

**NOMENCLATURE OF AMPHIBOLES: REPORT OF THE SUBCOMMITTEE ON
AMPHIBOLES OF THE INTERNATIONAL MINERALOGICAL ASSOCIATION,
COMMISSION ON NEW MINERALS AND MINERAL NAMES**

BERNARD E. LEAKE¹ (Chairman)

Department of Geology and Applied Geology, University of Glasgow, Glasgow G12 8QQ, U.K.

ALAN R. WOOLLEY (Secretary)

Department of Mineralogy, Natural History Museum, Cromwell Road, London SW7 5BD, U.K.

CHARLES E.S. ARPS* (The Netherlands; retired December 1994)

WILLIAM D. BIRCH* (Australia; from January 1995)

M. CHARLES GILBERT (U.S.A.; resigned 1994)

JOEL D. GRICE (Canada; *from January 1995)

Mineral Sciences Division, Canadian Museum of Nature, P.O. Box 3443, Station D, Ottawa, Ontario K1P 6P4, Canada

FRANK C. HAWTHORNE

Department of Earth Sciences, University of Manitoba, Winnipeg, Manitoba R3T 2N2, Canada

AKIRA KATO

Department of Geology, Natural Science Museum, 2-23-1 Hyakanin-cho, Shinjuku, Tokyo 160, Japan

HANAN J. KISCH

Department of Geology and Mineralogy, Ben Gurion University of the Negev, P.O. Box 653, 84105 Beer Sheva, Israel

VLADIMIR G. KRIVOVICHEV

Faculty of Geology, St. Petersburg University, University Emb. 7/9, 199034 St. Petersburg, Russia

KEES LINTHOUT

*Department of Ore Geology, Petrology and Mineralogy, Institute of Earth Sciences, Free University,
De Boelelaan 1085, 1081 HV Amsterdam, The Netherlands*

JO LAIRD

*Department of Earth Sciences, College of Engineering and Physical Sciences, University of New Hampshire,
Durham, New Hampshire 03824, U.S.A.*

JOSEPH A. MANDARINO* (Canada; retired December 1994)

WALTER V. MARESCH

Institut für Mineralogie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

ERNEST H. NICKEL* (Australia)

NICHOLAS M.S. ROCK (Australia; died February 1992)

JOHN C. SCHUMACHER

*Institut für Mineralogie-Petrologie-Geochemie der Albert-Ludwigs Universität zu Freiburg, Albertstrasse 23b,
D-79104 Freiburg, Germany*

DAVID C. SMITH (France; resigned 1994)

NICK C.N. STEPHENSON

Department of Geology and Geophysics, University of New England, Armidale, New South Wales 2351, Australia

LUCIANO UNGARETTI (Italy; resigned April 1993)

ERIC J.W. WHITTAKER

60 Exeter Road, Kidlington, Oxford OX5 2DZ, U.K.

GUO YOUZHI

Central Laboratory, Bureau of Geology and Mineral Resources of Hunnan Province, Dashiba, Kunming, P.R. China

* Indicates a nonvoting official of the CNMMN.

¹ E-mail address: bel@geology.gla.ac.uk

ABSTRACT

The International Mineralogical Association's approved amphibole nomenclature has been revised in order to simplify it, make it more consistent with divisions generally at 50%, define prefixes and modifiers more precisely, and include new species of amphibole discovered and named since 1978, when the previous scheme was approved. The same reference axes form the basis of the new scheme, and most names are little changed, but compound species names like tremolitic hornblende (now magnesiohornblende) are abolished, as are crossite (now glaucophane or ferroglaucophane or magnesioriebeckite or riebeckite), tirodite (now manganocummingtonite) and dannemorite (now manganogrunerite). The 50% rule has been broken only to retain tremolite and actinolite as in the 1978 scheme; the sodic-calcic amphibole range has therefore been expanded. Alkali amphiboles are now sodic amphiboles. The use of hyphens is defined. New amphibole names approved since 1978 include nyböite, leakeite, kornite, ungarettiite, sadanagaite and cannilloite. All abandoned names are listed. The formulae and source of the amphibole end-member names are listed, and procedures outlined to calculate Fe^{3+} and Fe^{2+} where not determined by analysis.

Keywords: amphibole nomenclature, crossite, dannemorite, tirodite.

SOMMAIRE

Le schéma de nomenclature approuvé de l'Association minéralogique internationale est ici révisé afin de le simplifier, de le rendre plus conforme à la règle des subdivisions à 50%, d'en définir plus précisément les préfixes et les qualificatifs, et d'y inclure les nouvelles espèces découvertes et approuvées depuis 1978, date de publication du rapport antérieur. Les mêmes axes de référence sont retenus dans le nouveau schéma, et la plupart des noms sont peu changés. En revanche, les noms d'espèce composés, par exemple hornblende trémolitique (désormais magnésiohornblende), sont abolis, de même que crossite (désormais glaucophane, ferroglaucophane, magnésioriebeckite ou riebeckite), tirodite (désormais manganocummingtonite) et dannemorite (désormais manganogrunerite). La règle de 50% n'est transgressée que pour le maintien des espèces trémolite et actinolite, dont la définition reste inchangée depuis le rapport de 1978, de telle sorte que le domaine occupé par les amphiboles sodiques-calciques s'en trouve agrandi. Les amphiboles alcalines sont maintenant appelées amphiboles sodiques. L'utilisation des traits d'union est précisée. Les espèces d'amphibole suivantes ont été approuvées depuis 1978: nyböite, leakeite, kornite, ungarettiite, sadanagaite et cannilloite. Tous les noms mis à l'écart sont indiqués. Nous donnons la formule chimique et l'origine des noms des pôles des amphiboles, ainsi que les procédures pour calculer la proportion de Fe^{3+} et de Fe^{2+} dans les cas où elle n'a pas été déterminée directement.

(Traduit par la Rédaction)

Mots-clés: nomenclature, amphiboles, crossite, dannemorite, tirodite.

INTRODUCTION

This report was produced in response to a motion at the IMA 1986 meeting in Stanford, California, asking the CNMMN to produce a more simplified nomenclature of amphiboles than that currently approved, which dates from 1978. The 1978 nomenclature (IMA 78) took over 13 years to formulate; a quicker response was attempted this time.

To ensure a fresh look at the nomenclature scheme, the Chairman of the Amphibole Subcommittee, Prof. B.E. Leake, with the agreement of the CNMMN officials, completely reconstituted the committee so that (1) representation was more international; (2) more than 80% of the voting members of the committee were not members of the committee that produced the 1978 report; in addition, none of the CNMMN officials was on the 1978 committee; (3) three members were retained from the 1978 committee to ensure that there was some continuity and collective memory of the main problems that had been dealt with previously; (4) representation included the principal proposer to the CNMMN of an improved scheme of nomenclature;

(5) representation was sought across the various fields concerned with amphibole nomenclature, from crystal-chemists, metamorphic and igneous petrologists to computer experts and ordinary broad-based petrologists. There were 18 voting members when the major framework of the revised scheme was approved.

The committee circulated over 1000 pages over nine years, and considered in detail all proposals made to it. Views were expressed that because the amphibole system is so complicated, adequate representation cannot be made with two- and three-dimensional diagrams, whereas four variables can represent the system adequately. However, the committee, by a very large majority, wanted to retain conventional nomenclature-diagrams because they are easier for most scientists to use. The committee considered a range of different schemes of nomenclature, but none was judged overall to be sufficiently better to justify abandoning the main basis of IMA 78, which has been widely accepted and is capable of simplification to provide an improved scheme. It must be remembered that over 95% of all amphibole analyses are currently obtained by electron microprobe, with no structural information, no knowledge

of the oxidation states of Fe, Ti and Mn, the H₂O content, or how the site populations are derived. What follows is a scheme of *nomenclature*, not one to determine at which position the ions really are located.

The proposed scheme involves reducing the number of subdivisions, especially in the calcic amphiboles, making the divisions generally follow the 50% rule (whereas IMA 78 uses divisions at 90%, 70%, 67%, 50%, 33%, 30% and 10%), and making the use of adjectival modifiers (additional to prefixes that are part of the basic names) optional. The new scheme has over 20 fewer names than IMA 78, and involves the abolition of only a few commonly used names, such as crossite. End-member formulae defined and approved in IMA 78 are generally retained, although the ranges to which they apply have commonly been changed. Information on the etymology, the type locality, and the unit-cell parameters of thirty end-members is provided in Appendix 1.

The principal reference-axes of IMA 78, namely Si, Na_B and (Na + K)_A (see below), are retained, but the primary divisions between the calcic, sodic-calcic and alkali (renamed sodic) amphiboles have been adjusted to divisions at Na_B < 0.50 and Na_B ≥ 1.50, instead of Na_B < 0.67 and Na_B ≥ 1.34. (Here, and elsewhere in this report, concentrations are expressed in atoms per formula unit of the standard formula of an amphibole given below.) Previously, the amphibole "box" was divided into three equal volumes with respect to Na_B. The new scheme enlarges the sodic-calcic amphiboles at the expense of the calcic and sodic amphiboles (Fig. 1) in order to make the divisions at 50% positions.

As with the 1978 scheme, the problem of what to do with analyses in which only the total iron is known (and not its division into FeO and Fe₂O₃) has been left to individual judgement, although a recommended procedure is given. This means that again an analysis may yield different names depending upon the procedure used to estimate Fe³⁺ and Fe²⁺. It clearly would be advantageous, *for purposes of naming* an amphibole, if the recommended procedure were followed, even if other procedures were used for other purposes.

General works dealing with the amphiboles include Deer *et al.* (1963, 1997), Ernst (1968), Chukhrov (1981), Veblen (1981), Veblen & Ribbe (1982), Hawthorne (1983) and Anthony *et al.* (1995), from which adequate general background summaries can be obtained.

GENERAL CLASSIFICATION OF THE AMPHIBOLES

As with the IMA 78 scheme, the proposed nomenclature is based on chemistry and crystal symmetry; where it is necessary to distinguish different polytypes or polymorphs, this may be done by adding the space group symbol as suffix. Anthophyllite having the symmetry *Pnmm* (as distinct from the more usual *Pnma* symmetry) may be prefixed proto.

The classification is based on the chemical contents of the standard amphibole formula AB₂^{VI}C₅^{IV}T₈O₂₂(OH)₂. It is to be noted, however, that possession of this formula does not define an amphibole. An amphibole must have a structure based on a double silicate chain: a biopyribole consisting of equal numbers of pyroxene chains and triple chains would have this formula, but would not be an amphibole.

The components of the formula conventionally described as A, B, C, T and "OH" correspond to the following crystallographic sites:

A	one site per formula unit;
B	two M4 sites per formula unit;
C	a composite of five sites made up of 2 M1, 2 M2 and 1 M3 sites per formula unit;
T	eight sites, in two sets of four, which need not be distinguished in this document;
"OH"	two sites per formula unit.

The ions considered *normally* to occupy these sites are in the following categories:

□ (empty site) and K	at A only
Na	at A or B
Ca	at B only
L-type ions: Mg, Fe ²⁺ , Mn ²⁺ , Li and rarer ions of similar size, such as Zn, Ni, Co	at C or B
M-type ions: Al	at C or T
Fe ³⁺ and, more rarely, Mn ³⁺ , Cr ³⁺	at C only
High-valency ions: Ti ⁴⁺	at C or T
Zr ⁴⁺	at C only
Si	at T only
Anions: OH, F, Cl, O	at "OH".

M-type ions normally occupy M2 sites and so are normally limited to two of the five C sites. Exceptions may occur to the above "normal" behavior, but are ignored for the present purposes of nomenclature.

Throughout this report, superscript arabic numerals refer to ionic charge (oxidation state), *e.g.*, Fe²⁺, superscript roman numerals, to coordination number, *e.g.*, ^{VI}Al, and subscript numerals, to numbers of atoms, *e.g.*, Ca₂.

To take account of these facts, it is recommended that the standard amphibole formula be calculated as follows, though it must be clearly appreciated that this is an arithmetic convention that assigns ions to convenient and reasonable site-occupancies. These cannot be confirmed without direct structural evidence.

- (1) If H₂O and halogen contents are well established, the formula should be calculated to 24(O,OH,F,Cl).
- (2) If the H₂O plus halogen content is uncertain, the formula should be calculated to the basis of 23(O) with 2(OH,F,Cl) assumed, unless this leads to an impossibility of satisfying any of the following criteria, in which case an appropriate change in the assumed number of (OH + F + Cl) should be made.
- (3) Sum T to 8.00 using Si, then Al, then Ti. For the sake of simplicity of nomenclature, Fe³⁺ is not allocated to T. The normal maximum substitution for Si is 2, but this can be exceeded.

- (4) Sum C to 5.00 using excess Al and Ti from (3), and then successively Zr, Cr^{3+} , Fe^{3+} , Mn^{3+} , Mg, Fe^{2+} , Mn^{2+} , any other L^{2+} -type ions, and then Li.
- (5) Sum B to 2.00 using excess Mg, Fe^{2+} , Mn^{2+} and Li from (4), then Ca, then Na.
- (6) Excess Na from (5) is assigned to A, then all K. Total A should be between 0 and 1.00.

The most common uncertainty results from lack of analyses for H_2O , Fe^{3+} and Fe^{2+} . The procedure adopted to divide the Fe into Fe^{3+} and Fe^{2+} can influence the resulting name, especially if a composition is near $\text{Mg}/(\text{Mg} + \text{Fe}^{2+}) = 0.50$ or $\text{Fe}^{3+}/(\text{Fe}^{3+} + \text{VIAl}) = 0.50$, *i.e.*, the same bulk composition may give rise to two or more names depending upon the allocation of the Fe. The committee was almost unanimous in not wanting to specify one compulsory procedure for allocating Fe^{3+} and Fe^{2+} , but in recommending that a common procedure be used for purposes of naming the amphibole. Rock & Leake (1984) showed that, on the basis of processing results of over 500 amphibole analyses, the IMA-favored procedure of adjusting the sum (Si + Al + Cr + Ti + Fe + Mg + Mn) to 13 by varying the Fe^{3+} and Fe^{2+} appropriately gave Fe^{3+} and Fe^{2+} values reasonably close to the true determined values in 80% of the compositions studied excluding those of kaersutite, for the calcic, sodic-calcic and sodic amphiboles. If this sum is adjusted to include Li and Zr, *i.e.*, (Si + Al + Cr + Ti + Zr + Li + Fe + Mg + Mn) = 13, and if for the Mg-Fe-Mn-Li amphiboles the sum (Si + Al + Cr + Ti + Zr + Li + Fe + Mg + Mn + Ca) = 15 is used, then only the Ti ≥ 0.50 amphiboles need special treatment, although it is recognized that Mn-rich amphiboles pose problems with the variable valence state of both the Fe and Mn and that, as shown by Hawthorne (1983, p. 183-185), both in theory and practice, any calculation of Fe^{3+} and Fe^{2+} values is subject to considerable uncertainty. A full discussion of the problem and a recommended procedure, both by J.C. Schumacher, are given as Appendix 2. Some analyses have given H_2O^+ contents that lead to more than $(\text{OH})_2$ in the formula, but the structure contains only two sites for independent OH^- ions, and the structural role of the extra H ions is uncertain.

The amphiboles are classified primarily into four groups depending on the occupancy of the B sites. These four principal groups of amphibole are slightly redefined as compared with IMA 78:

- (1) Where $(\text{Ca} + \text{Na})_B$ is < 1.00 and the sum of L-type ions $(\text{Mg}, \text{Fe}, \text{Mn}, \text{Li})_B$ is ≥ 1.00 , then the amphibole is a member of the *magnesium-iron-manganese-lithium group*.
- (2) Where $(\text{Ca} + \text{Na})_B$ is ≥ 1.00 and $\text{Na}_B < 0.50$, then the amphibole is a member of the *calcic group*. Usually, but not in every case, Ca_B is > 1.50 .
- (3) Where $(\text{Ca} + \text{Na})_B$ is ≥ 1.00 and Na_B is in the range 0.50 to 1.50, then the amphibole is a member of the *sodic-calcic group*.

- (4) Where Na_B is ≥ 1.50 , then the amphibole is a member of the *sodic group*, previously referred to as alkali amphiboles. The new name is more precise, as Na is the critical element, not any other alkali element such as K or Li.

Within each of these groups, a composition can then be named by reference to the appropriate two-dimensional diagram (Figs. 2-5). These are subdivided with respect to Si and $\text{Mg}/(\text{Mg} + \text{Fe}^{2+})$ or $\text{Mg}/(\text{Mg} + \text{Mn}^{2+})$, with *prefixes* to indicate major substitutions, and *optional modifiers* to specify less important substitutions.

Within the groups, the amphiboles are divided into individually named species distinguished from one another on the basis of the heterovalent substitutions: $\text{Si} = \text{IVAl}$, $\square = (\text{Na}, \text{K})_A$, $\text{Ca}_B = \text{Na}_B$, $\text{Li} = L^{2+}$, $\text{M}_C = L^{2+}_C$, $(\text{Ti}, \text{Zr}) = L_C$, $\text{O} = (\text{OH}, \text{F}, \text{Cl})$. These substitutions necessarily occur in pairs or multiplets to maintain neutrality. The species defined on this basis are shown in Figure 1 and along the horizontal axes of Figures 2-5. Different species defined in this way correspond to different distributions of charge over the A, B, C, T, and "OH" sites. Discovery of amphiboles with new or quantitatively extended distributions of charge over these sites would merit the introduction of new species names.

Within the species, there occur homovalent substitutions, most commonly $\text{Mg} = \text{Fe}^{2+}$, $\text{VIAl} = \text{Fe}^{3+}$ and $\text{OH} = \text{F}$. The end members of these ranges of substitution are distinguished by the use of prefixes, one or other end member usually having a traditional name without a prefix. These substitutions usually correspond to independent binary systems X - Y: the name of the X end member applies over the range $1.00 > X/(X + Y) > 0.50$, and the name of the Y end member, to $1.00 > Y/(X + Y) > 0.50$. For the boundaries of substitution ranges in ternary systems, see Nickel (1992).

The discovery of amphiboles with new or exotic homovalent substitutions never requires a new species name. They can always be named by use of an appropriate prefix. In future, one root or one trivial name ONLY should be approved for each charge arrangement in each amphibole group, and all species defined by homovalent substitutions should be designated by the relevant prefix. New species defined by heterovalent substitutions [including major replacement of (OH, F, Cl) by oxygen, and major entry of high-charge (>3+) cations into A, B or C] result in new root, or new trivial names.

The principal reference-axes chosen for the calcic, sodic-calcic and sodic amphiboles are as in IMA 78, namely Na_B , $(\text{Na} + \text{K})_A$, and Si, as shown in Figure 1, but the subdivision into the sodic-calcic group is now at $\text{Na}_B = 0.50$ (instead of 0.67), and $\text{Na}_B = 1.50$ (instead of 1.34). This increases the volume, and therefore the compositional range, assigned to the sodic-calcic amphiboles at the expense of the calcic and sodic amphibole groups, but is a logical consequence of

applying the 50% rule for all divisions rather than dividing the Na_B , $(Na + K)_A$ and Si box into equal volumes, as in IMA 78. The committee considered at length various proposals for the use of axes other than the three chosen, including four components, but eventually agreed, by a significant majority, that the IMA 78 axes be retained, despite their inability to represent R^{2+} and R^{3+} (i.e., usually *L*- and *M*-type ions) separately in the *C* group. The importance of the difference between R^{2+} and R^{3+} in the *C* group has, however, been recognized rather more formally than previously by the way in which the abundance of Fe^{3+} , Al^{3+} , Cr^{3+} or Mn^{3+} has been defined with prefixes, not modifiers, where they occupy 50% or more of the normal maximum of $2R^{3+}_C$, as shown in Table 1.

Following Nickel & Mandarino (1987), prefixes are an essential part of a mineral name (e.g., ferroglauco-phane and ferro-actinolite), whereas modifiers indicate a compositional variant, and may be omitted (e.g., potassian pargasite). Modifiers generally represent subsidiary substitutions, whereas prefixes denote major substitutions. In order to reduce the number of hyphens used, a single prefix is generally joined directly to the root name without a hyphen (e.g., ferrohornblende), unless two vowels would then adjoin (e.g., ferro-actinolite) or "an unhyphenated name is awkward, and a hyphen assists in deciphering the name" (Nickel & Mandarino 1987), e.g., ferric-nyböite. For all amphibole names involving multiple prefixes, a hyphen shall be inserted between the prefixes, but not between the last prefix and the root name, unless two vowels would be juxtaposed or the name would be difficult to decipher or awkward. This convention gives rise to alumino-ferrohornblende, chloro-ferro-actinolite and fluoro-ferri-cannilloite. Most (>90%) names will lack any hyphens, and less than 5% will have more than one prefix.

In general, excluding juxtaposed vowels, the prefixes (Table 1), which have *o*, *i* or *ic* endings, are either

TABLE 1. PREFIXES IN ADDITION TO THOSE IN THE FIGURES

Prefix	Meaning*	Applicable to
Alumino	${}^{VI}Al > 1.00$	Calcic and sodic-calcic groups only
Chloro	$Cl > 1.00$	All groups
Chromio	$Cr > 1.00$	All groups
Ferri	$Fe^{3+} > 1.00$	All groups except sodic
Fluoro	$F > 1.00$	All groups
Mangano	$1.00 < Mn^{2+} < 2.99$	All groups, except for kozoilite and ungariteite
Permangano	$3.00 < Mn^{2+} < 4.99$	All groups, except for kozoilite
Mangani	$Mn^{3+} > 1.00$	All groups, except for kornite and ungariteite
Potassic	$K > 0.50$	All groups
Sodic	$Na > 0.50$	Mg-Fe-Mn-Li group only
Titano	$Ti > 0.50$	All groups, except for kaersutite
Zinco	$Zn > 1.00$	All groups

The prefixes in the figures are ferro ($Fe^{2+} > Mg$) and magnesio ($Fe^{2+} < Mg$); in Figure 5a only, ferric is used as a prefix, as in ferri-nyböite, with ${}^{VI}Al < Fe^{3+}$ (not ferricynyböite, which is not clear). * Concentrations are expressed in atoms per formula unit.

attached directly to the root name (without a space or hyphen) or to a following prefix with a hyphen. All these characters distinguish them from modifiers.

All modifiers (Table 2) have an "ian" or "oan" ending to indicate moderate substitutions, as listed by Nickel & Mandarino (1987). Modifiers are not accompanied by a hyphen, and are invariably followed by a space and then the remainder of the name. The excluded applications follow from the fact that these groups will usually have substantial contents of these elements as part of the parameters that define them. The use of modifiers is optional and strictly qualitative (i.e., they can be used in other senses than in Table 2, but use as in Table 2 is strongly recommended).

THE NAMING OF AMPHIBOLES IN THIN SECTION AND HAND SPECIMEN

For amphiboles of which the general nature only is known, for instance from optical properties, without benefit of a chemical analysis, it is not generally possible to allocate a precise name. The nearest assigned amphibole name should then be made into an adjective, followed by the word amphibole, e.g., anthophyllitic amphibole, tremolitic amphibole, pargasitic amphibole, glaucophanic amphibole and richteritic amphibole. The familiar word *hornblende* can still be used where appropriate for calcic amphiboles in both hand specimen and thin section, because hornblende is never used without a prefix (ferro or magnesio) in the precise classification, such that confusion should not arise between colloquial use and precise use.

TABLE 2. MODIFIERS AND THEIR SUGGESTED RANGES

Modifier	Meaning*	Applicable to
Barian	$Ba > 0.10$	All groups
Borian	$B > 0.10$	All groups
Calcian	$Ca > 0.50$	Mg-Fe-Mn-Li group
Chlorian	$0.25 < Cl < 0.99$	All groups
Chromian	$0.25 < Cr < 0.99$	All groups
Ferrian	$0.75 < Fe^{3+} < 0.99$	All groups except sodic
Fluorian	$0.25 < F < 0.99$	All groups
Hydroxylian	$OH > 3.00$	All groups
Lithian	$Li > 0.25$	All groups, but excludes those species defined by the abundance of lithium (e.g., holmquistite)
Manganoan	$0.25 < Mn^{2+} < 0.99$	All groups, but excludes those species defined by the abundance of Mn^{2+}
Manganian	$0.25 < Mn^{3+} \text{ or } Mn^{4+} < 0.99$	All groups, but excludes those species defined by the abundance of Mn^{3+} (e.g., kornite)
Nickeloan	$Ni > 0.10$	All groups
Oxygenian	$(OH + F + Cl) < 1.00$	All groups, except for ungariteite
Potassian	$0.25 < K < 0.49$	All groups
Plumbian	$Pb > 0.10$	All groups
Sodian	$0.25 < Na < 0.49$	Mg-Fe-Mn-Li group only
Strontian	$Sr > 0.10$	All groups
Titanian	$0.25 < Ti < 0.49$	All groups
Vanadian	$V > 0.10$	All groups
Zincian	$0.10 < Zn < 0.99$	All groups
Zirconian	$Zr > 0.10$	All groups

* Concentrations are expressed in atoms per formula unit.

As in IMA 78, asbestiform amphiboles should be named according to their precise mineral name, as listed in this report, followed by the suffix -asbestos, e.g., anthophyllite-asbestos, tremolite-asbestos. Where the nature of the mineral is uncertain or unknown, asbestos alone or amphibole-asbestos may be appropriate. If the approximate nature of the mineral only is known, the above recommendations should be followed, but with the word amphibole replaced by asbestos, e.g., anthophyllitic asbestos, tremolitic asbestos.

Mg-Fe-Mn-Li AMPHIBOLES

The group is defined as possessing $(Ca + Na)_B < 1.00$ and $(Mg, Fe, Mn, Li)_B \geq 1.00$ in the standard formula; the detailed classification is shown in Figure 2. The main changes from IMA 78 are the adoption of divisions at $Mg/(Mg + Fe^{2+}) = 0.50$, the reduction of adjectives, and the abolition of tirodite and danemorite.

Orthorhombic forms of the Mg-Fe-Mn-Li amphiboles

(1) Anthophyllite series

$Na_xLi_z(Mg, Fe^{2+}, Mn)_{7-y-z}Al_y(Si_{8-x-y+z}Al_{x+y-z})O_{22}(OH, F, Cl)_2$, where $Si > 7.00$ (otherwise the mineral is gedrite) and $Li < 1.00$ (otherwise the mineral is holmquistite). Most samples of anthophyllite have the *Pnma* structure; those with the *Pnmm* structure may be prefixed proto without a hyphen.

End members

Anthophyllite	$\square Mg_7Si_8O_{22}(OH)_2$
Ferro-anthophyllite	$\square Fe^{2+}_7Si_8O_{22}(OH)_2$
Sodicanthophyllite	$NaMg_7Si_7AlO_{22}(OH)_2$
Sodic-ferro-anthophyllite	$NaFe^{2+}_7Si_7AlO_{22}(OH)_2$

Limits for the use of names of end members

Anthophyllite	$Mg/(Mg + Fe^{2+}) \geq 0.50$
Ferro-anthophyllite	$Mg/(Mg + Fe^{2+}) < 0.50$
Sodicanthophyllite	$Mg/(Mg + Fe^{2+}) \geq 0.50$; $Na \geq 0.50$
Sodic-ferro-anthophyllite	$Mg/(Mg + Fe^{2+}) < 0.50$; $Na \geq 0.50$

(2) Gedrite series

$Na_xLi_z(Mg, Fe^{2+}, Mn)_{7-y-z}Al_y(Si_{8-x-y+z}Al_{x+y-z})O_{22}(OH, F, Cl)_2$, where $(x + y - z) \geq 1.00$, so that $Si < 7.00$, this being the distinction from anthophyllite. $Li < 1.00$.

End members

Gedrite	$\square Mg_5Al_2Si_6Al_2O_{22}(OH)_2$
Ferrogedrite	$\square Fe^{2+}_5Al_2Si_6Al_2O_{22}(OH)_2$
Sodicgedrite	$NaMg_6AlSi_6Al_2O_{22}(OH)_2$

Sodic-ferrogedrite	$NaFe^{2+}_6AlSi_6Al_2O_{22}(OH)_2$
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Limits for the use of names of end members

Gedrite	$Mg/(Mg + Fe^{2+}) \geq 0.50$
Ferrogedrite	$Mg/(Mg + Fe^{2+}) < 0.50$
Sodicgedrite	$Mg/(Mg + Fe^{2+}) \geq 0.50$; $Na \geq 0.50$
Sodic-ferrogedrite	$Mg/(Mg + Fe^{2+}) < 0.50$; $Na \geq 0.50$

It should be noted that gedrite and ferrogedrite, with or without sodic as a prefix, extend down to at least Si 5.50. Discovery of homogeneous $Na(Fe, Mg)_5Al_2Si_5Al_3O_{22}(OH)_2$ will justify a new name.

(3) Holmquistite series

$\square [Li_2(Mg, Fe^{2+})_3(Fe^{3+}, Al)_2]Si_8O_{22}(OH, F, Cl)_2$. $Li \geq 1.00$ is critical.

End members

Holmquistite	$\square (Li_2Mg_3Al_2)Si_8O_{22}(OH)_2$
Ferroholmquistite	$\square (Li_2Fe^{2+}_3Al_2)Si_8O_{22}(OH)_2$

Limits for the use of names of end members

Holmquistite	$Mg/(Mg + Fe^{2+}) \geq 0.50$
Ferroholmquistite	$Mg/(Mg + Fe^{2+}) < 0.50$

Monoclinic forms of the Mg-Fe-Mn-Li amphiboles

(1) Cummingtonite-Grunerite series

$\square (Mg, Fe^{2+}, Mn, Li)_7Si_8O_{22}(OH)_2$. $Li < 1.00$. Most members of this series have space group *C2/m*; those with space group *P2/m* may optionally have this symbol added as a suffix at the end of the name.

End members

Cummingtonite	$\square Mg_7Si_8O_{22}(OH)_2$
Grunerite	$\square Fe^{2+}_7Si_8O_{22}(OH)_2$
Manganocummingtonite	$\square Mn_2Mg_5Si_8O_{22}(OH)_2$
Permanganogrunerite	$\square Mn_4Fe^{2+}_3Si_8O_{22}(OH)_2$
Manganogrunerite	$\square Mn_2Fe^{2+}_5Si_8O_{22}(OH)_2$

Limits for the use of names of end members

Cummingtonite	$Mg/(Mg + Fe^{2+}) \geq 0.50$
Grunerite	$Mg/(Mg + Fe^{2+}) < 0.50$
Manganocummingtonite	$Mg/(Mg + Fe^{2+}) \geq 0.50$; $1.00 < Mn < 3.00$
Permanganogrunerite	$Mg/(Mg + Fe^{2+}) < 0.50$; $3.00 < Mn < 5.00$
Manganogrunerite	$Mg/(Mg + Fe^{2+}) < 0.50$; $1.00 < Mn < 3.00$

Mg-Fe-Mn-Li amphiboles

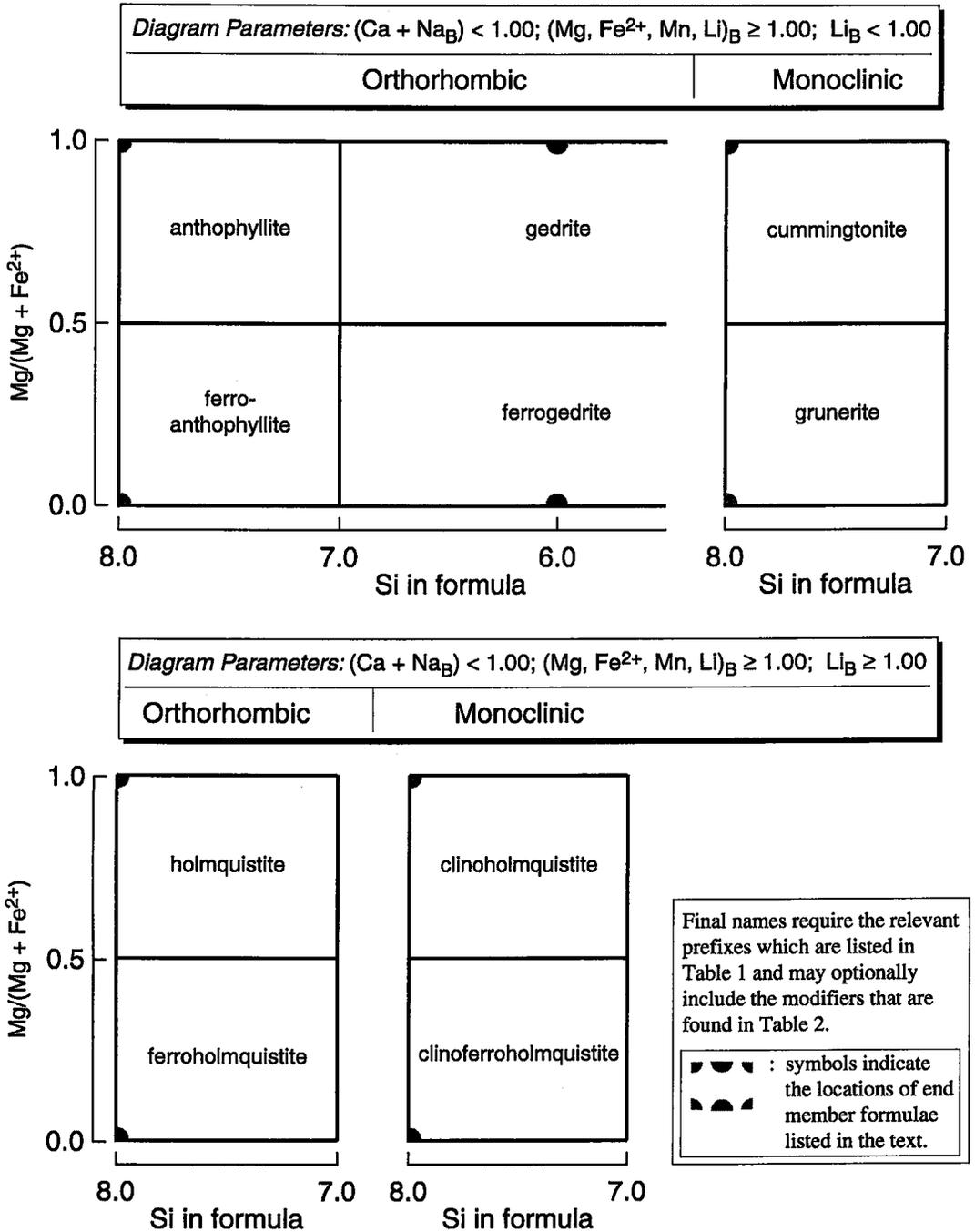
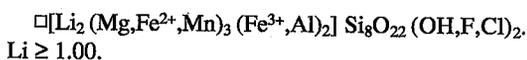


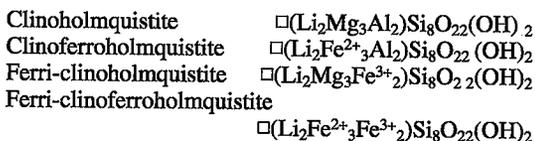
FIG. 2. Classification of the Mg-Fe-Mn-Li amphiboles.

It should be noted that the names given extend down to 7.00 Si. If a mineral with less than 7.00 Si is discovered, then it will justify a new name based on the end member $Mg_3Al_2Si_6Al_2O_{22}(OH)_2$.

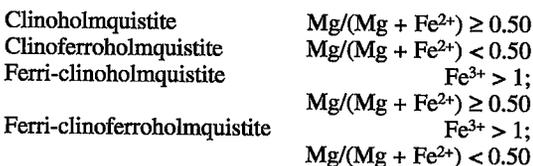
(2) *Clinoholmquistite series*



End members



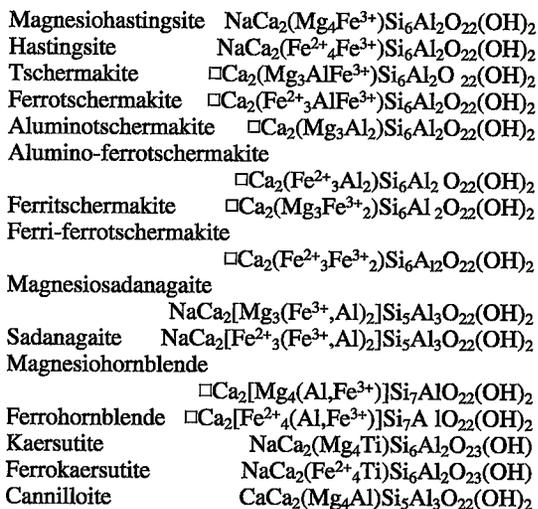
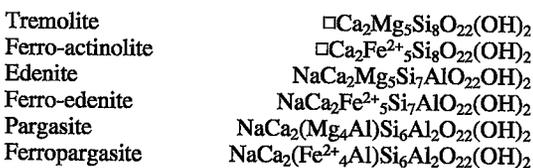
Limits for the use of names of end members



CALCIC AMPHIBOLES

The group is defined as monoclinic amphiboles in which $(Ca + Na)_B \geq 1.00$, and Na_B is between 0.50 and 1.50; usually, $Ca_B \geq 1.50$. The detailed classification is shown in Figure 3. The number of subdivisions used in IMA 78 has been more than halved; silicic edenite and compound names like tschermakitic hornblende have been abolished, sadanagaite (Shimazaki *et al.* 1984) and cannilloite (Hawthorne *et al.* 1996b) have been added, and the boundaries of the group have been revised. Hornblende is retained as a general or colloquial term for colored calcic amphiboles without confusion with respect to the precise range shown in Figure 3 because hornblende is always prefixed with "ferro" or "magnesio" in the precise nomenclature. Because of the strong desire, especially (but not solely) expressed by metamorphic petrologists, to retain the distinction of green actinolite from colorless tremolite, the subdivisions tremolite, actinolite, ferro-actinolite of IMA 78 are retained, as shown in Figure 3.

End members



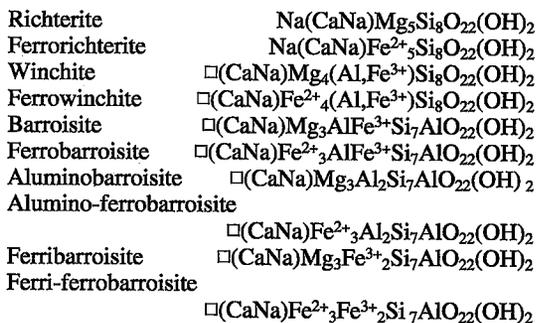
Limits for the use of the names of end members

These are summarized in Figure 3 with respect to Si, $(Na + K)_A$, $Mg / (Mg + Fe^{2+})$ and Ti. The prefixes ferri and alumino are only used where $Fe^{3+} > 1.00$ and $VI Al > 1.00$ (Table 1). For kaersutite and ferrokaersutite, Ti ≥ 0.50 ; any lower Ti content may optionally be indicated as in Table 2. Cannilloite requires $Ca_A \geq 0.50$.

SODIC-CALCIC AMPHIBOLES

This group is defined to include monoclinic amphiboles in which $(Ca + Na)_B \geq 1.00$ and $0.50 < Na_B < 1.50$. The detailed classification is shown in Figure 4. There are no significant changes from IMA 78 except for the 50% expansion of the volume occupied by the group in Figure 1. Because of the concentration of compositions relatively near the end members, the increase in the number of compositions in this group compared with the number classified in IMA 78 is quite small (much less than 50%). Nevertheless, a number of previously classified calcic and alkali amphiboles now become sodic-calcic amphiboles.

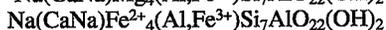
End members



Magnesiokatophorite



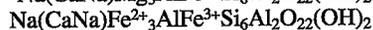
Katophorite



Magnesiotaramite



Taramite



calcic amphiboles

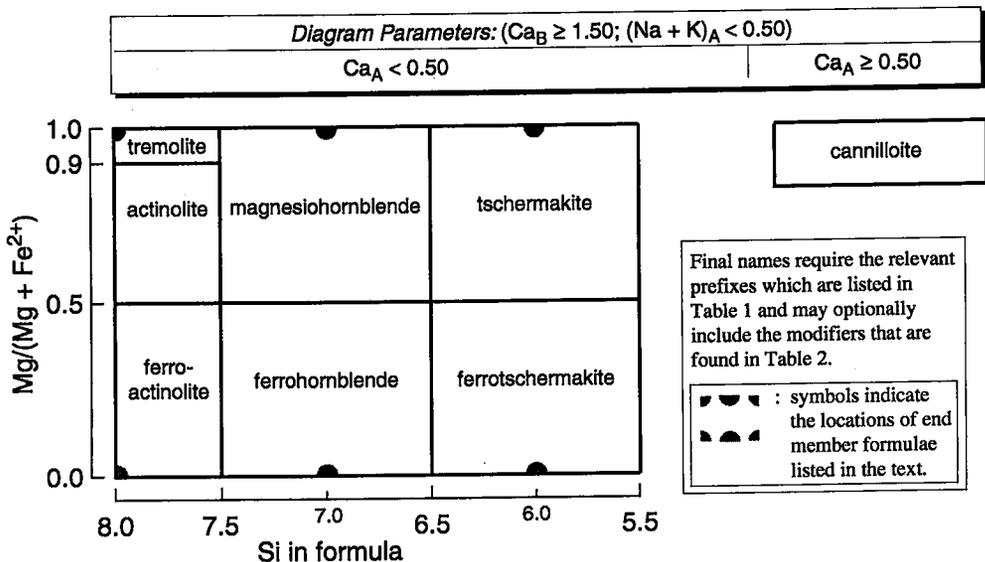
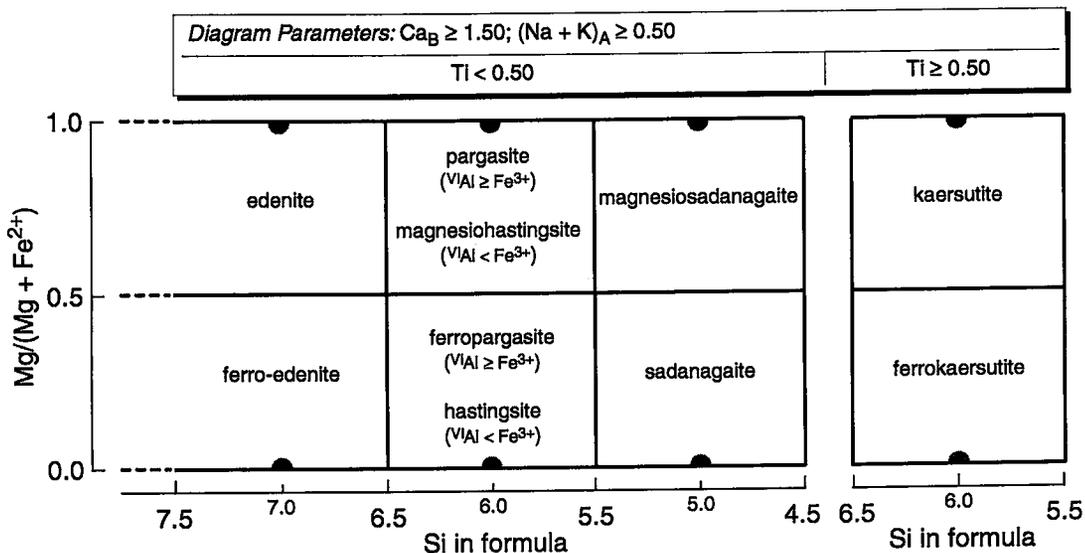
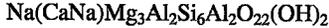


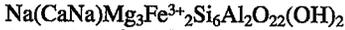
FIG. 3. Classification of the calcic amphiboles.

Alumino-magnesiotalarumite



Aluminotalarumite $\text{Na}(\text{CaNa})\text{Fe}^{2+}_3\text{Al}_2\text{Si}_6\text{Al}_2\text{O}_{22}(\text{OH})_2$

Ferri-magnesiotalarumite



Ferritalarumite $\text{Na}(\text{CaNa})\text{Fe}^{2+}_3\text{Fe}^{3+}_2\text{Si}_6\text{Al}_2\text{O}_{22}(\text{OH})_2$

Limits for the use of names of end members

These are summarized in Figure 4 with respect to Si, $(\text{Na} + \text{K})_A$ and $\text{Mg}/(\text{Mg} + \text{Fe}^{2+})$. Alumino and ferri are again restricted to ${}^{\text{VI}}\text{Al} > 1.00$ and $\text{Fe}^{3+} > 1.00$, being 50% of the normal maximum of $2R^{3+}_C$ sites.

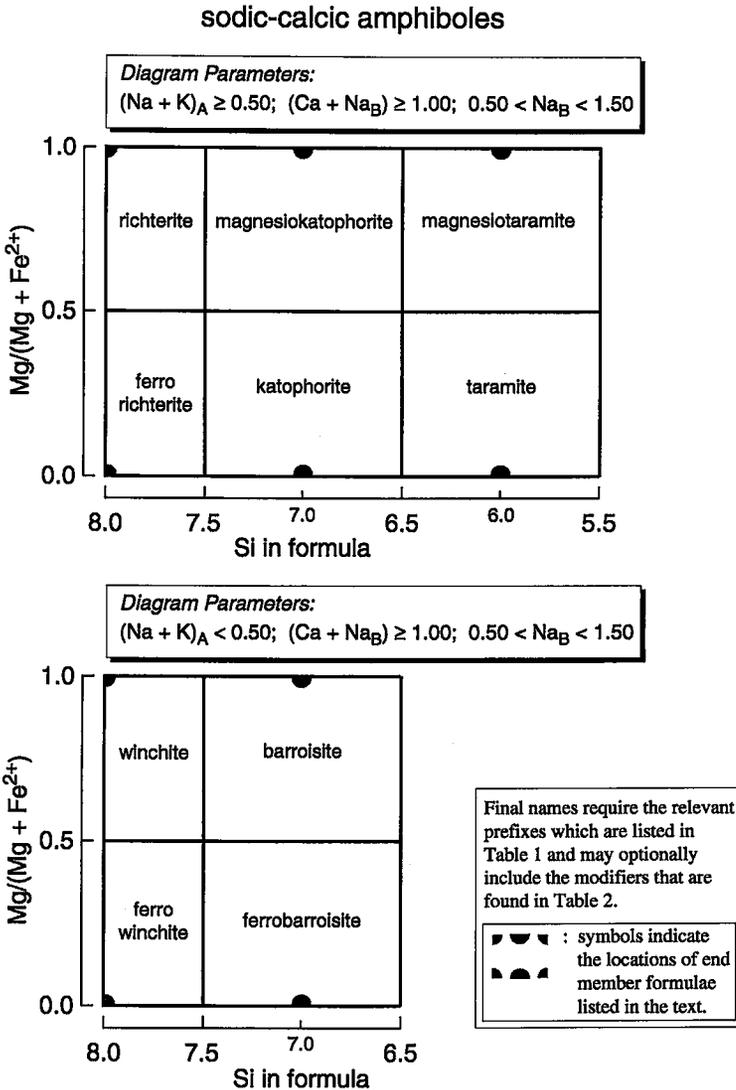


FIG. 4. Classification of the sodic-calcic amphiboles.

sodic amphiboles

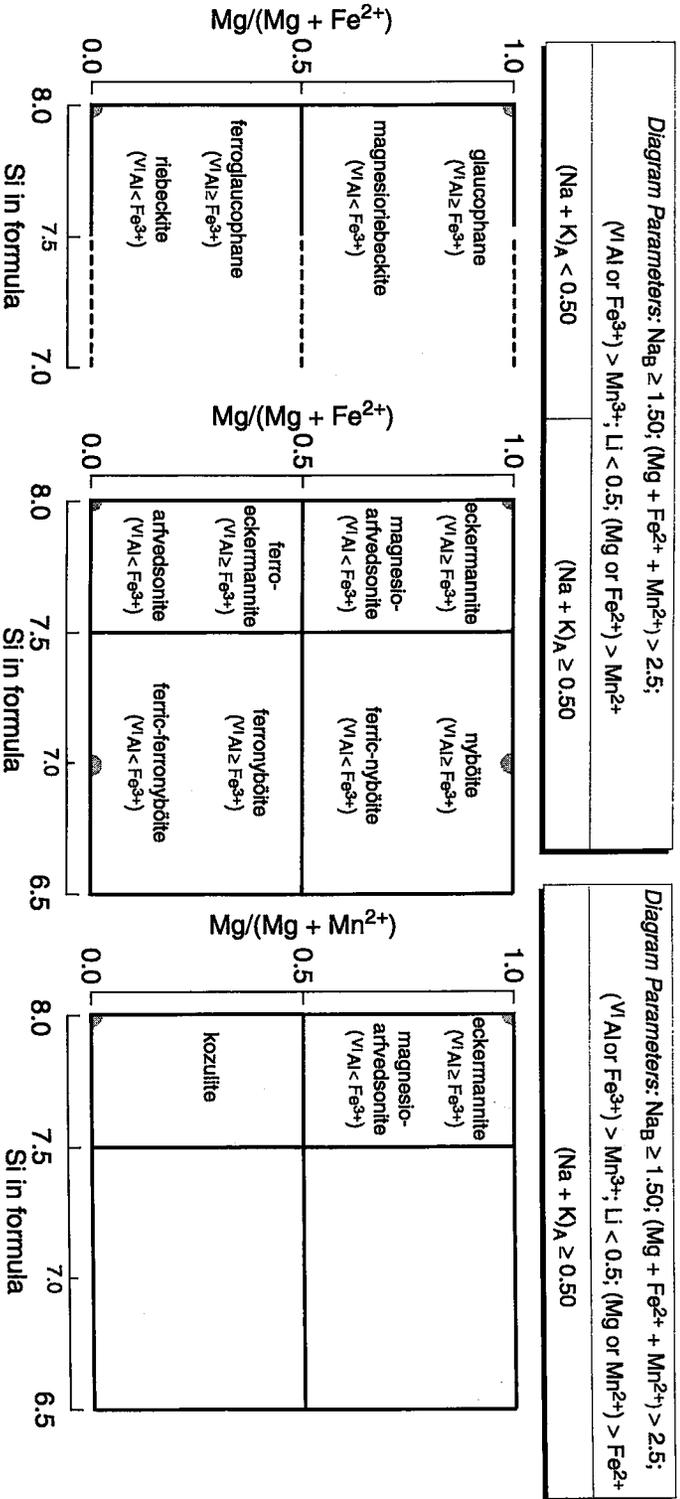
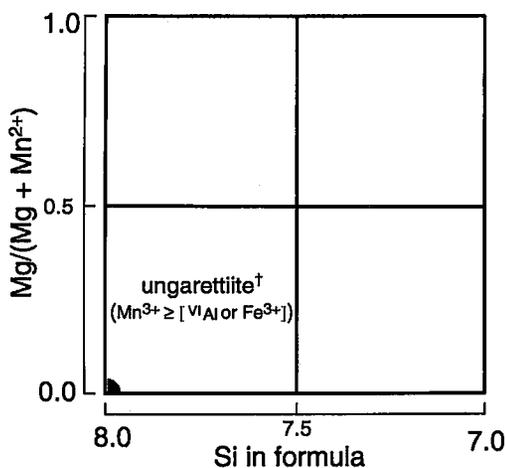
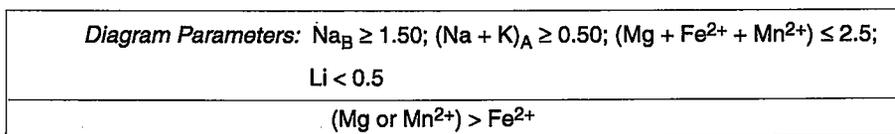
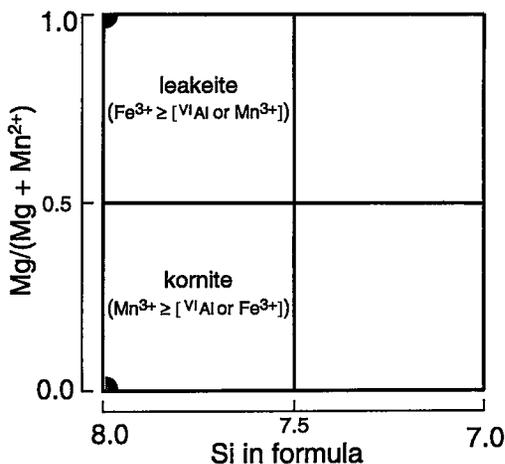
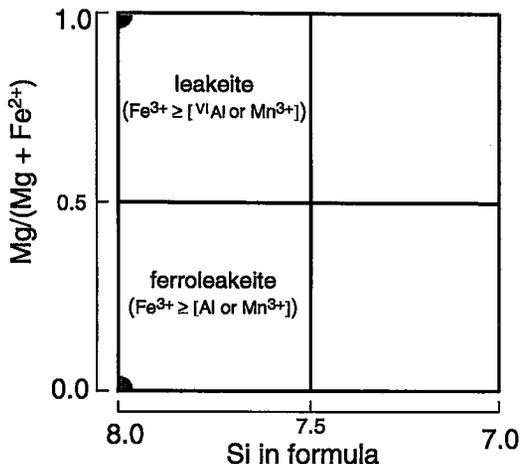
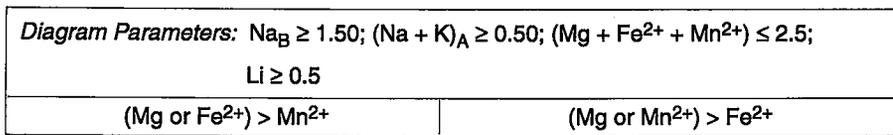


FIG. 5a. Classification of the sodic amphiboles with $(\text{Mg} + \text{Fe}^{2+} + \text{Mn}^{2+}) > 2.5$ apfu.

sodic amphiboles



Final names require the relevant prefixes which are listed in Table 1 and may optionally include the modifiers that are found in Table 2.

: symbols indicate the locations of end member formulae listed in the text.

†ideal formula is free of OH,F,Cl; the anion configuration is: ...O₂₂O₂

FIG. 5b. Classification of the sodic amphiboles with $(Mg + Fe^{2+} + Mn^{2+}) \leq 2.5$ apfu.

SODIC AMPHIBOLES

This group is defined to include monoclinic amphiboles in which $Na_B \geq 1.50$. The detailed classification is shown in Figures 5a and 5b. Apart from revision of the boundary at $Na_B \geq 1.50$ instead of $Na_B \geq 1.34$, and the abolition of crossite so that the 50% division is followed, the principal changes are the introduction of nyböite, with Si close to 7, as approved in 1981 (Ungaretti *et al.* 1981), ferric-nyböite (instead of the previously abandoned "anophorite"), leakeite (Hawthorne *et al.* 1992), ferroleakeite (Hawthorne *et al.* 1996a), kornite (Armbruster *et al.* 1993), and ungarettiite (Hawthorne *et al.* 1995).

End members

Glaucophane	$\square Na_2(Mg_3Al_2)Si_8O_{22}(OH)_2$
Ferroglaucophane	$\square Na_2(Fe^{2+}_3Al_2)Si_8O_{22}(OH)_2$
Magnesioriebeckite	$\square Na_2(Mg_3Fe^{3+}_2)Si_8O_{22}(OH)_2$
Riebeckite	$\square Na_2(Fe^{2+}_3Fe^{3+}_2)Si_8O_{22}(OH)_2$
Eckermannite	$NaNa_2(Mg_4Al)Si_8O_{22}(OH)_2$
Ferro-eckermannite	$NaNa_2(Fe^{2+}_4Al)Si_8O_{22}(OH)_2$
Magnesio-arfvedsonite	$NaNa_2(Mg_4Fe^{3+})Si_8O_{22}(OH)_2$
Arfvedsonite	$NaNa_2(Fe^{2+}_4Fe^{3+})Si_8O_{22}(OH)_2$
Kozulite	$NaNa_2Mn^{2+}_4(Fe^{3+}, Al)Si_8O_{22}(OH)_2$
Nyböite	$NaNa_2(Mg_3Al_2)Si_7AlO_{22}(OH)_2$
Ferronyböite	$NaNa_2(Fe^{2+}_3Al_2)Si_7AlO_{22}(OH)_2$
Ferric-nyböite	$NaNa_2(Mg_3Fe^{3+}_2)Si_7AlO_{22}(OH)_2$
Ferric-ferronyböite	$NaNa_2(Fe^{2+}_3Fe^{3+}_2)Si_7AlO_{22}(OH)_2$
Leakeite	$NaNa_2(Mg_2Fe^{3+}_2Li)Si_8O_{22}(OH)_2$
Ferroleakeite	$NaNa_2(Fe^{2+}_2Fe^{3+}_2Li)Si_8O_{22}(OH)_2$
Kornite	$(Na,K)Na_2(Mg_2Mn^{3+}_2Li)Si_8O_{22}(OH)_2$
Ungarettiite	$NaNa_2(Mn^{2+}_2Mn^{3+}_2)Si_8O_{22}O_2$

Limits for the use of names of end members

These are summarized in Figure 5 with respect to Si, $(Na + K)_A$ and $Mg/(Mg + Fe^{2+})$, Li and Mn parameters. Kozulite requires $Mn^{2+} > (Fe^{2+} + Fe^{3+} + Mg + {}^VI Al)$, with ${}^VI Al$ or $Fe^{3+} > Mn^{3+}$, $Li < 0.5$. Ungarettiite has both Mn^{2+} and $Mn^{3+} > (Fe^{2+} + Mg + Fe^{3+} + {}^VI Al)$, with $Li < 0.5$ and $(OH + F + Cl) < 1.00$. Leakeite and kornite require $Mg/(Mg + Fe^{2+}) \geq 0.50$, $Li \geq 0.50$, with $Fe^{3+} > Mn^{3+}$ in leakeite, and $Fe^{3+} < Mn^{3+}$ in kornite. Ferric-nyböite means $Fe^{3+} \geq {}^VI Al$, which should be clearly distinguished from ferri (meaning $Fe^{3+} > 1.00$), because neither aluminous (meaning ${}^VI Al > 1.00$) nor ferri are used as prefixes in the sodic amphiboles.

AMPHIBOLE NAMES RECOMMENDED
TO BE FORMALLY ABANDONED

The following names of amphiboles used in IMA 78 are recommended to be formally abandoned. IMA 78 listed 193 abandoned names.

Magnesio-anthophyllite	= anthophyllite
Sodium-anthophyllite	= sodicanthophyllite
Magnesio-gedrite	= gedrite
Sodium gedrite	= sodicgedrite
Magnesio-holmquistite	= holmquistite
Magnesio-cummingtonite	= cummingtonite
Tirodite	= manganocummingtonite
Dannemorite	= manganogrunerite
Magnesio-clinoholmquistite	= clinoholmquistite
Crossite	= glaucophane or ferroglaucophane or magnesioriebeckite or riebeckite
Tremolitic hornblende	= magnesiohornblende
Actinolitic hornblende	= magnesiohornblende
Ferro-actinolic hornblende	= ferrohornblende
Tschermakitic hornblende	= tschermakite
Ferro-tschermakitic hornblende	= ferrotschermakite
Edenitic hornblende	= edenite
Ferro-edenitic hornblende	= ferro-edenite
Pargasitic hornblende	= pargasite
Ferroan pargasitic hornblende	= pargasite or ferropargasite
Ferro-pargasitic hornblende	= ferropargasite
Ferroan pargasite	= pargasite or ferropargasite
Silicic edenite	= edenite
Silicic ferro-edenite	= ferro-edenite
Magnesio-hastingsitic hornblende	= magnesiohastingsite
Magnesian hastingsitic hornblende	= magnesiohastingsite or hastingsite
Hastingsitic hornblende	= hastingsite
Magnesian hastingsite	= magnesiohastingsite or hastingsite

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- _____, _____, OTTOLINI, L., GRICE, J.D. & CZAMANSKE, G.K. (1996a): Fluor-ferro-leakeite, $\text{NaNa}_2(\text{Fe}^{2+}_2\text{Fe}^{3+}_2\text{Li})\text{Si}_8\text{O}_{22}\text{F}_2$, a new alkali amphibole from the Cañada Pinabete pluton, Questa, New Mexico, U.S.A. *Am. Mineral.* **81**, 226-228.
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Received December 22, 1996.

APPENDIX 1. INFORMATION CONCERNING THE ETYMOLOGY, THE TYPE LOCALITY, AND THE UNIT-CELL PARAMETERS OF THIRTY AMPHIBOLE END-MEMBERS

Actinolite

Etymology: From the Greek, *aktin*, a ray, and *lithos*, a stone, alluding to the radiating habit.

Type locality: None.

X-ray data: a 9.884, b 18.145, c 5.294 Å, β 104.7° [powder-diffraction file (PDF) 25-157 on specimen from Sobotin, Czech Republic].

References: Kirwan, R. (1794): *Elements of Mineralogy* 1, 167 (actynolite). Modified by Dana, J.D. (1837): *Systematic Mineralogy* (1st ed.), 309.

Anthophyllite

Etymology: The name is derived from the Latin *anthophyllum*, clove, referring to its characteristic brown color.

Type locality: Described by Schumacher (1801, p. 96) as being from the Kongsberg area, Norway, the exact locality being kept secret, but later (Möller 1825) described it as being from Kjennerudvann Lake near Kongsberg.

X-ray data: a 18.5, b 17.9, c 5.28 Å (PDF 9-455 on specimen from Georgia, U.S.A.).

References: Möller, N.B. (1825): *Magazin for Naturvedenskaberne*. Christiania, Norway 6, 174. Schumacher, C.F. (1801): *Versuch Verzeich. Danisch-Nordisch Staat, Einfach Mineral.*, 96 and 165.

Arfvedsonite

Etymology: Named after J.A. Arfvedson.

Type locality: Kangerdluarsuk, Greenland.

X-ray data: a 9.94, b 18.17, c 5.34 Å. β 104.40° (PDF 14-633 on specimen from Nunarsuatsiak, Greenland).

References: Brooke, H.J. (1823): *Ann. Phil.* 21 (2nd ser., vol. 5), 381 (arfvedsonite). Amended by T. Thomson (1836): *Outlines of Mineralogy, Geology, and Mineral Analysis* 1, 483.

Barroisite

Etymology: Origin of name not found.

Type locality: Not traced.

References: Murgoci, G. (1922): *C.R. Acad. Sci. Paris* 175A, 373 and 426. Defined by Leake, B.E. (1978): *Can. Mineral.* 16, 514.

Cannilloite

Etymology: Named after Elio Cannillo of Pavia, Italy.

Type locality: Pargas, Finland.

X-ray data (for fluor-cannilloite): a 9.826, b 17.907, c 5.301 Å, β 105.41°.

Reference: Hawthorne, F.C., Oberti, R., Ungaretti, L. & Grice, J.D. (1996): *Am. Mineral.* 81, 995.

Clinoholmquistite

Etymology: Named as the monoclinic polymorph of holmquistite.

Type locality: Golzy, Sayany Mountain, Siberia, Russia.

X-ray data: a 9.80, b 17.83, c 5.30 Å, β 109.10° (PDF 25-498 on specimen from Siberia, Russia).

References: Ginzburg, I.V. (1965): *Trudy Mineral. Muz. Akad. Nauk SSSR* 16, 73. Defined by Leake, B.E. (1978): *Can. Mineral.* 16, 511. Forms a series with magnesio-clinoholmquistite and ferro-clinoholmquistite.

Cummingtonite

Etymology: Named after the discovery locality.

Type locality: Cummington, Massachusetts, U.S.A.

X-ray data: a 9.534, b 18.231, c 5.3235 Å, β 101.97° (PDF 31-636 on specimen from Wabush iron formation, Labrador, Canada).

References: Dewey, C. (1824): *Am. J. Sci.* 8, 58. Defined by Leake, B.E. (1978): *Can. Mineral.* 16, 511.

Eckermannite

Etymology: Named after H. von Eckermann.

Type locality: Norra Kärr, Sweden.

X-ray data: a 9.7652, b 17.892, c 5.284 Å, β 103.168° (PDF 20-386 on synthetic material).

References: Adamson, O.J. (1942): *Geol. Fören. Stockholm Förh.* 64, 329. See also Adamson, O.J. (1944): *Geol. Fören. Stockholm Förh.* 66, 194. Defined by Leake, B.E. (1978): *Can. Mineral.* 16, 515.

Edenite

Etymology: Named after the discovery locality.

Type locality: Eden (Edenville), New York, U.S.A.

X-ray data: a 9.837, b 17.954, c 5.307 Å, β 105.18° (PDF 23-1405 on specimen from Franklin Furnace, New Jersey, U.S.A.).

References: Not analyzed in original description. Two analyses of toptype material, reported by C.F. Rammsberg (1858): *Ann. Phys. Chem. (Pogg.)* 103, 441, and by Hawes, G.W. (1878): *Am. J. Sci.* 116, 397, differ considerably, and neither falls within the edenite range of Leake, B.E. (1978): *Can. Mineral.* 16, 512). The current definition was proposed by Sundius, N. (1946):

Årsbok Sver. Geol. Unders. **40**(4). Composition nearest to the end member may be that of Leake, B.E. (1971): *Mineral. Mag.* **38**, 405.

Gedrite

Etymology: Named after the discovery locality.

Type locality: Héas Valley, near Gèdre, France.

X-ray data: *a* 18.594, *b* 17.890, *c* 5.304 Å (PDF 13-506 on specimen from Grafton, Oxford County, Maine, U.S.A.).

References: Dufrénoy, A. (1836): *Ann. Mines, sér.* **3**, **10**, 582. Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 510.

Glaucophan

Etymology: From the Greek *glaukos*, bluish green, and *phainesthai*, to appear.

Type locality: Syra, Cyclades, Greece.

X-ray data: *a* 9.595, *b* 17.798, *c* 5.307 Å, β 103.66° (PDF 20-453 on specimen from Sebastopol Quadrangle, California, U.S.A. See also PDF 15-58 and 20-616).

Reference: Hausman, J.F.L. (1845): *Gel. Kön Ges. Wiss. Göttingen*, 125 (Glaukophan).

Grunerite

Etymology: Named after E.L. Gruner.

Type locality: Collobrières, Var, France.

X-ray data: *a* 9.57, *b* 18.22, *c* 5.33 Å (PDF 17-745 on specimen from White Lake, Labrador, Canada).

References: Described by Gruner, E.L. (1847): *C.R. Acad. Sci.* **24**, 794, but named by Kenngott, A. (1853): *Mohs'sche Mineral. Syst.*, 69. Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 511.

Hastingsite

Etymology: Named after the discovery locality.

Type locality: Hastings County, Ontario, Canada.

X-ray data: *a* 9.907, *b* 18.023, *c* 5.278 Å, β 105.058° (PDF 20-378 on specimen from Dashkesan, Transcaucasia, Russia. See also PDF 20-469).

References: Adams, F.D. & Harrington, B.J. (1896): *Am. J. Sci.* **151**, 212; Adams, F.D. & Harrington, B.J. (1896): *Can. Rec. Sci.* **7**, 81. Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 513).

Holmquistite

Etymology: Named after P.J. Holmquist.

Type locality: Utö, Stockholm, Sweden.

X-ray data: *a* 18.30, *b* 17.69, *c* 5.30 Å (PDF 13-401 on specimen from Barraute, Quebec, Canada).

References: Osann, A. (1913): *Sitz. Heidelberg Akad. Wiss., Abt. A, Abh.*, 23. Dimorphous with clinoholm-

quistite. Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 511.

Hornblende

Etymology: The name is from the German mining term *horn*, horn, and *blenden*, to dazzle.

Reference: The use of the term hornblende and its relationship to other calcic amphiboles was discussed by Deer *et al.* (1963): *Rock-Forming Minerals. 2. Chain Silicates*. Longmans, London (p. 265). Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 512-513.

Kaersutite

Etymology: Named after the discovery locality.

Type locality: Kaersut, Umanaksfjord, Greenland.

X-ray data: *a* 9.83, *b* 17.89, *c* 5.30 Å, β 105.18° (PDF 17-478 on specimen from Boulder Dam, Arizona, U.S.A.).

References: Lorenzen, J. (1884): *Medd. Grønland* **7**, 27. Defined and given species status by Leake, B.E. (1978): *Can. Mineral.* **16**, 513.

Katophorite

Etymology: From the Greek *kataphora*, a rushing down, in reference to its volcanic origin.

Type locality: Christiana District (now Oslo), Norway.

References: Brögger, W.C. (1894): *Die Eruptivgest. Kristianiagebietes, Skr. Vid.-Selsk. I, Math.-natur. Kl* **4**, 27. Frequently spelled catophorite, and other variants, but the accepted IMA spelling is katophorite. Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 514.

Kornite

Etymology: Named after H. Korn.

Type locality: Wessels mine, Kalahari Manganese Fields, South Africa.

X-ray data: *a* 9.94(1), *b* 17.80(2), *c* 5.302(4) Å, β 105.52°.

Reference: Armbruster, T., Oberhänsli, R., Bermanec, V. & Dixon, R. (1993): *Schweiz. Mineral. Petrogr. Mitt.* **73**, 349.

Kozulite

Etymology: Named after S. Kozu.

Type locality: Tanohata mine, Iwate Prefecture, Japan.

X-ray data: *a* 9.991, *b* 18.11, *c* 5.30 Å, β 104.6° (PDF 25-850).

References: Nambu, M., Tanida, K. & Kitamura, T. (1969): *J. Japan. Assoc. Mineral. Petrogr. Econ. Geol.* **62**, 311. Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 515.

Leakeite

Etymology: Named after B.E. Leake.

Type locality: Kajlidongri manganese mine, Jhabua district, Madhya Pradesh, India.

X-ray data: a 9.822, b 17.836, c 5.286 Å, β 104.37°.

Reference: Hawthorne, F.C., Oberti, R., Ungaretti, L. & Grice, J.D. (1992): *Am. Mineral.* **77**, 1112.

Nyböite

Etymology: Named after the discovery locality.

Type locality: Nybö, Nordfjord, Norway.

X-ray data: In Ungaretti *et al.* (1981), X-ray data are given for many specimens, and a single "type" specimen was not distinguished.

Reference: Ungaretti, L., Smith, D.C. & Rossi, G. (1981): *Bull. Minéral.* **104**, 400.

Pargasite

Etymology: Named after the discovery locality.

Type locality: Pargas, Finland.

X-ray data: a 9.870, b 18.006, c 5.300 Å, β 105.43° (PDF 23-1406, and PDF 41-1430 on synthetic material).

References: Von Steinheil, F. (1814) in *Tasch. Mineral.* (1815): **9**(1), 309. The name was widely used for green hornblende, but was redefined by Sundius, N. (1946): *Årsbok Sver. Geol. Unders.* **40**, 18, and Leake, B.E. (1978): *Can. Mineral.* **16**, 507 and 513.

Richterite

Etymology: Named after T. Richter.

Type locality: Långban, Värmland, Sweden.

X-ray data: a 9.907, b 17.979, c 5.269 Å, β 104.25° (PDF 25-808 on synthetic material; see also PDF 31-1284 for calcian richterite, and 25-675 and 31-1082 for potassian richterite).

References: An imperfect description by Breithaupt, A. (1865): *Bergmann Huttenmann. Z.* **24**, 364, was shown by Sjögren, H. (1895): *Bull. Geol. Inst. Univ. Uppsala* **2**, 71, to be an amphibole. Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 514.

Riebeckite

Etymology: Named after E. Riebeck.

Type locality: Island of Socotra, Indian Ocean.

X-ray data: a 9.769, b 18.048, c 5.335 Å, β 103.59° (PDF 19-1061 on specimen from Doubrutscha, Romania).

References: Sauer, A. (1888): *Z. Deutsch. Geol. Ges.* **40**, 138. Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 515.

Sadanagaite

Etymology: Named after R. Sadanaga.

Type locality: Yuge and Myojin islands, Japan.

X-ray data: a 9.922, b 18.03, c 5.352 Å, β 105.30°.

Reference: Shimazaki, H., Bunno, M. & Ozawa, T. (1984): *Am. Mineral.* **89**, 465.

Taramite

Etymology: Named after the discovery locality.

Type locality: Walitarama, Mariupol, Ukraine.

X-ray data: a 9.952, b 18.101, c 5.322, β 105.45° (PDF 20-734 on specimen of potassian taramite from Mbozi complex, Tanzania).

References: Morozewicz, J. (1923): *Spraw. Polsk. Inst. Geol., Bull. Serv. Géol. Pologne* **2**, 6. Redefined by Leake, B.E. (1978): *Can. Mineral.* **16**, 514.

Tremolite

Etymology: Named after the discovery locality.

Type locality: Val Tremola, St. Gotthard, Switzerland.

X-ray data: a 9.84, b 18.02, c 5.27 Å, β 104.95° (PDF 13-437 on specimen from San Gotardo, Switzerland, and PDF 31-1285 on synthetic material).

References: Pini, E. (1796) In Saussure, H.-B. (1923): *Voyages dans les Alpes* **4**, sect.). Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 512.

Tschermakite

Etymology: Named after G. Tschermak. Originally described as a hypothetical "Tschermak molecule".

References: Winchell, A.N. (1945): *Am. Mineral.* **30**, 29. Defined by Leake, B.E. (1978): *Can. Mineral.* **16**, 507 and 512.

Ungarettiite

Etymology: Named after L. Ungaretti.

Type locality: Hoskins mine, near Grenfell, New South Wales, Australia.

X-ray data: a 9.89(2), b 18.04(3), c 5.29(1) Å, β 104.6(2)°.

Reference: Hawthorne, F.C., Oberti, R., Cannillo, E., Sardone, N. & Zanetti, A. (1995): *Am. Mineral.* **80**, 165.

Winchite

Etymology: Named after H.J. Winch, who found the amphibole.

Type locality: Kajlidongri, Jhabua State, India.

X-ray data: a 9.834, b 18.062, c 5.300 Å, β 104.4° (PDF 20-1390).

References: Fermor, L.L. (1906): *Trans. Mining Geol. Inst. India* **1**, 79, named the amphibole described in 1904 (*Geol. Surv. India, Rec.* **31**, 236). Topotype material found by Leake, B.E., Farrow, C.M., Chao, F. & Nayak, V.K. (1986): *Mineral. Mag.* **50**, 174, proved to be very similar in composition to that originally documented by Fermor in 1909 (*Geol. Surv. India, Mem.* **37**, 149).

Editor's note: Readers interested in the etymology of amphibole names will find more information in Blackburn, W.H. & Dennen, W.H. (1997): *Encyclopedia of Mineral Names. Can. Mineral., Spec. Publ.* **1** (in press).

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APPENDIX 2. THE ESTIMATION OF THE PROPORTION OF FERRIC IRON IN THE ELECTRON-MICROPROBE ANALYSIS OF AMPHIBOLES

JOHN C. SCHUMACHER¹

*Institut für Mineralogie-Petrologie-Geochemie der Albert-Ludwigs Universität zu Freiburg,
Albertstrasse 23b, D-79104 Freiburg, Germany*

INTRODUCTION

Most users of the amphibole nomenclature will want to classify amphibole compositions that have been determined with the electron microprobe, which cannot distinguish among the valence states of elements. This situation is unfortunate, because it is clear that most amphiboles contain at least some ferric iron; see, for example, the compilations of Leake (1968) and Robinson *et al.* (1982). Consequently, the typical user of the amphibole nomenclature will need to estimate empirically ferric iron contents of amphiboles.

Empirical estimates of ferric iron are not just poor approximations that suffice in the absence of analytical determinations of the ratio Fe^{2+}/Fe^{3+} . Empirical estimates yield exactly the same results as analytical determinations of ferric iron, if (1) the analysis is complete (total Fe plus all other elements), (2) the analytical determinations are accurate, and (3) the mineral's stoichiometry (ideal anion and cation sums) is known. In the case of amphiboles, condition (3) cannot be uniquely determined because the A-site occupancy varies. However, knowledge of amphibole stoichiometry and element distribution can be used to estimate a range of permissible structural formulae and contents of ferric iron.

The most welcome circumstances will occur where the difference between the limiting structural formulae is trivial, and the entire range plots within the same field in the classification scheme. However, there will also be cases where the range of stoichiometrically allowable formulae is broad, *i.e.*, where it spans two or more fields in the classification scheme. Some users of the amphibole nomenclature may consider this a less than satisfactory solution, but until it is possible to determine ferric iron contents routinely with the same ease and convenience as with the electron microprobe, empirical estimates are probably the best alternative.

The procedure of estimating ferric iron will require at least one recalculation of the all-ferrous-iron analytical results to a different cation-sum. Consequently, familiarity with the calculation of mineral formulae is highly recommended for a fuller understanding of the procedure required to estimate the proportion of ferric iron. Thorough discussions of the calculation of mineral

formulae can be found in the appendices of Deer *et al.* (1966, 1992). The topic of ferric iron estimates in amphiboles has been discussed by Stout (1972), Robinson *et al.* (1982, p. 3–12), Droop (1987), Jacobson (1989), J.C. Schumacher (1991) and Holland & Blundy (1994). An example of the recalculation of the results of an electron-microprobe analysis and the procedure used to estimate minimum and maximum contents of ferric iron are given at the end of this appendix.

EMPIRICAL ESTIMATES OF FERRIC IRON IN AMPHIBOLES

The basic formula

Present knowledge of the crystal chemistry of amphiboles suggests that many of them contain essentially ideal stoichiometric proportions of 2 (OH) and 22 O. These anions can be rearranged to give the basis of recalculation of an anhydrous formula: 23 O (+ H₂O). Calculation of an anhydrous formula on this basis is the first basic assumption necessary to estimate the proportion of Fe³⁺. The ideal cation-sums in amphibole formulae are not fixed, but can vary between 15 and 16 cations per 23 O (anhydrous). Consequently, it is not possible to arrive at a unique estimation of Fe³⁺ on the basis of stoichiometry, as can be done for minerals with fixed ratios of cations to anions (*e.g.*, pyroxenes or the ilmenite-hematite series). Nevertheless, on the basis of present understanding of permissible and usual site-occupancies, limits can be placed on the maximum and minimum values of ferric iron contents, and these limits yield a range of acceptable formulae.

Critical examination of electron-microprobe data

The suitability of the results of an electron-microprobe analysis of an amphibole for an estimation of Fe³⁺ requires the evaluation of the all-ferrous-iron anhydrous formula calculated on a 23-oxygen-atom basis. The site assignments can be used to evaluate the data, and these are given in Figure A-1. From the site-assignment data, it is possible to define the important limits to the stoichiometry (cation subtotals) of the amphiboles (column 3, Fig. A-1). Acceptable formulae will satisfy all six of these criteria. Exceeding one or

¹ E-mail address: pogo@sun2.ruf.uni-freiburg.de

more of these limits in stoichiometry indicates that there are problems with the structural formula, and the identity of the unfulfilled condition will suggest the cause.

For minerals that bear ferric iron, the all-ferrous-iron structural formulae will have cation sums that are too high [for discussion, see J.C. Schumacher (1991) and references therein]. In amphiboles, this can result in violation of at least one of the criteria $Si \leq 8$, $\Sigma Ca \leq 15$ or $\Sigma K \leq 16$ (Fig. A-1). Violations of the other three criteria, $\Sigma Al \geq 8$, $\Sigma Mn \geq 13$ and $\Sigma Na \geq 15$ (Fig. A-1), **cannot** be due to failure to account for ferric iron, and usually indicate an analytical problem (too few cations

at some of the sites.) These analytical results should not be used for empirical estimates of the proportion of ferric iron. Note that exceptions do exist: potassium titanian richterite (Oberti *et al.* 1992) has Ti at the tetrahedral sites; cannilloite (Hawthorne *et al.* 1996) has one atom of Ca at the A position and two Ca atoms at the B (M4) position. These exceptions are rare.

Minimum and maximum estimates

In many cases, none of the criteria $Si \leq 8$, $\Sigma Ca \leq 15$ and $\Sigma K \leq 16$ will be exceeded by the all-ferrous-iron formula; the minimum estimate of the proportion of

Summary of site assignments and stoichiometric constraints					
Site and Occupancy	Cation*	Stoichiometric Limit	Correction		
			Minimum	Maximum	
T-site	Si	$Si \leq 8$	8Si	8SiAl	
	Al				$\Sigma Al \geq 8$
	Ti				
C-site	Cr				
	Fe ³⁺				
	Mg				
	Ni				
	Zn				
	B-site	Fe ²⁺			
		Mn	$\Sigma Mn \geq 13$		13eCNK
	Ca	$\Sigma Ca \leq 15$	15eNK		
A-site	Na	$\Sigma Na \geq 15$		15eK	
	K	$\Sigma K \leq 16$	16CAT		
	□				

* cations arranged according to increasing ionic radius (smallest, Si to largest, K)

Σ = cation subtotal (e.g. ΣMn = sum of all cations from Si through Mn in the list)

□ = vacancy at the A-site

FIG. A-1. Summary of ideal site-assignments, limits of various cation subtotals, and the type of correction (minimum or maximum) that can be obtained by calculating the formulae to these stoichiometric limits (after J.C. Schumacher 1991). Abbreviations of normalizations: 8Si: normalized such that total Si = 8; 8SiAl: normalized such that total Si + Al = 8; 13eCNK: normalized such that the sum of the cations Si through Mn (*i.e.*, all cations exclusive of Ca, Na, K) = 13; 15eNK: normalized such that the sum of the cations Si through Ca (*i.e.*, all cations exclusive of Na, K) = 15; 16CAT: normalized such that the sum of all cations = 16 (see also Robinson *et al.* 1982, p. 6-12).

Fe^{3+} is given by the all-ferrous-iron formula (*i.e.*, $Fe^{3+} = 0.000$, and the site occupancies of all-ferrous-iron formula are all allowable). If one (or more) of the three criteria $Si \leq 8$, $\Sigma Ca \leq 15$ and $\Sigma K \leq 16$ is exceeded, Fe^{3+} may be present, and a minimum estimate of its proportion can be made that will yield a formula with acceptable stoichiometry. The condition that is most greatly exceeded determines the basis of the recalculation. For example, if $Si = 8.005$, $\Sigma Ca = 15.030$ and $\Sigma K = 15.065$, then the ΣSi limit is exceeded by 0.005, and the ΣCa , by 0.030. Since ΣCa is in greatest excess, the minimum estimate of the proportion of ferric iron is obtained by recalculating the formula so that $\Sigma Ca = 15.000$ (15eNK estimate, Fig. A-1).

The maximum estimates of the proportion of ferric iron are obtained from the stoichiometric limits $\Sigma Al \geq 8$, $\Sigma Mn \geq 13$ and $\Sigma Na \geq 15$ (Fig. A-1). The condition that is nearest to the minimum value of one of these sums gives the maximum estimate of ferric iron. For example, if $\Sigma Al = 9.105$, $\Sigma Mn = 13.099$ and $\Sigma Na = 15.088$, then ΣAl is exceeded by 1.105, ΣMn , by 0.099, and ΣNa , by 0.088. The ΣNa is nearest the minimum value, and recalculating the formula so that $\Sigma Na = 15.000$ (15eK estimate, Fig. A-1) will give the formula with the maximum proportion of ferric iron.

Recalculation of the formulae

The recalculation procedure is described step-by-step at the end of this discussion, but some general aspects are discussed here. Table A-1 lists the hypo-

thetical results of an analysis (wt%) and four formulae that are based on 23 atoms of oxygen. Formulae were calculated for the two chemical limits (all iron as FeO or Fe_2O_3); the other two are the stoichiometric limits (Fig. A-1) that give the minimum (15eNK) and maximum (13eCNK) estimates of the proportion of ferric iron. All of the stoichiometric limits except $\Sigma Ca \leq 15$ (here $\Sigma Ca = 15.029$) are met by the all-ferrous-iron formula, which means that the minimum-ferric-iron formula is given by the 15eNK estimate (Table A-1).

Since ΣMn is nearest the lowest allowable sum, the maximum estimated proportion of ferric iron and the all-ferric-iron formula are obtained by recalculating as before, but in this case, the normalization must insure that $\Sigma Mn = 13.000$ (here the normalization factor is: $13 \div 13.201 = 0.9848$). The minimum values for ΣAl , ΣMn and ΣNa are, respectively, 8.000, 13.000 and 15.000, and the actual values are 9.139, 13.201 and 15.740.

These formulae for the minimum and maximum estimates of the proportion of ferric iron can be calculated in either of two ways: (1) by normalizing the proportion of all cations of the all-ferrous-iron formula that were calculated on a 23-oxygen-atom basis, such that $\Sigma Ca = 15.000$ and $\Sigma Mn = 13.000$ (*i.e.*, number of cations of each element multiplied by $15 \div \Sigma Ca$ or $13 \div \Sigma Mn$; here, $15 \div 15.029 = 0.9981$, and $13 \div 13.201 = 0.9848$, respectively), or (2) by using the normalization factor to determine the new sum of cations and then recalculating the entire formula on cation bases that set $\Sigma Ca = 15.000$ and $\Sigma Mn = 13.000$. The second method requires more calculation, but J.C. Schumacher (1991) has shown that this method leads to fewer rounding errors than normalizing the cations in the formula based on 23 atoms of oxygen.

The formula obtained from either recalculation method will have less than 23 atoms of oxygen. The proportion of cations of Fe^{3+} is found by calculating the number of moles of FeO that must be converted to $FeO_{1.5}$ to bring the sum of the oxygen atoms to 23; it equals $(23 - \Sigma O_x) \times 2$, where ΣO_x is the sum of the oxygen in the normalized formula ($\Sigma O_x = \Sigma R^{4+} \times 2 + \Sigma R^{3+} \times 1.5 + \Sigma R^{2+} + \Sigma R^{1+} \times 0.5$, where ΣR = the sums of cations with the same valence). The number of moles of FeO equal $Fe_T - Fe^{3+}$, where Fe_T = total Fe in the normalized formula. Following any recalculation, it is good practice to recheck to see that all six stoichiometric limits are also satisfied by the new formula.

Discussion of results of the recalculation

The variation in some cation values within the ranges of possible formulae (Table A-1) that are defined by the chemical and stoichiometric limits is compared in Figure A-2. In general, the range of possible formulae that are defined by the stoichiometric limits will be

TABLE A-1. A HYPOTHETICAL COMPOSITION OF AMPHIBOLE

Analyses (wt %)	Formulae			
	All Ferrous	15eNK	13eCNK	All Ferric
SiO ₂ 39.38	Si 6.093	6.081	6.000	5.714
Al ₂ O ₃ 16.70	Al 1.907	1.919	2.000	2.286
FeO 23.54	Σ 8.000	8.000	8.000	8.000
MgO 4.40				
CaO 11.03	Al 1.139	1.122	1.000	0.571
Na ₂ O 2.37	Fe ³⁺ 0.000	0.088	0.700	2.857
	Mg 1.015	1.014	1.000	0.952
Total 97.42	Fe ²⁺ 2.845	2.777	2.300	0.000
	Σ 5.000	5.000	5.000	4.380
	Fe ²⁺ 0.201	0.176	0.000	0.000
	Ca 1.799	1.824	1.800	1.714
	Na 0.000	0.000	0.200	0.286
	Σ 2.000	2.000	2.000	2.000
	Ca 0.029	0.000	0.000	0.000
	Na 0.711	0.709	0.500	0.381
	Sum 15.740	15.709	15.500	14.761

The structural formulae are based on the chemical and stoichiometric limits. The all-ferrous-iron formula assumes total Fe as FeO, and the all-ferric-iron formula assumes total Fe as Fe_2O_3 . The 13eCNK and 15eNK formulae are based on stoichiometric limits. See text for discussion.

Limits on ferric-Fe estimates in amphiboles

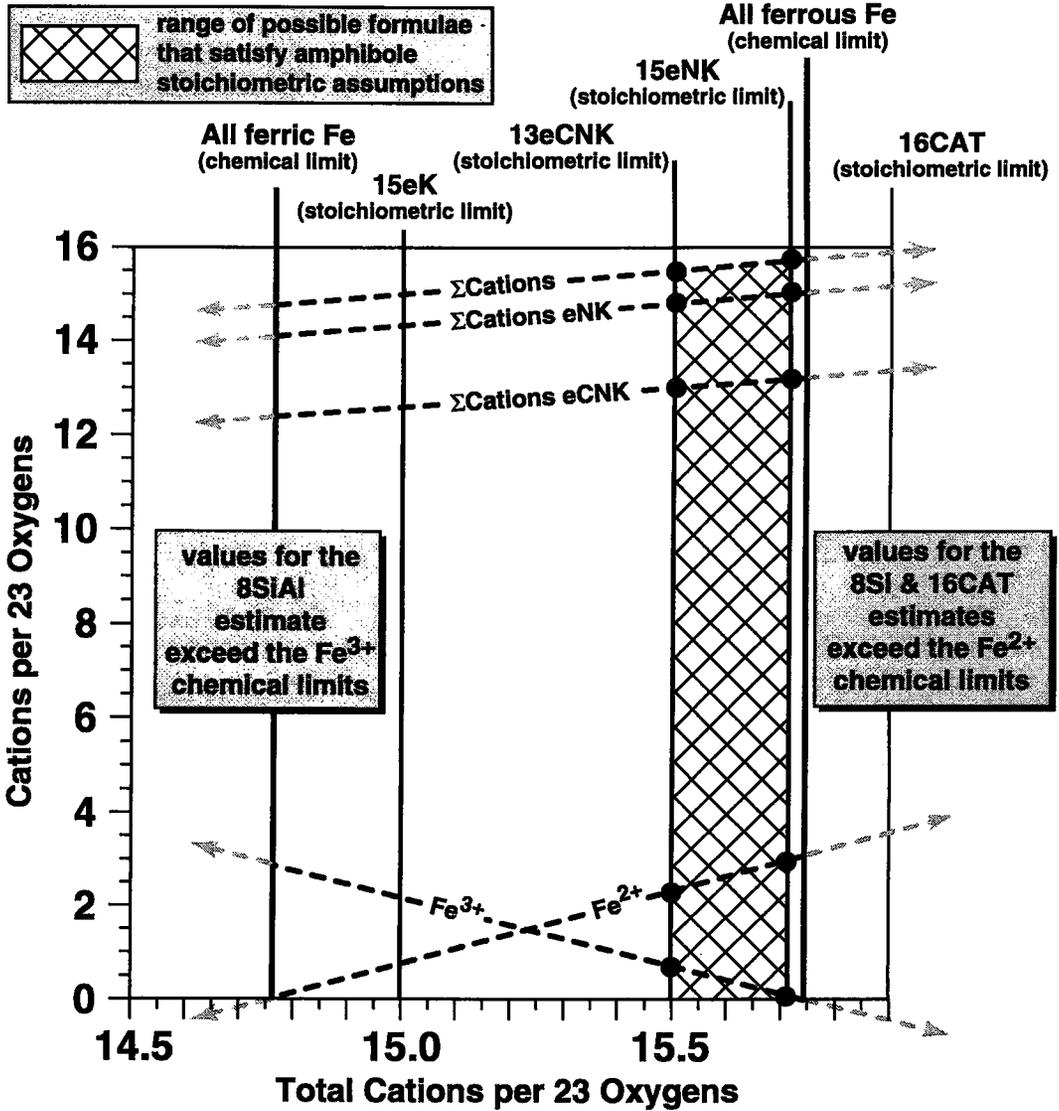


FIG. A-2. Plot of various cation values and sums *versus* total cations, which illustrates the continuous variation of these values relative to chemical and stoichiometric limits. The stoichiometric limits are given in Figure A-1, and the values are based on the amphibole composition given in Table A-1.

much narrower than the range obtained from the two chemical limits. A diagram like Figure A-1 could be constructed for every electron-microprobe data-set, and, on such a diagram, the range of both the chemical and the appropriate set of stoichiometric limits could vary greatly from example to example. It can be inferred from Figure A-2 that the range of permissible formulae could be, and commonly is, bounded by one of the chemical limits and one of the stoichiometric limits.

The relationships among cation sums that are illustrated in Figure A-2 show that comparison of some of the possible normalization-factors, which are obtained from the stoichiometric limits, can be used to (1) check the applicability of a specific estimate of the proportion of ferric iron, and (2) determine limits, chemical or stoichiometric, that give the minimum and maximum estimates of the proportion of ferric iron. To accomplish this, all the normalization-factors for all stoichiometric constraints and the chemical limits must be compared (Fig. A-1). The normalization-factors for the stoichiometric constraints, calculated from the all-ferrous-iron formula using the data in Table A-1, are:

Minimum estimate of the proportion of Fe^{3+} :

$$8\text{Si} = 8/\text{Si} = 8/6.093 = 1.313 \quad (1),$$

$$16\text{CAT} = 16/\Sigma\text{K} = 16/15.740 = 1.017 \quad (2),$$

$$\text{all ferrous iron (no change)} = 1.000 \quad (3),$$

$$15\text{eNK} = 15/\Sigma\text{Ca} = 15/15.029 = 0.998 \quad (4).$$

Maximum estimate of the proportion of Fe^{3+} :

$$13\text{eCNK} = 13/\Sigma\text{Mn} = 13/13.201 = 0.985 \quad (5),$$

$$15\text{eK} = 15/\Sigma\text{Na} = 15/15.740 = 0.953 \quad (6),$$

$$\text{all ferric iron} = 0.938 \quad (7),$$

$$8\text{SiAl} = 8/\Sigma\text{Al} = 8/9.139 = 0.875 \quad (8).$$

For the normalizations that yield minimum estimates (1 to 4), the recalculation that requires the lowest normalization-factor will give the minimum estimate of the proportion of ferric iron. For the normalizations that yield maximum estimates (5 to 8), the recalculation that requires the largest normalization-factor will give the maximum estimate of the proportion of ferric iron. All normalizations that lie between these values (in this example, 0.998 and 0.985) will give stoichiometrically acceptable formulae. If any of the normalization-factors for the maximum estimate (5 to 8) is greater than any of those for the minimum estimate (1 to 4), then the analytical data are not suitable for empirical estimations of the proportion of Fe^{3+} . Note that normalization-factors greater than 1.000 or less than the normalization-factor for the all-ferric-iron formula would yield impossible estimates of the proportion of Fe^{3+} , that lie beyond the chemical limits.

In addition to the stoichiometric constraints listed in Figure A-1, another constraint on maximum amount of Fe^{3+} can be defined if the C site in the formulation of

the amphibole nomenclature is further subdivided. The five C positions consist of three "mica-like" positions, two M1 octahedra and one M3 octahedron, and two "pyroxene-like" positions, the M2 octahedra. The cations Al, Fe^{3+} , Ti and Cr^{3+} are strongly partitioned into the M2 octahedra. Consequently, an additional estimate of the maximum amount of ferric iron can be obtained if one assumes that all the tetrahedral and M2 sites are completely filled with cations of valences 3+ and 4+. This normalization-factor (N) can be calculated by solving the two simultaneous equations for N: (1) $N \times (\text{Si} + \text{Ti} + \text{Al} + \text{Cr}) + \text{Fe}^{3+} = 10$, which describes the desired resulting stoichiometry, and (2) $\text{Fe}^{3+} = (23 - 23 \times N) \times 2$, which gives the amount of ferric iron for this normalization. The solution is: $N = 36/(46 - \text{Si} - \text{Ti} - \text{Al} - \text{Cr})$, where Si, Ti, Al and Cr are the amounts of these cations in the all-ferrous-iron formula. For the analytical results in Table A-1, this normalization-factor, here abbreviated $10\Sigma\text{Fe}^{3+}$, is 0.977, which is less than the 0.983 value of the 13eCNK factor, such that the $10\Sigma\text{Fe}^{3+}$ normalization will not give the maximum estimate of the amount of ferric iron in this case.

Most users of the nomenclature will want to report only a single formula and name for each amphibole analyzed; consequently, the overriding question is: which correction should be used? Unfortunately, there is no simple rule, and each group of similar analytical data may require individual treatment. Robinson *et al.* (1982, p. 11) and J.C. Schumacher (1991, p. 9-10) discussed some of these possibilities for Fe-Mg, calcic, sodic-calcic and sodic amphiboles in greater detail. The $10\Sigma\text{Fe}^{3+}$ correction discussed in the preceding paragraph will not likely be important in Ca-amphiboles, but in sodic amphibole (*e.g.*, riebeckite, glaucophane), it may commonly yield the maximum estimate of the proportion of ferric iron.

Choosing a single representative ferric-iron-bearing formula out of the range of possible formulae requires further justification or additional assumptions. One solution is to use the mean value between maximum and minimum contents of ferric iron (Spear & Kimball 1984). Other solutions can be obtained for restricted types of amphibole. For example, R. Schumacher (1991) derived a scheme of normalization that yields formulae intermediate between maximum- and minimum-ferric-iron formulae for samples of calcium-saturated metamorphic hornblende. Her scheme is based on regression analysis of hornblende compositions for which determinations of the proportion of ferric and ferrous iron were available.

In general, it will be desirable to determine the extent to which the minimum and maximum estimations of the proportion of ferric iron affects the classification of the amphibole in question by inspecting the formulae of both the maximum- and minimum-ferric-iron estimates. If the entire range of formulae gives a wide spectrum of possible names, this should probably at

least be mentioned wherever the amphibole is being described.

DEVIATIONS FROM THE BASIC ASSUMPTIONS

Incorporation of F and Cl

Both F and Cl may substitute for (OH) in the amphibole structure, but concentrations of these elements are not routinely determined at all electron-microprobe facilities. Although it is highly recommended that their concentrations also be determined, their presence has no effect on the procedure of estimation of ferric iron. Exchange of F or Cl for OH does not change the total number of negative charges (46) in the anhydrous formula, such that the proportions of cations required to give 46 positive charges will be independent of the proportions of OH, F or Cl that are present. The critical assumption is that exactly two anions [OH, F, Cl] are present for every 22 atoms of oxygen.

Coupled substitutions involving anions

The validity of a basic 23-oxygen-atom anhydrous formula (*i.e.*, exactly two OH + F + Cl) is an underlying assumption in the procedure to estimate the proportion of ferric iron in amphiboles. Any variation in these values will have a tremendous effect on the amount of ferric iron estimated. The partial replacement of [OH + F + Cl] by O in the amphibole structure is an example of this kind of variation, and has long been recognized. Amphiboles that are referred to in numerous textbooks on mineralogy and optical mineralogy as "basaltic hornblende" (Deer *et al.* 1966), or the kaersutite end-member of the IMA system of nomenclature, can show this type of compositional variation (see also Dyar *et al.* 1993).

Intuitively, one would expect analytical totals to be affected by variable proportions of O and OH; however, since these amphiboles tend to be richer in ferric iron, the increase in the sum from the partial exchange of O for OH tends to be offset by treating the larger amounts of Fe₂O₃ as FeO. Consequently, even in anhydrous amphiboles with a significant proportion of ferric iron, no compelling evidence of these substitutions will necessarily be seen in the results of the analyses. Ferric-iron estimation can still be carried out on compositions with variable proportions of O and OH, but an estimate of the H₂O and halogen contents will be an essential additional requirement.

CONCLUSIONS

Amphiboles typically contain at least some ferric iron, and may contain significant amounts; however, the most common analytical method, electron-microprobe analysis, cannot distinguish between valence states. The ferric iron contents of amphiboles can be estimated

provided that the chemical analysis is complete, and ideal stoichiometry (site occupancy) can be assumed. If these conditions hold, empirical estimates of ferric iron would have an accuracy and precision comparable to those associated with a determination of the ratio Fe²⁺/Fe³⁺. For amphiboles, stoichiometry cannot be uniquely determined, but various crystal-chemical constraints allow a range of possible formulae that give the minimum and maximum contents of ferric iron.

Selecting a single structural formula from the range of possibilities requires the application of an additional constraint or a further assumption, such as using the formula that gives minimum, maximum or the mean amount of ferric iron, or applying some petrological constraint. In written descriptions, it will be important to report the analytical results, which enables others to do their own recalculations, and a clear statement of the method and assumptions that were used to calculate the structural formula reported.

The users of the IMA amphibole nomenclature ought to explore the formulae to estimate the minimum and maximum amounts of ferric iron. This approach defines the range of possible formulae and possible names. Since some amphibole names carry special petrogenetic significance, care should be taken if the range of possible names is large.

WORKED-THROUGH EXAMPLE: CALCULATION OF AN AMPHIBOLE FORMULA AND AN ESTIMATE OF PROPORTION OF FERRIC IRON FROM RESULTS OF AN ELECTRON-MICROPROBE ANALYSIS

As an example (Table A-2), the composition that appears in Deer *et al.* (1992, p. 678) was chosen. To simulate analysis with an electron microprobe, the ferric iron was recast as ferrous iron, and results of the H₂O determination were ignored. The ferric iron estimate was made assuming that 2 (OH) are present rather than the 2.146 suggested by the actual determination of H₂O⁺. Any discrepancies in the final decimal places of the numbers that appear below and in Table A-2 are due to rounding effects.

(1) Divide the wt% of each constituent (column 1) by the molecular weight of the constituent, to yield the *molecular proportion* of each (column 2) [*e.g.*, for SiO₂: 51.63 ÷ 60.085 = 0.85928]. Data on the molecular weights were taken from Robie *et al.* (1978).

(2) Obtain *atomic proportions of the cations* (column 3) and *atomic proportions of oxygen* (column 4) by multiplying each *molecular proportion* value by the number of cations and oxygen atoms in the oxide [*e.g.*, for SiO₂: 0.85928 × 1 = 0.85928 and 0.85928 × 2 = 1.71857].

Note: If one assumes that 2 (OH) groups are present, one atom of oxygen is balanced by 2 H (*i.e.*, H₂O), such that the cation charges are balanced by the remaining

TABLE A-2. A WORKED-THROUGH EXAMPLE OF THE CALCULATION OF THE STRUCTURAL FORMULA OF AN AMPHIBOLE*

	1	2	3	4	5	6
	wt%	Molecular Proportions	Atomic Proportions (cations)	Atomic Proportions (oxygens)	anions on the basis of 23 oxygens	cations on the basis of 23 oxygens
		wt% ÷ mol. wt.	col. 2 × cations in oxide	col. 2 × oxygens in oxide	col. 4 × 8.45012	col. 3 × 8.45012
SiO ₂	51.63	0.85928	0.85928	1.71857	14.52208	7.261
TiO ₂	0.00	0.00000	0.00000	0.00000	0.00000	0.000
Al ₂ O ₃	7.39	0.07248	0.14496	0.21744	1.83736	1.225
Cr ₂ O ₃	0.00	0.00000	0.00000	0.00000	0.00000	0.000
FeO	7.55	0.10509	0.10509	0.10509	0.88799	0.888
MnO	0.17	0.00240	0.00240	0.00240	0.02025	0.020
MgO	18.09	0.44884	0.44884	0.44884	3.79274	3.793
CaO	12.32	0.21969	0.21969	0.21969	1.85641	1.856
Na ₂ O	0.61	0.00984	0.01968	0.00984	0.08317	0.166
K ₂ O	0.00	0.00000	0.00000	0.00000	0.00000	0.000
sum			1.79994	2.72185	23.0000	15.210

Factor for the recalculation of atomic proportions to 23 O basis: 23 ÷ 2.72185 = 8.45012

TABLE A-2 (CONTINUED)

Ideal site assignments	7	cations	8	9	Ideal site assignments	10	11	12	13
	Min. formula from col. 6		col. 6 × 0.99714	col. 8 × oxygen per cation		Formula (15eNK) minimum Fe ³⁺	Formula (15eK) maximum Fe ³⁺	Formula Average of Min. and Max. Fe ³⁺	Formula from DHZ
Si	7.261				Si	7.240	7.161	7.201	7.196
Al ^{IV}	0.739				Al ^{IV}	0.760	0.839	0.799	0.804
sum T	8.000	Si	7.2401	14.4802	sum T	8.000	8.000	8.000	8.000
Al ^{VI}	0.486	Al	1.2214	1.8321	Al ^{VI}	0.462	0.369	0.416	0.410
Fe ³⁺	0.000	Ti	0.0000	0.0000	Fe ³⁺	0.133	0.634	0.383	0.263
Cr	0.000	Cr	0.0000	0.0000	Cr	0.000	0.000	0.000	0.000
Mg	3.793	Mg	3.7818	3.7818	Mg	3.782	3.740	3.761	3.759
Fe ²⁺	0.721	Fe ²⁺	0.8854	0.8854	Fe ²⁺	0.624	0.242	0.440	0.618
Mn	0.000	Mn	0.0202	0.0202	Mn	0.000	0.015	0.000	0.000
sum C	5.000	Ca	1.8511	1.8511	sum C	5.000	5.000	5.000	5.000
Mg	0.000	Na	0.1659	0.0829	Mg	0.000	0.000	0.000	0.000
Fe ²⁺	0.167	K	0.0000	0.0000	Fe ²⁺	0.129	0.000	0.057	0.050
Mn	0.020	sum	15.1659	22.9337	Mn	0.020	0.005	0.020	0.020
Ca	1.856				Ca	1.851	1.831	1.841	1.840
Na	0.000				Na	0.000	0.164	0.082	0.090
sum B	2.043				sum B	2.000	2.000	2.000	2.000
Na	0.166				Na	0.166	0.000	0.083	0.074
K	0.000				K	0.000	0.000	0.000	0.000
sum A	0.166				sum A	0.166	0.000	0.073	0.074
total	15.210				total	15.166	15.000	15.083	15.074

ΣCa (col. 7)
 15 + 15.043 = 0.99714
 (23-22.9337) × 2
 = 0.1325
 0.885-0.133
 = 0.753

* Taken from Deer *et al.* (1992, p. 678). See text for a step-by-step discussion of this table.

23 atoms of oxygen, which is the basis of the anhydrous formula (see text for discussion; it can be shown that even if concentrations of F and Cl have not been determined, the 23-oxygen-atom formula will give the correct formula, as long as OH + F + Cl = 2).

(3) Obtain the *proportion of the anions based on 23 atoms of oxygen* (column 5) by multiplying each value in column 4 by 23 divided by the sum of column 4 [e.g., $23 \div 2.72185 = 8.45012$; for SiO₂: $1.71857 \times 8.45012 = 14.52208$].

(4) Obtain the *proportion of the cations on the basis of 23 atoms of oxygen* (column 6) by multiplying each value in column 3 by 23 ÷ the sum of column 4 [e.g., for SiO₂: $0.85928 \times 8.45012 = 7.261$].

Note: Column 6 is the all-ferrous-iron formula of the amphibole. Assignment of the cations to sites shows whether any deviations from ideal stoichiometry can be explained by failure to account for ferric iron.

(5) Ideal site-assignments (column 7) are made from the cation values in column 6. The general procedure is:

(a) *the eight tetrahedral (T) sites:*

- place all Si here; if Si < 8, fill the remaining sites with Al.
- if Si + total Al < 8, then place all Si + Al here.

(b) *the five octahedral (C) sites (M2, M1, M3)*

- place Al remaining from step (a), Ti, Fe³⁺ (initially = 0), and Cr here. In the following order, place enough Mg, Fe²⁺ and Mn to bring the total to 5.
- if $\Sigma(\text{VIAl...Mn}) < 5$, then place all these elements here.

(c) *the two (B) sites (M4)*

- place any Mg, Fe²⁺ or Mn and Ca remaining after step (b) here.
- if $\Sigma(\text{Mg...Ca})$ at B < 2, fill the remaining sites with Na to bring the total to 2.

(d) *the single large (A) site*

- place any remaining Na and K here.

(6) Evaluating the structural formula

If any site has less than their ideal values (*T* = 8.000, *C* = 5.000, *B* = 2.000, *A* = 0 to 1.000), then an estimate of the proportion of ferric iron is either impossible or only possible with additional constraining information. This situation could also indicate an analytical problem.

The suitability of the analytical data for an estimation of the proportion of ferric iron and the normalizations that yield the maximum and minimum estimates of ferric iron can be determined by calculating the normalization-factors for all the various stoichiometric and chemical limits. These are given in Table A-3 and are obtained from columns 6 or 7.

If the normalization-factors based on 8Si, 16CAT and 15eNK are greater than the normalization-factors based on 8SiAl, 15eK, 10ΣFe³⁺ and 13eCNK, then an estimate of a minimum and a maximum amount of

ferric iron can be calculated; if not, then no estimation is possible.

(7) Minimum estimates of the amount of ferric iron

The lowest normalization-factor among the four choices, 8Si, 16CAT, 15eNK and all ferrous iron, determines the formula that yields the minimum estimate of the amount of ferric iron. If the factors 8Si, 16CAT and 15eNK are all greater than 1.0000, then the all-ferrous-iron formula (Fe³⁺ = 0) is the lower limit. In this example, the 15eNK normalization-factor is the lowest.

To obtain the formula that gives the minimum estimate of the amount of ferric iron (column 8), multiply the proportion of the cations from column 6 by the 15eNK normalization-factor, 0.99714 ($15 \div 15.043$).

(8) Find the sum of oxygen atoms (22.9337) in the normalized formula by multiplying each single cation value (column 8) by the number of balancing atoms of oxygen [e.g., for SiO₂, $7.2401 \times 2 = 14.4802$; for AlO_{1.5}, $1.2214 \times 1.5 = 1.8321$; for MgO, $3.7818 \times 1 = 3.7818$; for NaO_{0.5}, $0.1659 \times 0.5 = 0.0829$].

(9) The amount of *ferric iron* equals the amount of ferrous Fe that must be converted to bring the total oxygen atoms up to 23. The amount is $(23 - 22.9337) \times 2 = 0.133$.

(10) The new *ferrous iron* value is the total Fe from column 8 minus the amount of ferric iron [e.g., $0.885 - 0.133 = 0.753$].

(11) Recast the normalized cations as in step 5 (column 10). This should yield a formula without violations of the ideal stoichiometry.

Note: Step 11 double-checks the correctness of the calculations. It also is a check on whether correction of the initial stoichiometric violation will produce another [here, insufficient cations to fill *T* or *C* could result from the 15eNK normalization. Such analytical data cannot

TABLE A-3. CALCULATION OF THE NORMALIZATION-FACTORS

Limit	Method of Calculation	Calculation	Normal factor
<i>Calculations of the estimated minimum amount of ferric iron</i>			
8Si	8 + Si	8 + 7.261	1.1018
16CAT	16 + ΣK	16 + 15.210	1.0519
all ferrous iron	—	—	1.0000
15eNK	15 + ΣCa	15 + 15.043	0.9971*
<i>Calculations of the estimated maximum amount of ferric iron</i>			
15eK	15 + ΣNa	15 + 15.210	0.9862*
13eCNK	13 + ΣMn	13 + 13.187	0.9858
all ferric iron	23 ÷ [23 + (0.5 × Fe ³⁺)]	23 + 23.444	0.9811
10ΣFe ³⁺	36 + (46 - Si - Al - Ti - Cr)	36 + 37.5141	0.9596
8SiAl	8 + ΣAl	8 + 8.486	0.9427

* Indicates the normalizations that yield the minimum and maximum estimated amounts of ferric iron, respectively.

be used to estimate the proportion of ferric iron (unfortunately, a lot of calculation is involved in determining this)].

(12) Maximum estimates of the proportion of ferric iron

The largest normalization-factor among the four choices, 8SiAl, 15eK, 13eCNK and all ferric iron, determines the formula that yields the maximum estimate of the proportion of ferric iron. If the factors 8SiAl, 15eK and 13eCNK are all less than the all-ferric-iron value, then the all-ferric-iron formula will give the maximum amount of Fe³⁺. In this example, the 15eK normalization-factor is the largest, and can be used to give the formula with the maximum amount of Fe³⁺.

To obtain the formula that gives the maximum estimated amount of ferric iron (column 11), repeat steps 7 through 10 using the 15eK normalization-factor 0.98621 (15 ÷ 15.210).

(13) Average of the maximum and minimum estimated amount of ferric iron

To obtain the formula that gives the average of the maximum and minimum estimated amount of ferric iron (columns 10 and 11), repeat steps 7 through 10 using the average of the normalization-factors that were obtained in steps 7 and 12. This normalization-factor is 0.99167 [(0.99714 + 0.98621) ÷ 2].

(14) The actual formula (column 12) given in Deer *et al.* (1992) lies approximately between the minimum estimate (15eNK) in column 10 and maximum estimate (15eK) in column 11, but is nearer the minimum.

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