

AMPH-IMA04: a revised Hypercard program to determine the name of an amphibole from chemical analyses according to the 2004 International Mineralogical Association scheme

A. MOGESSIE^{1,*}, K. ETTINGER¹ AND B. E. LEAKE²

¹ Institute of Mineralogy and Petrology, University of Graz, Universitaetsplatz 2, A-8010 Austria

² School of Earth, Ocean and Planetary Sciences, Cardiff University, P.O.Box 914 Cardiff CF1 3YE, UK

ABSTRACT

In 2004, the International Mineralogical Association (IMA) amended the IMA 97 amphibole classification and nomenclature scheme by adding a fifth group to include the recently discovered ^B(LiNa) amphiboles ferriwhittakerite and ferri-ottoloniite, which cannot be fitted into the four major amphibole groups. New root-names such as sodic-pedrizite in the Mg-Fe-Mn-Li group and obertiite and dellaventuraitite in the sodic group along with two new prefixes, parvo and magno have also been added. As result it has become necessary to modify the AMPH-IMA97 amphibole-naming program. The new program (AMPH-IMA04) allows single input or automatic input of as many amphibole analyses as are available following a set input format. Any of three different calculation schemes for dealing with an amphibole analysis can be chosen: (1) complete chemical analyses can be calculated to 24(O,OH,F,Cl); (2) analyses with determined FeO and Fe₂O₃, MnO and Mn₂O₃ but without H₂O can be calculated to 23(O); and (3) electron microprobe analyses with only total Fe determined and without H₂O can be calculated to 23(O) with IMA97-recommended normalization for Fe³⁺ and Fe²⁺ values. In addition a stoichiometric calculation of Mn²⁺ and Mn³⁺ is considered and implemented for the Mn-bearing sodic amphiboles in order to take care of electron microprobe analyses of such amphiboles where the total Mn is given as Mn²⁺.

KEYWORDS: Hypercard, amphibole classification, amphibole-naming, IMA-nomenclature.

Introduction

SINCE the first ever internationally agreed amphibole nomenclature (IMA78) was approved by the International Mineralogical Association (IMA), several computer programs have been written to classify and name amphiboles based solely upon the chemistry and crystal symmetry (orthorhombic or monoclinic). They include programs by Mogessie and Tessadri (1982), Rock and Leake (1984), Rock (1987), Gobel and Smith (1988), Mogessie *et al.* (1990), Richard and Clarke (1990), Currie (1991, 1997), Tindle

and Webb (1994), Yavuz (1996, 1999) and Mogessie *et al.* (2001).

More recently (Leake *et al.*, 2004), the IMA revised the 1997 amphibole nomenclature scheme, mainly in order to include recently discovered ^B(LiNa) amphiboles which necessitated defining a new fifth amphibole group (Na-Ca-Mg-Fe-Mn-Li) but also to include other newly discovered species in the sodic and Mg-Fe-Mn-Li groups.

The newly discovered amphiboles which were not described in 1997 and are included in the revised IMA04 scheme (Leake *et al.*, 2004), are sodic-ferripedrizite, NaLi₂(Mg₂Fe³⁺Li)Si₈O₂₂(OH)₂, (Oberti *et al.*, 2000), sodic-ferri-ferropedrizite, NaLi₂(Fe²⁺Fe³⁺Li)Si₈O₂₂(OH)₂ (Oberti *et al.*, 2004), ferri-ottoloniite, □NaLi(Mg₃Fe³⁺Li)Si₈O₂₂(OH)₂ (Oberti *et al.*, 2004), ferriwhittakerite, Na(NaLi)(Mg₂Fe³⁺Li)

* E-mail: aberra.mogessie@uni-graz.at
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$\text{Si}_8\text{O}_{22}(\text{OH})_2$ (Oberti *et al.*, 2004), obertiite $\text{NaNa}_2(\text{Mg}_3\text{Fe}^{3+}\text{Ti})\text{Si}_8\text{O}_{22}\text{O}_2$ (Hawthorne *et al.*, 2002) and dellaventurite $\text{NaNa}_2(\text{MgMn}_2^{3+}\text{TiLi})\text{Si}_8\text{O}_{22}\text{O}_2$. It should be noted that the name given to the ferripedrizite by Caballero *et al.* (2002), was changed to sodic-ferripedrizite in Leake *et al.* (2004), which may have caused confusion. The present scheme has five more root names than IMA97 and two new prefixes, as described below. Chemistry and crystal symmetry still control nomenclature (Leake *et al.*, 2004).

IMA04 amphibole classification

The standard amphibole formula unit of $A_{0-1}B_2C_5T_8\text{O}_{22}(\text{OH})_2$ is the basis of the classification. The allocation of ions to positions is as follows:

(1) Sum *T* to 8 using Si, then Al, then Ti.

(2) Sum *C* to 5 using excess Al, then excess Ti from (1) and then successively, Fe^{3+} , V, Cr, Mn^{3+} , Zr, Mg, Zn, Ni, Co, Fe^{2+} , Mn^{2+} , Li.

(3) Sum *B* to 2 using first any excess above 5.00 from C, in the reverse order of (2) starting with Li and then Mn^{2+} etc., and then follow with Ca, Sr, Ba and Na.

(4) Excess above 2.00 in *B* is assigned to *A* in the reverse order of (3), starting with Na and then finally all the K is allocated to *A*. Total *A* should be 0 to 1.00.

If the H_2O and halogen contents are well established, the formula should be calculated to 24(O,OH,F,Cl), but if these are uncertain, the formula should be calculated to 23(O) with 2(OH,F,Cl) assumed, unless this leads to an impossibility of satisfying any of the following criteria, in which instance an appropriate change in the number of (OH+F+Cl) should be made. This last point is considered in the AMPH-IMA04 program for sodic amphiboles which are anhydrous or with (OH+F+Cl) < 1, such as obertiite, ungarrettiite $\text{NaNa}_2(\text{Mn}_2^{2+}\text{Mn}_3^{3+})\text{Si}_8\text{O}_{22}\text{O}_2$, and dellaventurite, and the calcic amphibole, kaersutite, $\text{NaCa}_2(\text{Mg}_4\text{Ti})\text{Si}_6\text{Al}_2\text{O}_{23}(\text{OH})$, where the total oxygen is taken as 23.5 and (OH,F,Cl) = 1 (see calculated analysis of kaersutite in Table 1).

Before Leake *et al.* (2004), the amphiboles were primarily classified into 4 major groups: Group I – Mg-Fe-Mn-Li amphiboles; Group II – calcic amphiboles; Group III – sodic-calcic amphiboles; and Group IV – sodic amphiboles. Now the amphiboles are classified primarily into five groups, still based on occupancy of the *B* positions.

Group 1. Where the sum of the L-type ions ${}^B(\text{Mg}+\text{Fe}^{2+}+\text{Mn}^{2+}+\text{Li}) \geq 1.50$, then the amphibole belongs to the Mg-Fe-Mn-Li group.

Group 2. Where ${}^B(\text{Mg}+\text{Fe}^{2+}+\text{Mn}^{2+}+\text{Li}) \leq 0.50$, ${}^B(\text{Ca}+\text{Na}) \geq 1.00$ and ${}^B\text{Na} < 0.50$, then the amphibole is a member of the calcic group.

Group 3. Where ${}^B(\text{Mg}+\text{Fe}^{2+}+\text{Mn}^{2+}+\text{Li}) \leq 0.50$, ${}^B(\text{Ca}+\text{Na}) \geq 1.00$ and $0.50 \leq {}^B\text{Na} < 1.50$ then the amphibole is a member of the sodic-calcic group.

Group 4. Where ${}^B(\text{Mg}+\text{Fe}^{2+}+\text{Mn}^{2+}+\text{Li}) \leq 0.50$, ${}^B\text{Na} \geq 1.50$, then the amphibole is a member of the sodic group.

Group 5. Where $0.5 < {}^B(\text{Mg}+\text{Fe}^{2+}+\text{Mn}^{2+}+\text{Li}) < 1.50$, $0.50 \leq {}^B(\text{Ca}+\text{Na}) \leq 1.50$, then the amphibole is a member of the sodic-calcic-Mg-Fe-Mn-Li group.

Root names are envisaged based on charge arrangements and crystal symmetry. Prefixes (given in IMA97 and IMA04) indicate additional major substitutions while optional modifiers (listed in IMA97) specify less important substitutions. The new major amphibole Group 5 was established to give identity to the new ${}^B(\text{LiNa})$ amphiboles ferri-ottoliniite and ferriwhittakerite but a few Li-poor compositions also fall into this new group, and because IMA did not wish to see the already large number (34) of root names increased unless unavoidably, Group 5 Li-poor (defined as ${}^B\text{Li} \leq 0.50$) compositions retain the same root names that they had before Group 5 was established. Such compositions acquire one of two new prefixes, restricted in use to Group 5, parvo if they would have been calcic or sodic-calcic amphiboles and magno if they would have been Mg-Fe-Mn-Li amphiboles (Leake *et al.*, 2004). Because of chemical overlaps between some of the orthorhombic and monoclinic members of the Mg-Fe-Mn-Li group, two names are output, (e.g. anthophyllite and cummingtonite) and the crystal symmetry has to be known to decide the correct name.

Problems with IMA04

It is difficult to assign the correct name to an amphibole analysed with the electron microprobe, since it is difficult to know how much of the analysed Fe is FeO or Fe_2O_3 , i.e. Fe^{2+} and Fe^{3+} . A detailed discussion of the stoichiometric calculation of Fe^{2+} and Fe^{3+} from electron microprobe analyses is given by Mogessie *et al.* (2001) and will not be repeated here. For sodic amphiboles such as kornite, $(\text{Na,K})\text{Na}_2(\text{Mg}_2\text{Mn}_2^{3+}\text{Li})\text{Si}_8\text{O}_{22}(\text{OH})_2$, leakeite,

HYPERCARD AMPHIBOLE-NAMING PROGRAM

TABLE 1. An edited excel table for calculated amphiboles imported using the 'file' background icon. Original names are given in the first row and the calculated names using AMPH-IMA04 in the last row.

Sample	Obertiite	Kozulite	Leakeite	Kaersutite	Whittakerite	Ottoliniite	Sodic-ferripedrizite
SiO ₂	56.27	50.32	56.76	42.13	59.94	60.36	58.99
TiO ₂	9.35			9.33			
Al ₂ O ₃				11.92	6.36	6.4	
Mn ₂ O ₃							
Fe ₂ O ₃							
MgO	14.15		9.52	18.84	10.05	15.18	9.89
MnO		29.7					
FeO	8.41	7.52	16.97		8.96	9.02	17.64
CaO				13.11			
Li ₂ O			1.76		3.73	1.88	5.5
Na ₂ O	10.88	9.73	10.98	3.62	7.73	3.89	3.8
K ₂ O							
Total	99.06	97.27	95.99	98.95	96.77	96.73	95.82
-O=F,Cl	0	0	0	0	0	0	0
Total	99.06	97.27	95.99	98.95	96.77	96.73	95.82
H ₂ O calc.		1.886	2.127	2.105	2.247	2.262	2.211
Si	8	8	8	6	7.999	8	8
Al	0	0	0	2	0.001	0	0
Ti	0	0	0	0	0	0	0
sum T	8	8	8	8	8	8	8
Al	0	0	0	0.001	0.999	1	0
Ti	1	0	0	0.999	0	0	0
Fe ³⁺	1	1	2	0	1	1	2.001
Mn ³⁺	0	0.003	0	0	0	0	0
Mg	2.999	0	2	4	1.999	2.999	1.999
Fe ²⁺	0	0	0	0	0	0	0
Mn ²⁺	0	3.996	0	0	0	0	0
Li	0	0	0.998	0	1.002	0.001	1
sum C	4.999	4.999	4.998	5	5	5	5
Mg	0	0	0	0	0	0	0
Fe ³⁺	0	0	0	0	0	0	0
Mn ²⁺	0	0	0	0	0	0	0
Li	0	0	0	0	1	1.001	2
Ca	0	0	0	2	0	0	0
Na	2	2	2	0	1	0.999	0
sum B	2	2	2	2	2	2	2
Ca	0	0	0	0	0	0	0
Na	0.999	0.999	1	1	1	0.001	0.999
K	0	0	0	0	0	0	0
sum A	0.999	0.999	1	1	1	0.001	0.999
catsum	15.998	15.999	15.998	15.999	16	15	15.999
OH	0	2	2	0	2	2	2
Oxeq	24	23	23	23.5	23	23	23
AMPH-IMA04	Obertiite	Kozulite	Leakeite	Kaersutite	Whittakerite	Ottoliniite	Sodic-ferripedrizite

NaNa₂(Mg₂Fe³⁺Li) Si₈O₂₂(OH)₂ ungarrettiite and dellaventurite, the Mn³⁺ content is important for classification and nomenclature. However, most amphiboles are analysed with the electron microprobe and similar to the problem we have with Fe it is difficult to determine how much of the analysed Mn is MnO or Mn₂O₃, i.e. Mn²⁺ and Mn³⁺. Therefore, for such types of amphiboles it is important to calculate the Mn²⁺ and Mn³⁺ from the electron microprobe data using stoichiometric methods as employed to determine Fe²⁺ and Fe³⁺ (Stout, 1972; Droop, 1987; Schumacher, 1991, 1997). We have attempted to make a stoichiometric calculation for Mn²⁺ and Mn³⁺ after the calculation has been made to distribute Fe into Fe²⁺ and Fe³⁺ and the total calculated oxygen is found to be <23 or the charge balance is <48 when calculated to 24 oxygens. As far as we know this is the first time that an attempt has been made to calculate the Mn²⁺ and Mn³⁺ in addition to Fe²⁺ and Fe³⁺ from a microprobe analysis in order to take care of the Mn³⁺-rich sodic amphiboles.

Discussion

Compared with the previous AMPH-IMA97 program (Mogessie *et al.*, 2001), the new program extends the elements to include V, Co, Ni, Zr, Sr and Ba. There are three options for each analysis in the new program (Fig. 1) with some modifications to those stated in Mogessie *et al.* (2001). The three options are:

- (1) Complete (FeO, Fe₂O₃, H₂O) chemical analyses can be calculated to 24(O,OH,F,Cl).
- Analyses with zero Fe₂O₃ and Mn₂O₃ are automatically calculated using 23(O) and the FeO_{total} normalized.
- (2) Analyses with determined FeO, Fe₂O₃, MnO and/or Mn₂O₃ but not H₂O, can be calculated to 23(O).
- (3) Analyses without determined FeO, Fe₂O₃, MnO, Mn₂O₃ and H₂O, but with determined total Fe and Mn can be calculated to 23(O) with a normalization scheme.

It is important to note that the Mn-normalization is made only for sodic amphiboles where

wt%		cations		SAMPLE		AMPH-IMA 2004	
SiO2	50.47	Si	8.000	Ungarrettiite, EM		A. Mogessie, K. Ettinger & B.E. Leake	
TiO2		Ti	0.000			T	C
ZrO2		Zr	0.000			Si	8.000
Al2O3		Al	0.000			Al	0.000
V2O3		V	0.000	calculation scheme		Ti	0.000
Cr2O3		Cr	0.000	<input checked="" type="radio"/> 24 anions or 23 (O)-normalised <input type="radio"/> 23 (O) without normalisation <input type="radio"/> 23 (O)- Fe2O3 as FeO, Mn2O3 as MnO		Σ T	8.000
Mn2O3		Mn3+	2.998	normalised		Fe3+	0.000
Fe2O3		Fe3+	0.000	Fe2O3 calc	0.000	V	0.000
MgO		Mg	0.000	FeO calc	0.000	Cr	0.000
MnO	37.25	Mn	2.003	classification parameter		Mn3+	2.998
FeO		Fe	0.000	B(Mg+Fe ²⁺ +Mn ²⁺ +Li)	0.001	BNa	1.999
NiO		Ni	0.000	B(Ca+Na)	1.999	A(Na+K)	1.001
CoO		Co	0.000	Mg	0.000	Mg	0.000
ZnO		Zn	0.000	Mg+Fe ²⁺	0.000	Mg+Mn ²⁺	0.000
CaO		Ca	0.000	Mn ²⁺ +Mn ³⁺	5.001	VAl+Fe ³⁺ +Fe ²⁺ +Mg	0.000
SrO		Sr	0.000			Σ C	5.000
BaO		Ba	0.000			Ca	0.000
Li2O		Li	0.000			Sr	0.000
Na2O	9.76	Na	3.000			Ba	0.000
K2O		K	0.000			Na	1.999
H2O		Σ c	16.001			Σ B	2.000
F		OH	0.000			K	0.000
Cl		F	0.000			Σ A	1.001
Total	97.48	Cl	0.000	Ungarrettiite			
-O=F,Cl	0.00	Σ a	0.000				
Total	97.48	An, Ox	24.000				
H2O calc.		+Charge	48.000				

Home file import calculate new analysis delete sort print file
↔

FIG. 1. Output card after calculation of single or multiple amphibole analyses. This is also used as an input card for single or multiple amphibole analyses.

the concentrations of Mn^{2+} and Mn^{3+} are critical for naming the amphibole. We appreciate that the only satisfactory solution to determining Fe and Mn oxidation states is independent Mössbauer, wet chemical or structure refinement methods.

Nomenclature and the problem of Fe^{2+} and Fe^{3+} normalization

In the AMPH-IMA97 (Mogessie *et al.* 2001) for the normalization options, a Mg-Fe-Mn-Li group amphibole formula was calculated on the basis of the sum of all the cations, excluding Na and K = 15 ($\Sigma Ca = 15$), whereas for all the other groups the sum of all the cations, excluding Ca, Na and K = 13 ($\Sigma FM = 13$) was used. The new amphiboles in Group 5 and Li- and Mn-bearing sodic amphiboles were calculated using the above assumptions. The result was not satisfactory as there is a continuous chemical composition between Group 5 amphiboles and the rest. Therefore, it became necessary to change this fixed parameter for the normalization procedure and implement the Fe^{2+} and Fe^{3+} normalization parameters recommended by Schumacher (1997) which considers the minimum and maximum Fe^{3+} for a respective amphibole analysis.

The program is set to determine automatically the correct factor that fulfills the stoichiometric criteria and calculates the respective Fe^{2+} and Fe^{3+} . Apart from this, there were other problems to be considered and solved. These are (1) distribution of Mn^{2+} and Mn^{3+} in the sodic amphiboles as discussed above; (2) the calculation of amphibole analyses and nomenclature for sodic amphiboles where $(OH+F+Cl) < 1$, such as obertiite, ungarettiite and dellaventuraite; and (3) to assign the prefixes 'parvo' and 'magno' to Group 5 amphiboles with ${}^B Li \leq 0.50$ a.p.f.u. (see Table 1). Over 500 amphibole analyses cited in Deer *et al.* (1997) were calculated and named, proving that the new AMPH-IMA04 program works for all the amphibole groups recommended by Leake *et al.* (2004).

The AMPH-IMA04 program

The program is revised to include the recommended new names, the new amphibole group and the additional prefixes 'parvo' and 'magno'. However the description of the program remains the same (Mogessie *et al.*, 2001) only with minor modifications. Compared to the input card for AMPH-IMA97 (Mogessie *et al.*, 2001) the

present program has additional elements which include V, Co, Ni, Zr, Sr and Ba; and classification parameters (${}^B(Mg + Fe^{2+} + Mn^{2+} + Li)$, $(Mn^{2+} + Mn^{3+})$, $({}^{IV}Al + Fe^{3+} + Fe^{2+} + Mg)$) (Fig. 1). Buttons for 'comments' and 'parageneses' are left out.

It is important to note that one can import as many analyses as necessary using the 'file import' button and automatically calculate the imported data. The data should be in a tab-delimited input format where name, sample or oxides can be arranged in any order but should be in one line per analysis and the respective values must be given in the empty fields following the headings (e.g. SiO_2 50.5 etc.).

The program AMPH-IMA04 can be downloaded from the Mineralogical Society website: www.minersoc.org/pages/e_journals/dep_mat.htm

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