Mineralogical Magazine, October 2004, Vol. 68(5), pp. 825–830

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

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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 ferriwhittakeriite and ferri-ottoliniite, 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 dellaventuraite 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 Fe_2O_3, MnO and Mn_2O_3 but without H_2O can be calculated to 23(O); and (3) electron microprobe analyses with only total Fe determined and without H_2O can be calculated to 23(O) with IMA97-recommended normalization for Fe^{3+} and Fe^{2+} values. In addition a stoichiometric calculation of Mn^{2+} and Mn^{3+} 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 Mn^{2+}.

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, $NaLi_2(Mg_2Fe^{3+}_2Li)Si_8O_{22}(OH)_2$, (Oberti *et al*., 2000), sodic-ferri-ferropedrizite, $NaLi_2(Fe^{2+}_2Fe^{3+}_2Li)Si_8O_{22}(OH)_2$ (Oberti *et al*., 2004), ferri-ottoloniite, $\square NaLi(Mg_3Fe^{3+}Li)Si_8O_{22}(OH)_2$ (Oberti *et al*., 2004), ferriwhittakerite, $Na(NaLi)(Mg_2Fe^{3+}_2Li)$

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DOI: 10.1180/0026461046850223

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$Si_8O_{22}(OH)_2$ (Oberti *et al*., 2004), obertiite $NaNa_2(Mg_3Fe^{3+}Ti)Si_8O_{22}O_2$ (Hawthorne *et al*., 2002) and dellaventuraite $NaNa_2(MgMn_2^{3+}TiLi)Si_8O_{22}O_2$. 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 $A_{0-1}B_2C_5T_8O_{22}(OH)_2$ 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, ungarettiite $NaNa_2(Mn_2^{2+}Mn_3^{3+})Si_8O_{22}O_2$, and dellaventuraite, and the calcic amphibole, kaersutite, $NaCa_2(Mg_4Ti)Si_6Al_2O_{23}(OH)$, 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 $^B(Mg+Fe^{2+}+Mn^{2+}+Li) \geqslant 1.50$, then the amphibole belongs to the Mg-Fe-Mn-Li group.

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

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

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

Group 5. Where $0.5 < {}^B(Mg+Fe^{2+}+Mn^{2+}+Li) < 1.50$, $0.50 \leqslant {}^B(Ca+Na) \leqslant 1.50$, 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}(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 $^BLi \leqslant 0.50$) 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, $(Na,K)Na_2(Mg_2Mn_2^{3+}Li)Si_8O_{22}(OH)_2$, leakeite,

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_2O_3				11.92	6.36	6.4	
Mn_2O_3							
Fe_2O_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_2O			1.76		3.73	1.88	5.5
Na_2O	10.88	9.73	10.98	3.62	7.73	3.89	3.8
K_2O							
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_2O 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^{2+}	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

$NaNa_2(Mg_2Fe^{3+}_2Li)\ Si_8O_{22}(OH)_2$ ungarettiite and dellaventuraite, the Mn^{3+} 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 Mn_2O_3, i.e. Mn^{2+} and Mn^{3+}. Therefore, for such types of amphiboles it is important to calculate the Mn^{2+} and Mn^{3+} from the electron microprobe data using stoichiometric methods as employed to determine Fe^{2+} and Fe^{3+} (Stout, 1972; Droop, 1987; Schumacher, 1991, 1997). We have attempted to make a stoichiometric calculation for Mn^{2+} and Mn^{3+} after the calculation has been made to distribute Fe into Fe^{2+} and $Fe^{3+}$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 Mn^{2+} and Mn^{3+} in addition to Fe^{2+} and Fe^{3+} from a microprobe analysis in order to take care of the Mn^{3+}-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, Fe_2O_3, H_2O) chemical analyses can be calculated to 24(O,OH,F,Cl).

Analyses with zero Fe_2O_3 and Mn_2O_3 are automatically calculated using 23(O) and the FeO_{total} normalized.

(2) Analyses with determined FeO, Fe_2O_3, MnO and/or Mn_2O_3 but not H_2O, can be calculated to 23(O).

(3) Analyses without determined FeO, Fe_2O_3, MnO, Mn_2O_3 and H_2O, 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

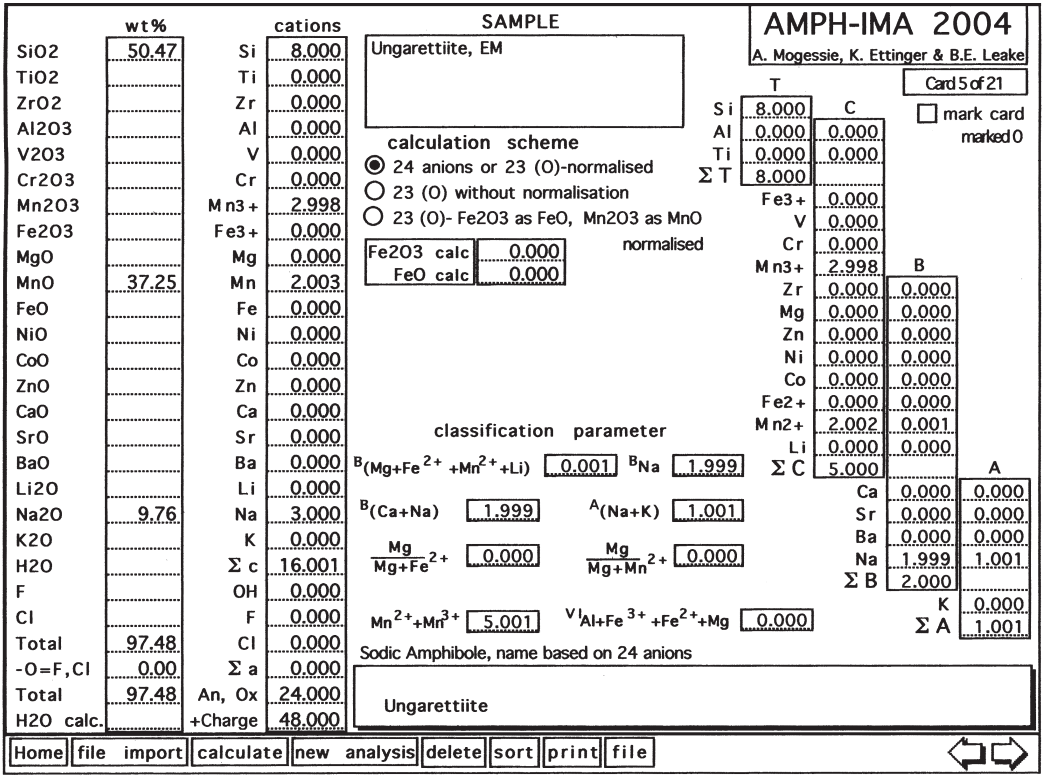

FIG. 1. Output card after calculation of single or multiple amphibole analyses.This is also used as an input card for single or multiple amphibole analyses.

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 fullfills 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 $^{B}Li \leqslant 0.50$ 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

Acknowledgements

We would like to thank F.C. Hawthorne for giving us permission to use the reference Tait *et al*. (in press) for the new sodic amphibole dellaventuraite. R. Oberti is thanked for the critical and constructive review of this paper.

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[*Manuscript received 14 April 2004: revised 27 August 2004*]