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Clarification of status of species in the pyrochlore supergroup

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ABSTRACT

After careful consideration of the semantics of status categories for mineral species names, minor corrections and disambiguations are presented for a recent report on the nomenclature of the pyrochlore supergroup. The names betafite, elsmoreite, microlite, pyrochlore and roméite are allocated as group names within the pyrochlore supergroup. The status of the names bindheimite, bismutostibiconite, jixianite, monimolite, partzite, stetefeldtite and stibiconite is changed from 'discredited' to 'questionable' pending further research.

KEYWORDS: pyrochlore, betafite, elsmoreite, microlite, roméite, bindheimite, partzite, stetefeldtite, stibiconite, mineral species status, mineral nomenclature.

Introduction

THE aims of this letter are to correct minor errors and resolve ambiguities in the recent Commission on New Minerals, Nomenclature and Classification (CNMNC) report on the classification and nomenclature of the pyrochlore supergroup (Atencio *et al*., 2010). These issues are primarily the result of the complex one-to-many and many-to-many mapping of older names onto new names. This has led to some uncertainty in the correspondence between old names and new names, and in the status of some old names and of type material. The discreditation of several old names appears to have been premature. To fully clarify the situation it should be stated explicitly that the 'status' applies to a species name, not to the population of specimens that physically represents the species. The status categories used here are defined as follows:

'A' (approved): the name has been approved by the CNMNC or its predecessor commission as a valid name for the mineral species.

'D' (discredited): the name is no longer the official name for a mineral species, it is now regarded as a synonym or varietal name, or was so poorly defined in the first place that it cannot be used in a reproducible fashion.

'G' (grandfathered): the name is an old one that pre-dates the requirement for approval by the CNMNC or its predecessors, and is generally accepted as valid.

'Group': the name refers to a group within the pyrochlore supergroup, defined on the basis of *B*-site occupancy. In the case of the pyrochlores, all such names are no longer valid as species names, and hence have the status 'D + Group'.

'N' (not approved): the name has been published without the approval of the CNMNC or its predecessors.

'Q' (questionable): the name refers to one or more mineral species which are probably valid, but type material was not well enough characterized for species to be unambiguously identified using current criteria. Further study is required for classification of the name into the 'A', 'D' or 'Rd' categories.

'Rd' (redefined): the current valid name now describes a chemical or structural variation for a species that is narrower, broader or otherwise different from that before the redefinition.

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TABLE 1. Status of old names for pyrochlore-supergroup minerals. Abbreviations are as defined in the text.

Mineral name	Status of name, Nickel and Nichols (2009)	Status of name, Atencio *et al.* (2010) Table 7	Correct status of name (2012)	Corresponding species names in the scheme of Atencio *et al.* (2010)
Alumotungstite	A	D	D	= Hydrokenoelsmoreite
Bariomicrolite	A	D	D	Probably hydrokenomicrolite
Bariopyrochlore	A	D	D	Zero-valent-dominant pyrochlore
Betafite	Rd	Possible new species	D + Group	Analysed instances = possible new species oxycalciobetafite, oxyuranobetafite
Bindheimite	G	D / Possible new species	Q	Analysed instance = possible new species oxyplumboroméite
Bismutomicrolite	A	D	D	Analysed instances = zero-valent-dominant microlite, or probable mixture.
Bismutopyrochlore	A	D / Possible new species	D	Analysed instances = possible new species oxynatropyrochlore,
zero-valent-dominant pyrochlore				
Bismutostibiconite	A	D	Q	Probably a Bi-dominant roméite species
Calciobetafite	A	D	D	Type material is Ca-dominant pyrochlore
Ceriopyrochlore-(Ce)	Rn	D / Possible new species	D	Analysed instances = possible new species fluorkenopyrochlore,
Ca- or zero-valent-dominant pyrochlore				
Cesstibtanite	A	Rd	D	Type material is now type hydroxykenomicrolite. Other occurrences may be other zero-valent-dominant microlite species
Elsemoreite	A	Rd	D + Group	Type material is now type hydrokenoelsmoreite
Ferritungstite	A	D	D	Hydrokenoelsmoreite
Fluornatromicrolite	-	A	A	IMA1998-018; full description published after delay as Witzke *et al.* (2011)
Jixianite	A	D	Q	Pb-dominant elsmoreite species.
Kalipyrochlore	A	Rd	D	Type material is now type hydropyrochlore
Lewisite	D	Rd	D	Type material is now type hydroxycalcioroméite
Microlite	A	Possible new species	D + Group	Analysed instances = possible new species fluorcalciomicrolite, oxycalciomicrolite
Monimolite	Q	D	Q	Probably "oxyplumboroméite"
Natrobistantite	A	D	D	Zero-valent-dominant microlite species
Partzite	G	D	Q	May be Cu-dominant roméite species
Plumbobetafite	A	D	D	Analysed instances = Pb-dominant betafite or zero-valent-dominant pyrochlore species

Plumbomicrolite	A	D/Possible new species	D	Analysed instances = possible new species kenoplumbomicrolite or zero-valent-dominant microlite species
Plumbopyrochlore	A	D/Possible new species	D	Analysed instances = possible new species oxyplumbopyrochlore, kenoplumbopyrochlore, unspecified Pb-dominant or zero-valent-dominant pyrochlore species
Pyrochlore	A	Possible new species	D + Group + Supergroup	Analysed instances = possible new species oxynatropyrochlore, hydroxycalciopyrochlore, fluorcalciopyrochlore, fluorkenopyrochlore
Roméite	G	Possible new species	D + Group	Analysed instances = possible new species fluornatroroméite, fluorcalcioroméite, oxycalcioroméite
Stannomicrolite	Rn	D / Rd	D	Type material of sukulaite is now type oxystannomicrolite. Other instances are Ca- or zero-valent-dominant microlite species
Stetefeldtite	Q	D	Q	May be Ag-dominant roméite species
Stibiconite	G	D	Q	May be Sb-dominant or other roméite species
Stibiobetafite	A	D / Rd	D	Type material is now type oxycalciopyrochlore
Stibiomicrolite	Rd	D / Rd / Possible new species	D	Type material is now type oxystibiomicrolite. Other analysed instances are possible new species oxycalciomicrolite, Ca- or zero-valent-dominant microlite species
Strontiopyrochlore	N	D / Possible new species	D	Analysed instances = possible new species fluorstrontiopyrochlore, fluorkenopyrochlore, or Ca- or zero-valent-dominant pyrochlore species
Uranmicrolite	Rn	D	D	Other microlite species
Uranpyrochlore	Rn	D / Possible new species	D	Analysed instances = possible new species oxynatropyrochlore, Na-dominant or U-dominant pyrochlore species
Yttrobetafite-(Y)	A	D / Possible new species	D	Analysed instances = possible new species oxycalciobetafite or zer-valent-dominant pyrochlore
Yttropyrochlore-(Y)	Rn	D / Possible new species	D	Analysed instances = possible new species oxyyttropyrochlore-(Y) or zero-valent-dominant pyrochlore

'Rn' (renamed): the current valid name replaced an earlier name without any change in species definition.

'Supergroup': the name now refers to the supergroup.

Note that 'Rn' and 'Rd' are special cases of 'A'. They are useful in that they highlight recent changes in status.

The pyrochlore-supergroup species names that were extant prior to the revision of Atencio *et al*. (2010), their status in the IMA–CNMNC list of mineral names compiled in October 2008 by E.H. Nickel and M.C. Nichols (which has been deposited with *Mineralogical Magazine* and can be downloaded from http://www.minersoc.org/pages/e_journals/dep_mat_mm.html), the status in Atencio *et al*. (2010) and the status as at November 2012, are listed in Table 1. If chemical analyses published for a particular mineral name allow identification of a species name or set of names that are consistent with the new nomenclature scheme, those names are also given.

The principal additions and changes to the scheme described by Atencio *et al*. (2010) are listed in the following text.

(1) The names betafite, elsmoreite, microlite, pyrochlore and roméite are reallocated as group names; these are defined on the basis of their *B*-site occupancy as described in Atencio *et al*. (2010). All except the elsmoreite group contain more than one approved species. Minerals that were formerly described using one of the group names require characterization of their *A*- and *Y*-site occupancies to be named to species level.

(2) If an old species name can be mapped unambiguously onto a new species name, and the structure and composition of the type material has been characterized to an appropriate standard, the old type specimen or specimens can be redefined to be types for the new species. Examples include type elsmoreite, which now corresponds to type hydrokenoelsmoreite; type cesstibtantite which now corresponds to type hydroxykenomicrolite; and type kalipyrochlore which now corresponds to type hydropyrochlore. None of the old pyrochlore-supergroup species names are valid in the new nomenclature scheme, and all are therefore discredited. The case of lewisite is unusual in that the name had been discredited prior to the creation of the pyrochlore supergroup as it was found to be synonymous with Ti-rich roméite (Burke, 2006), but the type material now serves as the type for hydroxycalcioroméite. However, it should be noted that other material with the same old species name may map onto a different new species.

(3) More than one old species may map onto the same new species. For example, alumotungstite and ferritungstite are no longer valid mineral names, both are synonyms of hydrokenoelsmoreite. All such redundant names are discredited.

(4) Some old names, including bindheimite, bismutostibiconite, jixianite, monimolite, partzite, stetefeldtite and stibiconite, probably correspond to one or more names in the new scheme, but the data available are insufficient to pinpoint the new species. In these cases, type material for the old names, if extant, cannot be redefined as type material for a specific new species name without further study. Many bindheimite specimens, for example, are probably the as yet unconfirmed mineral oxyplumboroméite, but further research is required to show that this is the case for the type specimen of bindheimite, or for all bindheimite specimens. The Sb-rich mineral stibiconite requires careful quantification of the oxidation state of its Sb for full characterization as although it may correspond to one or more Sb^{3+}-dominant roméite-group species; synthetic $Sb_2O_5 \cdot 1-3H_2O$ phases with the pyrochlore structure that contain no Sb^{3+} have also been reported (Natta and Baccaredda, 1936; England *et al*., 1980). Note that the Sb_2O_5 hydrate formulae can be rewritten to emphasize the pyrochlore structure as $\square_2Sb_2O_4(OH)_2\square$, $(H_2O\square)Sb_2O_4(OH)_2H_2O$ or $(H_3O\square)Sb_2O_6(OH)$. A structure refinement for $(Sb^{3+}\square)Sb_2^{5+}O_6(OH)$ was reported in a very early study by Dihlstroem and Westgren (1937) but the presence of significant Sb^{3+} remains to be demonstrated unequivocally in natural roméite-group minerals (P.A. Williams, pers. comm.). Partzite is complex in that some specimens may be multiphase mixtures, whereas others may contain one or more Cu-dominant roméite-group species. It is noteworthy that neither pyrochlore cation site is stereochemically favourable for occupation by Cu^{2+}, and that no synthetic Cu antimonates with the pyrochlore structure are known (Roper *et al*., 2012 and references therein). Artificial $CuSb_2O_6$ has the trirutile structure or a slight distortion thereof (Gieré *et al*., 1997). Stetefeldite is another interesting case. Synthetic $Ag_2Sb_2O_6$ with a pyrochlore structure is known (Mizoguchi *et al*., 2004) suggesting that phases that corresponding to one or more Ag-dominant roméite-group species might occur in nature. Natural and synthetic solid solutions with various Ag:Sb ratios that give pyrochlore-like

powder X-ray diffraction patterns have been described by Mason and Vitaliano (1953) and Stewart and Knop (1970), respectively. However, the existence of polymorphs of $Ag_2Sb_2O_6$ which do not have the pyrochlore structure (Hong *et al*., 1974), allows for the possibility that some old descriptions in this category, which were identified on the basis of their composition, may not be members of the pyrochlore supergroup.

The minerals described using the names in the foregoing paragraph require further study. If they are members of the pyrochlore supergroup, the nomenclature system of Atencio *et al*. (2010) prevents the old names being used either as species

TABLE 2. Species names in the pyrochlore supergroup according to Atencio *et al*. (2010) and new mineral descriptions published subsequently, with current status of species: 'A' = approved, 'P' = possible new species, 'T' = type material of an old name has been transferred to a new name (this is a special case of 'A'). References are given in Atencio *et al*. (2010), if not otherwise stated.

Mineral name	Best evidence for existence	Current status (October 2012)
Fluorcalciomicrolite	Andrade *et al*. (2012*b*); IMA2012-036	A
Fluorcalciopyrochlore	Published analyses	P
Fluorcalcioroméite	Published analyses	P
Fluorhydropyrochlore	Published analyses*	P
Fluorkenopyrochlore	Published analyses	P
Fluornatromicrolite	Witzke *et al*. (2011)	A
Fluornatropyrochlore	Unpublished analyses	P
Fluornatroroméite	Published structure determination	P
Fluorstrontiopyrochlore	Published analyses	P
Hydrokenoelsmoreite	Type specimen of former species elsmoreite transferred to new name	T
Hydrokenomicrolite	Andrade *et al*. (2012*a*); IMA2011-103	A
Hydromicrolite	Unpublished analyses	P
Hydropyrochlore	Type specimen of former species kalipyrochlore transferred to new name	T
Hydroxycalciopyrochlore	Yang *et al*. (2011); IMA2011-026	A
Hydroxycalcioroméite	Type specimen of former species lewisite transferred to new name	T
Hydroxykenomicrolite	Type specimen of former species cesstibtantite transferred to new name	T
Hydroxymanganopyrochlore	Chukanov *et al*. (2012); IMA2012-005	A
Kenoplumbomicrolite	Published structure determination	P
Kenoplumbopyrochlore	Published analyses	P
Oxycalciobetafite	Published analyses and structure	P
Oxycalciomicrolite	Published analyses	P
Oxycalciopyrochlore	Type specimen of former species stibiobetafite transferred to new name	T
Oxycalcioroméite	Biagioni and Orlandi (2012); IMA2012-022	A
Oxynatropyrochlore	Published analyses	P
Oxyplumbopyrochlore	Published analyses	P
Oxyplumboroméite	Published analyses	P
Oxystannomicrolite	Type specimen of former species sukulaite (= stannomicrolite) transferred to new name	T
Oxystibiomicrolite	Type specimen of former species stibiomicrolite transferred to new name	T
Oxyuranobetafite	Published analyses	P
Oxyyttropyrochlore-(Y)	Published analyses	P

* See discussion in text of Atencio *et al*. (2010)

names or root names, and it is for this reason that Atencio *et al*. (2010) classified them as discredited. However, the possibility remains that a future study might result in one or more of the old names being redefined as a species that does not belong to the pyrochlore supergroup. Unfortunately, the discreditation of the old names leaves extant specimens of compositionally distinctive material with no acceptable name, or forces the use of discredited names, which the CNMNC wishes to discourage. Therefore, it is preferable to amend the classification of the old names to 'questionable', which gives CNMNC sanction to their continued usage until sufficient data is available to either fully discredit them and replace their names by one or more pyrochlore supergroup names that are consistent with Atencio *et al*. (2010), or redefine them as a species that is not a member of the pyrochlore supergroup.

(5) One pre-2010 mineral species, fluornatromicrolite, is defined and named consistently with the 2010 scheme. Therefore, the name is listed in Table 1 as 'approved'.

(6) As the species names of Atencio *et al*. (2010) correspond to compositional ranges that are different from those of older schemes, all other names in the new scheme require explicit validation by the CNMNC. This was achieved for oxycalciopyrochlore, hydropyrochlore, hydroxykenomicrolite, oxystannomicrolite, oxystibiomicrolite, hydroxycalcioroméite and hydrokenoelsmoreite by reassigning the type material for well described former species to a new name (Atencio *et al*., 2010). As of November 2012, the new species, hydroxycalciopyrochlore (IMA 2011-026) and hydrokenomicrolite (IMA 2011-103), have also been approved by the CNMNC. Fluornatromicrolite was approved by the CNMNCs predecessor, the CNMMN (as IMA 1998-018), but controversies about its species status and the nomenclature of the pyrochlore supergroup delayed full publication. When the description of fluornatromicrolite was submitted for the first time, in 1998, problems arose as (although it was approved by the CNMMN−IMA) the name fluornatromicrolite was not in accord with the nomenclature of Hogarth (1977), which was then still *de rigueur*. The name fluornatromicrolite is, however, perfectly in line with the newly approved system

TABLE 3. Status of the names of Table 2, summarized in matrix form. Rows are ordered by *A*-site prefix, then *Y*-site prefix. Status symbols 'A','P' and 'T' are 'A' = approved, 'P' = possible new species, 'T' = type material of an old name has been transferred to a new name (this is a special case of 'A')..

Y-site prefix	*A*-site prefix	Betafite group (Ti^{4+} on *B*)	Elsmoreite group (W^{6+} on *B*)	Microlite group (Ta^{5+} on *B*)	Pyrochlore group (Nb^{5+} on *B*)	Roméite group (Sb^{5+} on *B*)
Fluor-	-calcio-			A	P	P
Hydroxy-	-calcio-				A	T
Oxy-	-calcio-	P		P	T	A
Fluor-	-hydro-				P	
Hydro-	(-hydro-)*			P	T	
Fluor-	-keno-				P	
Hydro-	-keno-		T			
Hydroxy-	-keno-			T		
Hydroxy-	-mangano-				A	
Fluor-	-natro-			A	P	P
Oxy-	-natro-				P	
Keno-	-plumbo-			P	P	
Oxy-	-plumbo-				P	P
Oxy-	-stanno-			T		
Oxy-	-stibio-			T		
Fluor-	-strontio-				P	
Oxy-	-urano-	P				
Oxy-	-yttro-...-(Y)				P	

* Omitted to avoid repetition.

TABLE 4. Composition ranges with inadequately analysed *Y*-site occupancies where there is evidence for additional new species are indicated by '×'.

A-site prefix	*A*-site species	Betafite group (Ti^{4+} on *B*)	Elsmoreite group (W^{6+} on *B*)	Microlite group (Ta^{5+} on *B*)	Pyrochlore group (Nb^{5+} on *B*)	Roméite group (Sb^{5+} on *B*)
-argento-	Ag^{+}					×
-bismuto-	Bi^{3+}					×
-calcio-	Ca^{2+}			×	×	
-cupro-	Cu^{2+}					×
-hydro- or -keno-	$H_2O/\square$			×	×	
-natro-	Na^{+}				×	
-plumbo-	Pb^{2+}	×	×		×	×
-stibio-	Sb^{3+}					×
-urano-	U^{4+}				×	

of nomenclature and the mineral description has been published recently (Witzke *et al*., 2011).

New species names discussed in Atencio *et al*. (2010) for which examples appear to exist, on the basis of analyses or crystal structure determinations, are listed in Table 2. Species that have been approved by the CNMNC since that report are also included. The status of the names is indicated as 'A' if the new species has already been approved by the CNMNC. To clarify the various status changes, two new categories have been created. The code 'T' (type transferred) is used if type material of a former species has been reassigned to be type material for a new species. In other words, if the type specimen has been transferred from an old discredited name to a valid new name. Note that this is quite distinct from the redefinition of a *name* as defined above. The category 'T' is not 'Rd', but a distinct special case of 'A'. The category 'P' (probable new species), is used if material exists that appears to correspond to a new species name, but no proposal has yet been made to the CNMNC. Note that this category is not equivalent to 'Q' as defined above. The category 'P' indicates that the name is currently *not* valid but would become so if a proposal was to be approved. The list of Table 2 is summarized by mineral groups in a more compact two-dimensional matrix form in Table 3; this complements Tables 1−5 of Atencio *et al*. (2010) but indicates the current status explicitly.

It is very probable that further new species exist, but they are not included in Tables 2−3 as their current state of chemical/structural characterization does not allow specification of the exact species name according to the new scheme. Atencio *et al*. (2010) require two prefixes in pyrochlore-supergroup species names, the first indicating the dominant species of the dominant valence in the *Y* sites, and the second indicating the dominant species of the dominant valency in the *A* site; in these cases, only the latter is known. On the basis of the names labelled 'Q' and comments on other names in Table 1, the composition fields in which such new species are likely to be found are summarized in Table 4. Material with such compositions includes the questionable species bismutostibiconite, bindheimite, jixianite, monimolite, partzite, stetefeldtite and stibiconite, and many other incomplete analyses of the betafite, microlite and pyrochlore groups.

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