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THE PYROCHLORE SUPERGROUP OF MINERALS: NOMENCLATURE

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Abstract

A new scheme of nomenclature for the pyrochlore supergroup, approved by the CNMNC–IMA, is based on the ions at the *A*, *B* and *Y* sites. What has been referred to until now as the pyrochlore group should be referred to as the pyrochlore supergroup, and the subgroups should be changed to groups. Five groups are recommended, based on the atomic proportions of the *B* atoms Nb, Ta, Sb, Ti, and W. The recommended groups are pyrochlore, microlite, roméite, betafite, and elsmoreite, respectively. The new names are composed of two prefixes and one root name (identical to the name of the group). The first prefix refers to the dominant anion (or cation) of the dominant valence [or H_2O or □] at the *Y* site. The second prefix refers to the dominant cation of the dominant valence [or H_2O or □] at the *A* site. The prefix "keno-" represents "vacancy". Where the first and second prefixes are equal, then only one prefix is applied. Complete descriptions are missing for the majority of the pyrochlore-supergroup species. Only seven names refer to valid species on the grounds of their complete descriptions: oxycalciopyrochlore, hydropyrochlore, hydroxykenomicrolite, oxystannomicrolite, oxystibiomicrolite, hydroxycalcioroméite, and hydrokenoelsmoreite. Fluornatromicrolite is an IMA-approved mineral, but the complete description has not yet been published. The following 20 names refer to minerals that need to be completely described in order to be approved as valid species: hydroxycalciopyrochlore, fluornatropyrochlore, fluorcalciopyrochlore, fluorstrontiopyrochlore, fluorkenopyrochlore, oxynatropyrochlore, oxyplumbopyrochlore, oxyyttropyrochlore-(Y), kenoplumbopyrochlore, fluorcalciomicrolite, oxycalciomicrolite, kenoplumbomicrolite, hydromicrolite, hydrokenomicrolite, oxycalciobetafite, oxyuranobetafite, fluornatroroméite, fluorcalcioroméite, oxycalcioroméite, and oxyplumboroméite. For these, there are only chemical or crystal-structure data. Type specimens need to be defined. Potential candidates for several other species exist, but are not sufficiently well characterized to grant them any official status. Ancient chemical data refer to wet-chemical analyses and commonly represent a mixture of minerals. These data were not used here. All data used represent results of electron-microprobe analyses or were obtained by crystal-structure refinement. We also verified the scarcity of crystal-chemical data in the literature. There are crystal-structure determinations published for only nine pyrochlore-supergroup minerals: hydropyrochlore, hydroxykenomicrolite, hydroxycalcioroméite, hydrokenoelsmoreite, hydroxycalciopyrochlore, fluorcalciopyrochlore, kenoplumbomicrolite, oxycalciobetafite, and fluornatroroméite. The following mineral names are now discarded: alumotungstite, bariomicrolite, bariopyrochlore, bindheimite, bismutomicrolite, bismutopyrochlore, bismutostibiconite, calciobetafite, ceriopyrochlore-(Ce), cesstibtantite, ferritungstite, jixianite, kalipyrochlore, monimolite, natrobistantite, partzite, plumbobetafite, plumbomicrolite,

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plumbopyrochlore, stannomicrolite, stetefeldtite, stibiconite, stibiobetafite, stibiomicrolite, strontiopyrochlore, uranmicrolite, uranpyrochlore, yttrobetafite-(Y), and yttropyrochlore-(Y).

Keywords: pyrochlore supergroup, nomenclature, pyrochlore group, microlite group, betafite group, roméite group, elsmoreite group.

SOMMAIRE

Nous proposons un nouveau système de nomenclature pour les minéraux du supergroupe du pyrochlore, sanctionné par le Comité des Noms de Minéraux, de Nomenclature et de Classification de l'Association internationale de Minéralogie, et fondé sur les ions se trouvant aux sites *A*, *B* et *Y*. Ce qui a déjà été considéré le groupe du pyrochlore devient le supergroupe du pyrochlore, et les sous-groupes deviennent dorénavant des groupes. Cinq groupes sont maintenant recommandés, selon la proportion des atomes Nb, Ta, Sb, Ti, et W au site *B*. Les groupes recommandés sont nommés pyrochlore, microlite, roméite, bétafite, et elsmoreïte, respectivement. Les nouveaux noms contiennent jusqu'à deux préfixes et un nom-racine, qui est identique au nom du groupe. Le premier préfixe fait allusion à l'anion prédominant (ou cation) de la valence dominante [ou H_2O ou □] au site *Y*. Le second se rapporte au cation prédominant de la valence dominante [ou H_2O ou □] au site *A*. Le préfix "kéno-" représente "lacune". Dans les cas où le premier et le second préfixe sont les mêmes, seul un préfixe suffira. Des descriptions complètes ne sont pas disponibles pour la majorité des espèces du supergroupe du pyrochlore. Seuls sept noms font référence à des espèces considérées valides à cause de leur description complète: oxycalciopyrochlore, hydropyrochlore, hydroxykénomicrolite, oxystannomicrolite, oxystibiomicrolite, hydroxycalcioroméite, et hydrokénoelsmoreïte. La fluornatromicrolite est une espèce approuvée, mais la description complète de cette espèce n'a pas encore été publiée. Les vingt noms suivants se rapportent à des espèces dont la description doit être complétée pour être considérées valides: hydroxycalciopyrochlore, fluornatropyrochlore, fluorcalciopyrochlore, fluorstrontiopyrochlore, fluorkénopyrochlore, oxynatropyrochlore, oxyplumbopyrochlore, oxyyttropyrochlore-(Y), kénoplumbopyrochlore, fluorcalciomicrolite, oxycalciomicrolite, kénoplumbomicrolite, hydromicrolite, hydrokénomicrolite, oxycalciobetafite, oxyuranobétafite, fluornatroroméite, fluorcalcioroméite, oxycalcioroméite, et oxyplumboroméite. Dans ces cas, il n'y a que des données chimiques ou des données sur la structure cristalline. On doit définir des échantillons-types. Dans plusieurs autres cas, des candidats potentiels existent, mais ils ne sont pas suffisamment bien caractérisés pour leur attribuer un statut officiel. Les données chimiques plus anciennes reposent sur des analyses par voie humide, et représenteraient en général des mélanges. De telles données n'ont pas été utilisées ici. Toutes les données représentent donc des résultats d'analyses obtenues avec une microsonde électronique ou bien des données établies par analyse de la structure cristalline. Nous avons aussi vérifié la rareté des données cristallochimiques dans la littérature. Nous avons trouvé des déterminations de la structure cristalline pour seulement neuf minéraux du supergroupe du pyrochlore: hydropyrochlore, hydroxykénomicrolite, hydroxycalcioroméite, hydrokénoelsmoreïte, hydroxycalciopyrochlore, fluorcalciopyrochlore, kénoplumbomicrolite, oxycalciobetafite, et fluornatroroméite. Les noms suivants deviennent désuets: alumotungstite, bariomicrolite, bariopyrochlore, bindheimite, bismutomicrolite, bismutopyrochlore, bismutostibiconite, calciobétafite, cériopyrochlore-(Ce), cesstibtantite, ferritungstite, jixianite, kalipyrochlore, monimolite, natrobistantite, partzite, plumbobétafite, plumbomicrolite, plumbopyrochlore, stannomicrolite, stetefeldtite, stibiconite, stibiobétafite, stibiomicrolite, strontiopyrochlore, uranmicrolite, uranpyrochlore, yttrobétafite-(Y), et yttropyrochlore-(Y).

(Traduit par la Rédaction)

Mots-clés: supergroupe du pyrochlore, nomenclature, groupe du pyrochlore, groupe du microlite, groupe de la bétafite, groupe de la roméite, groupe de l'elsmoreïte.

INTRODUCTION

In 1977, Hogarth presented a comprehensive classification and nomenclature for the pyrochlore supergroup, which represented the then-current body of knowledge on pyrochlore-supergroup minerals. The study produced a concise classification, and reduced the proliferation of synonyms to a handful of names. The IMA CNMMN (now CNMNC) has recently received a series of submissions for potentially new members of the pyrochlore supergroup. Some of the submissions invoked new interpretations or extensions of the approach of Hogarth (1977). In addition, some Commission members expressed concern about Hogarth's species and group divisions, which do not conform to current IMA criteria (Nickel 1992).

The official pyrochlore-supergroup system of classification (Hogarth 1977) does not follow the current IMA rules of mineralogical nomenclature, although that system is currently still approved by IMA. Hogarth (1977) assigned species prefixes according to the chemical composition of the *A* position of the pyrochlore formula. Species in which an exotic cation (*i.e.*, anything other than Ca or Na) made up more than 20% of the total number of *A* cations were assigned a special prefix indicating the presence of the cation. In such cases, the prefix was to apply to the dominant exotic cation. For example, a member of the pyrochlore group with 25% Pb and 20% Sr would be named plumbopyrochlore, with "strontian", as an optional (varietal) adjectival modifier. At the *A* site, Hogarth's (1977) system does not differentiate between occupancy by Ca and Na. In spite of this, the species *fluornatromicrolite* was approved on the basis of predominance of Na at the *A* site. The *natro-* prefix is also present in the name *natrobistantite*. The prefix *calcio-* was used for calciobetafite (Mazzi & Munno 1983). Regarding the *B*-site occupancy, the division among the groups is not made with a tripartite symmetrical classification (as suggested by Zurevinski & Mitchell 2004), nor is it based on the dominant-valence rule (as adopted in this proposal). The species with Nb + Ta > 2Ti and Nb > Ta are considered as pyrochlore-group minerals; if Nb + Ta > 2Ti and Ta ≥ Nb, the mineral is considered to belong to the microlite group, and if 2Ti ≥ Nb + Ta, the mineral belongs to the betafite group. Isostructural species with other predominant cations at the *B* site were not included in the pyrochlore supergroup (for example, roméite, with dominant Sb, and elsmoreite, with dominant W). The anions are not taken into account in the classification, but the predominance of fluorine was used for the approval of the species *fluornatromicrolite*. Other names that disagree with IMA recommendations, such as cesstibtantite and natrobistantite, were also introduced with IMA approval.

Many problematic features of pyrochlore-supergroup minerals and synthetic pyrochlores have been resolved since Hogarth (1977). The structural role of H_2O, very large cations (K, Cs, Rb), atypical *B* cations (Fe^{3+}, Zr, W), and cations with stereoactive lone-pair electrons (Sb^{3+}, Sn^{2+}) are now understood. In addition, modern electron-probe microanalysis (EPMA) permits routine determination of F, providing better-quality data on the anion content.

A new CNMMN subcommittee on pyrochlore (Chairman: Scott Ercit. Members: Petr Černý, Greg Lumpkin, Ernie Nickel, Milan Novák, and Roland Rouse) was established in 1998. One interim report was issued in 1999, but no additional report was presented formally to the Commission since then. This subcommittee was terminated in June 2008. An unofficial report prepared in 2003 by Scott Ercit was provided to the new subcommittee and served as a basis for the preparation of this report.

The following represents a modernization of Hogarth's (1977) system, in which we have taken into account the ideas presented in the paper by Hatert & Burke (2008). We believe that the new names being proposed are more rational, and their use should be preferred.

In order to make this report consistent with the recently approved definitions of group nomenclature by Mills *et al*. (2009), what is up to now referred to as the pyrochlore group should be referred to as the pyrochlore supergroup, and the subgroups should be changed to groups.

THE FORMULA

The pyrochlore-supergroup minerals crystallize in the isometric crystal system (space group $Fd\bar{3}m$ or its subgroups) and exhibit a unit cell characterized by a ≈ 10.4 Å and Z = 8 (Rouse *et al*. 1998). They conform to the general formula:

$$\boldsymbol{A}_{2-m}\,\mathbf{B}_2\,\boldsymbol{X}_{6-w}\,\mathbf{Y}_{1-n}.$$

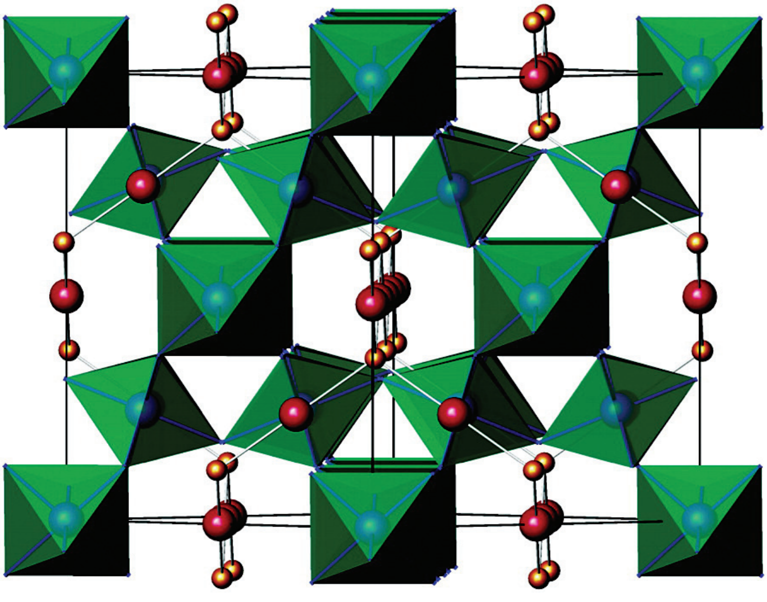

FIG. 1. Ideal pyrochlore crystal structure viewed along the [110] axis (*A* red, *Y* orange and BO_6 octahedra in green) (Henderson *et al*. 2007).

In this formula, ***A*** typically is a large [8]-coordinated cation with a radius of ~1.0 Å or a vacancy (□), but can also be H_2O (includes ions with or without lone-pair electrons on sites 16*d* or 96*g* in $Fd\bar{3}m$). The *A* site therefore may host **Na, Ca,** Ag, Mn, **Sr,** Ba, Fe^{2+}, **Pb^{2+}, Sn^{2+}, Sb^{3+},** Bi^{3+}, **Y**, Ce (and other REE), Sc, **U**, Th, **□, or H_2O**. The main constituents are shown in **bold**.

B is a [6]-coordinated cation (site 16*c*), typically of high field-strength. This site thus may contain **Ta, Nb, Ti, Sb^{5+}, W**, but also V^{5+}, Sn^{4+}, Zr, Hf, Fe^{3+}, Mg, Al and Si.

X typically is **O**, but can include subordinate OH and F (site 48*f*).

Y typically is an anion, but can also be a vacancy, H_2O, or a very large (>> 1.0 Å) monovalent cation (site 8*b*). Examples are **OH^-, F, O**, **□**, **H_2O**, K, Cs, Rb. Displacements to 96*g*, 32*e* and 192*i* positions were also located.

The symbols *m, w,* and *n* represent parameters that indicate incomplete occupancy of the *A*, *X* and *Y* sites, respectively. Vacancies have not been found to occur at the *B* site (Borodin & Nazarenko 1957, van Wambeke 1970). Compositions with a substantial concentration of vacancies at the *A* site have been described as "defect pyrochlores". However, it is undesirable to give this term official status in this context, since it is non-specific, and likely to be used to describe other deviations from the ideal structure and stoichiometry. Lumpkin & Ewing (1992, 1995), Ercit & Robinson (1994), Brugger *et al*. (1997), and Nasraoui & Waerenborgh (2001) noted vacancies at the *X* site in some extreme cases of secondary alteration. According to Lumpkin & Ewing (1995), the following ranges are encountered: $m = 0$ to 1.7, $w = 0$ to 0.7, and $n = 0$ to 1. Actually, *m* can range up to 2 (Ercit *et al*. 1994, Brugger *et al*. 1997).

Hogarth *et al.* (2000), among others, discussed the distribution of cations at the structural sites of pyrochlore-supergroup minerals. Synthetic pyrochlores have a much more variable chemical composition than natural examples (Subramanian *et al*. 1983).

For structural reasons, *A* can be subdivided into constituents without lone-pair electrons (*e.g*., Na, Ca), which occupy 16*d*, and stereoactive cations (*e.g*., Sb^{3+}), which occupy less symmetrical positions displaced slightly from 16*d*, *e.g*., 96*g*. For the purpose of this nomenclature, no subdivision is made. This approach has its analogues in the nomenclature of silicate minerals. For instance, the *A* site of the amphibole formula represents general or special positions, and the *C* "site" consists of the combination of the crystal-chemically similar *M*l to *M*3 sites.

The pyrochlore structure (Fig. 1) is an essential building block for other minerals and mineral groups, such as alunite (Goreaud & Raveau 1980) or pittongite (Grey *et al*. 2006).

THE NEW SCHEME OF NOMENCLATURE

In the present work, a new scheme of nomenclature based on the ions at the *A*, *B* and *Y* sites is presented. The new names are composed of two prefixes and one root name (identical to the name of the group). Five groups are recommended, on the basis of the atomic proportions of the *B*-site atoms Nb, Ta, Sb, Ti, and W. The recommended groups are **pyrochlore, microlite, roméite, betafite**, and **elsmoreite**, respectively. According to this new scheme, the pyrochlore supergroup now also includes mineral species with W or Sb^{5+} as the dominant cation at the *B* site. These species were once regarded as tungstates or antimonates rather than conventional oxides, but they contain W^{6+} or Sb^{5+} in octahedral coordination with oxygen, and the resulting octahedra are polymerized to form the framework of the pyrochlore structure. Furthermore, the W and Sb species show various degrees of solid solution with "conventional" members of the supergroup (Brugger & Gieré 1999). The determination of a proper group is made by the dominant valence at *B*, not by a single, dominant ion. That is, the numbers of all tetravalent cations are summed to give a total number of M^{4+}, the numbers of all pentavalent cations to give a sum M^{5+}, and so on. For this purpose, a group of atoms with the same valence state are considered to be a single constituent (Hatert & Burke 2008).

> If $M^{4+} > M^{5+}$ and $M^{4+} > M^{6+}$, then the group is:
> Betafite, if Ti is the dominant M^{4+} cation.
>
> If $M^{5+} > M^{4+}$ and $M^{5+} > M^{6+}$, then the group is:
> Pyrochlore, if Nb is the dominant M^{5+} cation,
> Microlite, if Ta is the dominant M^{5+} cation,
> Roméite, if Sb is the dominant M^{5+} cation.
>
> If $M^{6+} > M^{4+}$ and $M^{6+} > M^{5+}$, then the group is:
> Elsmoreite, if W is the dominant M^{6+} cation.

New root names were required for the new W- and Sb^{5+}-dominant pyrochlore groups. In accordance with Hogarth (1977), roméite will be the root name for species of the Sb^{5+}-dominant pyrochlore group because this is the name of the Ca–Na-dominant species. However, as no Ca–Na member has been established for the W-dominant pyrochlore group, we had to choose a root name among the four species that were considered valid: ferritungstite, alumotungstite, elsmoreite, and jixianite. The three first names are defined and distinguished on the basis of minor constituents at the *A* and *B* sites (*cf*. Ercit & Robinson 1994, Williams *et al*. 2005). In all three, vacancies are dominant at *A*, and W is the dominant species of the dominant valence at *B*, so by the criteria proposed here, these names refer to the same species. Ferritungstite would have historical precedence, as it was described in 1911 by Schaller.

Jixianite, described in 1979 by Liu Jianchang, refers to the mineral with Pb dominant at *A* and W at *B*. However, there is a problem with "ferritungstite" as the root name for a species of the W-dominant pyrochlore group: the name erroneously implies distinct crystallographic roles for W and Fe^{3+} in the structure of ferritungstite. In fact, Fe^{3+} is merely a subordinate cation at the W-dominant *B* site of the ferritungstite structure (Ercit & Robinson 1994), as is Al in the alumotungstite structure (≡ ferritungstite with subordinate Al: Ercit & Robinson 1994). The name could be jixianite, but in absence of a crystal-structure study, it is not possible to know the dominant anion of the dominant valence at the *Y* site of this mineral. Consequently, the name for this group, and the root name for all species of this group, will be **elsmoreite**. As a mineral group consists of two or more minerals (Mills *et al.* 2009), elsmoreite cannot really be considered, for now, as a mineral group. Hydrokenoelsmoreite should be designated as an unassigned member of the pyrochlore supergroup, because there is no other member to allow a group to be established.

Extensive solid-solution exists among Nb-, Ta-, and Ti-dominant pyrochlores. Hogarth (1977) delimited the betafite group from the Nb and Ta groups at the 33% mark in order to place more compositions in the sparsely populated field of betafite. We propose here that all group divisions be rearranged in accordance with the dominant valence at *B*, not by a single, dominant ion (see Fig. 2). Figures 2 and 3 were extracted from a preliminary version of this proposal made by the previous committee. Certainly, they include results of both microprobe and wet-chemical analyses. The two points near the Ti corner belong to betafite- and roméite-group minerals. Their apparent position in the far apex of the triangle is a projection artefact due to the absence of a Sb^{5+} corner in the diagram: Ti and Sb in nearly equal proportions are the dominant *B*-site cations in these minerals, with Nb and Ta almost completely absent. For example, one of the oxycalciobetafite compositions is $(Ca_{0.872}Ce_{0.609}Mn_{0.415}Na_{0.051}\square_{0.053})_{\Sigma 2.000}(Ti_{1.126}Sb_{0.783}Nb_{0.037}W_{0.033}Fe_{0.013}V_{0.008})_{\Sigma 2.000}O_6(O_{0.634}F_{0.068}\square_{0.053})$ (Brugger & Gieré 1999). Pyrochlore-type phases with *ca.* 2Ti are well known synthetically [*e.g.*, $CaUTi_2O_7$ (Dickson *et al.* 1989), $Y_2Ti_2O_7$ (Matteucci *et al.* 2007)], but the clustering of natural compositions near (Nb, Sb):Ti = 1:1 suggests entropy stabilization at the middle of the solid-solution series. Relative lack of Ti–Ta solid solution is an important and interesting difference between Ta and Nb.

The new scheme of nomenclature based on two prefixes and a root name allows one to use the root names without prefixes, or with only one prefix [*e.g.*,"plumboelsmoreite"] to specify at least a group for minerals that have not been fully analyzed. The first prefix will refer to the dominant anion (or cation) of the dominant valence [or H_2O or □] at the *Y* site. The second prefix will refer to the dominant cation of the dominant valence [or H_2O or □] at the *A* site. Given the Classical Greek derivation of "oxy-", "hydro-" and "hydroxy-", we suggest "keno-" to represent "vacancy", from the Greek κενος, meaning "empty". The term *keno-* has been previously suggested by Permingeat (in van Wambeke 1971) as a prefix modifier for cation-deficient members of the pyrochlore supergroup. Where the first and second prefixes are equal, then only one prefix is applied ("hydropyrochlore", not "hydrohydropyrochlore"). The only problem is that we might want to use "hydropyrochlore" to mean any pyrochlore in the group of species with H_2O at the *Y* sites and unspecified *A*-site occupancies.

Hogarth (1977) assigned species names incorporating prefixes that were determined by the *A*-site composition of the pyrochlore formula. These prefixes were used to define names of new species where a cation other than Ca or Na made up more than 20% of the total number of *A*-site cations. The prefix specified the dominant cation that is not Na or Ca. For example, a member of the pyrochlore group with 25% Pb would be named plumbopyrochlore. This approach has been modified in the new system of nomenclature to reflect current knowledge of the crystal chemistry of pyrochlore-supergroup minerals, and also to bring pyrochlore nomenclature into better consistency with current best practice for complex solid-solutions (Hatert & Burke 2008). Like the *B* sites, the *A* sites of pyrochlores can contain species of several different charges. They can also contain a neutral molecular species, H_2O, and vacancies. Consistent with the procedure for the *B* site, it is possible to group *A*-site species into valence groups M^{1+}, M^{2+} and so on, and a zero-charge group for H_2O and vacant sites. The second prefix is then determined by the dominant species of the dominant-valence group, as follows.

The zero-charge group

The occupancy of the *A* position in pyrochlore-supergroup minerals by cations is in some cases very low (<50%). Where the zero-charge group exceeds any valence group of the *A* site, the second prefix "keno" is proposed for species in which □ exceeds H_2O, and the second prefix "hydro" is proposed for species in which H_2O exceeds □.

The dominant valence rule

The Hogarth (1977) rules of nomenclature that reflect the chemical composition at the *A* position have been modified to conform to the **dominant-valence rule**. Consequently, where neutral species are not the largest valence-based group at the *A* position, a second prefix is now to be applied for the dominant cation of the dominant valence. There is a natural clustering of compositions near Na = Ca = 1 *apfu* (Fig. 3), a charge-balancing requirement for members of the B^{5+} groups.

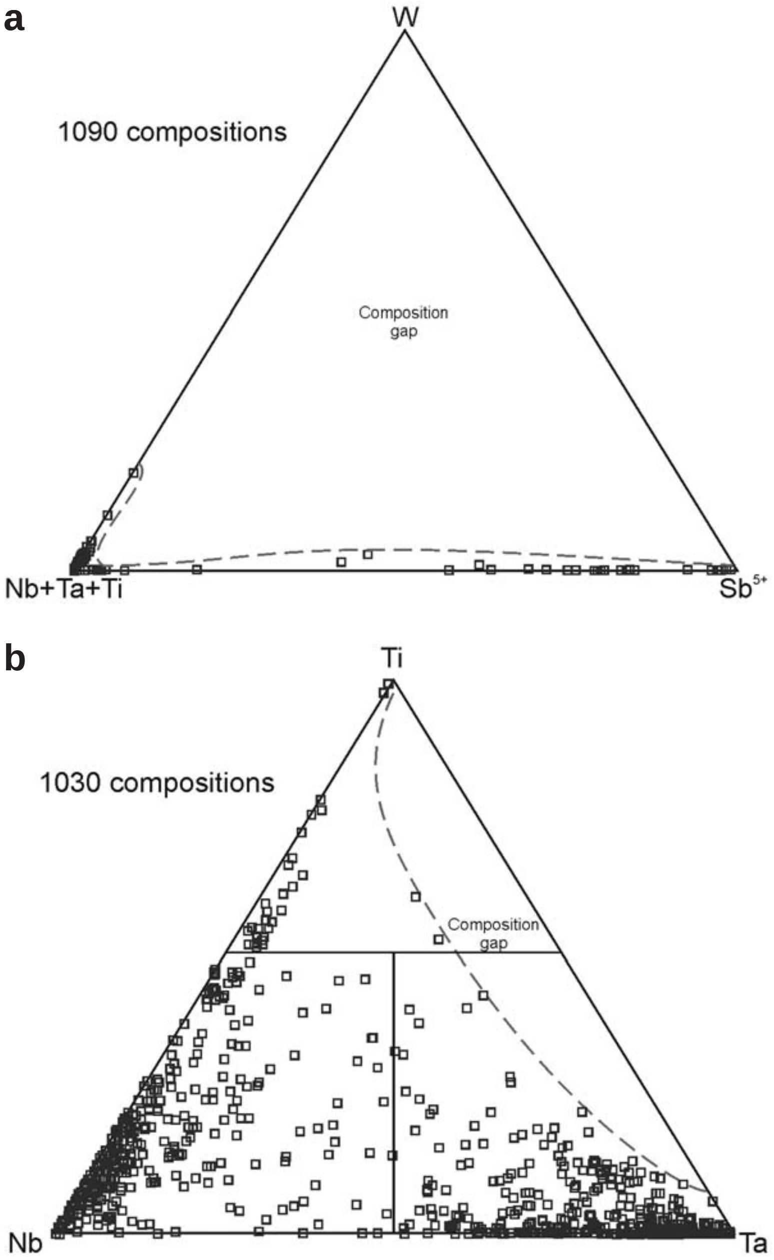

FIG. 2. Pyrochlore-supergroup minerals, *B*-site composition.

Hence, in Hogarth (1977), if the dominant cation was either Ca or Na, no prefix was used, and dominance of either of these cations was not indicated. Prefixes were only used to indicate substantial amounts of other cations. In order to regain consistency, it is proposed here to use second prefixes from now on in order to indicate Ca and Na predominance.

The pyrochlore supergroup presents complexities in the specification of end-member formulae, and also whether single-species names should correspond to single chemical end-members. For some species, a single unambiguous charge-balanced end-member formula cannot exist. For example, the fluornatromicrolite of Witzke *et al.* (IMA#98–018) exists with composition $(Na_{1.15}Ca_{0.70}Bi_{0.15})_{\Sigma 2}Ta_2O_6F$. Use of only dominant species at each site suggests the ideal "end-member" formula $Na_2Ta_2O_6F$, which is not electrostatically neutral and hence is physically impossible. In the real mineral, the heterovalent substitution $2Ca^{2+} = Bi^{3+} + Na^+$ takes place, so it is intermediate between the two charge-balanced end-members $NaCaTa_2O_6F$ and $Na_{1.5}Bi_{0.5}Ta_2O_6F$. These compositions have components of more than one valence on only one site, and thus are end-members in the sense of Hawthorne (2002). The boundary between these two end members is located at 50 mol.%, and corresponds to the composition $Na_{1.25}Ca_{0.5}Bi_{0.25}Ta_2O_6F$. The example above is close to this boundary, but has $NaCaTa_2O_6F$ predominant. Given the strong clustering of pyrochlore compositions near this end member, it is tempting to find a way to define this end member as corresponding to one species despite the 50:50 mixed occupancy of the *A* sites, in which case fluornatromicrolite would be a Bi-rich example of this species. We agree that it is unfortunate that a single composition field, with no major change in properties or paragenesis and with compositions clustering around the 50:50 mark, should be broken into Na-dominant and Ca-dominant halves. However, the division of the composition field does not really present a new nomenclatural difficulty. As the *A*-site and *Y*-site content of pyrochlore cannot be established without analysis, second prefixes can only be used with confidence for analyzed specimens. Compositions that are near the 50:50 composition can be explicitly flagged as being "near the 50:50 mark". Root names without prefixes are recommended for incompletely analyzed material.

Rigorous adherence to the principle of using a single dominant species in a dominant-valence group produces a mismatch between species and end members in pyrochlores. The charge-balanced end-member $NaCaTa_2O_6F$ is not at the center of the composition field of a species, but marks the boundary between fluornatromicrolite and fluorcalciomicrolite. Conversely, neither of these species names can be associated with a unique charge-balanced end-member. The formula $(Na_{1.5}Bi_{0.5})Ta_2O_6F$ is an example of one possible end-member for fluornatromicrolite, with neutrality maintained by the subordinate Bi^{3+} at the *A* site. The minor substituent need not be Bi: $(Na_{1.5}Y_{0.5})Ta_2O_6F$ and $(Na_{1.667}U_{0.333})Ta_2O_6F$ are examples of end members that would share

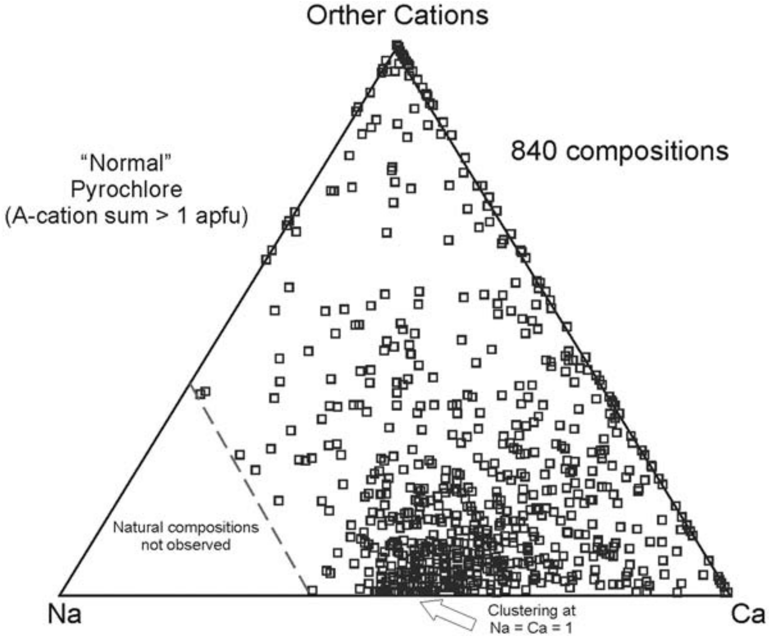

FIG. 3. Pyrochlore-supergroup minerals, *A*-site composition.

the same name in our scheme. In order to maintain simplicity and avoid proliferation of names, only the predominant Na is used to determine species, and we have a "one-to-many" mapping between names and some end members. These end members can collectively be represented as $(Na,\#)_2Ta_2O_6F$, where "#" is understood to mean a subordinate amount of an unspecified charge-balancing component. The situation is analogous for fluorcalciomicrolite, although the "#" components for that species would have a charge less than +1 rather than in excess of +2. In this scheme, the "fluornatromicrolite" composition above clearly pertains to fluornatromicrolite, with Ca and Bi as minor charge-balancing components. Mismatch of species and end members arises because the multiplicity of the *A* site (Na, Ca, *etc*.) is twice the multiplicity of the non-framework anion site (F, OH, O, H_2O), and the most common *B*-site and *Y*-site components require 50:50 occupancy of *A* by two different valences. This problem arises in many complex solid-solutions, and our solution for the pyrochlores may provide a template for the nomenclature of other mineral groups.

Nomenclature based on the dominant element in a dominant-valence group is simple and reproducible. This is not true for the alternative scheme of one end member is equal to one name, which is another reason for rejecting that model. In multidimensional coupled solutions, particularly where there are several different valence-groups at more than one site, it is not easy to define a rigorous, reproducible way of extracting a unique dominant end-member. An example is shown below.

Consider a formula such as $(Na_{1.1}Ca_{0.4}Y_{0.2}U_{0.2}\square_{0.1})(Nb_{1.7}Ti_{0.3})O_6(OH)$. Our rules quickly lead to the name "hydroxynatropyrochlore". However, it is possible to partition the various cations so as to find a great many end-members within it, for example:

$0.08\ (\square_{1.25}U_{0.75})Nb_2O_6(OH)$
$+ 0.14\ (NaU)Ti_2O_6(OH)$
$+ 0.02\ Ca_2(NbTi)O_6(OH)$
$+ 0.40\ (Na_{1.5}Y_{0.5})Nb_2O_6(OH)$
$+ 0.36\ (NaCa)Nb_2O_6(OH)$

but this is not a unique decomposition of the formula into "Hawthornian" end-members. The following decomposition also corresponds to the same overall formula:

$0.10\ (\square Y)Nb_2O_6(OH)$
$+ 0.60\ (Na_{1.67}U_{0.33})Nb_2O_6(OH)$
$+ 0.10\ (CaY)Ti_2O_6(OH)$
$+ 0.10\ Ca_2(NbTi)O_6(OH)$
$+ 0.10\ (NaCa)Nb_2O_6(OH)$

in which only two out of five end-members are the same, but their proportions are quite different! Even identifying the single dominant end-member unambiguously is not possible without careful definition of an elaborate procedure. The simplicity and reliability of our current scheme make it preferable.

Variability at the Y site

Pyrochlore-supergroup minerals show a variable *Y*-site composition. In the past, variations in *Y*-site occupancy were not reflected in species nomenclature, in part owing to a lack of knowledge of the structural chemistry of pyrochlore, but also owing to difficulties with the determination of some *Y* species. As the dominant constituent at the *Y* position can now commonly be established *via* EPMA and structure analysis, it is reasonable to indicate the composition of this site in the nomenclature. Rouse *et al*. (1998) demonstrated the presence of structural (OH) groups by infrared spectroscopy. The dominant-valence rule is also valid for anionic sites (Hatert & Burke 2008). Hence, a set of prefixes is to be used to indicate the dominant species of the dominant-valence group at the *Y* site. According to Lumpkin *et al*. (1986), a major difficulty is the determination of whether the "water" is present as OH or molecular H_2O. Borodin & Nazarenko (1957) assumed a total of seven anions and calculated the amount of OH necessary to achieve charge balance. Excess "water" was allocated as H_2O. In general, this procedure will not always be valid because of anion vacancies at the *Y* site (Pyatenko 1959, Aleshin & Roy 1962, Subramanian *et al*. 1983, Chakoumakos 1984). Assumptions involved in calculating structural formulae mainly affect O, OH, H_2O, and *Y*-site vacancies. The reader should be aware of these uncertainties in the following discussion. Some cases may be analyzed:

1) If the sum of cation valences is greater than 13.5, O will necessarily be the dominant species at the *Y* site, for reasons of charge balance.

2) If F exceeds 0.5 *apfu*, F will be considered as the dominant species at the *Y* site. The underlying assumption is that F orders at *Y*, which may not be correct in every case. A subset of data consisting of 32 oxyfluoride pyrochlores was considered separately by Chakoumakos (1984) to determine if any one of three possible anion configurations would yield better calculated values of the cell edge as compared with the observed values. The three anion configurations considered were: (1) $A_2B_2(O_6F)$, O and F disordered over *X* and *Y*; (2) $A_2B_2(O_5F)O$, O and F disordered over *X*, and O at *Y*, and (3) $A_2B_2X_6Y$, fully ordered with O at *X* and F at *Y*.

The regression statistics for the calculated *versus* the observed cell-edge for these three cases were not significantly different. Although arguments of electrostatic neutrality and calculations of Madelung energy rank the fully ordered case as the most likely distribution of anions, the cell edge does not appear to be sensitive enough to distinguish among the three configurations of anions.

3) If the sum of cation valences is less than 13.5 and F is less than 0.5 *apfu*, O, OH, F, H_2O or $\square$ can be the dominant species at the *Y* site. For example, an Na-dominant microlite sample with a valence sum of cations equal to 12.72 may have a formula ending with $\ldots O_{6.00}(\square_{0.45}F_{0.37}O_{0.17})_{\Sigma 1.00}$, $\ldots O_{6.00}[(H_2O)_{0.45}F_{0.37}O_{0.17}]_{\Sigma 1.00}$, $\ldots O_{6.00}[F_{0.37}(OH)_{0.35}\square_{0.28}]_{\Sigma 1.00}$, or $\ldots [O_{5.72}(OH)_{0.28}]_{\Sigma 6.00}[(OH)_{0.63}F_{0.37}]_{\Sigma 1.00}$. The name of this species would be kenonatromicrolite, hydronatromicrolite, fluornatromicrolite, or hydroxynatromicrolite, respectively. All these options may be equally correct without additional information. If, for some reason, it is not possible to know the dominant species of the dominant valence at the *Y* site, we suggest that a name with the anion prefix suppressed, such as "natromicrolite" be applied.

The new nomenclature system, therefore, results in mineral names of the type:

yaroot

where **root** is the name of the group, determined by the dominant species of the dominant-valence group at the *B* site, **y** indicates the dominant species of the dominant-valence group at the *Y* site, and **a** indicates the dominant species of the dominant-valence group at the *A* site.

CALCULATION OF THE FORMULA

Basis for formula calculation

Vacancies can occur at any of the *A*, *X* and *Y* sites, but have not been found to occur at the *B* site. Consequently, pyrochlore formulae should be calculated on the basis of an ideal number of *B* cations (2 *apfu*). See the section entitled "The formula" for a list of typical *B*-site cations to be used in the normalization.

The Si content

Pyrochlore-supergroup minerals that exhibit high Si contents are fairly common in geochemically evolved parageneses. The presence and structural role of Si in the structure of pyrochlore-supergroup minerals have been long debated but have been only partially resolved. Different explanations have been invoked to clarify the way in which Si is incorporated into natural pyrochlores, including the presence of Si as a dispersed crystalline or amorphous silicate phase (Hogarth 1977, Hogarth & Horne 1989, Voloshin *et al*. 1989), and its presence as an essential part of the structure. Despite the absence of tetrahedral sites suitable for Si incorporation in the pyrochlore structure, octahedral Si is possible: $Si(OH)_6^{2-}$ is stable at low pressure and temperature in thaumasite, $Ca_3[Si(OH)_6][SO_4][CO_3]\bullet 12H_2O$ (Edge & Taylor 1971). The real restriction on the occurrence of $^{[6]}Si$ in crystal structures is the crowding of cations around oxygen ions (O'Keeffe & Hyde 1981). Using TEM–EDX investigations combined with crystal-chemical considerations, Bonazzi *et al*. (2006) showed that a significant fraction (30–50%) of the Si detected by EMPA does in fact occupy the octahedral sites of the pyrochlore structure, whereas a larger fraction (50–70%) of Si is concentrated in radiation-damaged portions of the sample. On the basis of this observation, we could perhaps recommend that in the calculation of a formula, no more than 50% Si be attributed to *B*. Nevertheless, we prefer no recommendation on how to allot Si. The incorporation or not of Si into the pyrochlore-supergroup mineral structure should be investigated, but low Si contents can be included as a *B*-site cation or assumed to be due to contaminant phases, and this probably will not modify the name of the mineral. Synthetic pyrochlore-like phases have also been shown to contain Si at the *B* site (Reid *et al*. 1977). Results of two chemical analyses of pyrochlore-supergroup minerals presented by Uher *et al*. (1998) show Si as the dominant cation of the dominant valence at *B*. If it is proved that all the analyzed Si is really at this site, then a new pyrochlore group will exist and a new root name will have to be created.

The content of Cs, Rb and K

For stereochemical reasons, the very large Cs, Rb and K cations prefer the 8*b* (*Y*) site. They should not be assigned to the *A* position of the formula. Chemists refer to pyrochlore-supergroup minerals with very high numbers of vacancies at *A* and abundant Cs, Rb and K at *Y* as "inverse pyrochlores" (Ercit *et al*. 1993). No mineral with a predominance of these cations at *Y* has been described.

The content of F, OH and H_2O

The maximum amount of H_2O in the pyrochlore structure is controlled by the cation occupancy of the *A* site; the maximum content of H_2O ranges from 1.00 H_2O *pfu* for ideal pyrochlores (two *A* cations *pfu, i.e., m* = 0) to 1.75 H_2O *pfu* for *A*-deficient pyrochlores (no *A* cations, *i.e.*, *m* = 2; Ercit et al. 1994). Low *A*-site cation content, high displacement-parameters for the *Y*-site constituents, and the site splitting observed in some cases for the *Y* site indicate that the "O" at the *Y* sites can be H_2O. Ercit *et al*. (1994) found that H_2O molecules were actually displaced away from the ideal 8*b Y* sites, and partially occupied higher-multiplicity positions nearby. Displacements attained 0.57 Å along approximate <112> directions to 96*g Y*', or a similar distance along <111> to 32*e Y*" positions. A 192*i* position (*Y*"') very close to *Y*' was also located by Philippo *et al*.

(1995). Such displacements allow optimal distances between *A*- and *Y*-site species to be maintained.

For a normal pyrochlore AB_2X_6Y, in which *A* and *B* are cations, and *X* and *Y* are anions, there are no stereochemical constraints on the maximum occupancies of the *A* and *Y* sites. However, for pyrochlore-supergroup minerals with H_2O at both the *A* and *Y* sites, the maximum occupancies of both sites are limited owing to the short separation between the ideal *A* and *Y* sites, which is in the neighborhood of 2.3 Å (Ercit *et al.* 1994). Partial occupancy of the *A* site and positional disorder of H_2O at *A* and *Y* sites permit stable O...O separations for neighboring H_2O groups in pyrochlore. Ercit *et al.* (1994) found that positional disorder resulted in eight fractionally occupied *A'* sites around each *A* site, displaced from the ideal site by about 0.11 Å along <111> directions. Five of the eight are too close to the offset *Y'* and *Y"* positions to represent stable O...O separations for H_2O groups; however, three of the eight are sufficiently distant to represent stable intermolecular distances (averaging 2.74 Å). Philippo *et al.* (1995) reported a different scheme of displacement, in which H_2O partially occupies *A"* sites displaced from *A* by 0.75 Å along <100>. For synthetic *A*-cation-free pyrochlore, the maximum H_2O content *pfu* may be limited by the need to avoid close H_2O ... H_2O distances: if there is one H_2O group *pfu* at the *Y* site, then there can be only 3/8 H_2O groups at the *A* site. This constraint translates to a maximum of 1.75 H_2O *pfu* for *A*-cation-free pyrochlore. Previous refinements of the structures of H_2O-bearing pyrochlore have shown H_2O only in the vicinity of the *Y* site (*e.g.,* Groult *et al.* 1982). As no synthetic or natural pyrochlore has been found with all H_2O ordered at *A*, we presume that the *Y* site and its displaced variants are the preferred locations for H_2O, and that H_2O only enters the *A* sites if *Y* cannot accommodate more H_2O. The maximum amount of H_2O *pfu* in the pyrochlore structure is thus given as $1 + (3m/8)$. For an ideal pyrochlore with full *A*-site occupancies ($m = 0$), there can be no more than 1 H_2O *pfu*; as described above, the limit for *A*-deficient pyrochlore ($m = 2$) is 1.75 H_2O *pfu* (Ercit *et al.* 1994).

If there is a large deficit of cations at *A* and the analytical total is very low, we could suspect the presence of H_2O at *A* sites of the mineral. We can calculate the maximum possible amount of structural H_2O in the mineral and compare it with the analytical deficits in EPMA data. But one should neither assume that all H_2O in actinide-bearing, radiation-damaged pyrochlore-supergroup minerals is structural, nor that analytical deficits in EPMA data for pyrochlore-supergroup minerals are attributable to structural H_2O. Much of the H_2O in metamict or semi-metamict pyrochlore-supergroup minerals is adsorbed, and thus not structural. In this regard, it is interesting to note that chemical data on geologically young, non-metamict U-rich pyrochlore (Hogarth & Horne 1989) indicate low H_2O contents. If the H_2O content has been established directly and accurately, *e.g.,* by TGA, then it may indeed be shown that some H_2O must occupy the *A* sites. Unfortunately, we cannot monitor the content of a neutral species other than by density measurements, or from determination of the electron density in a structure, neither of which would be very accurate in the presence of significant heavy atoms. For nomenclature purposes, it will be important to know the H_2O content in *A* only if the total number of any valence group of *A*-site cations is exceeded by the zero-charge group. Two possibilities exist: (1) the cation deficit is comprised mainly of H_2O, and (2) the deficit mainly involves actual site-vacancies. If it is not possible to prove which of the two scenarios is correct, the expression "zero-valence-dominant species" can be used.

NAMES OF PYROCHLORE-SUPERGROUP SPECIES

The new names are presented below, in groups distinguished by the dominant *B* cation. For each group, a table is shown indicating the combinations of dominant species of the dominant-valence group at the *A* site and dominant species of the dominant-valence group at the *Y* site for which there is evidence of a mineral. With each table, a series of references is given for the corresponding species or potential species. Complete descriptions are missing for the majority of the pyrochlore-supergroup species. The seven names marked with an asterisk (*) refer to valid mineral species because of their complete descriptions. Fluornatromicrolite is an IMA-approved mineral, but the complete description has not yet been published. The other 20 names refer to minerals that need to be completely described in order to be approved as valid species. For these, there are only chemical or crystal-structure data. Type specimens need to be defined and deposited in public mineralogical museums. Potential candidates for several other species exist, but are not characterized well enough for any official status. Ancient chemical data derived by wet-chemical analyses commonly represent a mixture of minerals. These data were not used here. All data used were acquired by electron-microprobe analysis or were obtained by crystal-structure refinements. We also verified the scarcity of crystal-chemical data in the literature. Crystal-structure determination were made for only nine pyrochlore-supergroup minerals. The names of these species are marked with a dagger (†) in the tables. A serious problem is identified with the roméite-group minerals, because of an erroneous assumption that all the Sb is pentavalent.

Minerals of the pyrochlore group (Table 1)

In the listings that follow, the name attributed by the author or authors is shown is square brackets.

TABLE 1. PRESENT MEMBERS OF THE PYROCHLORE GROUP

Dominant at *A* site	Dominant species of the dominant-valence group at the *Y* site				
	OH	F	O	H_2O	□
Na		fluornatropyrochlore	oxynatropyrochlore		
Ca	hydroxycalciopyrochlore†	fluorcalciopyrochlore†	oxycalciopyrochlore*		
Sn^{2+}					
Sr		fluorstrontiopyrochlore			
Pb^{2+}			oxyplumbopyrochlore		kenoplumbopyrochlore
Sb^{3+}					
Y			oxyyttropyrochlore-(Y)		
U^{4+}					
H_2O				hydropyrochlore*†	
□		fluorkenopyrochlore			

In the left column are shown the dominant species of the dominant-valence group at the *A* site. An asterisk indicates a fully described species, and a dagger indicates that a structure refinement has been published.

fluornatropyrochlore

P.M. Kartashov (unpublished data)

oxynatropyrochlore

Hogarth & Horne (1989): anal. 3 [uranpyrochlore] is oxynatropyrochlore; anal. 1, 2 and 4 [uranpyrochlore], 5 and 6 [uranoan pyrochlore] are "natropyrochlore".
Knudsen (1989): at least three reported compositions are oxynatropyrochlore [pyrochlore].
Chukanov *et al*. (1999): the formula on page 41 [bismutopyrochlore].

hydroxycalciopyrochlore

Bonazzi *et al*. (2006) [pyrochlore]: only by crystal-structure study was it possible to confirm a hydroxycalciopyrochlore composition.

fluorcalciopyrochlore

There are several examples of analyzed fluorcalciopyrochlore [pyrochlore] in the literature, *e.g*., Hogarth (1961), Ohnenstetter & Piantone (1992), Nasraoui *et al*. (1999), Nasraoui & Bilal (2000), Seifert *et al*. (2000), Thompson *et al*. (2002), Lee *et al*. (2006). The crystal structure of fluorcalciopyrochlore was determined by Bonazzi *et al*. (2006).

oxycalciopyrochlore

There are several examples of analyzed oxycalciopyrochlore in the literature, *e.g*., Hogarth (1961), Černý *et al*. (1979) [the type "stibiobetafite"], Williams (1996), Chukanov *et al*. (1999) [formula on page 40], Mokhov *et al*. (2008) [Moon]. The type specimen of "stibiobetafite" described by Černý *et al*. (1979) should be considered as the type specimen of oxycalciopyrochlore.

fluorstrontiopyrochlore

Franchini *et al*. (2005): The “strontiopyrochlore” Ja–13 (first point) is fluorstrontiopyrochlore.

oxyplumbopyrochlore

Voloshin & Pakhomovskiy (1986), their anal. 1, Table 3.1.

kenoplumbopyrochlore

Voloshin & Pakhomovskiy (1986), their anal. 20, Table 3.1.

oxyyttropyrochlore-(Y)

Tindle & Breaks (1998): sample 96–29.

fluorkenopyrochlore

Kartashov *et al*. (1998): “strontiopyrochlore” 4, and “ceriopyrochlore” 8.
Schmitt *et al*. (2002): AM206 Pcl g1–s2 rim.

hydropyrochlore

The type sample of “kalipyrochlore” of van Wambeke (1978) and that of Ercit *et al*. (1994) [crystal structure determined] are hydropyrochlore. The type specimen of “kalipyrochlore” described by van Wambeke (1978) should be considered as the type specimen of hydropyrochlore.

Note that potential candidates for “fluorhydropyrochlore” exist [Nasraoui & Bilal (2000), the first “kalipyrochlore” and the first “ceriopyrochlore” samples of their Table 4; Xie *et al*. (2006), grain 1 Pyc–I and grain 3 Pyc–I)]

Minerals of the microlite group (Table 2)

TABLE 2. PRESENT MEMBERS OF THE MICROLITE GROUP

Dominant at *A* site	Dominant species of the dominant-valence group at the *Y* site				
	OH	F	O	H_2O	□
Na		fluornatromicrolite			
Ca		fluorcalciomicrolite	oxycalciomicrolite		
Sn^{2+}			oxystannomicrolite*		
Sr					
Pb^{2+}					kenoplumbomicrolite†
Sb^{3+}			oxystibiomicrolite*		
Y					
U^{4+}					
H_2O				hydromicrolite	
□	hydroxykenomicrolite*†			hydrokenomicrolite	

In the left column are shown the dominant species of the dominant-valence group at the *A* site. An asterisk indicates a fully described species, and a dagger indicates that a structure refinement has been published.

fluornatromicrolite

The IMA proposal 98–018 for fluornatromicrolite (Witzke *et al*. 1998) was approved, but the complete paper is only now in press. Some data were published by Atencio (2000). Chemical compositions that correspond to fluornatromicrolite from other occurrences are available in the papers by Ohnenstetter & Piantone (1992), Belkasmi *et al*. (2000), Huang *et al*. (2002) and Baldwin *et al*. (2005).

fluorcalciomicrolite

There are several compositions of fluorcalciomicrolite in the literature, *e.g*., Lumpkin *et al*. (1986), Baldwin (1989), Ohnenstetter & Piantone (1992), Tindle & Breaks (1998), Huang *et al*. (2002), Geisler *et al*. (2004), Tindle *et al*. (2005).

oxycalciomicrolite

Černý *et al*. (2004) [stibiomicrolite]; Guastoni *et al*. (2008) [microlite].

oxystannomicrolite

Vorma & Siivola (1967) [sukulaite]; Ercit *et al*. (1987) [stannomicrolite]. The type specimen of “sukulaite” described by Vorma & Siivola (1967) should be considered as the type for oxystannomicrolite.

kenoplumbomicrolite

Bindi *et al*. (2006b): crystal-structure study of kenoplumbomicrolite.

oxystibiomicrolite

Groat *et al*. (1987): the type sample of “stibiomicrolite”; Novák & Černý (1998). The type specimen of “stibiomicrolite” described by Groat *et al*. (1987) should be considered as the type specimen of oxystibiomicrolite.

hydrokenomicrolite

M.B. Andrade & D. Atencio (unpublished data).

hydromicrolite

M.B. Andrade & D. Atencio (unpublished data).

hydroxykenomicrolite

Ercit *et al*. (1993): crystal-structure study of “cesstibtantite”. The type specimen of “cesstibtantite” described by Voloshin *et al*. (1981) should be considered as the type specimen of hydroxykenomicrolite.

Minerals of the betafite group (Table 3)

TABLE 3. PRESENT MEMBERS OF THE BETAFITE GROUP

Dominant at *A* site	Dominant species of the dominant-valence group at the *Y* site				
	OH	F	O	H_2O	□
Na					
Ca			oxycalciobetafite†		
Sn^{2+}					
Sr					
Pb^{2+}					
Sb^{3+}					
Y					
U^{4+}			oxyuranobetafite		
H_2O					
□					

In the left column are shown the dominant species of the dominant-valence group at the *A* site. A dagger indicates that a structure refinement has been published.

oxycalciobetafite

Meyer & Yang (1988) [yttrobetafite-(Y)]: no H_2O reported in the analytical results, as this is a lunar mineral; Brugger & Gieré (1999); Cámara *et al*. (2004): crystal structure determined.

oxyuranobetafite

Mokhov *et al*. (2008), from the Moon.

Minerals of the roméite group (Table 4)

TABLE 4. PRESENT MEMBERS OF THE ROMÉITE GROUP

Dominant at *A* site	Dominant species of the dominant-valence group at the *Y* site				
	OH	F	O	H_2O	□
Na		fluornatroroméite†			
Ca	hydroxycalcioroméite*†	fluorcalcioroméite	oxycalcioroméite		
Sn^{2+}					
Sr					
Pb^{2+}			oxyplumboroméite		
Sb^{3+}					
Y					
U^{4+}					
H_2O					
□					

In the left column are shown the dominant species of the dominant-valence group at the *A* site. An asterisk indicates a fully described species, and a dagger indicates that a structure refinement has been published.

fluornatroroméite

Matsubara *et al*. (1996): crystal structure determined.

hydroxycalcioroméite

Rouse *et al*. (1998) and Zubkova *et al*. (2000): crystal structure determined ["lewisite"]. The type specimen of "lewisite" described by Hussak & Prior (1895) should be considered as the type specimen of hydroxycalcioroméite.

fluorcalcioroméite

Brugger *et al*. (1997), Uher *et al*. (1998), Brugger & Gieré (1999).

oxycalcioroméite

Christy & Gatedal (2005).

oxyplumboroméite

Christy & Gatedal (2005) [bindheimite].

Minerals of the elsmoreite group (Table 5)

TABLE 5. PRESENT MEMBER OF THE ELSMOREITE GROUP

Dominant at *A* site	Dominant species of the dominant-valence group at the *Y* site				
	OH	F	O	H_2O	□
Na					
Ca					
Sn^{2+}					
Sr					
Pb^{2+}					
Sb^{3+}					
Y					
U^{4+}					
H_2O					
□				hydrokenoelsmoreite*†	

In the left column are shown the dominant species of the dominant-valence group at the *A* site. An asterisk indicates a fully described species, and a dagger indicates that a structure refinement has been published.

hydrokenoelsmoreite

Schaller (1911) ["ferritungstite"]; Sahama (1981) ["alumotungstite"]; Ercit & Robinson (1994) ["ferritungstite"]: crystal structure determined; Williams *et al*. (2005) ["elsmoreite"]. The type specimen of "elsmoreite" described by Williams *et al*. (2005) should be considered as the type specimen of hydrokenoelsmoreite.

Correspondence Between Old and New Names

All the following mineral names shown in italics should be discarded, as they do not correspond to distinct species in the new classification. Note that there is not a one-to-one correlation between the new names and the traditional names in the literature.

Kalipyrochlore

Kalipyrochlore of van Wambeke (1978) is insufficiently K-rich to warrant the name "kalipyrochlore". The type sample and that of Ercit *et al.* (1994) are examples of hydropyrochlore, with H_2O dominant at both the *A* and *Y* sites. Additional data for samples from the type occurrence are given by Wall *et al.* (1996).

Strontiopyrochlore

Strontiopyrochlore of Lapin *et al.* (1986), Lottermoser & England (1988), Voloshin *et al.* (1989), Wall *et al.* (1996), Kartashov *et al.* (1998), Chakhmouradian & Mitchell (1998, 2002), and Franchini *et al.* (2005) [except fluorstrontiopyrochlore] are Ca- or zero-valent-dominant pyrochlore.

Bariopyrochlore

Bariopyrochlore of Jäger *et al.* (1959) ["pandaite"], Knudsen (1989), Wall *et al.* (1996), Williams *et al.* (1997), Subbotin & Subbotina (2000), and Bindi *et al.* (2006a) are all zero-valent-dominant pyrochlore.

Plumbopyrochlore

Plumbopyrochlore of Skorobogatova *et al.* (1966), Kartashov *et al.* (1992), Voloshin *et al.* (1993), Kovalenko *et al.* (1995), and Xie *et al.* (2006) is "plumbopyrochlore". Plumbopyrochlore of Chakhmouradian & Mitchell (2002), Wang *et al.* (2003), and Beurlen *et al.* (2005) is zero-valent-dominant pyrochlore. Plumbopyrochlore of Voloshin & Pakhomovskiy (1986) corresponds to oxyplumbopyrochlore [their anal. 1, Table 3.1], kenoplumbopyrochlore [their anal. 20, Table 3.1] and "plumbopyrochlore" [several compositions].

Bismutopyrochlore

Bismutopyrochlore of Chukanov *et al.* (1999) and Ercit *et al.* (2003) is zero-valent-dominant pyrochlore.

Ceriopyrochlore-(Ce)

Ceriopyrochlore-(Ce) of Weidmann & Lenher (1907), van Wambeke (1980), Wall *et al.* (1996), Chakhmouradian (1996), and Zurevinski & Mitchell (2004) is Ca- or zero-valent-dominant pyrochlore.

Yttropyrochlore-(Y)

Yttropyrochlore-(Y) of Kalita (1957) ["obruchevite"], and Ercit *et al.* (2003) is a zero-valent-dominant mineral. Yttropyrochlore-(Y) of Tindle & Breaks (1998) is oxyyttropyrochlore-(Y).

Uranpyrochlore

For all recorded cases of uranpyrochlore, U is not the dominant cation of the dominant valence at *A*, except for sample 9 from Khibina studied by Chakhmouradian & Mitchell (2002). Nevertheless, it is not possible to know the dominant anion of the dominant valence at the *Y* site of this mineral. It should be referred as "uranopyrochlore". Uranpyrochlore of Hogarth & Horne (1989) is "natropyrochlore".

Stannomicrolite

The stannomicrolite species of Ercit *et al.* (1987) ["sukulaite" of Vorma & Siivola (1967)] is oxystannomicrolite. The stannomicrolite of Uher *et al.* (2008) is Ca- or zero-valent-dominant microlite.

Plumbomicrolite

The plumbomicrolite of Safiannikoff & van Wambeke (1961), Beurlen *et al.* (2005) and Uher *et al.* (2008) is zero-valent-dominant microlite. The plumbomicrolite of Bindi *et al.* (2006b) is, by crystal-structure refinement, kenoplumbomicrolite.

Stibiomicrolite

The type sample for stibiomicrolite (Groat *et al.* 1987) and also the sample of Novák & Černý (1998) are now to be classified as oxystibiomicrolite. Two compositions by Černý *et al.* (2004) are oxycalciomicrolite, and one is "calciomicrolite". The stibiomicrolite of Beurlen *et al.* (2005) is zero-valent-dominant microlite.

Bismutomicrolite

The composition claimed for the original bismutomicrolite ["westgrenite"] (von Knorring & Mrose 1963) probably refers to a mixture. The bismutomicrolite studied by Erichsen de Oliveira *et al.* (1970) and Tindle & Breaks (1998) is zero-valent-dominant microlite.

Bariomicrolite

The bariomicrolite species of Hogarth (1977), the "rijkeboerite" of van der Veen (1963), is too poor in Ba to warrant this name. The type sample apparently has □ dominant at the A position and H_2O at the Y position, and as such is probably hydrokenomicrolite. The bariomicrolite studied by Beurlen *et al.* (2005) is probably also hydrokenomicrolite.

Uranmicrolite

No samples described as uranmicrolite ("djalmaite" of Guimarães 1939) (*e.g.,* Baldwin 1989, Rub *et al.* 1998, Tindle & Breaks 1998, Novák & Černý 1998, Zhang *et al.* 2004, Breiter *et al.* 2007, van Lichtervelde *et al.* 2007, Uher *et al.* 2007) are rich enough in U to warrant a status as a separate species.

Cesstibtantite

Cesstibtantite was described originally at Vasin Myl'k Mountain in Voronie Tundry, the Kola Peninsula, Russia, by Voloshin *et al.* (1981). Other occurrences were described in Manitoba, Canada, by Ercit *et al.* (1985), at Mt. Holland, Australia, by Nickel & Robinson (1985), and at Utö, Sweden, by Smeds *et al.* (1999). The crystal structure of cesstibtantite from Vasin Myl'k Mountain and Manitoba was solved by Ercit *et al.* (1993). Both are now to be classified as hydroxykenomicrolite. The two other samples are also zero-valent-dominant microlite, but it is not possible prove that they are hydroxykenomicrolite.

Natrobistantite

Natrobistantite studied by Voloshin *et al.* (1983) and by Beurlen *et al.* (2005) are both zero-valent-dominant microlite.

Calciobetafite

Hogarth (1977) defined betafite as a uranium-rich Ti-dominant pyrochlore, hence the origin of calciobetafite, a calcium-dominant Ti-rich pyrochlore (Mazzi & Munno 1983). However, all published analytical data on (non-defect) betafite have Ca in excess of U [except the mineral from the Moon studied by Mokhov *et al.* (2008) (oxyuranobetafite)]; consequently, by current standards, betafite is defined as a calcium-rich and Ti-dominant pyrochlore. This renders the name *calciobetafite* redundant, and has the added effect of bringing members of the betafite group in line with the other groups (furthermore, type calciobetafite is Nb-dominant, not Ti-dominant, and belongs to the pyrochlore group).

Stibiobetafite

Černý *et al*. (1979) defined stibiobetafite as the Sb^{3+} analogue of betafite; however, the type sample has Nb + Ta > Ti *apfu*, and Ca is the dominant species of the dominant-valence group at the *A* site. The type sample is now to be classified as oxycalciopyrochlore. It is not possible to calculate the formula of stibiobetafite studied by Tindle & Breaks (1998) owing to errors in the table of analytical data.

Plumbobetafite

Plumbobetafite of Ganzeev *et al*. (1969) is zero-valent-dominant pyrochlore. Plumbobetafite of Voloshin *et al*. (1993) is "plumbobetafite".

Yttrobetafite-(Y)

Yttrobetafite-(Y) of Kalita (1959) and Liferovich & Mitchell (2005) are zero-valent-dominant pyrochlore. Yttrobetafite-(Y) from the Moon (Meyer & Yang 1988) is oxycalciobetafite.

Lewisite

Crystal-structure studies (Rouse *et al*. 1998, Zubkova *et al*. 2000) proved "lewisite" to be hydroxycalcioroméite.

Stetefeldtite

Very old references (Riotte 1867, Mason & Vitaliano 1953). Probably "argento-roméite". This material needs to be examined chemically and structurally.

Stibiconite

Original material described by Beudant (1837). Probably "stibioroméite". No electron-microprobe data are available. This material needs to be examined chemically and structurally.

Bindheimite

Original material described by Dana (1868). Only with the data of Christy & Gatedal (2005) is it possible to correlate this mineral with oxyplumboroméite.

Monimolite

The problematical species monimolite (Igelström 1865, Mason & Vitaliano 1953) is almost certainly identical with oxyplumboroméite, but needs re-examination.

Bismutostibiconite

The mineral was described by Walenta (1983). The chemical data are considered inadequate owing to a standardless energy-dispersion spectroscopy (EDS), with all Sb assumed to be 5+, and results of the analysis normalized to 100%. It probably is "bismutoroméite". Needs a chemical and structural investigation.

Partzite

Arents (1867). Probably "cuproroméite". No electron-microprobe data. This material needs to be examined chemically and structurally.

Ferritungstite and alumotungstite

Ferritungstite (Schaller 1911, Ercit & Robinson 1994) and alumotungstite (Sahama 1981) are hydrokenoelsmoreite.

Jixianite

Jixianite (Liu 1979) is "plumboelsmoreite". In the absence of a crystal-structure study, it is not possible to know the dominant anion of the dominant valence at the *Y* site of jixianite.

THE FORMULA OF SELECTED SPECIES

Formulae are given in Table 6 for all 28 pyrochlore species for which we have analytical evidence. Note that subordinate components at the *A*, *B*, *X* or *Y* sites have no nomenclatural significance. We show specific examples here that are typical of the minor components observed, but any of these could be replaced by "#", indicating an unspecified heterovalent species required for charge balance.

TABLE 6. FORMULAE OF ALL 28 PYROCHLORE SPECIES FOR WHICH ANALYTICAL EVIDENCE IS DEEMED ADEQUATE

1	oxycalciopyrochlore*	$Ca_2Nb_2O_6O$
2	hydropyrochlore*†	$(H_2O,\square)_2Nb_2(O,OH)_6(H_2O)$
3	hydroxykenomicrolite*†	$(\square,Na,Sb^{3+})_2Ta_2O_6(OH)$
4	oxystannomicrolite*	$Sn_2Ta_2O_6O$
5	oxystibiomicrolite*	$(Sb^{3+},Ca)_2Ta_2O_6O$
6	hydroxycalcioroméite*†	$(Ca,Sb^{3+})_2(Sb^{5+},Ti)_2O_6(OH)$
7	hydrokenoelsmoreite*†	$\square_2W_2O_6(H_2O)$
8	fluornatromicrolite	$(Na,Ca,Bi)_2Ta_2O_6F$
9	hydroxycalciopyrochlore†	$(Ca,\square)_2Nb_2(O,OH)_6(OH)$
10	fluorcalciopyrochlore†	$(Ca,\square)_2Nb_2(O,OH)_6F$
11	kenoplumbopyrochlore†	$(Pb,\square)_2Nb_2O_6(\square,O)$
12	oxycalciobetafite†	$Ca_2(Ti,Nb)_2O_6O$
13	fluornatroroméite†	$(Na,Ca)_2Sb_2(O,OH)_6F$
14	fluornatropyrochlore	$(Na,REE,Ca)_2Nb_2(O,OH)_6F$
15	oxynatropyrochlore	$(Na,Ca,U)_2Nb_2O_6(O,OH)$
16	fluorstrontiopyrochlore	$(Sr,\square)_2Nb_2(O,OH)_6F$
17	oxyplumbopyrochlore	$Pb_2Nb_2O_6O$
18	oxyyttropyrochlore-(Y)	$(Y,\square)_2Nb_2O_6O$
19	fluorkenopyrochlore	$(\square,Na,Ce,Ca)_2(Nb,Ti)_2O_6F$
20	fluorcalciomicrolite	$(Ca,Na)_2Ta_2O_6F$
21	oxycalciomicrolite	$Ca_2Ta_2O_6O$
22	kenoplumbomicrolite	$(Pb,\square)_2Ta_2O_6(\square,O,OH)$
23	hydromicrolite	$(H_2O,\square)_2Ta_2(O,OH)_6(H_2O)$
24	hydrokenomicrolite	$(\square,H_2O)_2Ta_2(O,OH)_6(H_2O)$
25	oxyuranobetafite	$(U,Ca,\square)_2(Ti,Nb)_2O_6O$
26	fluorcalcioroméite	$(Ca,Sb^{3+})_2(Sb^{5+},Ti)_2O_6F$
27	oxycalcioroméite	$Ca_2Sb_2O_6O$
28	oxyplumboroméite	$Pb_2Sb_2O_6O$

An asterisk indicates a fully described species, and a dagger indicates that a structure refinement has been published, as indicated in Tables 1 to 5.

INDEX OF MINERAL NAMES

We show in Table 7 the correspondence between published names (with references) and the new names proposed, with an indication of the recommended fate of the old name.

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TABLE 7. THE CORRESPONDENCE BETWEEN PUBLISHED NAMES AND THE NEW NAMES PROPOSED

Current name	New name	Discredit, redefine, new species	References
–	"fluornatropyrochlore"	possible new species	P.M. Kartashov (unpublished data)
–	“hydromicrolite”	possible new species	Andrade & Atencio (unpublished data)
–	“hydrokenomicrolite”	possible new species	Andrade & Atencio (unpublished data)
alumotungstite	= hydrokenoelsmoreite	discredited	Sahama (1981)
bariomicrolite	probably “hydrokenomicrolite”	discredited	van der Veen (1963), Beurlen *et al.* (2005)
bariopyrochlore	= zero-valent-dominant pyrochlore	discredited	Jager *et al.* (1959), Knudsen (1989), Wall *et al.* (1996), Williams *et al.* (1997), Subbotin & Subbotina (2000), Bindi *et al.* (2006a)
betafite	“oxycalciobetafite”	possible new species	Brugger & Gieré (1999), Cámara *et al.* (2004)
betafite	“oxyuranobetafite”	possible new species	Mokhov *et al.* (2008)
bindheimite	“oxyplumboroméite”	possible new species	Christy & Gatedal (2005)
bindheimite	probably “plumboroméite”	discredited	Dana (1868)
bismutomicrolite	probably a mixture	discredited	Von Knorring & Mrose (1963)
bismutomicrolite	= zero-valent-dominant microlite	discredited	Erichsen de Oliveira *et al.* (1970), Tindle & Breaks (1998)
bismutopyrochlore	“oxynatropyrochlore”	possible new species	Chukanov *et al.* (1999)
bismutopyrochlore	= zero-valent-dominant pyrochlore	discredited	Chukanov *et al.* (1999), Ercit *et al.* (2003)
bismutostibiconite	probably “bismutoroméite”.	discredited	Walenta (1983)
calciobetafite	a pyrochlore-group mineral	discredited	Mazzi & Munno (1983)
ceriopyrochlore-(Ce)	“fluorkenopyrochlore”	possible new species	Kartashov *et al.* (1998)
ceriopyrochlore-(Ce)	= Ca- or zero-valent-dominant pyrochlore	discredited	Weidmann & Lenher (1907), van Wambeke (1980), Wall *et al.* (1996), Chakhmouradian (1996), Zurevinski & Mitchell (2004)
cesstibtantite	hydroxykenomicrolite	redefined	Voloshin *et al.* (1981), Ercit *et al.* (1993)
cesstibtantite	= zero-valent-dominant microlite	discredited	Nickel & Robinson (1985), Smeds *et al.* (1999)
elsmoreite	hydrokenoelsmoreite	redefined	Williams *et al.* (2005)
ferritungstite	= hydrokenoelsmoreite	discredited	Schaller (1911), Ercit & Robinson (1994)
fluornatromicrolite	“fluornatromicrolite”	approved (IMA#98-018)	Witzke *et al.* (1998), Ohnenstetter & Piantone (1992), Belkasmi *et al.* (2000), Huang *et al.* (2002), Baldwin *et al.* (2005)
jixianite	“plumboelsmoreite”.	discredited	Liu (1979)
kalipyrochlore	hydropyrochlore	redefined	van Wambeke (1978), Ercit *et al.* (1994)
lewisite	hydroxycalcioroméite	redefined	Hussak & Prior (1895), Rouse *et al.* (1998), Zubkova *et al.* (2000)
microlite	“fluorcalciomicrolite”	possible new species	Lumpkin *et al.* (1986), Baldwin (1989), Ohnenstetter & Piantone (1992), Tindle & Breaks (1998), Huang *et al.* (2002), Geisler *et al.* (2004), Tindle *et al.* (2005).
microlite	“oxycalciomicrolite”	possible new species	Guastoni *et al.* (2008)
monimolite	probably “oxyplumboroméite”	discredited	Igelström (1865), Mason & Vitaliano (1953)
natrobistantite	= zero-valent-dominant microlite	discredited	Voloshin *et al.* (1983), Beurlen *et al.* (2005)
partzite	probably “cuproroméite”	discredited	Arents (1867)
plumbobetafite	= zero-valent-dominant pyrochlore	discredited	Ganzeev *et al.* (1969)
plumbobetafite	= “plumbobetafite”	discredited	Voloshin *et al.* (1993)
plumbomicrolite	“kenoplumbomicrolite”	possible new species	Bindi *et al.* (2006b)
plumbomicrolite	zero-valent-dominant microlite	discredited	Safiannikoff & van Wambeke (1961), Beurlen *et al.* (2005), Uher *et al.* (2008)
plumbopyrochlore	“oxyplumbopyrochlore”	possible new species	Voloshin & Pakhomovskiy (1986)
plumbopyrochlore	“kenoplumbopyrochlore”	possible new species	Voloshin & Pakhomovskiy (1986)
plumbopyrochlore	= “plumbopyrochlore”.	discredited	Skorobogatova *et al.* (1966), Voloshin & Pakhomovskiy (1986), Kartashov *et al.* (1992), Voloshin *et al.* (1993), Kovalenko *et al.* (1995), Xie *et al.* (2006)
plumbopyrochlore	= zero-valent-dominant pyrochlore	discredited	Chakhmouradian & Mitchell (2002), Wang *et al.* (2003), Beurlen *et al.* (2005)
pyrochlore	“oxynatropyrochlore”	possible new species	Knudsen (1989)
pyrochlore	“hydroxycalciopyrochlore”	possible new species	Bonazzi *et al.* (2006)
pyrochlore	“fluorcalciopyrochlore”	possible new species	Hogarth (1961), Ohnenstetter & Piantone (1992), Nasraoui *et al.* (1999), Nasraoui & Bilal (2000), Seifert *et al.* (2000), Thompson *et al.* (2002), Lee *et al.* (2006), Bonazzi *et al.* (2006)
pyrochlore	“fluorkenopyrochlore”	possible new species	Schmitt *et al.* (2002)
roméite	“fluornatroroméite”	possible new species	Matsubara *et al.* (1996)

TABLE 7 (cont'd). THE CORRESPONDENCE BETWEEN PUBLISHED NAMES AND THE NEW NAMES PROPOSED

Current name	New name	Discredit, redefine, new species	References
roméite	"fluorcalcioroméite"	possible new species	Brugger *et al.* (1997), Uher *et al.* (1998), Brugger & Gieré (1999)
roméite	"oxycalcioroméite"	possible new species	Christy & Gatedal (2005)
stannomicrolite	oxystannomicrolite	redefined	Vorma & Siivola (1967), Ercit *et al.* (1987)
stannomicrolite	= Ca- or zero-valent-dominant microlite	discredited	Uher *et al.* (2008)
stetefeldtite	probably "argentoroméite"	discredited	Riotte (1867), Mason & Vitaliano (1953)
stibiconite	probably "stibioroméite"	discredited	Beudant (1837)
stibiobetafite	oxycalciopyrochlore	redefined	Černý *et al.* (1979)
stibiobetafite	? (errors in the table of analyses)	discredited	Tindle & Breaks (1998)
stibiomicrolite	"oxycalciomicrolite"	possible new species	Černý *et al.* (2004)
stibiomicrolite	oxystibiomicrolite	redefined	Groat *et al.* (1987), Novák & Černý (1998)
stibiomicrolite	calciomicrolite	discredited	Černý *et al.* (2004)
stibiomicrolite	= zero-valent-dominant microlite	discredited	Beurlen *et al.* (2005)
strontiopyrochlore	"fluorstrontiopyrochlore"	possible new species	Franchini *et al.* (2005)
strontiopyrochlore	"fluorkenopyrochlore"	possible new species	Kartashov *et al.* (1998)
strontiopyrochlore	= Ca or zero-valent pyrochlore	discredited	Lapin *et al.* (1986), Lottermoser & England (1988), Voloshin *et al.* (1989), Wall *et al.* (1996), Kartashov *et al.* (1998), Chakhmouradian & Mitchell (1998 and 2002), Franchini *et al.* (2005)
uranmicrolite	not sufficiently rich in U	discredited	Guimarães (1939), Baldwin (1989), Rub *et al.* (1998), Tindle & Breaks (1998), Novák & Černý (1998), Zhang *et al.* (2004), Breiter *et al.* (2007), van Lichtervelde *et al.* (2007), Uher *et al.* (2007)
uranpyrochlore	"oxynatropyrochlore"	possible new species	Hogarth & Horne (1989)
uranpyrochlore	= "uranopyrochlore"	discredited	Chakhamouradian & Mitchell (2002)
uranpyrochlore	natropyrochlore	discredited	Hogarth & Horne (1989)
yttrobetafite-(Y)	"oxycalciobetafite"	possible new species	Meyer & Yang (1988)
yttrobetafite-(Y)	= zero-valent-dominant pyrochlore	discredited	Kalita (1959), Liferovich & Mitchell (2005)
yttropyrochlore-(Y)	"oxyyttropyrochlore-(Y)"	possible new species	Tindle & Breaks (1998)
yttropyrochlore-(Y)	= zero-valent-dominant minerals	discredited	Kalita (1957), Ercit *et al.* (2003)

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