu.

(iii) Sum [Si + Al + Ti + $Fe^{3+}$ + $Fe^{2+}$ + $Mn^{2+}$ + Mg] = 13 apfu.

Criterion (i): This is not constrained by the structure and is not always correct. Richterite may contain $Ti^{4+}$ as a T cation, and in these circumstances, criterion i should not be used. However, in most rocks, this is not the case and criterion i may be applied (with caution).

Criterion (ii): With this criterion, one assumes that K does not occur as a B cation. This is not always correct, as K can occur as a B cation in richterite.

Criterion (iii): This criterion can be wrong if there is Li in the structure, or if there is ($Fe^{2+},Mn^{2+},Mg$) as a B cation [e.g., calcium amphiboles commonly contain small but significant amounts of $^B(Fe^{2+} + Mn^{2+} + Mg)$].

(*7*) *The formula [analysis 5, Appendix Table 1] is then inspected with regard to each of the above criteria:*

(i) Si + Al = 8.461 ≥ 8 apfu.

(ii) Sum [Si + Al + Ti + $Fe^{3+}$ + $Fe^{2+}$ + $Mn^{2+}$ + Mg + Ca + Na] = 15.165 > 15 apfu.

(iii) Sum [Si + Al + Ti + $Fe^{3+}$ + $Fe^{2+}$ + $Mn^{2+}$ + Mg] = 13.148 > 13 apfu.

(*8*) *The formula is normalized on each of equalities (ii) and (iii) in section (6) and $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ is adjusted for electroneutrality [analyses (6) and (7), Table A1].*

(i) Note that we cannot use equality (i) (Section 6) as the amount of $Fe_2O_3$ required for this constraint exceeds the maximum possible amount of $Fe^{3+}$ in the analysis (see analysis 4).

(ii) In analysis 6, [Si + Al + Ti + $Fe^{3+}$ + $Fe^{2+}$ + $Mn^{2+}$ + Mg + Ca + Na] = 14.994 < 15 apfu, indicating that this constraint cannot be used for this particular analysis.

(iii) In analysis 7, [Si + Al + Ti + $Fe^{3+}$ + $Fe^{2+}$ + $Mn^{2+}$ + Mg + Ca + Na] = 15.000 apfu and all other aspects of the formula are well behaved. Hence analysis 7 gives the maximum estimate of $Fe^{3+}$ in this amphibole.

*The minimum and maximum values of $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ are 0.149 (analysis 5) and 0.724 (analysis 7), respectively, and the mean value is 0.437, to be compared with the experimental value of 0.298 (analysis 2).*

Where experimental and measured values of $Fe^{3+}$ contents in amphiboles have been compared (e.g., Hawthorne 1983; Hawthorne and Oberti 2007), it can be seen that methods of estimation are not accurate. However, one must deal with this problem when calculating an amphibole formula. Even ignoring it means setting $Fe^{3+}$ = 0.00 apfu and hence an estimate of $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ is still made (i.e., 0.0). As $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ varies between 0.0 and 1.0 in amphiboles, in general an estimate using the techniques outlined here will give a better (i.e., closer to the true) value of $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ than setting $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ = 0.0.

## APPENDIX IV: PRINCIPAL VARIABLES USED IN THE CLASSIFICATION PROCEDURE

In most scientific problems, one focuses on the variables that show the greatest degree of relative variation, as these are the most informative. In addition, IMA procedures concerning the definition of distinct minerals focus on the dominant species (cation or anion) at a site. Of the A, B, C, T cations, and W anions, all except T show various dominant cations or anions in the set of all amphibole compositions; T is invariably dominated by Si (i.e., $^TAl$ <4.0 apfu). These issues indicate that the T cations should *not* be used as a primary parameter in an amphibole classification (of course, this does not preclude the use of T cations in showing graphically the variation in amphibole composition).

### The W anions

There is continuous variation in (OH,F,Cl) and O contents in amphiboles. Where $W_2 \approx (OH,F,Cl)_2$, the high-charge cations are ordered predominantly at the $M(2)$ site, whereas where $W_2 \approx O_2^{2-}$, the high-charge cations are distributed over the $M(1,2,3)$ sites, those at the $M(1,3)$ sites being associated with W = $O^{2-}$. Thus the presence of a significant oxo component (i.e., $W_2 \approx O_2^{2-}$) is accompanied by different patterns of order of C cations relative to amphiboles with $W_2 \approx (OH,F,Cl)_2$. This consideration suggests that the W constituents be used initially to divide amphiboles into two broad classes: **(1) hydroxy-fluoro-chloro-amphiboles** with (OH,F,Cl) ≥ 1.00 apfu, and **(2) oxo-amphiboles** with (OH,F,Cl) < 1.00 apfu (we do not use the term oxy as this has too many associations with the process of oxidation-dehydrogenation). Within these two classes, the A, B and C constituents are used to classify the amphiboles further.

### Hydroxy-fluoro-chloro-amphibole group

Hydroxy-fluoro-chloro-amphiboles are divided into subgroups according to the dominant B-cation or group of B cations. Let us write the sum of the small divalent cations as $\Sigma M^{2+} = ^BMg + ^BFe^{2+} + ^BMn^{2+}$, and the sum of the B cations as $\Sigma B = ^BLi + ^BNa$

$+ \Sigma M^{2+} + {}^{B}Ca$ (which generally is equal to 2.00 apfu). Thus the dominant B constituents may be represented as indicated in the main text of the report, giving rise to the following amphibole subgroups:

Magnesium-iron-manganese amphiboles
Calcium amphiboles
Sodium-calcium amphiboles
Sodium amphiboles
Lithium amphiboles
Sodium-(magnesium-iron-manganese) amphiboles
Lithium-(magnesium-iron-manganese) amphiboles
Lithium-calcium amphiboles.

The resulting supergroup-group-subgroup hierarchy is illustrated in Appendix Figure 2.

### Problems with the previous amphibole classification

There were many problems with this stage of the previous amphibole classification; some of these issues are discussed next.

**(1) The role of ${}^{B}Li$.** There is no good crystal-chemical or chemical reason for including Li amphiboles in the *magnesium-iron-manganese-lithium* group of IMA1997. Lithium is an alkali metal, is formally monovalent, and shows complete solid-solution with Na at the $M(4)$ site in monoclinic amphiboles, e.g., leakeite – ferri-pedrizite: $NaNa_2(Mg_2Fe_2^{3+}Li)Si_8O_{22}(OH)_2$ $- NaLi_2(Mg_2Fe_2^{3+}Li)Si_8O_{22}(OH)_2$, Oberti et al. (2003); magnesio-riebeckite – clino-ferri-holmquistite: $Na_2(Mg_3Fe_2^{3+})Si_8O_{22}(OH)_2$ $- Li_2(Mg_3Fe_2^{3+})Si_8O_{22}(OH)_2$, Oberti et al. (2004).

These points indicate that amphiboles with Li dominant at $M(4)$ should *not* be included as part of the magnesium-iron-manganese subgroup. There are two possible ways in which to treat such amphiboles: (1) recognize a separate subgroup of amphiboles with Li as the dominant B-cation (analogous to that with dominant ${}^{B}Na$), or (2) include ${}^{B}Li$ with ${}^{B}Na$ as a principal constituent of an alkali-amphibole subgroup. However, ${}^{B}Li$ amphiboles have some features that are not shared with ${}^{B}Na$ amphiboles; for instance, ${}^{B}Li$ amphiboles may occur with orthorhombic *Pnma* symmetry (holmquistite) and are also expected to occur with monoclinic $P2_1/m$ symmetry ("clino-holmquistite"). Hence, the simpler solution is to define a distinct subgroup of ${}^{B}Li$ amphiboles. Intermediate compositions between ${}^{B}Li$ and ${}^{B}\Sigma M^{2+}$ amphiboles fall in the lithium-(magnesium-iron-manganese) subgroup and give rise to root compositions analogous to those of sodium-calcium amphiboles (likewise the lithium-calcium amphiboles).

**(2) The names of the principal subgroups.** Having recognized a separate subgroup with Li as the dominant B-cation, it is obvious that the term "lithic", in accord with "calcic" and "sodic", is not a suitable name for this subgroup. Moreover, the names of the current five subgroups (IMA2003) are rather inhomogeneous, using both nouns (e.g., magnesium), element symbols (e.g., Mg) and adjectives (e.g., calcic, sodic). Here, we will use nouns to name the subgroups. The other inhomogeneity with regard to the names of these subgroups is the use of element symbols: the magnesium-iron-manganese subgroup is frequently referred to as the Mg-Fe-Mn subgroup (indeed, this is done in IMA1997), whereas the calcium subgroup is not referred to as

the Ca subgroup. Some sort of consistency is required in the use of these subgroup names; either element names or symbols may be used, but authors should maintain consistency of use in a single publication.

### The new classification

(1) The role of the sodium-calcium, lithium-calcium, sodium-(magnesium-iron-manganese), and lithium-(magnesium-iron-manganese) subgroups. A significant source of complexity in the classification of amphiboles is the recognition of the intermediate subgroups: sodium-calcium, lithium-calcium, sodium-(magnesium-iron-manganese), and lithium-(magnesium-iron-manganese) amphiboles. Let us consider the reason for these intermediate subgroups, considering the sodium-calcium subgroup as an example. The sodium-calcium subgroup was defined by IMA1978 and redefined by IMA1997, but its use was not justified from a nomenclature perspective. As noted above, IMA procedures involving the definition of distinct minerals focus on the dominant species at a site. Using this criterion, the sodium-calcium subgroup of amphiboles would not be recognized: amphiboles with $2.00 > Ca \geq 1.00$ apfu would belong to the calcium subgroup, and amphiboles with $2.00 > Na > 1.00$ apfu would belong to the sodium subgroup. Using this criterion to reduce the number of primary subgroups would certainly reduce both the complexity of the nomenclature and the number of distinct amphiboles. However, following this course will result in a problem with richterite (and other amphiboles with the same root-charge arrangement). This issue is investigated in Appendix Figure 3, which shows A-B-C compositional space for amphiboles with only Ca and Na as B cations (note that this excludes magnesium-iron-manganese and lithium amphiboles). Compositions of previous "end-members" are shown as black squares and white circles. Note that the compositions represented
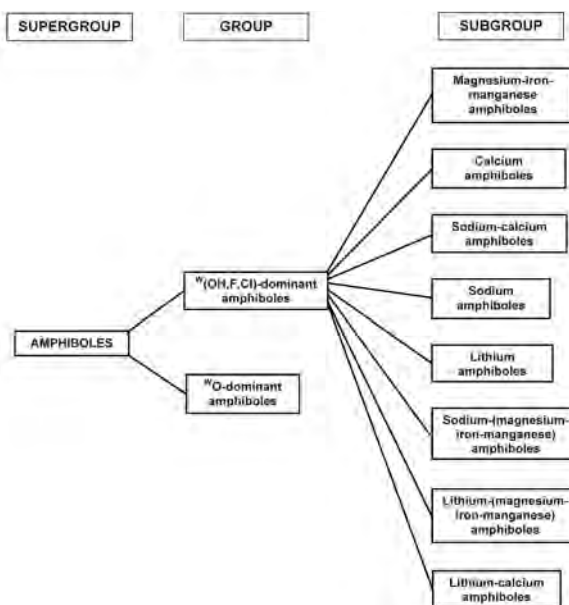


**APPENDIX FIGURE 2.** The supergroup-group-subgroup hierarchy of the amphiboles.

by white circles can always be represented as 50:50 mixtures of other "end-member" compositions. Thus magnesio-hornblende can be represented as 0.50 tremolite and 0.50 tschermakite, and barroisite can be represented as 0.50 tschermakite and 0.50 glaucophane. However, richterite cannot be represented by a combination of two end-members, as is apparent graphically from Appendix Figure 3; richterite is thus a true end-member according to the criteria of Hawthorne (2002). However, IMA criteria for the recognition of a valid mineral species do not involve its status as a valid end-member. The criteria include the dominance of a specific cation at a site or group of sites. This approach would definitely dispose of pargasite and magnesio-hornblende as distinct amphibole species. However, richterite cannot be resolved into a combination of two end-members; it is irreducible and hence a distinct species, and requires the existence of the sodium-calcium subgroup.

**(2) Lithium-calcium, sodium-(magnesium-iron-manganese), and lithium-(magnesium-iron-manganese) subgroups.** The above discussion concerning the sodium-calcium amphibole subgroup can be applied to all mixed-valence pairings of B cations. Thus $B_2 = (Li\ Ca)$, $(Li\ Mg)$, $(Na\ Mg)$, and their $^BFe^{2+}$ and $^BMn^{2+}$ analogues will all result in end-member compositions of the type $Na\ B_2\ Mg_5\ Si_8\ O_{22}\ W_2$ that cannot be decomposed into calcium-, lithium-, magnesium-iron-manganese-, or sodium-subgroup compositions. In this regard, consider the composition $^A(Na_{0.33}K_{0.03})_{\Sigma0.36}$ $^B(Na_{0.82}Ca_{0.39}Mn_{0.57}Mg_{0.22})_{\Sigma2.00}$ $^C(Mg_{3.83}Mn^{2+}_{0.37}Fe^{3+}_{0.73}Li_{0.07})_{\Sigma5.00}$ $^T(Si_{7.86}Al_{0.11})_{\Sigma7.97}$ $O_{22}$ $(OH_{1.60}F_{0.40})$, reported from Tirodi, India, by Oberti and Ghose (1993). This amphibole is close to the root composition $^A\square^B(Na\ Mn^{2+})^C(Mg_4\ Fe^{3+})\ ^TSi_8\ O_{22}\ (OH)_2$ and is named fluorian manganoan parvowinchite (IMA-CNMMN 2003-066), following IMA2003. This composition gives rise to a new root name, and hence requires definition of a new subgroup of $^B[Na\ (Mg,Fe,Mn)]$ amphiboles.

The $^B(Na\ Mg)$ and $^B(Li\ Mg)$ joins have been investigated by synthesis; intermediate compositions with a "richterite-like" charge-arrangement are stable and have $P2_1/m$ symmetry at room temperature (Cámara et al. 2003; Iezzi et al. 2004, 2005a, 2005b).

**(3) The A cations.** Having divided amphiboles with $1 < (OH,F,Cl) \leq 2$ apfu into eight subgroups based on the B cations, we have the A and C cations to classify within these subgroups and to assign specific names to specific compositional ranges and root compositions. For the A cations, the variation observed in Nature spans the complete range possible from a structural perspective: $\square$, Na, and K can vary over the range 0–1 apfu (at present, the maximum content of $^ACa$ observed only slightly exceeds 0.50 apfu). Thus we use the variable $^A(Na + K + 2Ca)$ in the classification graphs of this paper.

**(4) The C cations.** The situation for the C cations is more complicated, as these cations occur at three distinct sites in amphibole structures: $M(1)$, $M(2)$, and $M(3)$ in all common amphibole structure-types (but not in the $P2/a$ and $C\bar{1}$ structures, where there are five and eight $M$ sites, respectively, Hawthorne and Oberti 2007). Most heterovalent variations occur at the $M(2)$ site, where there is complete solid-solution among Mg, $Fe^{2+}$, Al, $Fe^{3+}$, and $Ti^{4+}$. Some Al can disorder over $M(2)$ and $M(3)$ in Mg-rich calcium amphiboles (Oberti et al. 1995), and some $Ti^{4+}$ and $Fe^{3+}$ can occur at $M(1)$ and at $M(1,3)$, respectively, but trivalent
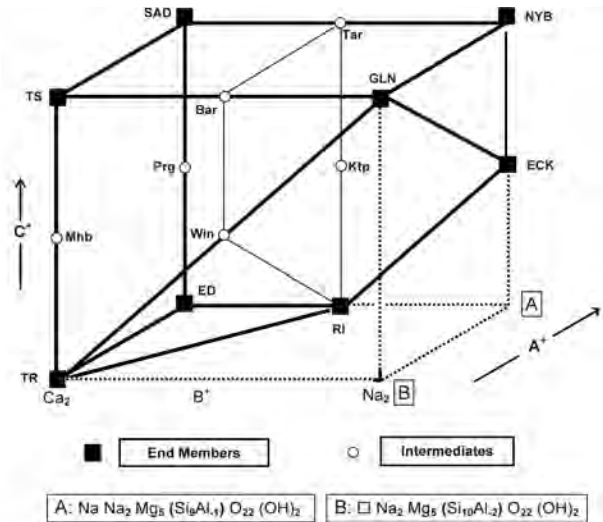


**APPENDIX FIGURE 3.** Compositional space for monoclinic Na-Ca-Mg-Al-Si amphiboles using $^BNa$, $^ANa$ and $^CAl$ as proxies for the aggregate charges of the B, A and C groups of cations. The heavy solid black lines indicate the limits of possible amphibole compositions. Filled black squares are the locations of end-members at the corners of the compositional space; open circles are the locations of end-members on the edges of compositional space. Bar = barroisite; Eck = eckermannite; Ed = edenite; Gln = glaucophane; Mhb = magnesio-hornblende; Ktp = katophorite; Nyb = nybøite; Prg = pargasite; Ri = richterite; Sad = sadanagaite; Tar = taramite; Tr = tremolite; Ts = tschermakite; Win = winchite. We use the symbols of Kretz (1983) for the amphiboles, and introduce new symbols for amphiboles not included in the original list of symbols. The full list of symbols used here for amphiboles is given as Appendix VII.

cations are never dominant at $M(1)$ or $M(3)$ in amphiboles with $(OH,F,Cl) \geq 1.00$ apfu. Lithium can become dominant at the $M(3)$ site, normally being accompanied by $Fe^{3+}$ at the $M(2)$ site.

We need to be able to represent the variation in C cations by a single variable, which therefore must be some function of their aggregate formal charge. The most common variation in C involves divalent and trivalent cations. The root composition for tremolite has $C = Mg_5$, and it is convenient to represent variation in C by the additional formal charge introduced by incorporation of trivalent and tetravalent cations as C cations, as the additional charge corresponds arithmetically to the amount of trivalent and tetravalent C-cations in the amphibole $(Al + Fe^{3+} + 2Ti^{4+})$. If we consider C cations of formal charge greater than $2^+$, i.e., Al, $Fe^{3+}$, $Cr^{3+}$, $V^{3+}$, $Ti^{4+}$, Sc, and Zr, we can express the additional C-cation charge as $M^{3+}$ where $M^{3+} = Al + Fe^{3+} + Cr^{3+} + V^{3+} + Sc + 2Ti^{4+} + 2Zr$; in most amphiboles, this reduces to $M^{3+} = Al + Fe^{3+} + 2Ti^{4+}$. If we are dealing with amphiboles in which $W = (OH,F,Cl)_2$, all of these cations will occur at the $M(2)$ site [except for some Al–Mg disorder over $M(2)$ and $M(3)$ in Mg-rich calcium amphiboles, which is immaterial to this argument], and thus the high-charge cations cannot exceed 2 apfu (i.e., the additional formal charge is at most $2^+$).

However, note that $M^{3+}$ can exceed 2.0 for some compositions. Where $^{O(3)}O^{2-}$ is not the dominant W anion, the behavior of $^CTi^{4+}$ also affects $M^{3+}$ because of the different roles that $^CTi^{4+}$ can

play in amphiboles: (a) $^C$Ti$^{4+}$ may occur at the $M(2)$ site where it contributes 2$^C$Ti$^{4+}$ to M$^{3+}$; (b) $^C$Ti$^{4+}$ may occur at the $M(1)$ site [coupled to the occurrence of O$^{2-}$ at the O(3) site, i.e., as a W anion] where it does not contribute to M$^{3+}$: i.e., M$^{3+}$ = Al + Fe$^{3+}$. The same is true for Fe$^{3+}$ at the $M(1)$ and $M(3)$ sites in calcic oxo-amphiboles (from volcanic environments, where dehydrogenation is related to post-crystallization oxidation processes). If known, the oxo component in amphiboles must be accounted for by subtracting the appropriate amount of Ti$^{4+}$ and Fe$^{3+}$ from M$^{3+}$ before classification. In addition, the same amount of Fe$^{3+}$ must be subtracted from the total amount of Fe$^{3+}$ in the formula with regard to the assignment of the prefix *ferri-*. Thus ferri- is assigned on the basis of [$^C$Fe$^{3+}$ $-$ $^{M(1,3)}$Fe$^{3+}$] if $^{M(1,3)}$Fe$^{3+}$ is known.

A correction to M$^{3+}$ is required also where Li is a C cation because $^C$Li enters the amphibole structure via the substitution $^{M(3)}$Li + $^{M(2)}$Fe$^{3+}$ → $^{M(2,3)}$Fe$^{2+}_2$. As $^C$Li is not incorporated into the A-B-C classification procedure but is considered separately, it is necessary to adjust the value of M$^{3+}$ for the effect of the substitution $^{M(3)}$Li + $^{M(2)}$Fe$^{3+}$ = $^{M(2,3)}$Fe$^{2+}_2$. This is done by subtracting an amount of trivalent cations equal to the amount of $^C$Li.

We use the variable $^C$(Al + Fe$^{3+}$ + 2Ti$^{4+}$) in the classification graphs of this paper. Note that this variable must be modified by adding [Cr$^{3+}$ + V$^{3+}$ + Sc + 2Zr] and subtracting [$^{M(3)}$Li + $^{M(1,3)}$Fe$^{3+}$ + $^{2M(1)}$Ti$^{4+}$] where appropriate (see above discussion). Major differences between this classification and the classifications of IMA1997 and IMA2003 are outlined in Appendix V.

**(5) Ti >0.50 apfu.** The occurrence of titanium as a C cation is not related to a homovalent substitution, and hence there is no titano- prefix. Titanium may be incorporated into the amphibole structure by heterovalent-cation substitution (e.g., $^C$Ti$^{4+}$ + 2$^T$Al = $^C$Mg + 2$^T$Si) or by oxo- substitution ($^C$Ti$^{4+}$ + 2$^W$O$^{2-}$ = $^C$Mg + 2$^W$OH). Both types of substitution lead to new charge arrangements and hence new root compositions, [e.g., NaCa$_2$(Mg$_4$Ti) (Si$_5$ Al$_3$)O$_{22}$(OH)$_2$ and NaCa$_2$(Mg$_4$Ti)(Si$_7$ Al)O$_{22}$O$_2$], both being derived from edenite by the substitutions $^C$Ti$^{4+}$ + 2$^T$Al = $^C$Mg + 2$^T$Si and $^C$Ti$^{4+}$ + 2$^W$O$^{2-}$ = $^C$Mg + 2$^W$OH]. Thus compositions with $^C$Ti >0.5 apfu involve new names, both in (OH,F,Cl) amphiboles and in oxo-amphiboles (e.g., dellaventuraite, kaersutite, obertiite). The occurrence of significant $^C$Ti, although less than 0.50 apfu in (OH,F,Cl) amphiboles, is important both for mineralogical and petrological reasons, and can be indicated using the modifier Ti-rich where 0.50 > $^C$Ti >0.30 apfu.

### Appendix V: Major differences between the new classification and IMA1997 and IMA2003

(1) We have changed the criterion to identify the different subgroups, bringing it more into accord with the *dominant-cation* criterion of current IMA-CNMNC nomenclature. IMA1997 and IMA2003 referred to specific atom contents in the formula unit to define the boundary between subgroups. Thus an amphibole was assigned to the calcium subgroup where the following conditions apply: $^B$(Mg,Fe$^{2+}$,Mn$^{2+}$, Li) ≤ 0.50, $^B$(Ca,Na) ≥ 1.50, and $^B$Na ≤0.50 apfu. In the present classification, amphiboles are assigned to various subgroups based on the *dominant cation* (or group of cations) at a site (or group of sites).

(2) IMA1997 and IMA2003 considered $^B$Li together with

$^B$(Mg,Fe$^{2+}$,Mn$^{2+}$). The crystal-chemical behavior of Li is very different from that of (Mg,Fe$^{2+}$,Mn$^{2+}$) and Ca, and is more similar to that of Na. Moreover, extensive recent work (Caballero et al. 1998, 2002; Oberti et al. 2003, 2004) has shown complete solid-solution between $^B$Li and $^B$Na, behavior that is different from that of the $^B$(Mg,Fe$^{2+}$,Mn$^{2+}$) amphiboles. The existence of $^B$Li amphibole with orthorhombic and monoclinic primitive symmetries indicates that $^B$Li-dominant amphiboles should be a distinct subgroup.

(3) IMA2003 defined a sodium-calcium-magnesium-iron-manganese-lithium group in which intermediate compositions require (1) a new root name if $^B$Li >0.50 apfu, or (2) the prefixes *parvo* and *magno* if $^B$Li ≤0.50 apfu. We have defined new subgroups: lithium-calcium, sodium-(magnesium-iron-manganese), and lithium-(magnesium-iron-manganese) amphiboles. These amphibole compositions have the same charge arrangement as richterite, and hence cannot be reduced to a combination of other end-members.

(4) IMA1997 AND IMA2003 used both nouns and adjectives to define the main groups (now subgroups) of amphiboles (e.g., magnesium-iron-manganese-lithium, calcic, sodic). Here we use nouns (e.g., magnesium-iron-manganese, calcium, sodium) or element or cation symbols in all cases.

(5) IMA1997 and IMA2003 used the A, B, and T cations for classification purposes. However, the dominant T-cation does not change: it is invariably Si, and hence compositional variation at T is not an appropriate variable to use for classification. All other groups show two or more cations as dominant, and hence the A, B, and C cations are more appropriate for classification purposes and accord with the dominant-cation principle currently used in IMA nomenclature. This point is the major difference between the two schemes. The use of C cations for classification has been implemented by considering the variation in $^C$M$^{3+}$ (the amount of highly charged C-cations not involved in the processes related to the oxo component) as a classification variable.

Three major crystal-chemical issues have been explored in detail since publication of the previous scheme of classification (IMA1997): (a) the behavior of $^C$Li, (b) the behavior of $^B$Li, and (c) the occurrence of dominant O$^{2-}$ at W. For (a) and (c), electroneutrality is maintained by incorporation of "unusual" cations at sites containing "normal" C-cations: (a) $^{M(3)}$Li is accompanied by $^{M(2)}$Fe$^{3+}$; (b) $^W$O$^{2-}$ is accompanied by $^{M(1)}$Ti$^{4+}$ or $^{M(1,3)}$(Fe$^{3+}$,Mn$^{3+}$). For classification purposes, these components are dealt with by subtracting the relevant amounts of Fe$^{3+}$ and Ti$^{4+}$ from $^C$M$^{3+}$ before using the standard compositional diagrams.

(6) The present classification recognizes a distinct group of amphiboles with O$^{2-}$ as the dominant W anion (oxo-amphiboles). These amphiboles contain high-charge C-cations, and have distinct root-names.

(7) We have adopted a different use of prefixes. Because some root compositions have been redefined as their magnesio-, alumino- analogues, the use of the prefixes *magnesio* and *alumino* has been restricted to a few root-names of petrological relevance (riebeckite, arfvedsonite, hastingsite, and hornblende), and the prefix *sodic* has been abolished. Appendix VI lists root-names that have been redefined in the present classification.

### APPENDIX VII: SYMBOLS FOR AMPHIBOLES*

**Act** Actinolite
**Ath** Anthophyllite
**Arf** Arfvedsonite
Bar Barroisite
Can Cannilloite
Cho Clino-holmquistite
**Cum** Cummingtonite
Del Dellaventuraite
**Eck** Eckermannite
**Ed** Edenite
**Ged** Gedrite
**Gln** Glaucophane
**Gru** Grunerite
**Hs** Hastingsite
Hol Holmquistite
**Krs** Kaersutite
**Ktp** Katophorite
Lkt Leakeite

Mhb Magnesio-hornblende
Nyb Nybøite
Ob Obertiite
**Prg** Pargasite
Ped Pedrizite
Ri Richterite
**Rbk** Riebeckite
Sad Sadanagaite
Tar Taramite
**Tr** Tremolite
**Ts** Tschermakite
Un Ungarettiite
Win Winchite.

Symbols in bold are from Kretz (1983); symbols in normal font are introduced here. Other lists of symbols have been published subsequent to that of Kretz (1983), but these are also incomplete with regard to amphibole names.