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How to name amphiboles after the IMA2012 report: rules of thumb and a new PC program for monoclinic amphiboles

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Abstract

Major changes have been introduced by the new scheme for amphibole classification and nomenclature for the amphibole supergroup recently approved by the Commission on New Minerals Nomenclature and Classification of the International Mineralogical Association, a scheme which adheres to the concepts of dominant group valency and dominant ion. The hierarchy of classification now proceeds through the W (→groups), B (→subgroups), and C and A (→rootnames) ions in a rational and comprehensive scheme which takes into account aspects of amphibole stability based on synthesis work. The new rules are here discussed in a simple and application-oriented manner, and the procedure to be followed to correctly classify and name amphibole compositions is outlined. A PC program (written in VisualBasic) for naming monoclinic amphiboles according to the new rules is now available by downloading from the website of CNR-IGG, UOS of Pavia: http://www_crystal.unipv.it /labcris/AMPH2012.zip.

Key words: Amphiboles; nomenclature; classification.

Introduction

Amphiboles are a very important supergroup of rock-forming minerals. Because of their high crystal-chemical compliance, amphiboles can incorporate many geochemically common anions and cations and hence are fairly ubiquitous in rocks. Furthermore, some cations may order over different sites so that their site partitioning can be used to derive *P*, *T* and fO_2 conditions of crystallization.

Monoclinic *C*2/*m* amphiboles are by far the most common and the most relevant for petrogenetic studies. Their structure (Figure 1) consists of a double chain of two topologically distinct corner-sharing tetrahedra (*T*(1) and *T*(2)) and a strip of three topologically distinct edge-sharing octahedra (*M*(1), *M*(2), *M*(3)), both extending parallel to the *c* direction. The *M*(4) site, with a coordination up to [8]-fold depending on the nature of the hosted cation, links these two building blocks. The *A* site is at the centre of a large cavity formed by the hexagonal rings of two back-to-back double-chains; it has a nominal

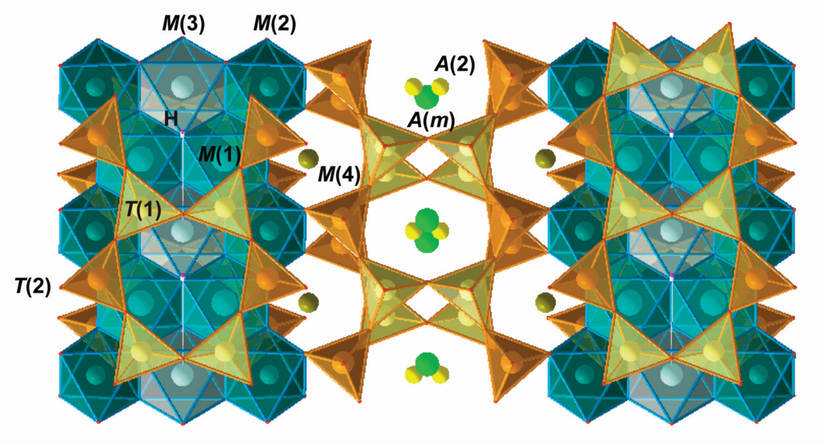

Figure 1. The structure of monoclinic C2/*m* amphiboles projected onto (100).

coordination of [12], but cations order between two (mutually incompatible) sub-sites, *A*(2) and *A*(*m*), which are shifted from the centre of the cavity along the relevant symmetry element. Besides the common space group *C*2/*m*, amphiboles may occur with different monoclinic space groups ($P2_1/m$ and *P*2/*a*) and with orthorhombic symmetry as well (space groups *Pnma* and *Pnmn*). Different systems imply different stacking behaviours, whereas different space groups imply different site multiplicities and hence independent behaviour, e.g. of two facing double chain of tetrahedra. Note that in this paper we deal only with monoclinic *C*2/*m* amphiboles, for which current site-nomenclature requires the use of italics and parentheses. In order to allow a distinction of structure type, parentheses shall not be used for sites in orthorhombic amphiboles.

The general chemical formula of the amphiboles should be written as $A_{0-1}B_2C_5T_8O_{22}W_2$, where: the main A cations (occurring at the *A* sites) are Na, K, and Ca; the main B cations (occurring at the *M*(4) site) are Na, Ca, Mg, Fe^{2+}, Mn^{2+} and Li; the main C cations (occurring at the *M*(1-3) sites) are Mg, Fe^{2+}, Mn^{2+}, Zn, Al, Fe^{3+}, Mn^{3+}, Cr^{3+}, Ti^{4+}, Zr and Li; the main T cations (occurring at the *T*(1-2) sites) are Si, Al, Ti^{4+} (only in richterite) and Be^{2+} (only in the rare *P*2/*a* amphibole joesmithite); the W anions (occurring at the O(3) site) are OH, F, Cl and O^2.

Due to our continuously increasing awareness of the complexity of amphibole compositional space, the International Mineralogical Association (IMA) has sequentially approved several classification schemes, which in this paper are referred as IMA78 (Leake, 1978), IMA 1997 (Leake et al., 1997) and IMA2003 (Leake et al., 2003). All these schemes were based on the nature and the amount of the A, B and T cations, and the nomenclature was based on combining a list of approved root-names with a series of prefixes defined on the basis of strict stoichiometric constraints (e.g., “ferri-“ implied ${}^{C}Fe^{3+} \geq 1.0$ atom per formula unit, apfu). Hawthorne and Oberti (2006) raised the issue that IMA2003 rules could be implemented by a major adherence to our present knowledge of amphibole crystal-chemistry and to the dominance criterion. They also pointed out that modern studies have shown that Li-bearing amphiboles and partly to completely dehydrogenated amphiboles are far more common than was previously thought, and that they need new rules for classification and nomenclature. A new Subcommittee on amphibole classification (co-chaired by F.C. Hawthorne and R. Oberti) was formed in 2006, and started to prepare a new classification scheme which significantly changed the rules for amphibole classification and nomenclature. This scheme was approved by the IMA Commission on New Minerals Nomenclature and Classification (CNMNC) in April 2012, and the report under publication (Hawthorne et al., 2012) is hereafter referred as IMA2012. In this paper, we provide a brief but accurate description of the rules to be used from now on to correctly classify and name monoclinic amphiboles. More details on the reasons why rules were changed and root-names were modified or introduced are beyond the scope of this paper, and can be found in IMA2012.

Several programs have been written for naming amphiboles, and the different releases have been adapted to changes in the rules for classification and nomenclature (Mogessie and Tessadri, 1982; Mogessie et al., 1990; 2001; Rock, 1987; Richard and Clarke, 1990; Currie, 1991; 1997; Yavuz, 1996; 1999). Here we introduce a simple program written in VisualBasic to be used to name amphiboles according to the IMA2012 rules; it can be appended to any program for the calculation of structural formulae. This program can be downloaded free of charge from the website of CNR-IGG, UOS of Pavia: http://www_crystal.unipv.it/labcris/AMPH2012.zip.

The new rules for amphibole classification and nomenclature

The IMA2012 report has adopted a new hierarchy for the amphibole supergroup (Figure 2), which adheres to the latest hierarchical rules of IMA-CNMMC (Mills et al., 2009) and uses criteria based on the dominant valency of group ions and the dominant ion within the group. This

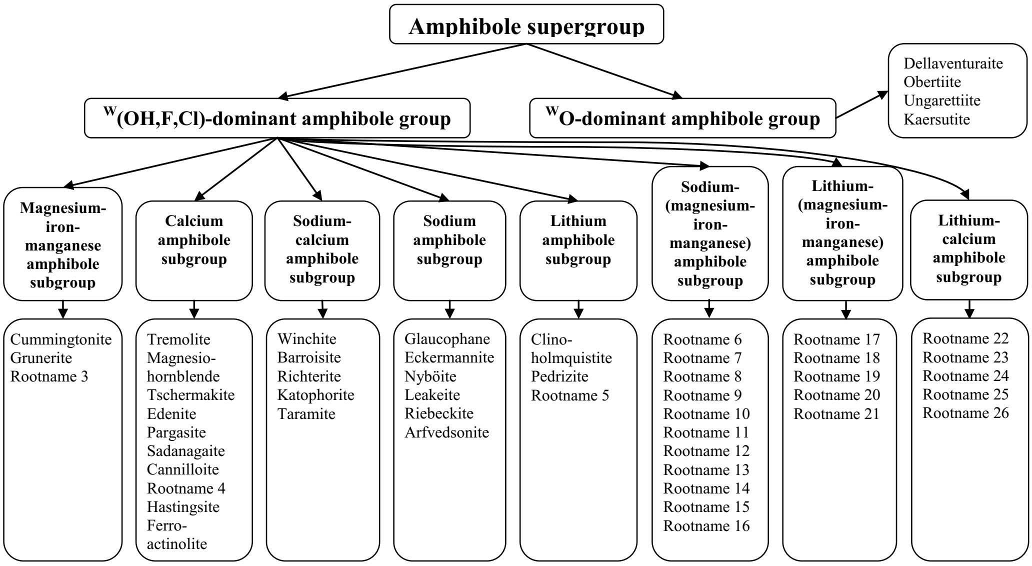

Figure 2. Classification hierarchy and root-names in the (monoclinic) amphibole supergroup (modified after Hawthorne et al., 2012).

approach was first unsuccessfully proposed during the 10 year discussion preceding IMA1987. However, these concepts germinated in the mineralogical literature and were accepted for smaller mineral groups (e.g., hellandite: Oberti et al., 2002; arrojadite: Chopin et al., 2006; epidote: Armbruster et al., 2006) and re-proposed for amphiboles by Hawthorne and Oberti (2006), until the dominance criterion was adopted in a more general vision of mineral nomenclature by the IMA-CNMCN (Hatert and Burke 2008).

The hierarchy of classification now proceeds through the W (→groups), B (→subgroups), and C and A (→rootnames) ions in a comprehensive scheme which takes into account aspects of amphibole stability based on synthesis work. As a consequence, amphibole compositions obtained or suggested during experimental work but not yet found as mineral species are listed with the code RootnameX, and will be given an appropriate rootname by the discoverers when found as minerals.

Groups: the first major division is between two groups, (OH,F,Cl)-dominant amphiboles and O^{2-} dominant (oxo-) amphiboles. This division is introduced to acknowledge the increasing importance and frequency of partial-to-dominant dehydrogenation in amphiboles, and recognises the fact that the dominance of either R^- or R^{2-} anions, respectively, at the W group in the unit formula has significant implications on the aggregate charge and ordering of C cations. Indeed, the high-charge cations related to dehydrogenation order at the *M*(1) and *M*(3) sites, whereas those not related to dehydrogenation order at the *M*(2) sites. Hence, high-charge cations at the *M*(1) and *M*(3) sites give rise to extra C positive charges, often well beyond the previously considered limit of 2.0 apfu. Only a few root compositions are known so far for oxo-amphiboles (Figure 1 and Table 1). The most common oxo-amphiboles have Ca dominant at B, are named kaersutites (with the end-member formula now redefined as $NaCa_2(Mg_3Ti^{4+}Al)(Si_6Al_2)O_{22}O_2$, and occur in high-*T*, high fO_2 environments; they have major petrogenetic relevance. In contrast, ^{B}Na oxo-amphiboles are rare, and are confined to unusual geological environments. Therefore, further division into subgroups has not been considered (yet) for oxo-amphiboles.

Subgroups: for (OH, F, Cl)-dominant amphiboles, different subgroups are defined based on the dominant B-group valency and the dominance of a given B cation or group of B cations, i.e. $^B(Mg + Fe + Mn)^{2+}$; ^{B}Ca, ^{B}Na and ^{B}Li. The compositional spaces of the eight resulting amphibole subgroups are defined as follow (where $^B\Sigma M^{2+} = {}^B(Mg + Fe + Mn)^{2+}$ and $\Sigma B = {}^BLi + {}^BNa + {}^B\Sigma M^{2+} + {}^BCa = 2$ apfu):

magnesium-iron-manganese
$^B(Ca + \Sigma M^{2+})/\Sigma B \geq 0.75$, $^B\Sigma M^{2+}/\Sigma B > {}^BCa/\Sigma B$;
calcium
$^B(Ca + \Sigma M^{2+})/\Sigma B \geq 0.75$, $^BCa/\Sigma B \geq {}^B\Sigma M^{2+}/\Sigma B$;
sodium-calcium
$0.75 > {}^B(Ca + \Sigma M^{2+})/\Sigma B > 0.25$, $^BCa/\Sigma B \geq {}^B\Sigma M^{2+}/\ \Sigma B$ and $0.75 > {}^B(Na + Li)/\Sigma B > 0.25$, $^BNa/\Sigma B \geq {}^BLi/\Sigma B$;
sodium
$^B(Na + Li)/\Sigma B \geq 0.75$, $^BNa/\Sigma B \geq {}^BLi/\Sigma B$;
lithium
$^B(Na + Li)/\Sigma B \geq 0.75$, $^BLi/\Sigma B > {}^BNa/\Sigma B$;
sodium-(magnesium-iron-manganese)
$0.75 > {}^B(Ca + \Sigma M^{2+})/\Sigma B > 0.25$, $^B\Sigma M^{2+}/\Sigma B > {}^BCa/\Sigma B$ and $0.75 > {}^B(Na + Li)/\Sigma B > 0.25$, $^BNa/\Sigma B \geq {}^BLi/\Sigma B$;
lithium-(magnesium-iron-manganese)
$0.75 > {}^B(Ca + \Sigma M^{2+})/\Sigma B > 0.25$, $^B\Sigma M^{2+}/\Sigma B > {}^BCa/\Sigma B$ and $0.75 > {}^B(Na + Li)/\Sigma B > 0.25$, $^BLi/\Sigma B > {}^BNa/\Sigma B$;
lithium-calcium amphiboles
$0.75 > {}^B(Ca + \Sigma M^{2+})/\Sigma B > 0.25$, $^BCa/\Sigma B \geq {}^B\Sigma M^{2+}/\Sigma B$ and $0.75 > {}^B(Na + Li)/\Sigma B > 0.25$, $^BLi/\Sigma B > {}^BNa/\Sigma B$.

In this way, the compositional tetrahedron defined by the vertices $^B\Sigma M^{2+}$, ^{B}Ca, ^{B}Na and ^{B}Li is divided into eight rational blocks, and their

Table 1. End-member compositions and root-names for monoclinic amphiboles after IMA2012. The composition of kaersutite has been redefined with respect to IMA1997, and root-names now refer to the C(Mg, Al) compositions, with the only exceptions of grunerite, riebeckite, arfvedsonite and hastingsite (cf. text).

^{W}(OH, F, Cl)-dominant group

Magnesium-iron-manganese subgroup:		*Lithium subgroup:*	
$Mg_2Mg_5Si_8O_{22}(OH)_2$	Cummingtonite	$Li_2(Mg_3Al_2)Si_8O_{22}(OH)_2$	Clino-holmquistite
$Fe^{2+}{}_2Fe^{2+}{}_5Si_8O_{22}(OH)_2$	Grunerite	$NaLi_2(Mg_2Al_2Li)Si_8O_{22}(OH)_2$	Pedrizite
$Mn^{2+}{}_2Mg_5Si_8O_{22}(OH)_2$	Rootname3	$Li_2(Mg_4Al)Si_8O_{22}(OH)_2$	Rootname 5
Calcium subgroup:		*Sodium-(magnesium-iron-manganese) subgroup:*	
$Ca_2Mg_5Si_8O_{22}(OH)_2$	Tremolite	$(NaMg)(Mg_4Al)Si_8O_{22}(OH)_2$	Rootname 6
$Ca_2(Mg_4Al)(Si_7Al)O_{22}(OH)_2$	Magnesio-hornblende	$(NaMg)(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$	Rootname 7
		$Na(NaMg)Mg_5Si_8O_{22}(OH)_2$	Rootname 8
$Ca_2(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$	Tschermakite	$Na(NaMg)(Mg_4Al)(Si_7Al)O_{22}(OH)_2$	Rootname 9
$NaCa_2Mg_5(Si_7Al)O_{22}(OH)_2$	Edenite	$Na(NaMg)(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$	Rootname 10
$NaCa_2(Mg_4Al)(Si_6Al_2)O_{22}(OH)_2$	Pargasite	$(NaMn^{2+})(Mg_4Al)Si_8O_{22}(OH)_2$	Rootname 11
$NaCa_2(Mg_3Al_2)(Si_5Al_3)O_{22}(OH)_2$	Sadanagaite	$(NaMn^{2+})(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$	Rootname 12
$CaCa_2(Mg_4Al)(Si_5Al_3)O_{22}(OH)_2$	Cannilloite	$Na(NaMn^{2+})Mg5Si_8O_{22}(OH)_2$	Rootname 13
$NaCa_2(Mg_4Ti)(Si_5Al_3)O_{22}(OH)_2$	Rootname 4	$Na(NaMn^{2+})(Mg_4Al)(Si_7Al)O_{22}(OH)_2$	Rootname 14
$NaCa_2(Fe^{2+}{}_4Fe^{3+})(Si_6Al_2)O_{22}(OH)_2$	Hastingsite	$Na(NaMn^{2+})(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$	Rootname 15
$Ca_2Fe^{2+}{}_5Si_8O_{22}(OH)_2$	Ferro-actinolite	$(NaFe^{2+})(Fe^{2+}{}_4Al)Si_8O_{22}(OH)_2$	Rootname 16
$PbCa_2(Mg_3Fe^{3+}{}_2)(Si_6Be_2)O_{22}(OH)_2$	Joesmithite	*Lithium-(magnesium-iron-manganese) subgroup:*	
Sodium-calcium subgroup:		$(LiMg)(Mg_4Al)Si_8O_{22}(OH)_2$	Rootname 22
$(NaCa)(Mg_4Al)Si_8O_{22}(OH)_2$	Winchite	$(LiMg)(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$	Rootname 23
$(NaCa)(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$	Barroisite	$Na(LiMg)Mg_5Si_8O_{22}(OH)_2$	Rootname 24
$Na(NaCa)Mg_5Si_8O_{22}(OH)_2$	Richterite	$Na(LiMg)(Mg_4Al)(Si_7Al)O_{22}(OH)_2$	Rootname 25
$Na(NaCa)(Mg_4Al)(Si_7Al)O_{22}(OH)_2$	Katophorite	$Na(LiMg)(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$	Rootname 26
$Na(NaCa)(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$	Taramite	*Lithium-calcium subgroup:*	
Sodium subgroup:		$(LiCa)(Mg_4Al)Si_8O_{22}(OH)_2$	Rootname 22
$Na_2(Mg_3Al_2)Si_8O_{22}(OH)_2$	Glaucophane	$(LiCa)(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$	Rootname 23
$NaNa_2(Mg_4Al)Si_8O_{22}(OH)_2$	Eckermannite	$Na(LiCa)Mg_5Si_8O_{22}(OH)_2$	Rootname 24
$NaNa_2(Mg_3Al_2)(Si_7Al)O_{22}(OH)_2$	Nybøite	$Na(LiCa)(Mg_4Al)(Si_7Al)O_{22}(OH)_2$	Rootname 25
$NaNa_2(Mg_2Al_2Li)Si_8O_{22}(OH)_2$	Leakeite	$Na(LiCa)(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$	Rootname 26
$Na_2(Fe^{2+}{}_3Fe^{3+}{}_2)Si_8O_{22}(OH)_2$	Riebeckite		
$NaNa_2(Fe^{2+}{}_4Fe^{3+})Si_8O_{22}(OH)_2$	Arfvedsonite		

$^{W}O^{2-}$-dominant group

$NaNa_2(Mg_3Fe^{3+}Ti^{4+})Si_8O_{22}O_2$	Ferri-obertiite
$NaNa_2(MgMn^{3+}{}_2Ti^{4+}Li)Si_8O_{22}O_2$	Mangani-dellaventuraite
$NaNa_2(Mn^{2+}{}_2Mn^{3+}{}_3)Si_8O_{22}O_2$	Mangano-mangani-ungarettiite
$NaCa_2(Mg_3Ti^{4+}Al)(Si_6Al_2)O_{22}O_2$	Kaersutite

extension and mutual relations are shown in Figure 3. Mineral compositions belonging to the last three blocks have not been found yet; however, these joins have been the object of extensive synthesis and characterization, which confirmed amphibole stability. Hence, they have been inserted in IMA2012 in order to make the new amphibole nomenclature conformable with possible discovery of new amphiboles in the future.

Rootnames: within each group, amphiboles are classified based on the proximity to integer aggregate ionic charge of the A and C cations, and rootnames identify integer-charge arrangements related to coupled heterovalent exchanges involving the A, C and T cations. The choice of C cations instead of T cations for classification purposes is a major issue of the new scheme and allows a better consideration of compositional complexity while adhering strictly to the dominance rule. Silicon is always the dominant T cation in the unit formula (and the formula of sadanagaite, $NaCa_2(Mg_3Al_2)(Si_5Al_3)O_{22}(OH)_2$, acknowledges for this fact), whereas several cations of major crystal-chemical significance may become dominant at the C group. Tremolite ($^{A}\ \ {}^{B}Ca_2{}^{C}Mg_5{}^{T}Si_8O_{22}{}^{W}(OH)_2$) is taken as the origin of amphibole compositional space, so that amphiboles are classified based on the aggregate ionic charge of the A cations ($^{A}R^{+}$) and the aggregate excess charge of the C cations ($^{C}R^{3+}$).

For classification purposes, the value of $^{A}R^{+}$ is calculated as $^{A}(Na + K + 2Ca)$. The value of $^{C}R^{3+}$ is calculated taking into account the following factors: 1) high-charge cations in amphiboles are commonly ordered at the *M*(2) site, so that their stoichiometric limit is 2.0 apfu; 2) high-charge cations involved in dehydrogenation are ordered at the *M*(1) and *M*(3) sites, and should therefore be considered separately; 3) the amount of Fe^{3+} at *M*(2) locally balancing the presence of ^{C}Li at

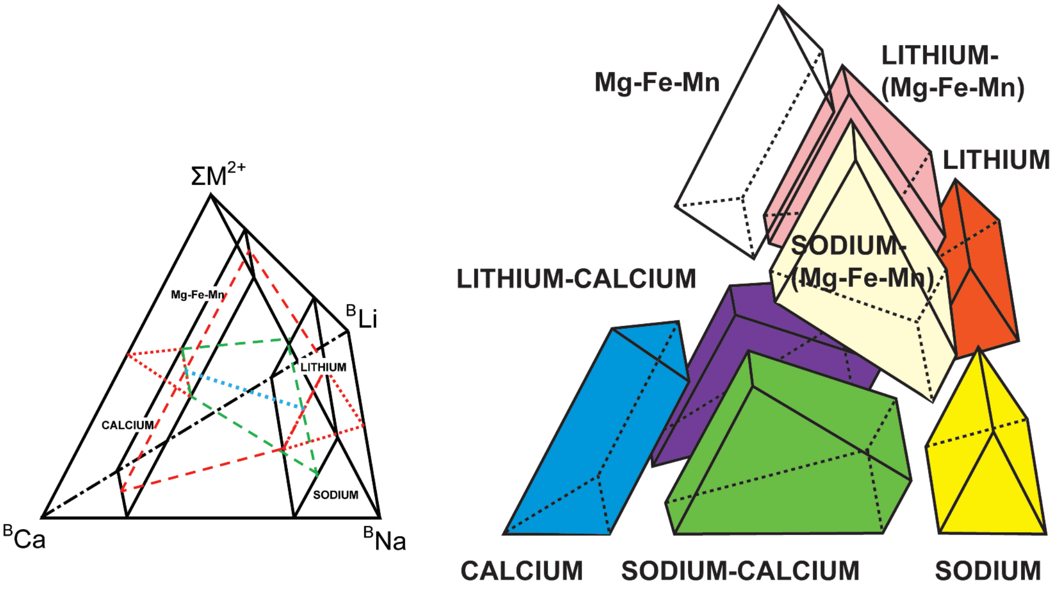

Figure 3. The compositional space of the $^{W}(OH, F, Cl)$-amphibole group. Mutual relations and boundaries among the different sub-groups are made clearer in the exploded tetrahedron (right).

the *M*(3) site should also not be considered because this exchange is internal to the C group in the unit formula. Hence, $^{C}R^{3+}$ is calculated as $^{C}(Al + Fe^{3+} + Mn^{3+} + (Sc, V, Cr, \dots)^{3+} + 2Ti^{4+} - Li - O^{2-})$. This correction to the raw $^{C}R^{3+}$ value is also one of the most significant innovations of this scheme, and must be done properly. Indeed, the crucial issue in this regard is the quantification of O^{2-}. Leake (1968) and Saxena and Ekström (1970) first noted a correlation between the Ti content and the oxo-component in calcic amphiboles, and further studies have confirmed that $^{M(1)}(Fe, Mn)^{2+} + 2OH^{-} \rightarrow {}^{M(1)}Ti^{4+} + 2O^{2-}$ accounts for most of the partial dehydrogenation occurring in amphiboles crystallised in upper-mantle and deep-crust geological environments (cf. Oberti et al., 2007 for a review). In contrast, H loss following oxidation of C cations, $^{M(1,3)}(Fe, Mn)^{2+} + OH^{-} \rightarrow {}^{M(1,3)}(Fe, Mn)^{3+} + O^{2-}$ is a often a signal of post-crystallisation processes. Hence, $^{C}Ti^{4+}$ can generally be considered as a proxy for dehydrogenation, and should be subtracted first, while $^{C}Fe^{3+}$ is subtracted only when the measured O^{2-} content is higher than $2Ti^{4+}$. It is important to state that $O^{2-} = 2Ti$ is the *maximum* value in most mantle amphiboles. Crystal-chemical studies confirm that only $^{C}Fe^{3+}$ must be subtracted from $^{C}R^{3+}$ to account for the presence of ^{C}Li.

Root names are assigned based on the integer values of reference for $^{A}R^{+}$ and $^{C}R^{3+}$; they all refer to the Mg, Al compositions, except for grunerite, riebeckite, arfvedsonite and hastingsite, which retain their former definitions because they are strongly embedded in petrological literature and rock nomenclature. Similarly, the general name "hornblende" is maintained, but is always accompanied by at least one prefix. A further important innovation in the IMA2012 scheme concerns magnesium-iron-manganese monoclinic amphiboles. Because Mn^{2+} is preferentially a B cation, compositions with $Mn^{2+} > 1.0$ apfu now deserve a new rootname, rootname 3. In contrast, because the site preference of Mg and Fe^{2+} is not so clear, and it is difficult to determine, the boundary between cummingtonite, $Mg_2Mg_5Si_8O_{22}(OH)_2$, and grunerite, $Fe^{2+}{}_2Fe^{2+}{}_5Si_8O_{22}(OH)_2$ has been put at $Fe_{tot}{}^{2+} = 3.5$ apfu. A comprehensive list of expected end-member compositions and rootnames for monoclinic amphiboles is reported in Table 1. Note that several rootnames have been abolished: ottoliniite, $(NaLi)(Mg_3Al_2)Si_8O_{22}(OH)_2$, and whittakerite, $Na(NaLi)(Mg_2Al_2Li)Si_8O_{22}(OH)_2$, because former Group 5 (Na-Ca-Mg-Mn-Fe-Li) amphiboles are now treated in a different way; kornite, $KNa_2(Mg_2Mn^{3+}{}_2Li)Si_8O_{22}(OH)_2$, and ehimeite, $NaCa_2(Mg_4Cr)(Si_6Al_2)O_{22}(OH)_2$, because the new definition of prefixes does no longer allow the use of a distinct rootname for composition differing only by homovalent substitutions; sodic-pedrizite, $NaLi_2(Mg_2Al_2Li)Si_8O_{22}(OH)_2$, because that was an anomalous use of the prefix "sodic" (as it implied a heterovalent substitution, $^{A}\ {}_{-1}{}^{A}Na_1$), a prefix that has been abolished in IMA2012. Note also that several end-members have been abolished, i.e., all those belonging to the former Group 5 which were not given a new rootname but only the parvo-prefix by IMA2003 (e.g., parvo-mangano-edenite and parvo-mangano-tremolite).

Prefixes. The use of prefixes is a further major difference from previous classifications, which considered fixed stoichiometric thresholds. Prefixes are now assigned based on the dominance among ions with the same charge (i.e., to A and C cations and W anions involved in homovalent substitutions). This choice emphasises the presence of many solid-solutions in amphiboles, and gives the proper weight to the dominant cation. For instance, the prefix "ferri" is now used when: a) the root name has an integral number of $^{C}R^{3+}$ cations, and b) $^{C}Fe^{3+} > {}^{C}Al, {}^{C}Cr, {}^{C}Mn^{3+}$. Note that the $^{C}Fe^{3+}$ value to be used is the one obtained after correction for ^{C}Li and O^{2-}, as discussed above.

The major consequence of the new rules is the fact that they recognises the presence of significant "exotic" substitutions (e.g., $^{C}Cr^{3+}$) but do not allow the use of a different rootname for homovalent substitution, as happened in the case of pargasite, $NaCa_2(Mg_4Al)(Si_6Al_2)O_{22}(OH)_2$, and its $^{C}Cr^{3+}$ counterpart (previously named ehimeite, Nishio-Hamane et al. (2012) and now named chromio-pargasite). Note also that "titano-" is no longer an approved prefix for amphiboles, because variation of $^{C}Ti^{4+}$ is not related to any homovalent substitution. Hence, in both the amphibole subgroups, the presence of $^{C}Ti^{4+} > 0.5$ apfu implies use of a new root-name. Note also that the prefix "sodium-" (formerly "sodic") is abolished (because it does not concern C cations), and the prefix "magnesium-" is limited to grunerite, riebeckite, arfvedsonite and hastingsite. The list of allowed prefixes and their definitions is reported in Table 2. The inconsistent prefixes "parvo" and "magno" introduced for Group 5 amphiboles in IMA2003 (now abolished) are no longer valid.

IMA2012 also specifies a new sequence of prefixes, which now follows the order of the amphibole formula itself: $AB_2C_5T_8O_{22}W_2$; hence, potassic-ferro-ferri-fluoro- followed by the root name. Prefixes related to symmetry (e.g., proto-) must precede those related to composition. Moreover, all prefixes must now be followed by a hyphen, so that root names are easily identified in the complete name (which makes computer search more straightforward).

Calculation of the unit formula and the AMPH2012 program

The new rules described above are quite rational and have only very few exceptions concerning root-names that are well embedded in the petrological and geochemical literature. However, they imply some treatment of the data, especially when significant amounts of ^{C}Li or O^{2-} are present in the amphibole under consideration. Indeed, a proper treatment of both these components requires very careful evaluation of the Fe^{3+}/Fe^{2+} ratio in the calculation of the formula unit. Calculation of Fe^{3+} strongly depends on the completeness, accuracy and precision of the analysis, with special reference to ^{C}Li and $^{W}O^{2-}$, and also on the normalization procedures. It is therefore strongly suggested that independent determinations of the Fe^{3+} content (e.g., Mössbauer or structure refinement analysis) are done when dealing with geological environments where Li incorporation and/or partial dehydrogenation are possible. If this is not the case, calculations based on 24(O, OH, Cl, F), with H_2O calculated so as to have 2(OH, F, Cl) pfu are suggested. Deviations from the correct group stoichiometry (especially of the C cations) should be taken into careful account because they can be signals of the presence of $^{B,C}Li$ or $^{W}O^{2-}$, which requires higher Fe^{3+} contents and Fe^{3+}/Fe_{tot} ratios. In this case, the use of independent information becomes crucial, and recalculation must be done taking into account increasing amounts of dehydrogenation (i.e., lower H_2O contents).

Although crystal-chemical studies have made us aware of a number of exceptions, the correlations presented by Leake (1968) and Saxena and Ekström (1970) for Ti-rich amphiboles support the general applicability of the relations $^{M(1)}Ti = Ti$ and $O^{2-} = 2Ti^{4+}$, with the limit of [2– (OH,F)]. Thus in the absence of a direct estimate of the (OH,F,Cl) content, we recommend that amphibole formulae be calculated on the basis of 24(O, OH, F, Cl) with (OH, F, Cl) = (2 - 2 Ti) apfu (being aware that this choice yields the maximum possible value of O^{2-}). Higher O^{2-} contents are however possible in all those petrogenetic environments where post-crystallization oxidation is feasible, for instance during subduction or interaction with metasomatic fluids. In all those cases, however, dehydrogenation is balanced by oxidation of $^{M(1,3)}Fe^{2+}$ to $^{M(1,3)}Fe^{3+}$.

Table 2. Prefixes to be used for amphiboles according to IMA2012.

Prefix	*Definition (apfu)*	*Not applicable to*
Chloro	$^{W}Cl > {}^{W}OH, {}^{W}F$	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	$^{C}Fe^{2+} > {}^{C}Mg, {}^{C}Mn^{2+}, {}^{C}Zn$	Any amphibole whose ferro-end-member has a trivial name: tremolite, cummingtonite, grunerite, hastingsite, riebeckite, arfvedsonite, rootname16
Fluoro	$^{W}F > {}^{W}OH, {}^{W}Cl$	Oxo-amphiboles
Magnesio	$^{C}Mg > {}^{C}Fe^{2+}, {}^{C}Mn^{2+}, {}^{C}Zn$	All amphiboles except riebeckite, arfvedsonite, hastingsite, hornblende
Mangano	$^{C}Mn^{2+} > {}^{C}Mg, {}^{C}Fe^{2+}, {}^{C}Zn$	
Mangani	$^{C}Mn^{3+} > {}^{C}Al, {}^{C}Cr, {}^{C}Fe^{3+}$	Amphiboles which do not contain trivalent cations in their root formulae
Oxo	$^{W}O^{2-} > {}^{W}(OH + F + Cl)$	Oxo-amphiboles where Ti = 1 apfu in the root formula, plus ungarettiite
Potassic	$^{A}K > {}^{A}Na$	Amphiboles which do not contain A-site cations in their root formulae
Zinco	$^{C}Zn > {}^{C}Mg, {}^{C}Fe^{2+}, {}^{C}Mn^{2+}$	

Spreadsheets for formula recalculation are presently available to any researcher, and are usually deeply modified accordingly to one's requirements. Hence, we have decided that the classification routine should start from a standard input of a crystal-chemical reasonable distribution of the constituents in the formula unit. This latter can be obtained by assigning, in this sequence, Si, Al and Ti (the latter only in the case of richterite) to the T cations up to the limit of 8.0 apfu; Al, Ti and all the other high-charge cations, Zn, Ni, Mg, Fe^{2+}, and Mn^{2+} to the C cations up to the limit of 5.0 apfu; residual Mn^{2+}, Fe^{2+}, Mg, and Ca and Na to the B cations up to a limit of 2.0 apfu, and the remainder (Na, K and -rarely - Ca) to the A cations.

When a structure refinement (SREF) is available, a more accurate redistribution of the cations (which can take into account also Li and O^{2-}) can be obtained by comparison of the refined site-scattering values (ss, epfu; cf. Hawthorne et al., 1995, for a definition) calculated for the B- and C-cations and the << *M*-O >> distance calculated based on the ionic radii of the C cations and their measured contents. SREF data also allow calculation of the maximum ^{C}Li content by the relation [ss*M*(1)-ss*M*(3)]/23, and of the O^{2-} content in calcium and sodium-calcium amphiboles from the relations (3.076-*M*(1)*M*(2))/0.054 and (3.120-*M*(1)*M*(2))/

0.051, respectively, where *M*(1)*M*(2) is the distance (in Å) between the two sites (Oberti et al., 2007).

The AMPH2012 program is written in Microsoft VisualBasic 6, and runs on all PCs working in the Windows operating system more recent than Windows2000. It can be downloaded free of charge from the website of CNR-IGG, UOS of Pavia: http://www_crystal.unipv.it/labcris/AMPH2012.zip.

The input consists of a string listing: ^{A}Na, ^{A}K, ^{A}Ca, ^{B}Na, ^{B}Ca, ^{B}Mg, ^{B}Fe^{2+}, ^{B}Mn^{2+}, ^{B}Li, ^{C}Mg, ^{C}Fe^{2+}, ^{C}Mn^{2+}, ^{C}Zn, ^{C}Al, ^{C}Fe^{3+}, ^{C}Mn^{3+}, ^{C}Cr^{3+}, ^{C}Ti^{4+}, ^{C}Zr^{4+}, ^{C}Li, ^{T}Si, ^{T}Al, ^{T}Ti, ^{W}O^{2-}, ^{W}F, ^{W}Cl, ^{W}OH. All these values can be also inserted manually in the opening frame.

The program takes into consideration in the correct logical sequence all the choices and requirements considered in the new classification scheme described above. The output gives the crystal-chemical formula, the correct amphibole group and the correct name (prefixes + rootname). When the result depends on the scientist's knowledge of site partitioning, as it is the case of magnesium-iron-manganese amphiboles, a message informs the user about the possible ambiguity and provides alternative solutions. At the end of each session, a report is printed listing all the amphibole compositions examined.

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