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An Excel spreadsheet to classify chemical analyses of amphiboles following the IMA 2012 recommendations

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ABSTRACT

A Microsoft Excel spreadsheet has been programmed to assist with classification of chemical analyses of orthorhombic and monoclinic amphiboles following the 2012 nomenclature recommended by the International Mineralogical Association. The spreadsheet is intended for use only with compositional data (wt% oxides and halogens, rather than atomic proportions) and provides options for the estimation of $Fe^{3+}/\Sigma Fe$ and $Mn^{3+}/\Sigma Mn$ ratios and OH content. Various cation normalization schemes can be automatically or manually selected. For each analysis, the output includes the group, subgroup (or B-occupancy for the oxo-amphiboles), and species name including any mandatory chemical prefixes, along with a formula based on 24 anions. The formula results can be exported in a form suitable for the AMPH2012 program. Prefixes related to space groups (proto-) and suffixes ($-P2_1/m$) are not assigned in the spreadsheet. Large data sets (up to 200 analyses at a time) can be accommodated by the spreadsheet, which is accompanied by results calculated for more than 650 amphibole analyses taken from the literature.

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1. Introduction

The compositional complexity of amphiboles has driven several previous attempts by the International Mineralogical Association to organize their nomenclature (Leake, 1978; Leake et al., 1997, 2003; Burke and Leake, 2004). Continued investigation of amphibole crystal chemistry has necessitated revisions to these guidelines (Hawthorne and Oberti, 2006, 2007b), and has culminated in the establishment of the amphibole supergroup (Hawthorne et al., 2012; Oberti et al., 2012). Computer-based implementation of the various IMA guidelines has developed in parallel with ongoing changes in amphibole nomenclature. Several programs and spreadsheets were published following each round of nomenclatural changes, and these are reviewed in Yavuz (2007), Esawi (2011) and Oberti et al. (2012). Most recently, a Visual Basic program, AMPH2012, has been published (Oberti et al., 2012) and classifies amphiboles based on the already-calculated formula proportions of the constituent ions. The AMPH2012 program is the official tool endorsed for amphibole nomenclature by the IMA-CNMNC Subcommittee on Amphiboles (Hawthorne et al., 2012; Oberti et al., 2012).

The conversion from compositional data (percent by weight) to formula proportions – a formula expressed in atoms per formula unit (apfu) – is not as straightforward for an amphibole as it is for many other rock-forming minerals. The general amphibole formula from Hawthorne et al. (2012) is: $AB_2C_5T_8O_{22}W_2$, where A=□, Na, K, Ca, Pb, Li; B=Na, Ca, Mn^{2+}, Fe^{2+}, Mg, Li; C=Mg, Fe^{2+}, Mn^{2+}, Zn, Ni^{2+}, Co^{2+}, Fe^{3+}, Mn^{3+}, Cr^{3+}, V^{3+}, Sc, Al, Ti, Zr, Li; T=Si, Al, Ti^{4+}, Be; W=(OH), F, Cl, O^{2-}. The calculation from wt% to apfu is made more complex by the range of the A cations from complete occupancy to complete vacancy, and the possibility of occupancy of W by anions of different charge: $(OH)^-$, F^-, Cl^-, O^{2-}. This variability results in a potential range from 15 to 16 non-H cations, and from 46 to 48 negative charges, per formula unit (pfu), e.g., tremolite $□Ca_2(Mg_5)(Si_8)O_{22}(OH)_2$, and kaersutite $NaCa_2(Mg_3TiAl)(Si_6Al_2)O_{22}O_2$. The challenges inherent in calculation of amphibole formulas have been discussed most notably by Stout (1972), Hawthorne (1983), Schumacher (1991, 2007), Appendix 2 of Leake et al. (1997), Hawthorne and Oberti (2007a), Oberti et al. (2012) and Hawthorne et al. (2012).

At present, most analyses of amphiboles are obtained solely with the use of an electron microprobe, which cannot measure some of the important light elements involved in amphibole classification (H, Li), and which does not routinely measure the valence state (oxidation state) of Fe (or Mn). Hawthorne et al. (2012) drew attention to the inaccuracy of amphibole formulas that lack data for H, Li and Fe^{3+}, and summarized the various modern analytical methods that can measure these quantities (Appendix II of Hawthorne et al. (2012)). In the absence of results from such techniques and despite the consequent potential for

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significant inaccuracy, classification of large amounts of electron microprobe data is still needed, and so Hawthorne et al. (2012) reviewed methods for calculating the Fe^{3+} and OH content of amphiboles in their Appendix III.

It must be emphasized that the spreadsheet described herein is limited to using only chemical data to implement the nomenclature (referred to henceforward as IMA 2012) of the amphibole supergroup (Hawthorne et al., 2012). The limitations of the input chemical data therefore limit the results from this spreadsheet (e.g., Li-rich amphiboles will not be properly handled if lithium has not been analyzed). For a comprehensive understanding of a given amphibole, a structure refinement and spectroscopic data should be acquired.

Elements that occur in amphibole only in low abundance (such as Ba or Ge) and that were not considered in IMA 2012 are not included here, with the exceptions of Sr and P. The spreadsheet can accommodate up to 200 analyses, and includes results calculated for more than 650 amphibole analyses from the literature and over 130 end-members and hypothetical compositions.

2. IMA 2012 nomenclature of the amphibole supergroup

The IMA 2012 nomenclature is described in detail by Hawthorne et al. (2012) and Oberti et al. (2012). The nomenclature follows the dominant-constituent and dominant-valence principles elucidated by Hatert and Burke (2008), and is based on the occupancy of the W, B, A and C groups of crystallographic sites (Hawthorne et al., 2012; Oberti et al., 2012). The amphibole supergroup is divided into two formal groups based on the anions that are dominant at W, resulting in ^{W}(OH,F,Cl)-dominant amphiboles and ^{W}O-dominant amphiboles. The hydroxy-fluoro-chloro-amphiboles are formally divided into eight subgroups on the basis of the occupancy of the B cations. Within each subgroup, distinct formal charge-arrangements yield distinct rootnames. Substitution by homovalent ions is indicated by the use of mandatory prefixes, resulting in distinct species names. The A and C groups of cations are used to distinguish species using ranges of compositions within the formal subgroups. The expression used here for classification purposes related to the A cations is $^{A}(Li+Na+K+2Ca+2Pb)$. The expression used here for classification purposes related to the C cations is $^{C}(Al+Fe^{3+}+Mn^{3+}+Cr+V+Sc+2Ti+2Zr)-(^{W}O)-(^{C}Li)$; see Hawthorne et al. (2012) and Oberti et al. (2012). As a result of the new subgroups, the prefixes parvo and magno are no longer required in amphibole nomenclature (Leake et al., 2003; Hawthorne et al., 2012; Oberti et al., 2012). Ghoseite (IMA-CNMNC, 2013a), suenoite (IMA-CNMNC, 2013b), and oxo-magnesio-hastingsite (Zaitsev et al., 2013) have been approved subsequently by the IMA Commission on New Minerals, Nomenclature and Classification (CNMNC).

Only five distinct root-compositions of oxo-amphiboles (amphiboles with O dominant at W) have been described. However, the possibility of further oxo-species analogous to the ^{W}(OH,F,Cl)-dominant amphiboles has been recognized. Substitution by homovalent ions in the oxo-amphiboles is also handled by mandatory prefixes.

3. Formula normalization and Fe^{3+} estimation

3.1. Basis for formula normalization

Following IMA 2012, the formula, $AB_2C_5T_8O_{22}W_2$ should be normalized on the basis of 24 anions (O,OH,F,Cl), with the assumption of (OH,F,Cl)=2 pfu at W for analyses where H_2O+ content (water of crystallization corresponding to hydroxyl content) is not known. This basis can be expressed as 22O+2(OH,F,Cl) and formally yields 46 negative charges, which is equivalent in charge to 23O pfu (23 O-equivalents). Alternatively, as the occurrence of significant Ti (but not Zr) into the amphibole structure is commonly accompanied by the replacement of ^{W}(OH) by ^{W}O, IMA 2012 recommends that the OH content in such cases be estimated by the expression: (OH,F,Cl)=2–2Ti pfu (Hawthorne et al., 2012; Oberti et al., 2012). They caution that this will produce the maximum value of O at W, as the expression effectively also corresponds to: WO=2Ti apfu. However, they also caution that Fe^{3+} may balance the loss of H, especially when post-crystallization oxidation is feasible. The estimation of the W contents based on the amount of Ti gives a maximum basis of 24O (for 1Ti apfu), e.g., kaersutite $NaCa_2(Mg_3TiAl)(Si_6Al_2)O_{22}O_2$. Three options can therefore be considered for handling the anion content at W:

1. Use the (OH,F,Cl) content derived from the input composition, regardless of whether it exceeds, equals, or does not reach, 2 pfu.
2. Estimate (OH,F,Cl)=2–2Ti pfu, and therefore, ^{W}O=2Ti apfu.
3. Assume 2(OH,F,Cl) pfu.

Depending on the anion content, the basis for normalization of an amphibole analysis thus varies from 23 O-equivalents: 22O+2(OH,F,Cl), to 24 O-equivalents: 22O+2O. In analyses where the OH content slightly exceeds 2 pfu, the O-equivalents will be slightly lower than 23O. [Although amphibole is generally considered to have a stoichiometric limit of 2 (OH,F,Cl) pfu, some wet-chemical analyses report results in excess of this limit, and the present spreadsheet is designed to accommodate this possibility for comparative purposes, at the option of the user.] This variable basis has implications for the calculation of Fe^{3+} based on expressions of cation sums.

3.2. Lithium

Li is a significant component in some amphibole species (Oberti et al., 2003), although it is not a common constituent of ordinary rock-forming amphiboles (Deer et al., 1997). In the end-member amphiboles of IMA 2012, Li can occur either as a B or a C cation (or both), for example holmquistite $\square Li_2(Mg_3Al_2)Si_8O_{22}(OH)_2$, mangani-dellaventuraite $NaNa_2(MgMn^{3+}_2Ti^{4+}Li)Si_8O_{22}O_2$, and pedrizite $NaLi_2(Mg_2Al_2Li)Si_8O_{22}(OH)_2$ (Hawthorne et al., 2012; Oberti et al., 2012). Lithium only rarely occurs as an A cation – to date, it has only been found in synthetic amphiboles (e.g., Iezzi et al., 2004) – and therefore no end-members with this assignment were established in IMA 2012.

It is recommended that Li should be measured by techniques such as SIMS, LA-ICP-MS, or structure refinement (Hawthorne and Oberti, 2007a; Marks et al., 2008; Hawthorne et al., 2012; Oberti et al., 2012). If Li has been measured, such data can be used in the spreadsheet. If Li has not been measured but is actually present in abundance (approximately >0.8 wt% Li_2O), the spreadsheet will not give correct results. As shown by Oberti et al. (2003), for amphibole analyses with $Si>8$ apfu and/or $C<5$ apfu, the presence of Li may be suspected, and in certain favorable cases, estimated. Estimation of Li content is not implemented in the current spreadsheet because such estimation lacks sufficient accuracy for many amphiboles. The user is, of course, free to use trial-and-error methods to approximate Li content by judging the suitability of the resulting stoichiometry, but such methods propagate considerable uncertainty from the entire chemical analysis into the approximation (Giaramita and Day, 1990).

3.3. Estimation of Fe^{3+} content

Amphibole classification generally requires that the valence state of Fe be known or estimated. In analyses where the valence

state of Fe has not been measured, the $Fe^{3+}/\Sigma Fe$ ratio can be calculated by constraining the sum of a set of cations to a particular value and assuming electroneutrality for the entire formula (Hawthorne et al., 2012). The various cation sums and constraints proposed for this calculation have been discussed in detail: Hawthorne (1983), Schumacher (1991, 2007), Appendix 2 of Leake et al. (1997), Hawthorne and Oberti (2007a), and Hawthorne et al. (2012). For the purposes of classification, following IMA 2012, an amphibole analysis with the formula $AB_2C_5T_8O_{22}W_2$ can be considered to have the following non-hydrogen cations as possible constituents: Si, P, Ti, Zr, Al, Sc, V^{3+}, Cr, Mn^{2+}, Mn^{3+}, Fe^{2+}, Fe^{3+}, Co, Ni, Zn, Be, Mg, Ca, Sr, Li, Na, Pb, K. The elements Sr and P were not included in the IMA 2012 classification; Sr is included here as a B cation and assumed to play the same role in cation sums as Ca, and P is assigned as a T cation. The following cation sums discussed in the IMA 2012 nomenclature are commonly used for normalization of an amphibole formula (for which the cations are considered in the order listed above):

1. Sum of all cations from Si to K = 16 apfu.
2. Sum of cations from Si to Na = 15 apfu.
3. Sum of cations (includes Li) from Si to Ca = 15 apfu.
4. Sum of cations (includes Li) from Si to Mg = 13 apfu.

The application of these cation sums is discussed in the description of the spreadsheet below. Additional stoichiometric constraints for metamorphic amphiboles are detailed in Appendix 1 of Schumacher (2007). As these latter constraints are not explicitly discussed in the IMA 2012 nomenclature, they are not implemented for charge-balance purposes in the current spreadsheet. However, users of the present spreadsheet should be aware of these the limits on the compositions of common amphiboles, and examine their results with some care.

Methods of estimation of Fe^{3+} (and Mn^{3+}) contents of amphibole are generally inaccurate in comparison to measured values (Appendix 3 of Hawthorne et al. (2012); Appendix 1 of Schumacher (2007)), but are better than no estimate at all. In the current spreadsheet, simple scoring criteria are used to determine which cation sums are used for estimation of Fe^{3+} (and Mn^{3+}) contents, as detailed in Section 4.3 below. In cases where the scores are equal for two or more cation sums, their results are averaged, even if those results differed considerably from each other. It is up to the user to decide whether such averaging is acceptable; the option exists instead to force the use of one or more cation sums.

4. Spreadsheet description

The Excel spreadsheet consists of nine worksheets:

1. **Instructions** worksheet.
2. **Input_Output** worksheet that contains both the input chemical data and the output (group, subgroup, species, and formula) for each analysis.
3. **Calculation** worksheet in which the details of the algorithm have been programmed.
4. **Literature** worksheet tabulates the data and results for over 650 analyses from the literature as well as data for more than 130 end-members.
5. **References** worksheet lists bibliographic entries for more than 150 literature references from which the chemical analyses were obtained.
6. **apfu_wt%** worksheet can be used to calculate compositional data from the input of formula proportions for amphiboles and lists ideal chemical data for end-members.
7. **Elements** worksheet can be used to transform concentration data from weight percent element to weight percent oxide.
8. **How to Export** worksheet gives the steps necessary to export the formula proportions in a form suitable for the AMPH2012 program (Oberti et al., 2012) using the **9. AMPH2012** worksheet.
9. **AMPH2012** worksheet lists the formula proportions taken automatically from the **3. Calculation** worksheet in a form suitable to be exported as a MS-DOS text file for use with the AMPH2012 program (Oberti et al., 2012).

4.1. Data input

Compositions are entered in the columns of the **2. Input_Output** worksheet (Table 1). Iron and manganese can be entered either as the monoxides FeO and MnO, or as the sequioxides Fe_2O_3 and Mn_2O_3, or in both valence states; note that for reasons of redox equilibria FeO and Mn_2O_3 should not both be present in the same analysis. The correction for the oxygen equivalence of fluorine and chlorine (O = F, Cl), the total, and the initial values for $Fe^{3+}/\Sigma Fe$ and $Mn^{3+}/\Sigma Mn$ are calculated by the worksheet.

Up to 200 analyses can be entered (one per column) in the **2. Input_Output** worksheet. For each analysis, a label should be assigned. In Table 1, the labels correspond to publications and sample names. In addition to entering the data and labels, the user is required to make four decisions for each analysis that influence how the calculation will proceed (Table 1). These include whether:

1. the amphibole has orthorhombic symmetry, "orthorhombic? (TRUE/FALSE)";
2. the initial values for the valence states of Fe and Mn should be retained throughout the algorithm, "use initial $M^{3+}/\Sigma M$? (TRUE/FALSE)";
3. the hydroxyl content should be estimated based on the Ti content of the analysis, "estimate OH = 2–2Ti? (TRUE/FALSE)";
4. the initial value for water of crystallization should be retained throughout the algorithm, "Require initial H_2O+? (TRUE/FALSE)".

Each choice should be answered with TRUE or FALSE. If any other entry is made in the decision cell, or if the cell is left blank, then Excel defaults to FALSE. The consequences of these choices are described below.

The symmetry of an amphibole can be determined by petrography or diffraction techniques, and this information is needed as some of the orthorhombic amphiboles have different rootnames from the corresponding monoclinic amphiboles. However, it is up to the user to recognize and label monoclinic amphiboles that have space group $P2_1/m$ (with the suffix $-P2_1/m$), and equally to recognize and label orthorhombic amphiboles that have $a \sim 9.4$ Å and space group *Pnmn* (Sueno et al., 1998) with the principal prefix proto-, as recommended by IMA 2012.

To retain the initial valence states of Fe and Mn throughout the algorithm, the entry for the decision cell "use initial $M^{3+}/\Sigma M$? (TRUE/FALSE)" must be TRUE. If TRUE, the calculation will be based on 24 anions using the input values for FeO, MnO, Fe_2O_3 and Mn_2O_3. Otherwise, the spreadsheet will try to achieve charge balance by normalizing the formula to one or more sets of cation sums.

If the water of crystallization (corresponding to structural OH) has not been measured, or if the result of such a measurement is considered unreliable, then the OH content can be estimated on the basis of the Ti content (see Section 3.1 above). If so, the entry for the cell "estimate OH = 2–2Ti? (TRUE/FALSE)" must be TRUE. Hawthorne et al. (2012) introduced this approximation, and along

Table 1
Examples of input data for amphibole analyses.

INPUT	J Petrol 13 99 Stout (1972)	Can Min 21 173 Hawthorne (1983)	RiMG 67 1 Hawthorne and Oberti (2007a)	Deer et al. (1966)
Identifier/label	161A	Table 7	745	Appendix 1
Orthorhombic? (TRUE/FALSE)	FALSE	FALSE	FALSE	FALSE
Use initial $M^{3+}/\Sigma M$ (TRUE/FALSE)	FALSE	**TRUE**	**TRUE**	**TRUE**
Estimate OH=2–2Ti? (TRUE/FALSE)	FALSE	FALSE	FALSE	FALSE
Require initial H_2O+? (TRUE/FALSE)	FALSE	**TRUE**	**TRUE**	**TRUE**
Analysis (wt%)				
SiO_2	45.40	40.85	52.47	51.63
TiO_2		0.65	6.51	
ZrO_2				
Al_2O_3	13.30	14.45	0.09	7.39
Sc_2O_3				
V_2O_3				
Cr_2O_3				
MnO	0.30	0.35	0.15	0.17
Mn_2O_3				
FeO	12.70	18.53	18.43	5.30
Fe_2O_3		5.59	4.54	2.50
CoO				
NiO				
ZnO				
BeO				
MgO	13.80	5.11	5.74	18.09
CaO	11.20	10.86	0.90	12.32
PbO				
Li_2O			0.17	
Na_2O	1.60	1.48	8.70	0.61
K_2O		0.61	1.51	
H_2O+		1.62	0.58	2.31
F			0.51	
O=F,Cl (calc)			−0.21	
Initial total	98.30	100.10	100.09	100.32
$Fe^{3+}/\Sigma Fe$ initial	0.000	0.213	0.181	0.298
$Mn^{3+}/\Sigma Mn$ initial	0.000	0.000	0.000	0.000
Manual choice of normalization procedure(s): use initial $M^{3+}/\Sigma M$=false				
Require Si–Ca&Li ≤ 15? (TRUE/FALSE)				
Require Si–Mg&Li ≥ 13? (TRUE/FALSE)				
Require Si–Na ≥ 15? (TRUE/FALSE)				
Require Si–K ≤ 16? (TRUE/FALSE)				

For clarity, some vacant rows present in the spreadsheet have been omitted from this table.

with Oberti et al. (2012) noted that this yields a minimum value for OH, as not all of the Ti is necessarily involved in a deprotonation substitution. In addition, they noted that post-crystallization deprotonation may occur by oxidation of Fe. Hence, modulation of the $Fe^{3+}/\Sigma Fe$ ratio should be attempted by the user when the results of the estimation of OH by Ti content are not satisfactory (Oberti, personal communication, June 2013).

Alternatively, if the initial value for H_2O+ is accepted, then the entry for the decision cell "Require initial H_2O+? (TRUE/FALSE)", must be TRUE. In this circumstance, the initial value of H_2O+ is retained throughout the algorithm, even if this value was zero. If the entry is not TRUE, and if the OH content is *not* estimated on the basis of Ti content, then the spreadsheet defaults to sufficient OH content to reach 2(OH,F,Cl) pfu.

If the proportions of both FeO and Fe_2O_3 (or both MnO and Mn_2O_3) are not determined, or if the initial valence states of Fe and Mn are not considered reliable, the spreadsheet automatically attempts to achieve charge balance while normalizing the formula to one or more sets of cation sums. However, a user may wish to employ one or more particular cation sum (or sums) for such normalization (especially if some independent sense of the oxidation state of the amphibole is known). If a particular cation normalization scheme is used, the entry for the decision cell "use initial $M^{3+}/\Sigma M$? (TRUE/FALSE)" *cannot* be TRUE. There are four cation sum constraints to select from (Table 1):

1. Require Si–Ca&Li ≤ 15? (TRUE/FALSE).
2. Require Si–Mg&Li ≥ 13? (TRUE/FALSE).
3. Require Si–Na ≥ 15? (TRUE/FALSE).
4. Require Si–K ≤ 16? (TRUE/FALSE).

The value TRUE must be entered in the corresponding decision cell to ensure use of a specific cation sum; the spreadsheet defaults to FALSE for any other entry including a blank cell.

4.2. Formula proportions

The calculations take place in the **3. Calculation** worksheet with data copied automatically from the **2. Input_Output** worksheet.

To determine the formula proportions, the compositional data in weight percent are divided by the atomic weights (Wieser and Berglund, 2009) of the corresponding oxides and halogens to yield molar proportions. The molar proportions of cations and anions are determined, and the formula proportions are calculated by normalizing the formula on the basis of 24 anions (O,OH,F,Cl). For amphiboles with W=2(OH,F,Cl), this basis is equivalent to 23O (23 O-equivalents). However, for amphibole analyses in which O^{2-} occupies part or all of W, this basis ranges up to 24O (24 O-equivalents). The spreadsheet begins its calculations with the O-equivalents that are calculated from the input data.

4.3. Charge balance

The description below of charge balance applies only to those analyses where the initial values for the valence states of Fe and Mn are *not* retained throughout the calculation process.

As the valence state of Fe (and Mn) is not commonly measured in contemporary analyses, but is needed for classification purposes, it is usually necessary to normalize the analysis on the basis of the sum of a set of cations. This cation sum is constrained to a particular value, and the ratio $Fe^{3+}/\Sigma Fe$ and/or $Mn^{3+}/\Sigma Mn$ is adjusted with the assumption of electroneutrality. The cation sums used are listed in Section 3.3. In the **3. Calculation** worksheet, after the initial formula proportions have been determined, the formula proportions are then recalculated on the basis of the following cation normalization schemes (sums): Si to Ca+Li=15 apfu; Si to Mg+Li=13 apfu; Si to Na=15 apfu; and Si–K=16 apfu.

How should an algorithm determine which schemes are most appropriate for a given analysis? Hawthorne et al. (2012) showed that the constraints on the amphibole formula arising from the various cation normalization schemes could be treated as criteria. As the criteria are not each satisfied by every amphibole end-member, and as real analyses are imperfect, there will usually be deviations from the criteria. In the spreadsheet, for each of the four normalization schemes, the maximum magnitude of the deviations of the formula proportions from the following criteria is determined: Si < 8 apfu; non-H cations < 16 apfu; sum Si to Ca (+Li) < 15 apfu; sum Si to Mg (+Li) > 13 apfu; sum Si to Na > 15 apfu. The normalization schemes with the smallest maximum deviations are used. To allow for the imperfection of real data, a threshold of 0.005 apfu is used for the deviations, and for the separation of the normalization schemes. Having automatically determined which normalization schemes should be used

(based on the smallest maximum deviations from the criteria), the spreadsheet calculates the appropriate formula proportions based on the number of oxygen equivalents and then normalizes the formula proportions to 24 anions (O,OH, F,Cl).

For an amphibole with between 23 and 24 O-equivalents – that is, if (OH,F,Cl) is <2 pfu, such as occurs with some measured H_2O+ contents, or if OH is estimated based on non-zero Ti content – the format of the input data (e.g., total iron input as FeO or as Fe_2O_3) affects the magnitude of the anion basis that is initially computed. For analyses in which the relative proportions of both FeO and Fe_2O_3 (and both MnO and Mn_2O_3) are calculated by normalization rather than retained from the input data, the differing magnitudes of the anion basis may lead to slightly differing formula proportions. To avoid this discrepancy, the entire algorithm completed to this point is repeated using the ratios $Fe^{3+}/\Sigma Fe$ and $Mn^{3+}/\Sigma Mn$ that were first calculated by normalization. This procedure, although inelegant, avoids iteration within the spreadsheet, as the option of iterative calculation must be set up explicitly by each user in Excel.

4.4. Assignment of cations

The final formula proportions are used in the assignment of the A, B, C, and T cations, and the W anions. Use of the spreadsheet requires that cations be assigned in a specific order. The following procedure is used to allocate the ions to the groups of sites:

- T: Si, P, Be, and Al as needed to reach 8 apfu. If Al is insufficient, Ti is added. If Ti is insufficient, Fe^{3+} is added to reach 8 apfu. Note that $^{[4]}Ti$ is only expected in certain richterite-rich amphiboles (Oberti et al., 1992); authors should carefully examine their data if this assignment is made in the spreadsheet. Similarly, the assignment in amphibole of $^{[4]}Fe^{3+}$ is controversial (Deer et al., 1997), although supported by some spectroscopic data (Homonnay et al., 1990), and is not given in IMA 2012.
- C: all remaining Al, Ti, Fe^{3+}, Zr, Sc, V, Cr, Mn^{3+}, Co, Ni, Zn, and Mg to reach 5 apfu. If Mg is insufficient, it is followed by Fe^{2+}, then Mn^{2+}, and finally Li to reach 5 apfu.
- B: any remaining Mn^{2+}, Fe^{2+}, Mg, any Sr and enough Li to reach 2 apfu. If Li is insufficient, it is followed by Ca, and then by Na, to reach 2 apfu.
- A: all remaining Li, Ca, Na, Pb and K, ideally to a maximum of 1 apfu.
- W: OH, F and Cl are assigned here, with sufficient O to reach 2 apfu.

A more accurate cation distribution for a given amphibole can only be obtained by including independent data such as the results of structure refinement or spectroscopy. However, the procedure implemented in the present spreadsheet yields results that are in very good agreement with published amphibole structure refinements. In particular, the cation distributions of Li-rich amphiboles ($Li>0.5$ apfu) were tested for 31 unique structure refinements from release 2012-2 of the Inorganic Crystal Structure Database (Belsky et al., 2002). For this set, the results from the spreadsheet agree with the charge-balanced formulas from the refined structures to within 0.01 apfu, with the exception of the relative partitioning of Mg and Fe^{2+} between the C and B cation groups. Such Mg–Fe^{2+} partitioning can only be determined properly with additional constraints from structure refinement or spectroscopy. It must be stressed that the limitations of the input data limit the results from the spreadsheet; Li-rich amphiboles cannot be properly classified by the spreadsheet if lithium contents have not been provided.

4.5. Determination of group, subgroup, rootname, prefixes and formula

From the allocated ions, an amphibole analysis is assigned to the (OH,F,Cl)-group of amphiboles or the oxo-amphibole group based on the dominant occupancy of W. This assignment relies heavily on accurate analysis of H_2O+ (and F and Cl), or on reliable estimation of OH (and thus O) content based on Ti content (and possibly on Fe^{3+} content related to deprotonation). Within the (OH,F,Cl)-group, one of eight subgroups is assigned based on the dominant occupancy of B: (Mg–Fe–Mn), Ca, Na–Ca, Na, Li, Na–(Mg–Fe–Mn), Li–(Mg–Fe–Mn), and Li–Ca subgroups. For the oxo-amphiboles, the dominant B occupancy is listed instead. As recommended by IMA 2012, the A- and C-groups of cations are used to assign rootnames based on specific compositional ranges (see Section 2). Mandatory prefixes (if any) are assigned to describe symmetry (clino-), and the homovalent variations in the dominant ions of the root compositions. Space-group-related prefixes (proto-) and suffixes ($-P2_1/m$) are not assigned in the spreadsheet. As clino-holmquistite *sensu stricto* was formally discredited as a species (Oberti et al., 2005) but is a compositional field in IMA 2012 (Hawthorne et al., 2012), compositions that fall in this field are labeled 'clino-holmquistite'; the use of single quotation marks helps indicate the lack of accreditation of this name.

A formula is generated for each analysis, with sums for each ion set: A, B, C, T, O, and W. Within each set, the contents are listed in order of decreasing abundance regardless of valence state. Because of the format limitations in Excel for generated text, numerical values cannot be given automatically as superscripts or subscripts. Thus, ferric iron is shown as FeIII and ferrous iron as Feii, and trivalent manganese is given as MnIII with divalent manganese as Mnii; these valence-state indicators in the formula are given for the C cations only (Fe^{3+} and Mn^{3+} do not occur as B cations).

4.6. Data output

The results (group, subgroup, species, and formula) calculated by the algorithm in the **3. Calculation** worksheet are copied to the **2. Input_Output** worksheet below the corresponding input composition for each analysis (Table 2). The output includes the normalization procedures that were used. For analyses where the initial values for the valence states of Fe and Mn were retained throughout the algorithm, the result "per 24 (O,OH,F,Cl)" is given instead. If one or more cation-sum normalization schemes were used (see Section 3.3), these are listed (Table 2). For each analysis the values used in the final formula proportions of the ratios $Fe^{3+}/\Sigma Fe$ and $Mn^{3+}/\Sigma Mn$ are given, along with the final values in weight percent of MnO, Mn_2O_3, FeO, Fe_2O_3, H_2O+ and the final total of the weight percent data.

The assignments of the ions are tabulated for T, C, B, A, non-W O, and W with subtotals for each, and an overall cation sum. The group, subgroup (or B-occupancy for the oxo-amphiboles) and species name (including mandatory chemical prefixes) is given, along with the chemical formula derived from the analysis (Table 2). As a result of rounding in the presentation of the results, the formula proportions and sums are valid only to ± 0.001 apfu.

Several warnings are programmed into the spreadsheet to assist with the recognition of data of inferior quality, or conflicting instructions. Nevertheless, it is incumbent upon the user to ensure the quality of their data and the interpretation of the results – this spreadsheet must not be treated as a "black box". The **2. Input_Output** worksheet outputs a warning (Table 2) if:

- the final analytical total (including any calculated proportion of H_2O+) is outside the range 98–102 wt%;

Table 2
Examples of output for amphibole analyses.

Identifier/label	J Petrol 13 99 Stout (1972) 161A	Can Min 21 173 Hawthorne (1983) Table 7	RiMG 67 1 Hawthorne and Oberti (2007a) 745	Deer et al. (1966) Appendix 1
Normalization procedures used for average formula (apfu)	Si–Ca&Li = 15 Si–Mg&Li = 13	per 24 (O,OH,F,Cl)	per 24 (O,OH,F,Cl)	per 24 (O,OH,F,Cl)
$Fe^{3+}/\Sigma Fe$ used	0.499	0.213	0.181	0.298
$Mn^{3+}/\Sigma Mn$ used	0.000	0.000	0.000	0.000
Final wt% values				
MnO	0.30	0.35	0.15	0.17
Mn_2O_3	0.00	0.00	0.00	0.00
FeO	6.36	18.54	18.44	5.30
Fe_2O_3	7.04	5.58	4.53	2.50
H_2O+	2.09	1.62	0.58	2.31
Total	101.10	100.10	100.09	100.32
Formula Assignments				
T (ideally 8 apfu)				
Si	6.447	6.252	7.992	7.196
Al	1.553	1.748	0.008	0.804
T subtotal	8.000	8.000	8.000	8.000
C (ideally 5 apfu)				
Ti		0.075	0.746	
Al	0.673	0.859	0.009	0.410
Fe^{3+}	0.753	0.644	0.520	0.262
Mn^{2+}			0.019	
Fe^{2+}	0.652	2.257	2.348	0.569
Mg	2.921	1.166	1.303	3.759
Li			0.055	
C subtotal	4.999	5.001	5.000	5.000
B (ideally 2 apfu)				
Mn^{2+}	0.036	0.045		0.020
Fe^{2+}	0.103	0.115		0.049
Li			0.050	
Ca	1.704	1.781	0.147	1.840
Na	0.157	0.058	1.803	0.091
B subtotal	2.000	1.999	2.000	2.000
A (from 0 to 1 apfu)				
Na	0.284	0.381	0.766	0.074
K		0.119	0.293	
A subtotal	0.284	0.500	1.059	0.074
O (non-W)	22.000	22.000	22.000	21.852
W (ideally 2 apfu)				
OH	2.000	1.654	0.589	2.148
F			0.246	
Cl				
O		0.346	1.165	
W subtotal	2.000	2.000	2.000	2.148
Sum T,C,B,A	15.283	15.500	16.059	15.074
Group	OH,F,Cl	OH,F,Cl	oxo	OH,F,Cl
Subgroup of (OH,F,Cl)	Ca	Ca	B = Na	Ca
Species	Magnesio-ferri-hornblende	Ferro-hornblende	Ferro-ferri-obertiite	Magnesio-hornblende
Formula	(Na0.284)Σ0.284 (Ca1.704Na0.157Fe0.103Mn0.036)Σ2 (Mg2.921FeIII0.753Al0.673Feii0.652)Σ4.999 (Si6.447Al1.553)Σ8 O22 ((OH)2)Σ2	(Na0.381K0.119)Σ0.5 (Ca1.781Fe0.115Na0.058Mn0.045)Σ1.999 (Feii2.257Mg1.166Al0.859FeIII0.644Ti0.075)Σ5.001 (Si6.252Al1.748)Σ8 O22 ((OH)1.654O0.346)Σ2	(Na0.766K0.293)Σ1.059 (Na1.803Ca0.147Li0.05)Σ2 (Feii2.348Mg1.303Ti0.746FeIII0.52Li0.055Mnii0.019Al0.009)Σ5 (Si7.992Al0.008)Σ8 O22 (O1.165(OH)0.589F0.246)Σ2	(Na0.074)Σ0.074 (Ca1.84Na0.091Fe0.049Mn0.02)Σ2 (Mg3.759Feii0.569Al0.41FeIII0.262)5 (Si7.196Al0.804)Σ8 O21.852 ((OH)2.148)Σ2.148
Warnings				
Final total < 98 or > 102 wt%				
A > 1			High A sum: 1.059	
C < > 5				
T < > 8				
W < > 2				High W sum: 2.148

For clarity, some vacant rows present in the spreadsheet have been omitted from this table.

Table 3
Examples of the effects of select normalizations for an amphibole analysis.

Notes	Deer et al. (1966) Original	Deer et al. (1966) All ferrous iron	Deer et al. (1966) All ferric iron	Deer et al. (1966) Si–Ca&Li = 15	Deer et al. (1966) Si–Na = 15	Deer et al. (1966) Automatic: mean of Si–Ca&Li = 15 and Si–Na = 15
use initial $M^{3+}/\Sigma M$? (TRUE/FALSE)	**TRUE**	**TRUE**	**TRUE**	FALSE	FALSE	FALSE
Require initial H_2O+? (TRUE/FALSE)	**TRUE**	FALSE	FALSE	FALSE	FALSE	FALSE
Analysis (wt%)						
SiO_2	51.63	51.63	51.63	51.63	51.63	51.63
Al_2O_3	7.39	7.39	7.39	7.39	7.39	7.39
MnO	0.17	0.17	0.17	0.17	0.17	0.17
FeO	5.30	7.55	–	5.30	5.30	5.30
Fe_2O_3	2.50	–	8.39	2.50	2.50	2.50
MgO	18.09	18.09	18.09	18.09	18.09	18.09
CaO	12.32	12.32	12.32	12.32	12.32	12.32
Na_2O	0.61	0.61	0.61	0.61	0.61	0.61
H_2O+	2.31	2.31	2.31	2.31	2.31	2.31
Initial total	100.32	100.07	100.91	100.32	100.32	100.32
$Fe^{3+}/\Sigma Fe$ initial	0.298	0.000	1.000	0.298	0.298	0.298
Normalization procedures used for formula (apfu)	per 24 (O,OH,F,Cl)	per 24 (O,OH,F,Cl)	per 24 (O,OH,F,Cl)	Si–Ca&Li = 15	Si–Na = 15	Si–Ca&Li = 15 and Si–Na = 15
$Fe^{3+}/\Sigma Fe$ used	0.298	0.000	1.000	0.150	0.724	0.435
Final wt% values						
MnO	0.17	0.17	0.17	0.17	0.17	0.17
FeO	5.30	7.55	0.00	6.42	2.08	4.27
Fe_2O_3	2.50	0.00	8.39	1.26	6.07	3.65
H_2O+	2.31	2.13	2.16	2.14	2.15	2.14
Total	100.32	99.89	100.76	100.03	100.52	100.27
T (ideally 8 apfu)						
Si	7.196	7.261	7.124	7.240	7.161	7.201
Al	0.804	0.739	0.876	0.760	0.839	0.799
T subtotal	8.000	8.000	8.000	8.000	8.000	8.000
C (ideally 5 apfu)						
Al	0.410	0.486	0.325	0.462	0.369	0.415
Fe^{3+}	0.262		0.871	0.132	0.634	0.383
Mn^{2+}			0.020		0.015	
Fe^{2+}	0.569	0.721		0.624	0.242	0.440
Mg	3.759	3.793	3.721	3.782	3.740	3.761
C subtotal	4.999	5.000	4.937	5.000	5.000	4.999
B (ideally 2 apfu)						
Mn^{2+}	0.020	0.020		0.020	0.005	0.020
Fe^{2+}	0.049	0.167		0.129		0.057
Ca	1.840	1.813	1.821	1.851	1.831	1.841
Na	0.091		0.163		0.164	0.082
B subtotal	2.000	2.000	1.984	2.000	2.000	2.000
A (from 0 to 1 apfu)						
Ca		0.043				
Na	0.074	0.166		0.166		0.083
A subtotal	0.074	0.209	0.000	0.166	0.000	0.083

Table 3 (*continued*)

Notes	Deer et al. (1966) Original	Deer et al. (1966) All ferrous iron	Deer et al. (1966) All ferric iron	Deer et al. (1966) Si–Ca&Li = 15	Deer et al. (1966) Si–Na = 15	Deer et al. (1966) Automatic: mean of Si–Ca&Li = 15 and Si–Na = 15
O (non-W)	21.852	22.000	22.000	22.000	22.000	22.000
OH	2.148	2.000	2.000	2.000	2.000	2.000
Sum T,C,B,A	15.074	15.209	14.921	15.166	15.000	15.082
Group	OH,F,Cl	OH,F,Cl	OH,F,Cl	OH,F,Cl	OH,F,Cl	OH,F,Cl
Subgroup of (OH,F,Cl)	Ca	Ca	Ca	Ca	Ca	Ca
Species	Magnesio-hornblende	Actinolite	Magnesio-ferri-hornblende	Magnesio-hornblende	Magnesio-ferri-hornblende	Magnesio-hornblende
Formula	(Na0.074)Σ0.074 (Ca1.84Na0.091Fe0.049Mn0.02)Σ2 (Mg3.759Feii0.569Al0.41FeIII0.262)Σ5 (Si7.196Al0.804)Σ8 O21.852 ((OH)2.148)Σ2.148	(Na0.166Ca0.043)Σ0.209 (Ca1.813Fe0.167Mn0.02)Σ2 (Mg3.793Feii0.721Al0.486)Σ5 (Si7.261Al0.739)Σ8 O22 ((OH)2)Σ2	()Σ0 (Ca1.821Na0.163)Σ1.984 (Mg3.721FeIII0.871Al0.325Mnii0.02)Σ4.937 (Si7.124Al0.876)Σ8 O22 ((OH)2)Σ2	(Na0.166)Σ0.166 (Ca1.851Fe0.129Mn0.02)Σ2 (Mg3.782Feii0.624Al0.462FeIII0.132)Σ5 (Si7.24Al0.76)Σ8 O22 ((OH)2)Σ2	()Σ0 (Ca1.831Na0.164Mn0.005)Σ2 (Mg3.74FeIII0.634Al0.369Feii0.242Mnii0.015)Σ5 (Si7.161Al0.839)Σ8 O22 ((OH)2)Σ2	(Na0.083)Σ0.083 (Ca1.841Na0.082Fe0.057Mn0.02)Σ2 (Mg3.761Feii0.44Al0.415FeIII0.383)Σ4.999 (Si7.201Al0.799)Σ8 O22 ((OH)2)Σ2
Warnings						
B < > 2			Low B sum: 1.984			
C < > 5			Low C sum: 4.937			
W < > 2	High W sum: 2.148					

For clarity, some vacant rows present in the spreadsheet have been omitted from this table.

- the totals for any of A, B, C, T or W are outside the expected stoichiometric values;
- ferrous iron and trivalent manganese are both present; this would have had to been input by the user and retained throughout the algorithm;
- both of the mutually exclusive choices "estimate OH=2–2Ti? (TRUE/FALSE)" and "Require initial H_2O+? (TRUE/FALSE)" are entered as TRUE; the spreadsheet defaults to using the measured value of H_2O+;
- one or more of the normalization schemes (Si to Ca+Li=15 apfu; Si to Mg+Li=13 apfu; Si to Na=15 apfu; and Si–K=16 apfu) has been manually selected and the option "use initial $M^{3+}/\Sigma M$? (TRUE/FALSE)" has been entered as TRUE; the spreadsheet defaults to using the initial valence states of iron and manganese;
- Ca or Li are present as A cations – these assignments are possible, but very rare;
- the sum of high valence (M^{3+} and M^{4+}) C cations exceeds 2 apfu – this is possible, but not expected in common amphiboles.

In addition to these explicit warnings, a user of the spreadsheet should carefully consider the validity of any uncommon cation assignments, including ^{A}Ca, ^{A}Li, ^{T}Ti, or $^{T}Fe^{3+}$ (cf. Appendix 1 of Schumacher, 2007). It is possible that in many cases, such assignments are artifacts of the calculation procedure in combination with the effects of propagated analytical uncertainty.

The effects of different choices of Fe valence state or normalization scheme on the results are shown in Table 3 using the analysis from Appendix 1 of Deer et al. (1966). This analysis was used previously as an example for calculations in both IMA 2012 (Hawthorne et al., 2012) and in the 1997 IMA amphibole nomenclature (Leake et al., 1997; Schumacher, 1997). Along with the formula proportions determined for the original analysis, Table 3 presents formula proportions (assuming 2 OH pfu) calculated with $Fe^{3+}/\Sigma Fe=0$, $Fe^{3+}/\Sigma Fe=1$, and the cation normalizations Si–Ca&Li=15, Si–Na=15, and the average of these two normalizations that is the automatic choice of the spreadsheet for this analysis. The results of Table 3 are in good agreement with Appendix III of Hawthorne et al. (2012).

4.7. Data export

The AMPH2012 program endorsed by the IMA-CNMNC Subcommittee on Amphiboles does not accept chemical data, but uses atomic proportions of the cation and anion sites (Oberti et al., 2012). The formula results from the present spreadsheet can be exported as a MS-DOS text file for use with the AMPH2012 program. Instructions are given in the **8. How to Export** worksheet, and the **9. AMPH2012** worksheet lists the formula proportions in a form suitable for such export. Note that the formula proportions are not recalculated for such export. As AMPH2012 only accepts a certain range of elements, the exported data may only be a subset of the complete analysis.

5. Testing of the spreadsheet

More than 650 analyses, mostly from the recent literature, were compiled in the **4. Literature** worksheet to test the utility and validity of the spreadsheet. This compilation is extensive, but not exhaustive, and omits elements (such as Ba or Ge) that were not included in IMA 2012 as possible constituents. The application of the IMA 2012 nomenclature to the compiled analyses results in 141 distinct names because of homovalent substitution and/or differing symmetry. These are listed, each with a selected reference, in Table 4 (divided by group and/or subgroup, and organized semi-alphabetically by rootname). This table is only representative of the compiled analyses and is not a comprehensive list of all possible species. The complete bibliographic entries for the references cited in Table 4 can be found in the **5. References** worksheet. Some of the species listed in Table 4 have not received formal approval from the IMA; these are *named amphiboles* (Burke and Leake, 2004), including the currently discredited 'clino-holmquistite'.

Most of the variation in Table 4 results from the application of chemistry-specific mandatory prefixes, along with symmetry-specific prefixes and suffixes; only 33 trivial (common) rootnames are tabulated. Five rootnames in IMA 2012 correspond to Fe^{2+} or Fe^{3+} equivalents (homovalent substitution of Mg or Al by Fe) of common amphiboles: actinolite, arfvedsonite, grunerite, hastingsite and riebeckite. A number of the compiled analyses yield compositions that have no trivial name defined in the IMA 2012 guidelines, e.g., rootname2 (Table 4). Rootname2 was introduced in IMA 2012 in place of sodicgedrite, as the formula differs from the previous (Leake et al., 1997) and because the term "sodic" is not a valid mandatory prefix in IMA 2012 (Hawthorne et al., 2012). Compositions that appear to require new trivial names include rootname2, rootname4 and rootname14 (Table 4). Further investigation of these compositions, including structure refinement and possibly acquisition of spectroscopic data, is needed to verify these species, and in some cases, is already underway (Oberti and Hawthorne, personal communications, May 2013).

Analytical uncertainty is propagated and magnified in a complex fashion during the calculation of a (multisite, multivalent) structural formula from oxide concentrations (Giaramita and Day, 1990). One result of such error magnification is that the naming of a given amphibole may be less definite than it first appears. Detailed consideration of error propagation is beyond the scope of the present work. However, the user of the spreadsheet is cautioned that the propagated errors resulting from calculation of $Fe^{3+}/\Sigma Fe$ ratios with differing normalization schemes may introduce considerable uncertainty into the classification of an amphibole analysis (e.g., Table 3). Particularly where a formula is close to a boundary between species, it is fitting to recall that the word amphibole is derived from the Greek term *amphibolos*, meaning ambiguous (Deer et al., 1997).

6. System requirements and program availability

The spreadsheet has been tested with Excel 2000 and the OpenOffice program Calc using the Windows XP operating system, with Excel 2010 using the Windows 7 operating system, and with Microsoft Excel for Mac 2011 using the Mac OS X (V10.5.6) operating system. The spreadsheet is available from github.com as a release: https://github.com/cageo/Locock-2013/releases, or from the author.

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Table 4
Amphiboles and selected references; $n=141$ entries.

Group: oxo-amphiboles	
Mangani-dellaventuraite	Tait et al. (2005)
Oxo-edenite	Deer et al. (1997) Table 11, #22
Oxo-magnesio-hastingsite	Zaitsev et al. (2013)
Kaersutite	Jarosewich et al. (1980)
Ferri-kaersutite	Dyar et al. (1993)
Ferri-obertiite	Hawthorne et al. (2000)
Ferro-ferri-obertiite	Hawthorne et al. (2010)
Oxo-pargasite	Leake (1971)
Oxo-ferri-pargasite	Dyar et al. (1993)
Mangani-ungarettiite	Ashley (1986)
Mangano-mangani-ungarettiite	Hawthorne et al. (1995)
Group: OH–F–Cl; subgroup Mg–Fe–Mn	
Orthorhombic	
Anthophyllite	Welch et al. (2011)
Ferro-anthophyllite	Mücke et al. (2006)
Gedrite	Schindler et al. (2008)
Ferro-gedrite	Linthout et al. (1995)
Ferro-ferri-gedrite	Mücke et al. (2006)
Rootname2	Tsunogae et al. (2007)
Ferro-rootname2	Damman (1988)
Proto-anthophyllite	Konishi et al. (2003)
Proto-ferro-anthophyllite	Sueno et al. (1998)
Proto-ferro-suenoite	Sueno et al. (1998)
Monoclinic	
Cummingtonite	Ishida and Hawthorne (2003)
Grunerite	Nayak et al. (2011)
Clino-suenoite	Klein and Ito (1968)
Clino-ferro-suenoite	Vassileva et al. (2001)
Cummingtonite-$P2_1/m$	Kisch (1969)
Group: OH–F–Cl; subgroup Ca	
Actinolite	Ernst (2002)
Ferro-actinolite	Leake et al. (1995)
Mangano-actinolite	Damman and Lustenhouwer (1992)
Fluoro-cannilloite	Hawthorne et al. (1996)
Edenite	Oberti et al. (2006)
Ferro-edenite	Giret et al. (1980)
Fluoro-edenite	Gianfagna and Oberti (2001)
Potassic-ferro-chloro-edenite	Pan and Fleet (1992)
Hastingsite	Uvarova et al. (2007)
Magnesio-hastingsite	McCanta et al. (2008)
Magnesio-fluoro-hastingsite	Bojar and Walter (2006)
Potassic-magnesio-hastingsite	Dawson and Smith (1982)
Potassic-hastingsite	Oberti et al. (1993)
Potassic-fluoro-hastingsite	Lupulescu et al. (2009)
Potassic-chloro-hastingsite	Léger et al. (1996)
Ferro-hornblende	Sautter et al. (2006)
Ferro-ferri-hornblende	Nawaz and Ryback (1989)
Magnesio-hornblende	Ernst (2002)
Magnesio-ferri-hornblende	Ernst (2002)
Joesmithite	Moore et al. (1993)
Pargasite	Ishida and Hawthorne (2006)
Ferro-pargasite	Oberti et al. (1993)
Chromio-pargasite	Nishio-Hamane et al. (2012)
Mangani-pargasite	Hålenius and Bosi (2012)
Fluoro-pargasite	Ishida and Hawthorne (2006)
Potassic-pargasite	Robinson et al. (1997)
Potassic-ferro-pargasite	Ishida and Hawthorne (2006)
Potassic-fluoro-pargasite	Oberti et al. (2010)
Potassic-chloro-pargasite	Chukanov et al. (2002)
Rootname4	Dyar et al. (1993)
Ferro-rootname4	Deer et al. (1997) Table 21, #19
Ferri-rootname4	Lamb et al. (2012)
Potassic-ferro-rootname4	Shimazaki et al. (1984)
Sadanagaite	Hawthorne et al. (2008)
Ferro-sadanagaite	Deer et al. (1997) Table 16, #9
Ferri-sadanagaite	Dawson and Smith (1982)
Ferro-ferri-sadanagaite	Deer et al. (1997) Table 16, #3
Ferro-chloro-sadanagaite	Kullerud and Erambert (1999)
Potassic-sadanagaite	Shimazaki et al. (1984)
Potassic-ferro-sadanagaite	Shimazaki et al. (1984)
Potassic-ferri-sadanagaite	Shimazaki et al. (1984)
Potassic-ferro-ferri-sadanagaite	Hawthorne et al. (2008)
Potassic-ferro-chloro-sadanagaite	Kullerud and Erambert (1999)
Tremolite	Valley et al. (1982)
Group: OH–F–Cl; subgroup Na–Ca	
Barroisite	Horak and Gibbons (1986)
Ferri-barroisite	Deer et al. (1997) Table 23, #6
Ferro-ferri-barroisite	Deer et al. (1997) Table 23, #8
Katophorite	Mével and Kiénast (1986)
Ferro-katophorite	Leake et al. (1995)
Ferri-katophorite	Hawthorne et al. (2008)
Ferro-ferri-katophorite	Borley (1963)
Fluoro-katophorite	Hawthorne et al. (1998)
Ferri-fluoro-katophorite	Hawthorne et al. (1993)
Chromio-fluoro-katophorite	Olsen et al. (1973)
Potassic-ferri-katophorite	Hawthorne et al. (1998)
Potassic-ferri-fluoro-katophorite	Robinson et al. (1998)
Richterite	Hawthorne et al. (1998)
Ferro-richterite	Deer et al. (1997) Table 22, #21
Fluoro-richterite	Hawthorne et al. (1998)
Potassic-richterite	Mottana and Griffin (1986)
Potassic-fluoro-richterite	Mazdab (2003)
Taramite	Oberti et al. (2007)
Ferro-taramite	Oberti et al. (2007)
Ferri-taramite	Pushcharovskiĭ et al. (2003)
Ferro-ferri-taramite	Deer et al. (1997) Table 26, #1
Fluoro-taramite	Oberti et al. (2007)
Potassic-ferro-taramite	Oberti et al. (2008)
Potassic-ferro-ferri-taramite	Deer et al. (1997) Table 26, #3
Winchite	Horak and Gibbons (1986)
Ferri-winchite	Sokolova et al. (2001)
Ferro-ferri-winchite	Nysten and Skogby (1994)
Group: OH–F–Cl; subgroup Na	
Arfvedsonite	Hawthorne et al. (2001)
Magnesio-arfvedsonite	Hawthorne et al. (1994)
Mangano-arfvedsonite	Nambu et al. (1969)
Fluoro-arfvedsonite	Hawthorne et al. (1993)
Magnesio-fluoro-arfvedsonite	Hawthorne et al. (1993)
Potassic-arfvedsonite	Hawthorne et al. (1993)
Potassic-magnesio-arfvedsonite	Robinson et al. (2008)
Potassic-magnesio-fluoro-arfvedsonite	Robinson et al. (2008)
Eckermannite	Mével and Kiénast (1986)
Ferro-eckermannite	Wallace et al. (1990)
Chromio-eckermannite	Mével and Kiénast (1986)
Glaucophane	Enders et al. (2000)
Ferro-glaucophane	Enders et al. (2000)
Ferri-leakeite	Hawthorne et al. (1992)
Ferro-ferri-leakeite	Borley (1963)
Fluoro-leakeite	Oberti et al. (2009)
Ferri-fluoro-leakeite	Cámara et al. (2010)
Ferro-ferri-fluoro-leakeite	Hawthorne et al. (1993)
Potassic-ferri-leakeite	Matsubara et al. (2002)
Potassic-mangani-leakeite	Armbruster et al. (1993)
Nybøite	Oberti et al. (2003)
Ferro-ferri-nybøite	Foord et al. (1996)
Fluoro-nybøite	Oberti et al. (2003)
Ferro-ferri-fluoro-nybøite	Borg (1967)
Riebeckite	Enders et al. (2000)
Magnesio-riebeckite	Hawthorne et al. (2008)
Fluoro-riebeckite	Hawthorne (1978)
Magnesio-fluoro-riebeckite	Robinson et al. (2008)
Group: OH–F–Cl; subgroup Li	
Orthorhombic	
Holmquistite	Cámara and Oberti (2005)
Ferro-holmquistite	Cámara and Oberti (2005)
Monoclinic	
'Clino-holmquistite'	Deer et al. (1997) Table 3, #1
Clino-ferri-holmquistite	Oberti et al. (2003c)
Clino-ferro-ferri-holmquistite	Oberti et al. (2003b)
Ferri-pedrizite	Oberti et al. (2000)
Ferro-ferri-pedrizite	Oberti et al. (2003b)
Ferro-fluoro-pedrizite	Oberti et al. (2009)
Fluoro-pedrizite	Oberti et al. (2005)
Group: OH–F–Cl; subgroup Na–(Mg–Fe–Mn)	
Ferri-ghoseite	Oberti and Ghose (1993)
Ferri-rootname14	Ishida and Hawthorne (2001)

Table 4 (*continued*)

Fluoro-tremolite	Valley et al. (1982)	
Tschermakite	Leake (1971)	
Ferro-tschermakite	Hawthorne and Grundy (1973)	Notes: table and analysis # specified for Deer et al. (1997);
Ferri-tschermakite	Deer et al. (1997) Table 12, #14	'Clino-holmquistite' has been discredited as a species: Oberti et al. (2005)
Ferro-ferri-tschermakite	Mücke et al. (2006)	

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Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.cageo.2013.09.011.

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