

## Nomenclature of the apatite supergroup minerals

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**Abstract:** The apatite supergroup includes minerals with a generic chemical formula  $^{IX}M_1^{VI}M_2^{IV}M_3^{IV}(TO_4)_3X$  ( $Z = 2$ ); chemically they can be phosphates, arsenates, vanadates, silicates, and sulphates. The maximum space group symmetry is  $P6_3/m$ , but several members of the supergroup have a lower symmetry due to cation ordering and deviations from the ideal topology, which may result in an increase of the number of the independent sites. The apatite supergroup can be formally divided into five groups, based on crystal-chemical arguments: apatite group, hedyphane group, belovite group, britholite group, and ellestadite group. The abundance of distinct ions which may be hosted at the key-sites [ $M = Ca^{2+}, Pb^{2+}, Ba^{2+}, Sr^{2+}, Mn^{2+}, Na^+, Ce^{3+}, La^{3+}, Y^{3+}, Bi^{3+}$ ;  $T = P^{5+}, As^{5+}, V^{5+}, Si^{4+}, S^{6+}, B^{3+}$ ;  $X = F^-, (OH)^-, Cl^-$ ] result in a large number of compositions which may have the status of distinct mineral species. Naming of apatite supergroup minerals in the past has resulted in nomenclature inconsistencies and problems. Therefore, an *ad hoc* IMA-CNMNC Subcommittee was established with the aim of rationalizing the nomenclature within the apatite supergroup and making some order among existing and potentially new mineral species. In addition to general recommendations for the handling of chemical (EPMA) data and for the allocation of ions within the various sites, the main recommendations of this subcommittee are the following:

1. Nomenclature changes to existing minerals. The use of adjectival prefixes for anions is to be preferred instead of modified Levinson suffixes; accordingly, six minerals should be renamed as follows: apatite-(CaF) to *fluorapatite*, apatite-(CaOH) to *hydroxylapatite*, apatite-(CaCl) to *chlorapatite*, ellestadite-(F) to *fluorellestadite*, ellestadite-(OH) to *hydroxyllelestadite*, phosphohedyphane-(F) to *fluorophosphohedyphane*. For the apatite group species these changes return the names that have been used in thousands of scientific paper, treatises and museum catalogues over the last 150 years. The new mineral IMA 2008-009, approved without a name, is here named *stronadelphite*. Apatite-(SrOH) is renamed *fluorstrophite*. Deloneite-(Ce) is renamed *deloneite*. The new mineral IMA 2009-005 is approved with the name *fluorbritholite-(Y)*.

2. Potentially new mineral species. The following end-member compositions are eligible for status as distinct mineral species; the approved name, if any, is given in parentheses:  $Ca_2Pb_3(AsO_4)_3(OH)$  (hydroxylhedyphane);  $Ca_2Pb_3(PO_4)_3(OH)$  (hydroxylphosphohedyphane);  $Ca_2Sr_3(PO_4)_3F$  (new root name);  $Mn_2Ca_3(PO_4)_3Cl$  (new root name);  $Pb_5(SiO_4)_{1.5}(SO_4)_{1.5}(OH)$  (hydroxylmattheddleite).

3. Minerals and mineral names which could be discredited. The mineral ellestadite-(Cl) is not thought to exist and should be discredited; the name melanocerite-(Ce) should be discontinued [= tritomite-(Ce)].

4. Changes of status from distinct species to polymorphic variants. Fermorite is the monoclinic polymorph of johnbaumite (= johnbaumite-*M*); clinohydroxylapatite is the monoclinic polymorph of hydroxylapatite (= hydroxylapatite-*M*); clinomimetite is the monoclinic polymorph of mimetite (= mimetite-*M*).

5. Recognition of a new polymorphic variant. A new monoclinic polymorph of apatite is recognized (chlorapatite-*M*).

6. Changes to end-member formulae. The ideal chemical formula of morelandite is  $Ca_2Ba_3(AsO_4)_3Cl$  instead of  $Ba_5(AsO_4)_3Cl$ ; the ideal chemical formula of deloneite is  $(Na_{0.5}REE_{0.25}Ca_{0.25})(Ca_{0.75}REE_{0.25})Sr_{1.5}(CaNa_{0.25}REE_{0.25})(PO_4)_3F_{0.5}(OH)_{0.5}$ .

**Key-words:** nomenclature, apatite supergroup, apatite group, hedyphane group, belovite group, britholite group, ellestadite group.

### 1. Introduction

Apatite is a generic name, first introduced in the mineralogical literature by Werner (1786), and used to describe calcium

phosphates with simplified formula  $Ca_5(PO_4)_3X$  ( $X = F, Cl, OH$ ). The name originates from the Greek *απατάω*, which means “to deceive”, because the mineral was often mistaken for other species (Fig. 1). Since 1856–1860, these minerals



Fig. 1. Fluorapatite crystal exhibiting the common forms {001}, {100} and {101} on a matrix of albite and muscovite, from a granitic pegmatite in the Nagar area, Gilgit district, Northern Areas, Pakistan (Jeff Scovil photograph).

have been named fluorapatite, chlorapatite, and hydroxylapatite, depending on the dominant  $X^-$  anion. As the number of new species increased over the years, several comprehensive reviews on the crystal chemistry of the “apatite group” were published (*e.g.*, McConnell, 1938 and 1973; Nriagu & Moore, 1984; Elliott, 1994; Kohn *et al.*, 2002). Recently, in the context of a revision of the mineralogical nomenclature initiated by then chairman of the IMA Commission on New Minerals, Nomenclature and Classification E.A.J. Burke, and aimed at adopting, as far as possible, modified Levinson suffixes instead of adjectival prefixes such as “fluor-”, “chlor-”, and “hydroxyl-”, the above minerals were renamed apatite-(CaF), apatite-(CaCl), and apatite-(CaOH), respectively (Burke, 2008). One of the rationales for that change was the benefit of having the names of these minerals appear consecutively in alphabetical listings and databases.

The changes introduced by Burke (2008) to the nomenclature of these and other minerals with the apatite structure, *e.g.* strontium-apatite and “ellestadites”, did not fully consider the structural complexities of these minerals. The apatite structure type is flexible enough to allow a wide degree of substitutions among cations (*cf.* White & Dong, 2003; White *et al.*, 2005), and this fact, coupled with the possible lowering of symmetry related to ordering of cations and anions, dramatically increases the number of end-members which are potentially eligible as individual mineral species.

The recently approved nomenclature scheme of Burke (2008) could logically be extended to the renaming of other apatite group minerals, changing, *e.g.*, pyromorphite into apatite-(PbCl), or alforsite into apatite-(BaCl). And one could be tempted to include also the various tetrahedral cations (P, As, or V), into the extended suffix [*e.g.*, apatite-(PbAsCl) instead of mimetite, apatite-(CaAsOH) instead of johnbaumite]. The

result would be mineral names that are more similar to chemical formulae. The limit of such an approach would be to adopt chemical formulae throughout, instead of mineral names. However, a nomenclature based extensively upon modified Levinson-style suffixes is likely to be rejected by the mineralogical community, since many would argue that multiple suffixes are difficult to be read, almost impossible to be spoken, not immediately self-explanatory, and unpleasant to the eye. Furthermore, such naming replaces many traditional names given to honour worthy individuals.

A specific example of a nomenclature problem resulting from ordering in the apatite structure is presented by the recently approved Sr end-member of apatite *lato sensu*,  $Sr_5(PO_4)_3F$  (IMA 2008-009). While “strontioapatite” would have been an appropriate name for this species, a mineral with essentially the same name already exists, strontium-apatite [which has just been renamed apatite-(SrOH) after Burke (2008)]. Furthermore, the latter mineral has a cation-ordered structure, and it is actually F-dominant, with the ideal formula  $SrCaSr_3(PO_4)_3F$  (Efimov *et al.*, 1962; Klevtsova, 1964; Pushcharovsky *et al.*, 1987); therefore, its renaming as apatite-(SrOH) is incorrect. To make the issue even more complicated, there is also another cation-ordered member along the join  $Ca_5(PO_4)_3F \Leftrightarrow Sr_5(PO_4)_3F$ , namely fluorcaphite,  $SrCaCa_3(PO_4)_3F$ .

For the above reasons the former chairman of the IMA CNMNC, E.A.J. Burke, asked us (MP & ARK) to convene a subcommittee to re-evaluate the nomenclature of minerals belonging to the “apatite group”, to propose a new consistent nomenclature and to rationalize all existing mineral names in this group.

The “apatite group” traditionally includes phosphate, arsenate and vanadate minerals. Other minerals belonging to different chemical classes, namely silicates (*e.g.*, britholite), silicate-sulphates (*e.g.*, ellestadite), and sulphates (*e.g.*, cesanite) display the structural topology of apatite. In accordance with the newly approved standardisation of mineral group hierarchies (Mills *et al.*, 2009), all of these minerals can be included in the broader apatite supergroup. Because the same nomenclature questions are relevant for all members of the supergroup, they will all be considered in this report. All valid species within the apatite supergroup are listed in Table 1. Their ideal chemical formulae are also given, as they should appear in the official IMA List of Minerals. The minerals have here been divided into five groups on the basis of their crystallographic and/or chemical similarities. This report has been approved by the IMA Commission on New Minerals, Nomenclature and Classification.

## 2. Crystal-chemistry of apatite supergroup minerals

The archetype structure of apatite is hexagonal with space group  $P6_3/m$  and unit-cell parameters  $a = 9.3 - 9.6$ ,  $c = 6.7 - 6.9$  Å. The generic crystal-chemical formula may be also written in its doubled form, which corresponds to the unit cell content, as follows:  ${}^{IX}M1_4 {}^{VII}M2_6 ({}^{IV}TO_4)_6 X_2$  ( $Z = 1$ ),

Table 1. Existing names (after the IMA List of Minerals), approved names and end-member formulae for minerals within the apatite supergroup. The approved changes are set in bold. Names in quotes are the most appropriate names we would recommend for potential new minerals.

Existing name (IMA list of minerals)	Approved name (this subcommittee)	End-member formula
<i>Apatite group</i>		
Apatite-(CaF)	<b>Fluorapatite</b>	Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> F
Apatite-(CaCl)	<b>Chlorapatite</b> <sup>a</sup>	Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl
—	<b>Chlorapatite-M</b> <sup>b</sup>	Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl
Apatite-(CaOH)	<b>Hydroxylapatite</b> <sup>a</sup>	Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> OH
Apatite-(CaOH)-M	<b>hydroxylapatite-M</b> <sup>b</sup>	Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> OH
Svabite	Svabite	Ca <sub>5</sub> (AsO <sub>4</sub> ) <sub>3</sub> F
Turneaureite	Turneaureite	Ca <sub>5</sub> (AsO <sub>4</sub> ) <sub>3</sub> Cl
Johnbaumite	Johnbaumite <sup>a</sup>	Ca <sub>5</sub> (AsO <sub>4</sub> ) <sub>3</sub> OH
Fermorite	<b>Johnbaumite-M</b> <sup>b</sup>	Ca <sub>5</sub> (AsO <sub>4</sub> ) <sub>3</sub> OH
2008-009 <sup>c</sup>	<b>Stronadelphite</b>	Sr <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> F
Pyromorphite	Pyromorphite	Pb <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl
Mimetite	Mimetite <sup>a</sup>	Pb <sub>5</sub> (AsO <sub>4</sub> ) <sub>3</sub> Cl
Clinomimetite	<b>Mimetite-M</b> <sup>b</sup>	Pb <sub>5</sub> (AsO <sub>4</sub> ) <sub>3</sub> Cl
Alforsite	Alforsite	Ba <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl
Vanadinite	Vanadinite	Pb <sub>5</sub> (VO <sub>4</sub> ) <sub>3</sub> Cl
<i>Hedyphane group</i>		
Hedyphane	Hedyphane	Ca <sub>2</sub> Pb <sub>3</sub> (AsO <sub>4</sub> ) <sub>3</sub> Cl
—	<b>“Hydroxylhedyphane”</b> <sup>d</sup>	Ca <sub>2</sub> Pb <sub>3</sub> (AsO <sub>4</sub> ) <sub>3</sub> OH
Phosphohedyphane <sup>e</sup>	Phosphohedyphane	Ca <sub>2</sub> Pb <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl
Phosphohedyphane-(F)	<b>Fluorophosphohedyphane</b>	Ca <sub>2</sub> Pb <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> F
—	<b>“Hydroxylphosphohedyphane”</b> <sup>d</sup>	Ca <sub>2</sub> Pb <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> OH
—	<b>New root name</b> <sup>d</sup>	Ca <sub>2</sub> Sr <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> F
Morelandite	Morelandite	<b>Ca<sub>2</sub>Ba<sub>3</sub>(AsO<sub>4</sub>)<sub>3</sub>Cl</b>
—	<b>New root name</b> <sup>d</sup>	Mn <sub>2</sub> Ca <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl
Cesanite	Cesanite	Ca <sub>2</sub> Na <sub>3</sub> (SO <sub>4</sub> ) <sub>3</sub> OH
Caracolite	Caracolite	Na <sub>2</sub> (Pb <sub>2</sub> Na)(SO <sub>4</sub> ) <sub>3</sub> Cl
Aiolosite	Aiolosite	Na <sub>2</sub> (Na <sub>2</sub> Bi)(SO <sub>4</sub> ) <sub>3</sub> Cl
<i>Belovite group</i>		
Fluorcapthite	Fluorcapthite	SrCaCa <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> F
Apatite-(SrOH)	<b>Fluorstrophite</b>	SrCaSr <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> F <sup>f</sup>
Deloneite-(Ce)	<b>Deloneite</b>	<b>(Na<sub>0.5</sub>REE<sub>0.25</sub>Ca<sub>0.25</sub>)(Ca<sub>0.75</sub>REE<sub>0.25</sub>)Sr<sub>1.5</sub> (CaNa<sub>0.25</sub>REE<sub>0.25</sub>)(PO<sub>4</sub>)<sub>3</sub>F<sub>0.5</sub>(OH)<sub>0.5</sub></b>
Belovite-(Ce)	Belovite-(Ce)	NaCeSr <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> F
Belovite-(La)	Belovite-(La)	NaLaSr <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> F
Kuannersuite-(Ce)	Kuannersuite-(Ce)	NaCeBa <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> F <sub>0.5</sub> Cl <sub>0.5</sub>
<i>Britholite group</i>		
Britholite-(Ce)	Britholite-(Ce)	(Ce,Ca) <sub>5</sub> (SiO <sub>4</sub> ) <sub>3</sub> OH
Britholite-(Y)	Britholite-(Y)	(Y,Ca) <sub>5</sub> (SiO <sub>4</sub> ) <sub>3</sub> OH
Fluorbritholite-(Ce)	Fluorbritholite-(Ce)	(Ce,Ca) <sub>5</sub> (SiO <sub>4</sub> ) <sub>3</sub> F
2009-005 <sup>g</sup>	<b>Fluorbritholite-(Y)</b>	(Y,Ca) <sub>5</sub> (SiO <sub>4</sub> ) <sub>3</sub> F
Fluorcalciobritholite	Fluorcalciobritholite	(Ca,REE) <sub>5</sub> (SiO <sub>4</sub> ,PO <sub>4</sub> ) <sub>3</sub> F
Melanocerite-(Ce)	— <sup>h</sup>	
Tritomite-(Ce)	Tritomite-(Ce)	Ce <sub>5</sub> (SiO <sub>4</sub> ,BO <sub>4</sub> ) <sub>3</sub> (OH,O)
Tritomite-(Y)	Tritomite-(Y)	Y <sub>5</sub> (SiO <sub>4</sub> ,BO <sub>4</sub> ) <sub>3</sub> (O,OH,F)
<i>Ellestadite group</i>		
Ellestadite-(OH)	<b>Hydroxyllelestadite</b>	Ca <sub>5</sub> (SiO <sub>4</sub> ) <sub>1.5</sub> (SO <sub>4</sub> ) <sub>1.5</sub> OH
Ellestadite-(F)	<b>Fluorellestadite</b>	Ca <sub>5</sub> (SiO <sub>4</sub> ) <sub>1.5</sub> (SO <sub>4</sub> ) <sub>1.5</sub> F
Ellestadite-(Cl)	— <sup>i</sup>	
Mattheddleite	Mattheddleite	Pb <sub>5</sub> (SiO <sub>4</sub> ) <sub>1.5</sub> (SO <sub>4</sub> ) <sub>1.5</sub> Cl
—	<b>“Hydroxylmattheddleite”</b> <sup>d</sup>	Pb <sub>5</sub> (SiO <sub>4</sub> ) <sub>1.5</sub> (SO <sub>4</sub> ) <sub>1.5</sub> OH

<sup>a</sup>Whenever necessary and convenient, the suffix *-H* could be used to denote the hexagonal polymorph.

<sup>b</sup>Name for the monoclinic polymorph. It should no longer be considered a distinct species.

<sup>c</sup>Mineral approved by the IMA CNMNC without a name.

<sup>d</sup>A potentially new mineral species.

<sup>e</sup>The change of the name into phosphohedyphane-(Cl) has been approved by the IMA CNMNC, but this is not yet of public domain. In the IMA List of Minerals the original name phosphohedyphane is still reported.

<sup>f</sup>There is a mistake in the IMA List of minerals. The mineral with ideal formula Sr<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>(OH) is named apatite-(SrOH) and is marked as Rn (renamed); the given reference is Burke (2008). Clearly, the above entry refers to the old strontium-apatite, which has the formula SrCaSr<sub>3</sub>(PO<sub>4</sub>)<sub>3</sub>F, and was incorrectly renamed apatite-(SrOH) by Burke (2008), and not to the newly approved IMA 2008-009, which has the formula Sr<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>F, and is the true strontium end-member (see text for more detail).

<sup>g</sup>Mineral and name approved by the IMA CNMNC; publication delayed.

<sup>h</sup>To be potentially discredited [= tritomite-(Ce)].

<sup>i</sup>To be discredited (a mineral with ideal end-member formula Ca<sub>5</sub>(SiO<sub>4</sub>)<sub>1.5</sub>(SO<sub>4</sub>)<sub>1.5</sub>Cl is assumed not to exist).



where the left superscripts indicate the ideal coordination numbers. In this report we will generally use the reduced formula with  $Z = 2$ , which is commonly adopted in the mineralogical literature. Despite the rather simple formula, with only four key sites (M1, M2, T, and X) besides those (O1, O2, and O3) which are known to be occupied by  $O^{2-}$  only, the number of distinct species based on cationic and anionic substitutions is quite large. This number increases further, because in some cases the M1 sites are split into pairs of non-equivalent sites with corresponding lowering of the space group symmetry. Concerning the coordination numbers, M1 has nine-fold ( $6 + 3$ ) coordination with the innermost six ligands forming a polyhedron that is often referred to as a metaprism (White & Dong, 2003; Dong & White, 2004a and b; Mercier *et al.*, 2005). When the three more distant ligands are included, the M1 coordination polyhedron is often described as a tri-capped trigonal prism. The M2 site is considered to be seven-fold coordinated whenever Ca is the central cation; such a polyhedron can be described as a distorted pentagonal bipyramid (Dolivo-Dobrovolsky, 2006); in other cases, *e.g.*, when the site is occupied by Pb and/or the X site is occupied by Cl, the coordination of M2 sites may be more irregular and the central cation may be considered to be eight- or nine-fold coordinated. A drawing of the apatite structure-type is shown in Fig. 2. The relationships among ionic sites and multiplicity and Wyckoff positions in all known space groups of apatite supergroup minerals are shown in Table 2.

Species-forming M and T cations thus far known among minerals are: M =  $Ca^{2+}$ ,  $Pb^{2+}$ ,  $Ba^{2+}$ ,  $Sr^{2+}$ ,  $Mn^{2+}$ ,  $Na^+$ ,

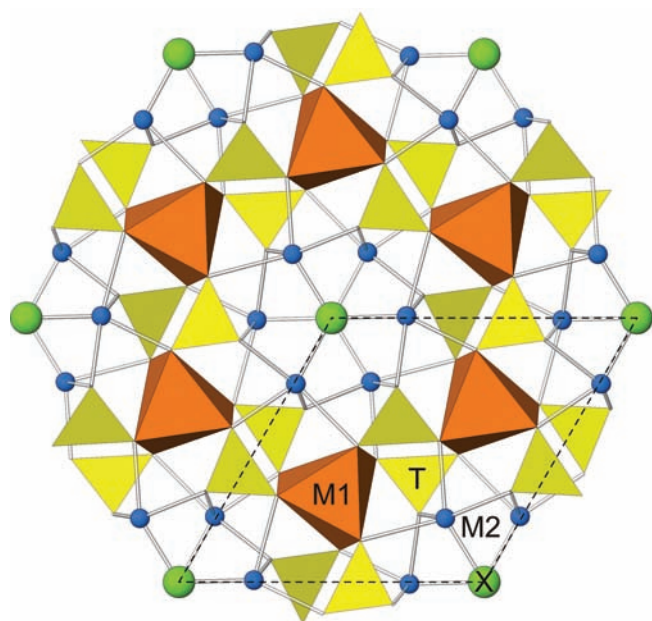


Fig. 2. The crystal structure of apatite, as seen along  $c$ . The unit cell is outlined. The M1-centred polyhedra are represented as six-fold coordinated metaprisms (the bonded O3 ligands are not included in this polyhedral representation). Two out of the seven bonds to M2 overlap in this projection, therefore only five are visible in the figure.

$Ce^{3+}$ ,  $La^{3+}$ ,  $Y^{3+}$ ,  $Bi^{3+}$ ; T =  $P^{5+}$ ,  $As^{5+}$ ,  $V^{5+}$ ,  $Si^{4+}$ ,  $S^{6+}$ ,  $B^{3+}$ . Species-forming substitutions at the X anionic site are limited to the monovalent anions  $F^-$ ,  $Cl^-$ , and  $(OH)^-$ . This implies – for all minerals known thus far – a total of 50 negative charges per unit cell throughout [*i.e.*,  $24 O^{2-} + 2 (F, Cl, OH)^-$ ]. In addition, many studies of synthetic compounds with the apatite structure have demonstrated that the X site can be occupied by  $O^{2-}$  (which would increase the total negative charges) as well as vacancies and  $H_2O$  molecules (which would decrease the total negative charges), that the M site can be occupied by Cd, Co, K, and almost all *REE* and that the T site can be occupied by Be, Cr, Ge, and  $Mn^{5+}$ .

Even though in the present report we limit ourselves to natural compounds, the presence of M cations with charge 1+, 2+, and 3+, and of T cations with charge 4+, 5+, and 6+, implies a great number of possible combinations of different atoms, and thus of potentially different species.

### 3. Minerals of the apatite supergroup: state of the art

The valid, IMA-accepted mineral species within the apatite supergroup can be divided into five groups. Although we are aware that different groupings could be chosen, *e.g.* based upon purely chemical grounds, we prefer for our purposes a subdivision based on a combination of crystallographic and chemical criteria. Our five groups are as follows:

(1) *Apatite group*: hexagonal and pseudo-hexagonal phosphates, arsenates, and vanadates containing the same prevailing (species-defining) cation at both the M1 and M2 sites.

(2) *Hedyphane group*: hexagonal and pseudo-hexagonal phosphates, arsenates and sulphates containing different prevailing (species-defining) cations at the M1 and M2 sites.

(3) *Belovite group*: hexagonal and trigonal phosphates with the M1 site split into the M1 and M1' sites containing different prevailing (species-defining) cations.

(4) *Britholite group*: hexagonal and pseudo-hexagonal silicates, typically with partially ordered M1 and M2 cations.

(5) *Ellestadite group*: hexagonal and pseudo-hexagonal sulphato-silicates with the ideal ratio  $(SiO_4)^{4-} : (SO_4)^{2-} = 1 : 1$ .

#### 3.1. Apatite group

##### 3.1.1. Apatite-(CaF), apatite-(CaOH), apatite-(CaCl)

These three minerals have ideal formulas  $Ca_5(PO_4)_3F$ ,  $Ca_5(PO_4)_3OH$ , and  $Ca_5(PO_4)_3Cl$ , respectively. They were formerly known as fluorapatite, hydroxylapatite, and chlorapatite and were recently renamed as apatite-(CaF), apatite-(CaOH), apatite-(CaCl) (Burke, 2008). The birth of the three distinct names to denote the F-, OH-, and Cl-dominant variants, and their distinction with respect to the original “apatite” *sensu lato* is uncertain, but is generally ascribed to Damour (1856) for “hydroxylapatite” and

Table 2. Structure site multiplicities and Wyckoff positions for all known space groups of apatite supergroup minerals.

Site	$P6_3/m$	$P6_3$	$P\bar{6}$	$P\bar{3}$	$P3$	$P2_1/m$	$P2_1$
M1	4f	$2 \times 2b$	2i, 2h	$2 \times 2d$	$2 \times 1b, 2 \times 1c$	4f	$2 \times 2a$
M2	6h	6c	3k, 3j	6g	$2 \times 3d$	$2a, 2 \times 2e$	$3 \times 2a$
T	6h	6c	3k, 3j	6g	$2 \times 3d$	$3 \times 2e$	$3 \times 2a$
O	$2 \times 6h, 12i$	$4 \times 6c$	$2 \times 3k, 2 \times 3j, 2 \times 6l$	$4 \times 6g$	$8 \times 3d$	$6 \times 2e, 3 \times 4f$	$12 \times 2a$
X	$2a$ or $2b$ or $4e$ ( $\times 0.5$ )	$2a$	$1a, 1b$ or $2g$	$1a, 1b$	$2 \times 1a$	$2a$ or $2e$	$2a$

Rammelsberg (1860) for “fluorapatite” and “chlorapatite”. The crystal structure of “apatite” was first solved by Mehmel (1930) and Náray-Szabó (1930) in the space group  $P6_3/m$ , and typically all apatites crystallize in that space group. However, crystal structure refinement in lower symmetry space groups have been carried out on synthetic  $\text{Ca}_5(\text{PO}_4)_3\text{Cl}$  (Mackie *et al.*, 1972),  $\text{Ca}_5(\text{PO}_4)_3\text{OH}$  (Elliott *et al.*, 1973) and natural apatite-(CaCl) (Hughes *et al.*, 1990). This latter mineral, a monoclinic chlorapatite from Jackson Peak, Gunkock, Washington Co., Utah, USA is structurally identical (space group  $P2_1/b$ , with a doubled  $b$ -axis, and  $\gamma \approx 120^\circ$ ;) to apatite-(CaOH)-*M* (see below), of which it represents the Cl-dominant analogue.

### 3.1.2. Apatite-(CaOH)-*M*

The mineral was referred to as clinohydroxylapatite by Chakhmouradian & Medici (2006), and subsequently renamed apatite-(CaOH)-*M* (Burke, 2008). Its monoclinic symmetry (non standard space group  $P2_1/b$ , evidently chosen so as to maintain the typical axial setting of apatites) probably results from orientational ordering of  $(\text{OH})^-$  anions within  $[00z]$  anionic columns, with consequent doubling of the periodicity along  $[010]$ . The following unit-cell parameters are given:  $a$  9.445(2),  $b$  18.853(4)  $c$  6.8783(6) Å,  $\gamma$  120.00(2)°. All chemical analyses point to the ideal formula  $\text{Ca}_5(\text{PO}_4)_3(\text{OH})$ . A coupled substitution of  $\text{Ca}^{2+}$  by  $\text{Na}^+$  and of  $(\text{PO}_4)^{3-}$  by  $(\text{SO}_4)^{2-}$  has been reported. The formula of the most Na- and S-rich apatite-(CaOH)-*M* is ca.  $(\text{Ca}_{4.4}\text{Na}_{0.6})(\text{PO}_4)_{2.4}(\text{SO}_4)_{0.6}(\text{OH})$ .

### 3.1.3. Svabite

Svabite,  $\text{Ca}_5(\text{AsO}_4)_3\text{F}$ , was first described by Sjögren (1892) from the Hartsigen mine, Värmland, Sweden. It is the arsenate analogue of apatite-(CaF). In the mineralogical literature svabite is commonly reported as hexagonal,  $P6_3/m$ . However, a crystal structure refinement of natural svabite is lacking. The structure of the synthetic analogue of svabite has been recently refined in the triclinic space group  $P\bar{1}$  (Baikie *et al.*, 2007).

### 3.1.4. Johnbaumite

The hydroxyl analogue of svabite was observed as early as 1944 at the Franklin mine, New Jersey, USA, but was not formally described as a new mineral until 36 years later (Dunn *et al.*, 1980). Its chemical composition is not far from the end-member formula  $\text{Ca}_5(\text{AsO}_4)_3(\text{OH})$ . Johnbaumite has the cell parameters  $a$  9.70,  $c$  6.93 Å.

With the lack of a crystal structure refinement, the space group is speculated to be either  $P6_3/m$  or  $P6_3$ . Because of its similarity to other related compounds,  $P6_3/m$  is most likely the correct space group.

### 3.1.5. Turneaureite

This is the chlorine analogue of svabite, discovered at Långban, Sweden, Franklin, New Jersey, USA, and Balmat, New York, USA (Dunn *et al.*, 1985a). The chemical analysis for turneaureite from Långban, which is considered the type locality, yields the following formula:  $(\text{Ca}_{4.88}\text{Mn}_{0.17}\text{Pb}_{0.02})(\text{As}_{2.44}\text{P}_{0.54})\text{O}_{12.04}\text{Cl}_{0.56}\text{F}_{0.40}$ . Turneaureite has the cell parameters  $a$  9.810,  $c$  6.868 Å, and the space group  $P6_3/m$  is inferred by analogy with the other members of the apatite group.

### 3.1.6. Fermorite

Fermorite was first described as a Sr-bearing calcium phosphate-arsenate, with hexagonal symmetry (Smith & Prior, 1911). The original chemical analysis by Smith & Prior (1911) carried out on a sample from the Sitapar manganese ore deposit (Chhindwara district, Madhya Pradesh state, India) yields the following chemical formula, conventionally recalculated on the basis of 13 total anions:  $(\text{Ca}_{4.75}\text{Sr}_{0.58})(\text{P}_{1.70}\text{As}_{1.32})\text{O}_{12.74}\text{F}_{0.26}$ . This formula has an excess of M cations, very low fluorine, and  $\text{P} > \text{As}$ . The anion content is a bit problematic.  $\text{H}_2\text{O}$  was analytically determined and is given as “trace” in the chemical analysis, and it is explicitly stated that no chlorine was detected in the mineral. If the above figures are correct, the analysis would indicate an “oxy-apatite”, *i.e.* a mineral with  $\text{O}^{2-}$  as the dominant anion at the X site. A more recent chemical analysis (electron microprobe data) by Hughes & Drexler (1991), carried out on the type material, gave the formula:  $(\text{Ca}_{4.21}\text{Sr}_{0.80})(\text{As}_{1.48}\text{P}_{1.45})\text{O}_{12}(\text{OH}_{0.65}\text{F}_{0.35})$ , with the hydroxyl content calculated by difference. There is a slight dominance of As over P. A crystal structure analysis showed the mineral to have monoclinic symmetry (space group  $P2_1/m$ ,  $a$  9.594,  $b$  6.975,  $c$  9.597 Å,  $\beta$  119.97°; Hughes & Drexler, 1991) and provided clear evidence that  $(\text{OH})^-$  and not  $\text{O}^{2-}$  is the dominant anion at the X site; therefore, fermorite should be considered the monoclinic polymorph of johnbaumite. The deviations from the hexagonal symmetry are admittedly small, given “the three non equivalent monoclinic tetrahedral sites are similar in their chemical composition and bond lengths” (Hughes & Drexler, 1991).

### 3.1.7. IMA 2008-009

A Sr-dominant analogue of apatite-(CaF), close to the Sr end-member of the series  $\text{Ca}_5(\text{PO}_4)_3\text{F} - \text{Sr}_5(\text{PO}_4)_3\text{F}$ , with space group  $P6_3/m$ , was studied in detail by Pekov *et al.* (Pekov, pers. comm.) and recently approved by the CNMNC (IMA 2008-009) without a name.

As mentioned above, the existence of the ordered (on M1 and M1') Sr-Ca apatite mineral with formula  $\text{SrCaSr}_3(\text{PO}_4)_3\text{F}$  bearing the original name strontium-apatite makes the choice of a name for the new Sr apatite with formula  $\text{Sr}_5(\text{PO}_4)_3\text{F}$  problematic.

### 3.1.8. Pyromorphite

Pyromorphite is the lead phosphate, with ideal formula  $\text{Pb}_5(\text{PO}_4)_3\text{Cl}$ , widespread in nature. The mineral was named by Hausmann (1813). A crystal structure refinement of pyromorphite was carried out in the space group  $P6_3/m$  by Dai & Hughes (1989). In pyromorphite, the dominant X anion is typically chlorine. This may be related to the presence of lead as the dominant cation at both the M1 and M2 sites, which results in larger unit-cell dimensions and makes chlorine (whose ionic radius is markedly greater than those of fluorine and hydroxyl) the best candidate to occupy the X site. Similar reasons are also valid for alforsite, the barium-dominant member of the apatite group (see below).

Stalder & Rozendaal (2002) presented EPMA data of a mineral from the Gamsberg Pb-Zn deposit, Namaqua province, South Africa. It is described as a "calcian pyromorphite", but has a very low Cl + F content (and presumably ordering of Ca and Pb in the M1 and M2 sites, respectively).

### 3.1.9. Mimetite

Mimetite is the lead arsenate, with ideal formula  $\text{Pb}_5(\text{AsO}_4)_3\text{Cl}$ . The mineral was named by von Haidinger (1845). The crystal structure of mimetite was solved in the space group  $P6_3/m$  by Sokolova *et al.* (1982) and refined by Dai *et al.* (1991). In the structure of mimetite, the special position of chlorine at (0, 0, 1/2) results in two equidistant Cl ions around Pb (M2 site) and in an eightfold coordination for the cation.

### 3.1.10. Clinomimetite

Clinomimetite is the monoclinic polymorph of mimetite. It was formally described as a mineral species by Dai *et al.* (1991), although it was already known as both a synthetic and natural phase. It crystallizes in the space group  $P2_1/b$ , with  $a$  10.189(3)  $b$  20.372(8),  $c$  7.456 (1) Å,  $\gamma$  119.88(3)°. Unit-cell parameters and space group are consistent with those of the other accepted apatite group mineral with monoclinic symmetry, apatite-(CaOH)-M.

### 3.1.11. Alforsite

Alforsite was described as the barium analogue of "apatite" (Newberry *et al.*, 1981). The single crystal X-ray diffraction study was carried out on synthetic material: long-exposure

Weissenberg and precession photographs indicated the  $P6_3/m$  space group and did not reveal any superstructure reflections. All known chemical analyses of alforsite point to the ideal end-member formula  $\text{Ba}_5(\text{PO}_4)_3\text{Cl}$ .

### 3.1.12. Vanadinite

Vanadinite, ideally  $\text{Pb}_5(\text{VO}_4)\text{Cl}$ , is the only vanadium-dominant member of the apatite group. Known for more than two centuries (the type locality is Zimapán, Hidalgo, Mexico), it was first given its present name by von Kobell (1838). Crystal structure studies for vanadinite have been published, all in the space group  $P6_3/m$ , by Trotter & Barnes (1958), Dai & Hughes (1989), and Laufek *et al.* (2006).

## 3.2. Hedyphane group

### 3.2.1. Hedyphane

Hedyphane was originally described from Långban, Sweden (Breithaupt, 1830). Another important occurrence for the mineral is the Franklin mine, New Jersey, USA (Foshag & Gage, 1925). Rouse *et al.* (1984) carried out a careful crystal-chemical study of hedyphane from both occurrences, which showed that Ca and Pb are ordered at M1 and M2, respectively. This led to the redefinition of the ideal formula of the mineral as  $\text{Ca}_2\text{Pb}_3(\text{AsO}_4)_3\text{Cl}$ . Shortly thereafter, Dunn *et al.* (1985b) described another halogen-deficient hedyphane sample from the type locality, which contained 0.34 wt.  $\text{H}_2\text{O}$  (determined by Penfield method). The empirical formula of that sample is  $(\text{Ca}_{1.69}\text{Ba}_{0.28})\text{Pb}_{3.01}(\text{As}_{2.69}\text{P}_{0.20}\text{Si}_{0.15})\text{O}_{12}[(\text{OH})_{0.44}\text{Cl}_{0.42}\text{F}_{0.12}\text{O}_{0.02}]$ . Although very close to the compositional boundary, and despite some analytical uncertainties, *e.g.* the somewhat high total of T cations, this mineral has  $\text{OH} > \text{Cl}$  and should, therefore, be considered a separate species, the hydroxyl analogue of hedyphane.

### 3.2.2. Phosphohedyphane

The new mineral was described by Kampf *et al.* (2006) from the Capitana mine, Atacama Province, Chile. New EDS analyses on numerous samples from world-wide localities and examination of earlier reported analyses for "calcium-rich pyromorphite" revealed that phosphohedyphane occurs at numerous other localities. The ideal end-member formula is  $\text{Ca}_2\text{Pb}_3(\text{PO}_4)_3\text{Cl}$ . Single crystal X-ray diffraction data confirmed that Ca and Pb are ordered at the M1 and M2 sites, respectively. The mineral was approved with the name phosphohedyphane, and then changed into phosphohedyphane-(Cl) after the discovery of phosphohedyphane-(F) (see below) and the concurrent recognition of "phosphohedyphane" as a series name. This change has been approved by IMA, but is not yet of public domain, since the publication of the paper with the description of phosphohedyphane-(F) is being delayed pending the outcome of this report.

### 3.2.3. Phosphohedyphane-(F)

The F-dominant analogue of phosphohedyphane from the Blue Bell claims, San Bernardino County, California, USA



was recently approved by the CNMNC (IMA 2008-068; Kampf & Housley, 2008). Chemical analysis showed the X site to be entirely occupied by F and structure analysis confirmed the ordering of Ca and Pb as well as the shorter Pb–F bonds of 2.867 Å in contrast with the Pb–Cl bond lengths of 3.068 Å in phosphohedyphane-(Cl).

#### 3.2.4. Morelandite

This mineral is a bit problematic, because of the unknown partitioning of cations among the M1 and M2 sites. First described by Dunn & Rouse (1978), the original chemical analysis yields the formula  $(\text{Ba}_{2.25}\text{Ca}_{1.65}\text{Pb}_{1.16}\text{Fe}_{0.06}\text{Mn}_{0.06})[(\text{AsO}_4)_{2.56}(\text{PO}_4)_{0.30}]\text{Cl}_{1.09}$ .

In that paper, as well as in the IMA list of minerals, the ideal formula is given as  $\text{Ba}_5(\text{AsO}_4)_3\text{Cl}$ , but this would imply that barium is the dominant cation at both the M1 and M2 sites, which is impossible given the above stoichiometric ratios and the characteristics of the apatite structure. Assuming that the space group is  $P6_3/m$ , the most likely ideal formula is  $\text{Ca}_2\text{Ba}_3(\text{AsO}_4)_3\text{Cl}$ , resulting from a cation allocation as described in § 4.1. (see below).

#### 3.2.5. Mn-rich apatite

Pieczka (2007) recently described a sample of “Mn-rich apatite” from the Szklary granitic pegmatite, Lower Silesia, Poland, which has the highest manganese content ever reported for an apatite (31.5 wt%, corresponding to 2.43 apfu). The chemical formula provided for that sample is  $(\text{Mn}_{2.43}\text{Ca}_{2.29}\text{Fe}^{2+}_{0.23}\text{Mg}_{0.04}\text{Na}_{0.01})(\text{PO}_4)_{3.00}(\text{Cl}_{0.48}\text{F}_{0.32}\text{OH}_{0.20})$ . In the absence of a structural study, this potentially new mineral species is tentatively included in the hedyphane group, under the assumption that Ca and Mn are ordered between the two M sites. This assumption is based on several studies that show a marked preference for the M1 site by  $\text{Mn}^{2+}$  in Mn-rich apatites (Suitch *et al.*, 1985; Hughes *et al.*, 2004).  $\text{Mn}^{5+}$  has also been identified in apatite, substituting for P on the T site, however at very low concentrations (Johnson *et al.*, 1963; Dardenne *et al.*, 1999; Hughes *et al.*, 2004).

#### 3.2.6. Cesanite

First described by Cavarretta *et al.* (1981) and named after the type locality (the Cesano geothermal field, Latium, Italy), cesanite is a sulphate with the apatite structure. It is related to apatite by the coupled heterovalent substitution  $\text{Na}_1(\text{SO}_4)_1\text{Ca}_{-1}(\text{PO}_4)_{-1}$ . The only available chemical analysis points to the empirical formula  $(\text{Na}_{3.42}\text{Ca}_{1.53}\text{Sr}_{0.03}\text{K}_{0.02})\text{S}_{2.99}\text{O}_{12}[(\text{OH})_{0.44}\text{F}_{0.06}\text{Cl}_{0.06}(\text{H}_2\text{O})_{0.44}]$ . Cavarretta *et al.* (1981) proposed revision of the general formula of apatites to allow substantial incorporation of  $\text{H}_2\text{O}$  at the X anionic sites in order to allow for the reduced positive charge associated with cations, due to the presence of  $\text{Na}^+$  as a major element. An initial crystal structure refinement was carried out in the space group  $P6_3/m$  by Tazzoli (1983), and seemed to support this proposal, resulting in the structural formula  $(\text{Na}_{3.51}\text{Ca}_{1.49})\text{S}_3\text{O}_{12}[(\text{OH})_{0.49}(\text{H}_2\text{O})_{0.45}]$ . A more recent refinement of both

natural and synthetic cesanite was carried out in the space group  $P\bar{6}$  (Piotrowski *et al.*, 2002). In this latter space group, each of the M1 and M2 sites are split into two because of the lower symmetry. The refinement in  $P\bar{6}$  determined  $\text{Ca} > \text{Na}$  at the M1' site only (Wyckoff 3j), whereas M1'', M2' and M2'' (Wyckoff 3k, 2h, and 2l, respectively) have  $\text{Na} > \text{Ca}$ . The resulting formula is similar to that obtained by Tazzoli (1983), and requires that the X site is occupied in equal parts by hydroxyls and water molecules  $\text{Na}_4(\text{Na}_3\text{Ca}_3)(\text{SO}_4)_6(\text{OH})(\text{H}_2\text{O})$ .

#### 3.2.7. Caracolite

The mineral was first described by Websky (1886). According to a crystal structure refinement (Schneider, 1967), the ideal formula of caracolite is  $\text{Na}_3\text{Pb}_2(\text{SO}_4)_3\text{Cl}$ . However, the distribution of M cations in the basic  $P6_3/m$  structure type is as follows:  $4\text{Na}^+$  in the M1 site,  $4\text{Pb}^{2+} + 2\text{Na}^+$  in the M2 site, yielding the formula  $\text{Na}_2(\text{Pb}_2\text{Na})(\text{SO}_4)_3\text{Cl}$ . A second refinement carried out in the monoclinic  $P2_1/m$  space group is characterized by the ordering of Pb (eight atoms per unit cell:  $4 \times 2e$ ) and Na (12 atoms per unit cell:  $2 \times 4f + 2 \times 2e$ ) and the concurrent doubling of the *a*-axis (Schneider, 1969).

#### 3.2.8. Aiolosite

Aiolosite was recently approved as a new mineral from Vulcano, Aeolian Islands, Italy (Demartin *et al.*, 2010). Its ideal formula is  $\text{Na}_2(\text{Na}_2\text{Bi})(\text{SO}_4)_3\text{Cl}$ . Aiolosite crystallizes in the space group  $P6_3/m$ , with *a* 9.626, *c* 6.880 Å. Similarly to caracolite, Na enters the M1 site, whereas Na and Bi occupy the M2 site.

### 3.3. Belovite group

#### 3.3.1. Fluorcaphite

Fluorcaphite was originally described from Mt. Koashva, Khibiny, Kola peninsula, Russia (Khomyakov *et al.*, 1997). A crystal structure analysis carried out in the space group  $P6_3$  (Rastsvetaeva & Khomyakov, 1996a) points to the formula  $(\text{Sr}_{0.52}\text{Na}_{0.32})\text{Ca}(\text{Ca}_{2.16}\text{Sr}_{0.64}\text{LREE}_{0.33})(\text{P}_{2.96}\text{Si}_{0.06})\text{O}_{12}\text{F}_{0.66}(\text{OH})_{0.34}$ , ideally  $\text{SrCaCa}_3(\text{PO}_4)_3\text{F}$ .

More recently, Chakhmouradian *et al.* (2005) described a second occurrence of “fluorcaphite” from Lovozero, Kola peninsula, Russia. Their refinement, again in space group  $P6_3$ , provided the structural formula  $(\text{Ca}_{0.48}\text{Na}_{0.29}\text{Sr}_{0.12}\text{Ce}_{0.11}\text{La}_{0.05})(\text{Ca}_{0.58}\text{Na}_{0.29}\text{Ce}_{0.11}\text{Nd}_{0.02})(\text{Sr}_{1.48}\text{Ca}_{1.39}\text{La}_{0.13})(\text{PO}_4)_3\text{F}$ . Moreover, they also performed a further refinement for a “fluorcaphite” sample from Khibiny for comparative purposes, yielding  $(\text{Ca}_{0.59}\text{Sr}_{0.21}\text{Na}_{0.19}\text{La}_{0.01})(\text{Ca}_{0.88}\text{Ce}_{0.07}\text{Pr}_{0.04}\text{Nd}_{0.01})(\text{Ca}_{1.83}\text{Sr}_{0.84}\text{La}_{0.16}\text{Ce}_{0.12}\text{Nd}_{0.05})(\text{PO}_4)_3\text{F}$ .

Neither of these formulae match the presently accepted formula for fluorcaphite. The ideal composition of the crystal from Lovozero is  $\text{CaCaSr}_3(\text{PO}_4)_3\text{F}$  (a potentially new end-member), that of the crystal from Khibiny is  $\text{CaCaCa}_3(\text{PO}_4)_3\text{F}$  (chemically a fluorapatite in which the symmetry is lowered due to selected occupancy by subordinate cations).

### 3.3.2. Apatite-(SrOH)

The mineral was first described from the Inagli alkaline complex, South Yakutia, Siberia, Russia. The given name was strontium-apatite. Initially, it was considered to be the Sr-dominant analogue of fluorapatite, with the simplified formula  $(\text{Sr,Ca})_5(\text{PO}_4)_3(\text{F,OH})$ , and this was the rationale for its name (Efimov *et al.*, 1962). However, a structural study of the holotype specimen demonstrated its cation-ordered structure and, consequently, the space group symmetry  $P6_3$  (Klevtsova, 1964). In strontium-apatite, the M1 site, of multiplicity 4 in space group  $P6_3/m$ , is transformed into two sites, M1 and M1', each of multiplicity 2. The M1 site is mainly occupied by Sr and the M1' site is mostly occupied by Ca; in the M2 site, Sr prevails over Ca. The crystal-chemical formula of the holotype specimen of strontium-apatite is  $^{\text{M1}}[(\text{Sr,Ba})]^{\text{M1}'}[\text{Ca}]^{\text{M2}}[\text{Sr,Ca,REE,Na}]_3(\text{PO}_4)_3(\text{F,OH})$ .

Later, the crystal structure of strontium-apatite from Mt. Rasvumchorr, Khibiny, was studied. The same space group  $P6_3$  and the same type of cation arrangement were found. The crystal-chemical formula of this latter sample is  $^{\text{M1}}[\text{Sr}_{0.75}\text{Ca}_{0.25}]^{\text{M1}'}[\text{Ca}_{0.7}\text{Sr}_{0.3}]^{\text{M2}}[\text{Sr}_{2.6}\text{Ca}_{0.4}](\text{PO}_4)_3\text{F}$  (Pushcharovsky *et al.*, 1987). Thus, the idealized (end-member) formula of the mineral is  $\text{SrCaSr}_3(\text{PO}_4)_3\text{F}$ .

Recently, the mineral was renamed apatite-(SrOH) (Burke, 2008). However, the name should have been changed to apatite-(SrF) given that fluorine is the dominant  $X^-$  anion.

### 3.3.3. Belovite-(Ce), belovite-(La)

Belovites have the ideal formula  $\text{NaREESr}_3(\text{PO}_4)_3\text{F}$ . Belovite-(Ce) was first described from Mt. Malyi Punkaruaiiv, Lovozero, Kola Peninsula, Russia, with formula  $(\text{Sr,Ce,Na,Ca})_5(\text{P}_3\text{O}_{12})(\text{OH,O})$  (Borodin & Kazakova, 1954). Fluorine was not determined in this sample. Klevtsova & Borisov (1964) studied its structure and found ordering of Sr, Na and REE and space group  $P\bar{3}$ . Nadezhina *et al.* (1987) studied the structure of belovite-(Ce) from Mt. Karnasurt, Lovozero, confirmed the model found by Klevtsova & Borisov (1964) with space group  $P\bar{3}$ , and suggested the idealized formula  $\text{NaCeSr}_3(\text{P}_3\text{O}_{12})\text{OH}$  (despite the fact that  $F > 0.5$  apfu). The results of a detailed study of belovite-(Ce) from different localities, including the reinvestigation of the holotype from Mt. Malyi Pukaruaiiv, Lovozero, established its idealized end-member formula as  $\text{NaCeSr}_3(\text{PO}_4)_3\text{F}$  and confirmed the space group  $P\bar{3}$  (Pekov *et al.*, 1995). These results were confirmed by Rakovan & Hughes (2000). Belovite-(La) was described as a new species by Pekov *et al.* (1996) from Mounts Kukisvumchorr and Eveslogchorr, Khibiny, Russia. A structural study of a crystal from the type specimen (Kabalov *et al.*, 1997) showed that belovite-(La) is isostructural with belovite-(Ce).

In belovites, Sr substitutes for Ca in the M2 site, and Na + REE substitute for Ca in the M1 site. The strict ordering of Na and REE at the M1 site lowers the symmetry from  $P6_3/m$  to  $P\bar{3}$ . In this latter space group there are two independent sites (M1 and M1', occupied by REE and

Na, respectively) which correspond to the unique M1 site in the archetype apatite structure. Another consequence of the reduced space group symmetry is the splitting of O3 sites into a pair of non-equivalent sites (O3 and O4). These atoms represent the capping anions in the tri-capped trigonal prism coordination around M1 and M1' sites. The M1-O3 and M1'-O4 distances (which are equivalent in the  $P6_3/m$  structure) are markedly different in the  $P\bar{3}$  structure, and reflect the different occupancy by REE and Na. Therefore the reduced symmetry results not only in the selected occupancy of M1 and M1' sites by REE and Na, but also in a significant variation in the dimensions of the corresponding coordination polyhedra.

### 3.3.4. Kuannersuite-(Ce)

Kuannersuite-(Ce) is the Ba analogue of belovite-(Ce). As in belovite-(Ce), the ordering of REE and Na in kuannersuite-(Ce) lowers the symmetry from  $P6_3/m$  to  $P\bar{3}$ ; however, there is another difference. F and Cl are ordered at distinct anionic sites ( $\text{F}_{1.00}$  and  $\text{Cl}_{0.59}\text{F}_{0.41}$ , respectively). Consequently, the ideal formula should be written (in its doubled form with  $Z = 1$ ) as  $\text{Ce}_2\text{Na}_2\text{Ba}_6(\text{PO}_4)_6\text{FCl}$  (Friis *et al.*, 2004).

### 3.3.5. Deloneite-(Ce)

Deloneite-(Ce) was described as a new mineral from Mt. Koashva, Khibiny, in syntactic intergrowths with fluorcaphite and belovite-(Ce). Its simplified formula was given as  $\text{NaCa}_2\text{SrCe}(\text{PO}_4)_3\text{F}$  (Khomyakov *et al.*, 1996); however, this formula reflects only the rough cation ratios and not the cation arrangement. According to Rastsvetaeva & Khomyakov (1996b), deloneite-(Ce), with space group  $P3$ , is the most cation-ordered apatite-like mineral. In its structure, which is a derivative of the belovite structure type, the M1 and M1' sites are split into two pairs: (1)  $\text{M1}^1$  and  $\text{M1}^2$ , and (2)  $\text{M1}'^1$  and  $\text{M1}'^2$ , respectively. Unlike other apatite group members, the M2 and T sites are also split into corresponding pairs: (1) M2 and M2', and (2) T and T'. The X site is also split, similar to kuannersuite-(Ce), into X and X'. The crystal-chemical formula of the mineral based on 26 total anions is thus  $^{\text{M1}1}[\text{Na}_{0.5}\text{REE}_{0.3}\text{Ca}_{0.2}]^{\text{M1}2}[\text{Na}_{0.5}\text{REE}_{0.25}\text{Ca}_{0.25}]^{\text{M1}'1}[\text{Ca}_{0.7}\text{REE}_{0.3}]^{\text{M1}'2}[\text{Ca}_{0.7}\text{REE}_{0.3}]^{\text{M2}}[\text{Sr}_{2.3}\text{Ca}_{0.7}]^{\text{M2}'}[\text{Ca}_{1.0}\text{Na}_{1.0}\text{REE}_{1.0}]^{\text{T}}[\text{P}_3]^{\text{T}'}[(\text{P,Si})_3]\text{O}_{24}^{\text{X}}[\text{F}]^{\text{X}'}[(\text{OH},\text{F})]$  (Rastsvetaeva & Khomyakov, 1996b). The simplified form of this formula is  $^{\text{M1}}[\text{Na,REE,Ca}]_2^{\text{M1}'}[\text{Ca,REE}]_2^{\text{M2}}[\text{Sr,Ca}]_3^{\text{M2}'}[\text{Ca,Na,REE}]_3(\text{P}_6\text{O}_{24})^{\text{X}}[\text{F}]^{\text{X}'}[\text{OH}]$ , or  $(\text{Na,REE,Ca})_2(\text{Ca,REE})_2\text{Sr}_3(\text{Ca,Na,REE})_3(\text{PO}_4)_6\text{F}(\text{OH})$ .

The crystal-chemical formula shows that no sites exist with REE prevailing over other cations; therefore, the -(Ce) suffix is incorrect and the mineral should be renamed deloneite.

## 3.4. Britholite group

### 3.4.1. Britholite-(Ce)

Britholite-(Ce) was first described from Ilimaussaqaq complex, Narsaq, Kitaa, West Greenland, by Winther (1901). Its formula is  $(\text{REE,Ca})_5(\text{Si,P})\text{O}_4\text{I}_3(\text{OH},\text{F})$  or, in simplified form,  $(\text{Ce,Ca})_5(\text{SiO}_4)_3(\text{OH})$ , or, assuming cation



ordering,  $(\text{Ce}_3\text{Ca}_2)(\text{SiO}_4)_3(\text{OH})$ . This mineral is typically Th-bearing and metamict. Some crystalline samples are hexagonal with space group  $P6_3/m$  or  $P6_3$  (Gay, 1957; Kalsbeek *et al.*, 1990; Genkina *et al.*, 1991; Noe *et al.*, 1993), or monoclinic pseudo-hexagonal with space group  $P2_1$  (Noe *et al.*, 1993). REE prevail over Ca generally, but the M cations can be disordered or partially ordered in the M1 and M2 sites. For instance, structurally studied samples demonstrate two major types of cation arrangements,  $(\text{REE}, \text{Ca})_2(\text{REE}, \text{Ca})_3[(\text{Si}, \text{P})\text{O}_4]_3(\text{OH}, \text{F})$  (Genkina *et al.*, 1991; Noe *et al.*, 1993) or  $(\text{Ca}, \text{REE})_2(\text{REE}, \text{Ca})_3[(\text{Si}, \text{P})\text{O}_4]_3(\text{OH}, \text{F})$  (Noe *et al.*, 1993).

### 3.4.2. Britholite-(Y)

Britholite with a predominance of Y among the M cations and  $\text{OH} > \text{F}$  was first described under the name abukumalite by Hata (1938) from the Suishoyama pegmatite, Abukuma massif, Fukushima Prefecture, Japan. Later, it was reinvestigated in detail by Omori & Hasegawa (1953) who confirmed the predominance of Y among the M cations and of OH over F. Then, abukumalite was renamed britholite-(Y) as part of the general changes in the nomenclature of rare-earth minerals (Levinson, 1966). Although the mineral is typically metamict, studies of crystal structures of rare crystalline samples show monoclinic pseudo-hexagonal symmetry with space group  $P2_1$  and partial cation ordering at the M1 and M2 sites (Zhang *et al.*, 1992; Noe *et al.*, 1993). The simplified formula can be presented as  $(\text{Y}, \text{Ca}, \text{Ln})_5[(\text{Si}, \text{P})\text{O}_4]_3(\text{OH})$  or, considering the cation ordering, as  $(\text{Y}_3\text{Ca}_2)(\text{SiO}_4)_3(\text{OH})$ .

### 3.4.3. Fluorbritholite-(Ce)

Fluorbritholite-(Ce) was described as a new mineral from Mont Saint-Hilaire, Québec, Canada (Gu *et al.*, 1994). It is considered the F-dominant analogue of britholite-(Ce). In the original paper, Gu *et al.* (1994) proposed the concurrent renaming of britholite-(Ce) and britholite-(Y) into hydroxylbritholite-(Ce) and hydroxylbritholite-(Y), respectively. The proposal has been ignored; however, it must be observed that a number of chemical analyses of minerals referred to as “britholites” actually have  $\text{F} > \text{OH}$  (e.g., Oberti *et al.*, 2001) and, therefore, should be considered “fluorbritholites”.

### 3.4.4. IMA 2009-005

The F-dominant analogue of britholite-(Y) was studied recently in detail by Pekov *et al.* (Pekov, pers. comm.) and a proposal for its approval as a new mineral was submitted to the CNMNC, IMA 2009-005. The mineral and its name were approved, and the authors have agreed to postpone publication of the description of the new mineral pending completion of the present nomenclature report. A crystalline sample from Lagmannsvik, Hamarøy, Nordland, Norway, is considered the holotype material for IMA 2009-005 and all important characteristics, namely chemical composition, X-ray single-crystal and powder data, crystal structure, IR spectrum and optical data, were obtained from this specimen. Note that

britholite with Y dominant among the M cations and  $\text{F} > \text{OH}$  was first described from Mt. Vyuntspakhk, Western Keivy, Kola Peninsula, Russia, by Lunts (1962). This metamict sample was re-studied using electron probe and IR spectroscopy, its Y- and F-dominant character was confirmed, and it was included in the IMA 2009-005 proposal as the cotype. The mineral IMA 2009-005 has the simplified formula  $(\text{Y}, \text{Ca}, \text{Ln})_5[(\text{Si}, \text{P})\text{O}_4]_3\text{F}$ , or, ideally,  $(\text{Y}_3\text{Ca}_2)(\text{SiO}_4)_3\text{F}$ . The holotype from Lagmannsvik has the archetype space group  $P6_3/m$ , with predominance of  $(\text{Y} + \text{Ln})$  over Ca in both the M1 and M2 sites.

### 3.4.5. Fluorcalciobricholite

This mineral was defined as a distinct species by Pekov *et al.* (2007) with a unique combination of dominant cations at M and T sites in the space group  $P6_3/m$ . In fact, fluorcalciobricholite has the T site occupancy  $(\text{T}^{4+}_2\text{T}^{5+})$ , i.e.  $\text{Si}_2\text{P}$ , and thus differs from both “britholite” and “apatite”. Britholite has  $\text{T}^{4+}_3$ , i.e.  $\text{Si}_3$ , must have at least 3 trivalent cations in M, and actually is a REE-dominant mineral. Apatite has  $\text{T}^{5+}_3$ , i.e.  $\text{P}_3$ , with only divalent cations at the M sites. The ideal chemical formula for fluorcalciobricholite may be written as  $(\text{Ca}_3\text{REE}_2)[(\text{SiO}_4)_2(\text{PO}_4)]\text{F}$ . In view of the coupled heterovalent substitutions occurring at the M and T sites in the series apatite – calciobricholite – britholite, it is more practical in this case for nomenclature purposes to consider the total abundance of M cations as a single, composite site (Fig. 3).

## 3.5. Ellestadite group

### 3.5.1. Ellestadite-(OH), ellestadite-(F), ellestadite-(Cl)

Ellestadites *lato sensu* are sulphato-silicates. For stoichiometric reasons, the incorporation of the sulphate anion  $(\text{SO}_4)^{2-}$  in the structure of apatite in the place of  $(\text{PO}_4)^{3-}$  or  $(\text{AsO}_4)^{3-}$  must be coupled with a concurrent substitution by silicate anions  $(\text{SiO}_4)^{4-}$ . This holds in all cases in which the M sites are occupied by divalent cations. Pure sulphates with the apatite structure may occur only by reducing the overall positive charge associated with the M cations, as is the case in cesanite and caracolite.

Ellestadite was first described from Crestmore, Riverside County, California, USA (McConnell, 1937). Based on the original chemical analysis, the type specimen

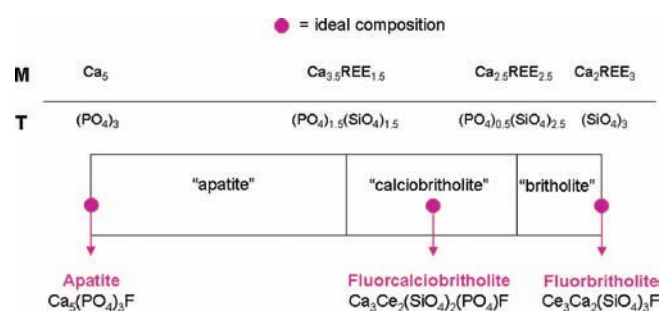


Fig. 3. Coupled heterovalent substitutions at the M and T sites in the series apatite – calciobricholite – britholite.

should be considered ellestadite-(OH). Later, Harada *et al.* (1971) redefined ellestadite from Chichibu mine, Saitama Prefecture, Japan as the OH-dominant calcium silicate-sulphate, and called it hydroxyllelestadite, based on the wrong assumption that type ellestadite from Crestmore had  $\text{Cl} > (\text{OH}), \text{F}$ . Although analyses of natural ellestadite-(F) are known (*e.g.*, Rouse & Dunn, 1982), the Cl-dominant analogue, which has been synthesized (Pliego-Cuervo & Glasser, 1978), has never been found in nature (as far as we know); therefore, it should not be considered a mineral. Ellestadite-(F) was formally described as a new mineral species from Kopeisk, South Urals, Russia (Chesnokov *et al.*, 1987). The given name was fluorellestadite. The crystal structure of ellestadite-(OH) was refined in the space group  $P2_1/m$  by Sudarsanan (1980) and by Hughes & Drexler (1991), and later in the space group  $P6_3/m$  by Onac *et al.* (2006).

The names hydroxyllelestadite, fluorellestadite, and chlor-ellestadite were changed into the suffixed names ellestadite-(OH), ellestadite-(F), ellestadite-(Cl) by Burke (2008).

### 3.5.2. Mattheddleite

This mineral was first described from Leadhills Dod, Strathclyde region, Scotland, UK (Livingstone *et al.*, 1987). The original chemical analyses are a bit odd in that they display a marked excess of lead and, hence, a Si/S ration greater than 1, and point to the chemical formula  $\text{Pb}_{5.49}(\text{SiO}_4)_{1.87}(\text{SO}_4)_{1.09}\text{O}_{0.16}\text{Cl}_{0.99}$ . Nevertheless, new electron microprobe data and a single-crystal structure refinement (Steele *et al.*, 2000) confirmed that mattheddleite can be ascribed to the apatite group, with the structural formula  $\text{Pb}_5(\text{SiO}_4)_{1.5}(\text{SO}_4)_{1.5}\text{Cl}_{0.57}(\text{OH})_{0.43}$ , space group  $P6_3/m$ ,  $a = 10.006$ ,  $c = 7.496$  Å.

More recently, another set of electron microprobe data on samples from the type locality (Essene *et al.*, 2006) confirmed the excess of Si over S in mattheddleite. The resulting charge imbalance is adjusted assuming small vacancies at the O sites, leading to an average formula  $\text{Pb}_5(\text{Si}_{1.8}\text{S}_{1.2}\text{O}_{11.7}\square_{0.3})(\text{Cl}, \text{OH})$ . Moreover, the possible existence of an (OH)-dominant analogue of mattheddleite is mentioned.

## 3.6. Other minerals with the apatite structure

### 3.6.1. Tritomite-(Ce), melanocerite-(Ce), tritomite-(Y)

The three minerals tritomite-(Ce), melanocerite-(Ce), and tritomite-(Y) (Frondel, 1961) are listed as valid species in the IMA list of minerals. Tritomite-(Y) has been renamed, its original name being spencite (Jaffe & Molinski, 1962). All of these minerals are metamict; X-ray powder diffraction patterns were recorded on annealed material. Their chemical compositions are: tritomite-(Ce),  $\text{Ce}_5(\text{SiO}_4, \text{BO}_4)_3(\text{OH}, \text{O})$ ; melanocerite,  $(\text{Ce}, \text{Ca})_5(\text{SiO}_4, \text{BO}_4)_3(\text{OH}, \text{F}) \cdot n\text{H}_2\text{O}$ ; tritomite-(Y),  $\text{Y}_5(\text{SiO}_4, \text{BO}_4)_3(\text{O}, \text{OH}, \text{F})$ . Therefore, these minerals can be considered borosilicates, with REEs strongly prevalent over calcium in the M sites for stoichiometric reasons. Clearly melanocerite-(Ce) and

tritomite-(Ce) are probably the same mineral, and tritomite-(Y) could be the Y-dominant analogue. According to Dana (Gaines *et al.*, 1997), type localities and year of discovery are as follows: tritomite-(Ce)–Låven Island, Langesundfjord, Norway (1849); melanocerite-(Ce) – Kjeøy Island, Langesundfjord, Norway (1887); tritomite-(Y) – Cranberry Lake, Sussex, Co., New Jersey, USA (1962). Although commonly ascribed to the apatite group, the available chemical analyses (Engstrom, 1877; Jaffe & Molinski, 1962) do not conform to the usual M/T stoichiometric ratio, indicating either conspicuous vacancies at the M sites or, more likely, analytical inaccuracies and admixtures with other phases. Formally, tritomite-(Ce), melanocerite-(Ce) and tritomite-(Y) could be included, as REE silicates in the britholite subgroup. The relationships and the possible identity of tritomite-(Ce) and tritomite-(Y) with britholite-(Ce) and britholite-(Y), respectively, deserve further study.

### 3.6.2. Carbonate-fluorapatite, carbonate-hydroxylapatite

Although the above names are extensively used in literature, *e.g.*, to denote the mineral portion of bones and teeth of vertebrates, their validity as distinct mineral species belonging to the apatite group has always been under question.  $(\text{CO}_3)^{2-}$  anion is known to occur as a subordinate component in members of the apatite group (*e.g.*, Knudsen & Gunter, 2002; Pan & Fleet, 2002). A paper by Baumer *et al.* (1990) reports infrared absorption spectra of a natural “carbonate-fluorapatite”; however, neither chemical nor X-ray diffraction data are given. Ivanova *et al.* (2001), Fleet *et al.* (2004) and Fleet & Liu (2008) presented Rietveld and single-crystal X-ray diffraction data describing a possible substitution mechanism of  $(\text{PO}_4)$  by  $(\text{CO}_3)$  in synthetic fluorapatite and hydroxylapatite. After Burke (2008), both “carbonate-fluorapatite” and “carbonate-hydroxylapatite” have been discredited.

## 4. Chemical composition of apatite supergroup minerals

### 4.1. Calculation of crystal-chemical formulae

Determining the correct placement of a mineral within the apatite supergroup can be a difficult task, requiring a high-quality crystal structure refinement, mainly in those cases where ordering may occur. In most cases, the available analytical data consist of electron microprobe chemical analyses without any direct determination of the  $\text{H}_2\text{O}$  content (which may play a crucial role in some apatites). Hence, although the unequivocal identification of some existing apatite group minerals (or the recognition of potential new end-members) is impossible without structural information, we think it is useful to provide a series of suggestions for the handling of EMPA data, which can be used in most straightforward cases.

Given a set of chemical analyses within a group of minerals with similar crystal-chemical features, the

formula calculation basis may be more or less arbitrarily chosen; in the cases of apatites, for example, the following criteria may be selected:

(a) Calculation on the basis of 13 total anions. If the analytical value for H<sub>2</sub>O is available, this will not result in exactly 12 O and 1 (F + Cl + OH). Typically, the total amounts of O and (F + Cl + OH) should not dramatically shift from the above values; however, in some cases, depending on the overall positive charges associated with cations, it could also be that some O<sup>2-</sup> substitutes for monovalent anions at the X crystallographic site. If the analytical value for H<sub>2</sub>O is lacking, it is reasonable to assume a calculated wt% H<sub>2</sub>O so as to give 13 total anions (O + F + Cl + OH), with O = 12 and (F + Cl + OH) = 1, unless (F + Cl) ≥ 1 (in those cases H<sub>2</sub>O<sub>calc</sub> can be omitted).

(b) Calculation on the basis of 8 total (M + T) cations.

(c) Calculation on the basis of 3 T cations (*i.e.*, P + As + V + Si + S).

In principle, criterion (a) is preferable to criteria (b) and (c). In fact, calculation based on any subset of all atoms does not affect the stoichiometric ratios between them, but automatically shifts any analytical error to the atoms not belonging to that subset. Criteria (b) and (c) would be best to use in cases in which structural vacancies are possible at some sites, but this does not seem to be the case for any apatite supergroup mineral.

For cation allocation, P<sup>5+</sup>, As<sup>5+</sup>, V<sup>5+</sup>, Si<sup>4+</sup> and S<sup>6+</sup> can be assumed to be in tetrahedral coordination and assigned to the T site, where they should sum up to 3. In cases of a marked deviation from the ideal value of 3 apfu (say more than 3 %), it may be inferred that the analysis is in error, or unreliable due to admixture with other phases or another such issue.

All remaining cations will enter the M1 and M2 sites. Elucidation of partitioning between these two sites (or more, in cases of split sites) is almost impossible without an accurate evaluation of the electron density at each of them, which makes a structural study mandatory. On the basis of both the historical appraisal of all available structural studies within the apatite supergroup and general crystal-chemical considerations, for cases where structural data are not available, we suggest allocation of M cations in order of increasing ionic radius, filling M1 sites (Wyckoff positions 4f in the P6<sub>3</sub>/m structure) with smaller cations (in particular Ca), and putting larger cations (Ba, Pb, etc.) in M2 sites (Wyckoff positions 6h in the P6<sub>3</sub>/m structure). This should result in correct allocations of cations in most cases, which can be used for identification or naming; however, this approach is not infallible in that some doubts remain regarding cation partitioning trends in

apatite (*sensu lato*), mainly in the partitioning of Ca and REE between M1 and M2.

#### 4.2. Effect of charge compensation on the idealized formulae

Cations with charges of +4, +5 and +6 can occupy the T site in the apatite structure and cations with charges of +1, +2 and +3 can occupy the M sites. Given the basic stoichiometry of apatite supergroup minerals, M<sub>1</sub><sub>2</sub>M<sub>2</sub><sub>3</sub>(TO<sub>4</sub>)<sub>3</sub>X (or M1M1' M<sub>2</sub><sub>3</sub>(TO<sub>4</sub>)<sub>3</sub>X), and assuming, for the sake of simplicity, that the overall charge associated with anions is -25 [*i.e.*, 12 O<sup>2-</sup> + 1 (F, Cl, OH)<sup>-</sup>], charge compensation dictates the combinations of T and M site occupancies provided in Table 3.

Due to the symmetry of apatites, and to the existence of a single independent T site, the overall charge associated with T cations is, as a rule, a multiple of 3. The only exception to this rule is fluorcalciobriholite.

### 5. General nomenclature rules for apatite supergroup minerals

The crystal chemistry of apatites has important implications on nomenclature. After careful consideration of the intricacies of apatite crystal chemistry as described above, we propose the following basic guidelines for the nomenclature of apatite supergroup minerals:

(1) As a rule, each combination of M1, M2, and T dominant cations deserves a specific root name.

(2) Adjectival prefixes for the X anions are to be preferred over modified Levinson suffixes for two main reasons:

(i) Historical – Most minerals within the apatite group were originally named using the adjectival prefixes and some of these (*esp.* chlorapatite, fluorapatite and hydroxylapatite) have long histories of usage in the scientific literature. Renaming them at this point creates needless disruption in historical continuity, which is certainly not outweighed by issues of convenience, *e.g.* alphabetical listing.

(ii) Practical – There are members of the apatite supergroup which are REE-dominant minerals and in those cases, according to general nomenclature rules, the root name must be followed by the Levinson suffix denoting the most abundant among REEs [*e.g.*, belovite-(La), briholite-(Ce)]. The adoption of the suffix nomenclature for

Table 3. Possible combinations of cation site occupancies based upon cation charge.

T site occupancy	T charge	M1, M2 sites occupancy	M charge
T <sup>4+</sup> <sub>3</sub>	12	M <sup>2+</sup> <sub>2</sub> M <sup>3+</sup> <sub>3</sub>	13
T <sup>4+</sup> <sub>2</sub> T <sup>5+</sup>	13	M <sup>2+</sup> <sub>3</sub> M <sup>3+</sup> <sub>2</sub>	12
T <sup>5+</sup> <sub>3</sub>	15	M <sup>2+</sup> <sub>2</sub> M <sup>2+</sup> <sub>3</sub> or (M <sup>1+</sup> M <sup>3+</sup> ) M <sup>2+</sup> <sub>3</sub>	10
T <sup>4+</sup> <sub>1.5</sub> T <sup>6+</sup> <sub>1.5</sub>	15	M <sup>2+</sup> <sub>2</sub> M <sup>2+</sup> <sub>3</sub>	10
T <sup>6+</sup> <sub>3</sub>	18	M <sup>1+</sup> <sub>2</sub> (M <sup>2+</sup> <sub>2</sub> M <sup>1+</sup> ) or M <sup>1+</sup> <sub>2</sub> (M <sup>1+</sup> <sub>2</sub> M <sup>3+</sup> )	7



X-dominant anions would require a double Levinson suffix in some cases [*e.g.*, britholite (YF), instead of fluorbritholite-(Y)] and we believe that such mixed cation-anion suffixes are awkward.

Aiming to avoid unnecessary changes in the existing nomenclature, the use of adjectival prefixes should not be applied retroactively; in other words, it is not recommended to rename pyromorphite,  $\text{Pb}_5(\text{PO}_4)_3\text{Cl}$ , as chlorpyromorphite. If in the future the F analogue of pyromorphite,  $\text{Pb}_5(\text{PO}_4)_3\text{F}$ , is described, the name “fluorpyromorphite” could be logically adopted for it. There are plenty of examples of pairs of mineralogical names, in which only one has the adjectival prefix, *e.g.*, phlogopite – fluorphlogopite, clinohumite – hydroxylclinohumite, bartonite – chlorbartonite, etc. In general, a given mineral name is not meant to reveal the details of the chemical composition.

Neither is it recommended to adopt a prefix-based nomenclature for the calcium arsenates svabite, johnbaumite, and turneaureite, although the two latter minerals would have been better named hydroxylsvabite and chlorsvabite, respectively.

(3) Minerals with the same ideal chemical composition and different space group symmetries should be denoted with the same name, and with italicized suffixes denoting the crystalline system (*e.g.*, mimetite-*H*, mimetite-*M*). Thus far, among all known minerals of the apatite supergroup, there are only three such cases, and a fourth one has been recognized (see § 6.4. and 6.5.). According to the general IMA-CNMNC guidelines on nomenclature (Nickel & Grice, 1998), these are cases of polymorphic minerals with essentially the same structural topologies and should not be regarded as separate species. As happens with similar cases (*e.g.*, analcime, muscovite, sapphirine) for which topologically identical polymorphs (or polytypes) with different crystal systems are known, in the IMA List of Minerals only the basic, unsuffixed name need be used and this will be considered the official name for the mineral. The “-*H*” or “-*M*” will only be used in cases where there is a need to distinguish or identify the specific polymorph, *e.g.*, in papers discussing the crystallographic variants of a given mineral. We are aware that the pronunciation of such names may be a bit clumsy, but we anticipate that in verbal form most people will choose to use only the root name, *i.e.* mimetite, and when referring specifically to monoclinic polymorph, can preface the root name with “monoclinic”, *i.e.* “monoclinic mimetite”.

(4) In addition to monovalent anions (F, Cl, OH),  $\text{O}^{2-}$  may also enter the X site. For example, a structural model for a synthetic compound  $\text{Ca}_{10}(\text{PO}_4)_6\text{O}$ , obtained by dehydration of  $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$  under electron microscope conditions, has been designed on the basis of simulated high resolution lattice images (Henning *et al.*, 1999). For the definition of a potential new mineral with  $\text{O}^{2-}$  as the dominant anion, it is required that the fraction of  $^{\text{X}}\text{O}^{2-}$  is  $> 50\%$ . Here we refer to the concept of “charge compensating anion”, according to which monovalent anions may be considered as a whole. In other words, for nomenclature purposes, if  $^{\text{X}}\text{O}^{2-} > (\text{F} + \text{Cl} + \text{OH})^-$ , the mineral will have

the adjectival prefix “oxy” (sometimes in literature the hypothetical “oxyapatite” component is mentioned for natural compounds, whereas synthetic end-members are well known; *e.g.*, Ito, 1968); if  $(\text{F} + \text{Cl} + \text{OH})^- > ^{\text{X}}\text{O}^{2-}$  the mineral could have the adjectival prefix corresponding to the dominating anion of the dominant valency state (Hatert & Burke, 2008). As far as we are aware, as yet no reliable analyses of apatite supergroup minerals have been reported in the literature with  $^{\text{X}}\text{O}^{2-} > (\text{F} + \text{Cl} + \text{OH})^-$ .

(5) Similar arguments may be valid for the possible substitution of monovalent anions by water molecules (the hypothetical “hydroapatite” component). Although the structural role of water molecules within the framework of apatite is yet to be clarified, in a single case, that of cesanite (Cavarretta *et al.*, 1981), the water content points to a formula which has substantial  $\text{H}_2\text{O}$  entering the X site. However, the reported formula still has  $(\text{OH} + \text{F} + \text{Cl}) > \text{H}_2\text{O}$ .

## 6. Approved changes

With the intent of rationalizing the nomenclature of minerals within the apatite supergroup, we propose a number of changes, which are listed in detail below and are also summarized in Table 1. In this endeavour, our two guiding principles have been: (1) to make a completely self-consistent nomenclature system, and (2) to reduce, as much as possible, changes to existing mineral names. Clearly, these two principles are not fully reconcilable with one another, and our final product represents the best compromise we could find between them. Overall, within the broad apatite supergroup, we have made six types of recommendations: (1) nomenclature changes to existing minerals, (2) potentially new mineral species, (3) minerals and mineral names which could be discredited, (4) changes of status from distinct species to polymorphic variants, (5) recognition of a new polymorphic variant, and (6) changes to end-member formulae.

### 6.1. Nomenclature changes to existing minerals

(1) In keeping with our suggestion to use adjectival prefixes instead of modified Levinson suffixes for the dominant X anion, a number of mineral names should be changed as follows: apatite-(CaF) to **fluorapatite**; apatite-(CaOH) to **hydroxylapatite**; apatite-(CaCl) to **chlorapatite**; ellestadite-(F) to **fluorellestadite**; ellestadite-(OH) to **hydroxyllellestadite**; phosphohedyphane-(F) to **fluorphosphohedyphane**. Therefore, for “apatites” the historical names, adopted in the XIX century and occurring in thousands of mineralogical and non-mineralogical publications, should be reintroduced. The same holds for “ellestadites”, although these minerals have a more recent history and are not as widespread as apatites.

Phosphohedyphane, which was renamed phosphohedyphane-(Cl) after the description of phosphohedyphane-(F), should be re-assigned its original name, with neither “chlor-” prefix nor “-(Cl)” suffix.

(2) **Stronadelphite** (given name for IMA 2008-009): The new mineral IMA 2008-009,  $\text{Sr}_5(\text{PO}_4)_3\text{F}$ , was approved without a name. Now we (MP & IP), being among the authors of the IMA 2008-009 proposal and of this nomenclature report, in agreement with the whole apatite subcommittee herewith propose for this mineral a new root name, namely stronadelphite. It is a compound word after the chemical element *strontium* and  $\alpha\delta\epsilon\lambda\phi\acute{o}\sigma$ , Greek for “brother”; the mineral is the full strontium analogue of fluorapatite, the most widespread member of the apatite group. We wish to avoid the constructions strontioadelphite or strontio-adelphite, because of the inconvenient fragment *oa* or *o-a*, and strontiadelphte because of the possibility that it might be misspelled as strontiodelphte by somebody unfamiliar with Greek roots.

(3) **Fluorstrophite** instead of apatite-(SrOH): To have a mineral named either apatite-(SrOH) (the new name) or “strontium-apatite” (the old name) after the discovery of a mineral (IMA 2008-009) which is more Sr-rich than strontium-apatite itself is clearly misleading. The original name strontium-apatite was given before the structural study of the mineral and incorrectly reflects its relationship with apatite; therefore, we propose to change its name to fluorstrophite. This seems a proper name for a mineral with ideal composition  $\text{SrCaSr}_3(\text{PO}_4)_3\text{F}$ , due to its parallelism, in both the name and the ideal formula, with the related mineral fluorcaphite,  $\text{SrCaCa}_3(\text{PO}_4)_3\text{F}$ . The root name originates from the combination of elements: *fluorine*, *strontium* (at the M2 site), and *phosphorus*. Fluorcaphite is a similar acronym, with *calcium* instead of *strontium*.

(4) **Deloneite** instead of deloneite-(Ce): The detailed structural analysis carried out by Rastsvetaeva & Khomyakov (1996b) showed that none of the four independent M sites has REE as the dominant cation, therefore deloneite should not be considered a REE mineral, and the Levinson suffix should be omitted.

(5) For the newly approved mineral IMA 2009-005, the originally proposed name, **fluorbritholite-(Y)**, perfectly fits with our nomenclature scheme; therefore, we recommend its adoption for the mineral with composition  $(\text{Y}_3\text{Ca}_2)(\text{SiO}_4)_3\text{F}$ , which is actually the F-dominant analogue of britholite-(Y) and the Y-dominant analogue of fluorbritholite-(Ce).

## 6.2. Potentially new mineral species

(1) Hedyphane has ideal formula  $\text{Ca}_2\text{Pb}_3(\text{AsO}_4)_3\text{Cl}$ . Dunn *et al.* (1985b) described a mineral, which was called “hydroxyl-bearing hedyphane”, that has (OH) as the dominant anion at the X site. This mineral deserves distinct species status, with ideal formula  $\text{Ca}_2\text{Pb}_3(\text{AsO}_4)_3(\text{OH})$ . The most logical name for it would be “hydroxylhedyphane”. Aiming at reducing, as far as possible, the changes to existing names, we do not see any need for the concurrent renaming of hedyphane to chlorhedyphane, if this potentially new mineral is approved.

(2) Stalder & Rozendaal (2002) report a “calcian pyromorphite” with a very low content of Cl and F. Assuming

ordering of Pb and Ca in the two M sites, one of their analyses (#5 in their Table 4) is consistent with this being close to the OH end-member of phosphohedyphane,  $\text{Ca}_2\text{Pb}_3(\text{PO}_4)_3(\text{OH})$ . According to the naming approach recommended herein, the most logical name for this potentially new species would be “hydroxylphosphohedyphane”.

(3) The mineral studied structurally by Chakhmouradian *et al.* (2005) and reported as the second occurrence of fluorcaphite has the ideal chemical formula  $\text{CaCaSr}_3(\text{PO}_4)_3\text{F}$ , or more simply  $\text{Ca}_2\text{Sr}_3(\text{PO}_4)_3\text{F}$ . This mineral is different from both fluorcaphite,  $\text{SrCaCa}_3(\text{PO}_4)_3\text{F}$ , and fluorstrophite,  $\text{SrCaSr}_3(\text{PO}_4)_3\text{F}$ , and deserves distinct species status and a new root name.

(4) The “Mn-rich apatite” described by Pieczka (2007) deserves distinct species status. This would be the only mineral within the entire apatite supergroup having Mn as an essential element, but more significantly, it would be the only mineral in which a normally octahedrally-coordinated cation is an essential element. Although the ordering of Mn and Ca between the M1 and M2 sites cannot be confirmed without a structural study, one might expect Mn to go into the M1 site (*cf.* also § 4.1.). If this were the case, this mineral would have the ideal formula  $\text{Mn}_2\text{Ca}_3(\text{PO}_4)_3\text{Cl}$ .

(5) Mattheddleite has ideal formula  $\text{Pb}_5(\text{SiO}_4)_{1.5}(\text{SO}_4)_{1.5}\text{Cl}$ . Essene *et al.* (2006) re-analyzed samples from the type locality and found zones in some crystals with (OH) > Cl, although (OH) was admittedly calculated as 1 – Cl. This would represent a potentially new mineral, the OH-analogue of mattheddleite, for which the most logical name would be “hydroxylmattheddleite”. As for hedyphane, also in the case that “hydroxylmattheddleite” will be approved as a valid species, we do not see any need to rename mattheddleite into “chlormattheddleite”.

## 6.3. Minerals and mineral names which could be discredited

(1) Ellestadite-(Cl): As far as we are aware, no reliable chemical analyses were ever published for any “ellestadite” mineral having  $\text{Cl}^-$  as the dominant  $\text{X}^-$  anion; therefore, ellestadite-(Cl), formerly known as “chlorellestadite”, is not thought to exist and we herewith propose to discredit the mineral and its name.

(2) Melanocerite-(Ce): Both the “melanocerite” and “tritomite” root names indicate REE-rich silicoborate minerals within the apatite supergroup. Although all these minerals are inadequately characterized, the existence of two distinct root names seems unnecessary. For priority reasons, the root name “tritomite” should be maintained; therefore, the name melanocerite-(Ce) for an apatite-like silicoborate having cerium as the dominant REE, could be potentially discredited, once its identity with tritomite-(Ce) is ascertained.

## 6.4. Changes of status from distinct species to polymorphic variants

(1) Fermorite is the monoclinic polymorph of johnbaumite,  $\text{Ca}_5(\text{AsO}_4)_3(\text{OH})$ , but the two structures are topologically

equivalent. Therefore, according to existing IMA-CNMNC guidelines (Nickel & Grice, 1998), johnbaumite and fermorite should not be considered two distinct species. It could be a matter of discussion which of the above names has priority. In strictly chronological terms, the name fermorite (1911) existed before johnbaumite (1980); however, the original characterization of fermorite (Smith & Prior, 1911) was incorrect in two critical respects: the mineral was described as hexagonal (like johnbaumite) and the given chemical formula did not correspond to that of a calcium arsenate mineral. A complete characterization of fermorite as the monoclinic polymorph of  $\text{Ca}_5(\text{AsO}_4)_3(\text{OH})$  was presented by Hughes & Drexler (1991) after the description of hexagonal johnbaumite by Dunn *et al.* (1980). Within the entire apatite supergroup, the hexagonal structures can be generally considered as “parents” upon which the lower symmetry polymorphic structures are based. Moreover, in this specific case, the deviations from hexagonal symmetry are very limited (Hughes & Drexler, 1991). Therefore, we propose to maintain “johnbaumite” as the root name for the calcium arsenate, and to rename fermorite as johnbaumite-*M*. Concurrently, the hexagonal polymorph of johnbaumite should be renamed johnbaumite-*H*.

(2) Clinohydroxylapatite was described by Chakhmouradian & Medici (2006) as the monoclinic polymorph of  $\text{Ca}_5(\text{PO}_4)_3(\text{OH})$ . According to existing IMA-CNMNC guidelines (Nickel & Grice, 1998), hydroxylapatite and clinohydroxylapatite should not be considered two distinct minerals, but two polymorphic variants of the same species. It is therefore recommended that clinohydroxylapatite be renamed hydroxylapatite-*M*. Concurrently, the hexagonal polymorph of hydroxylapatite should be renamed hydroxylapatite-*H*.

(3) Clinomimetite was described by Dai *et al.* (1991) as the monoclinic polymorph of mimetite. According to existing IMA-CNMNC guidelines (Nickel & Grice, 1998), mimetite and clinomimetite should not be considered two distinct minerals, but two polymorphic variants of the same species. It is, therefore, recommended that clinomimetite be renamed as mimetite-*M*. Concurrently, the hexagonal polymorph of mimetite should be renamed mimetite-*H*.

For the sake of convenience, the suffix -*H* will be generally omitted in the name of the hexagonal polymorphs, by far more common in nature than the monoclinic polymorphs.

## 6.5. Recognition of a new polymorphic variant

Hughes *et al.* (1990) refined the structure of a sample of monoclinic chlorapatite from Jackson Peak, Gunkock, Washington Co., Utah, USA, which is analogous to the monoclinic hydroxylapatite described by Chakhmouradian & Medici (2006). Therefore, as in the case of hydroxylapatite, the hexagonal and the monoclinic forms of chlorapatite are to be considered as polymorphs. The sample from Jackson Peak should be named chlorapatite-*M*. Concurrently, the hexagonal polymorph of chlorapatite should be renamed chlorapatite-*H* (see also § 6.4.).

## 6.6. Changes to end-member formulae

(1) Morelandite. The only available chemical analysis for morelandite yields the empirical formula  $(\text{Ba}_{2.25}\text{Ca}_{1.65}\text{Pb}_{1.16}\text{Fe}_{0.06}\text{Mn}_{0.06})[(\text{AsO}_4)_{2.56}(\text{PO}_4)_{0.30}]\text{Cl}_{1.09}$  (Dunn & Rouse, 1978). In the IMA List of Minerals, morelandite is given the formula  $\text{Ba}_5(\text{AsO}_4)_3\text{Cl}$ . To conform with this ideal, “end-member” formula  $[\text{M}^1\text{Ba}_2\text{M}^2\text{Ba}_3(\text{AsO}_4)_3\text{Cl}]$ , barium would have to be the dominant cation at both the M1 and M2 sites ( $\text{Ba} > 2.50$  apfu), but it is not. Therefore, the ideal chemical formula of morelandite should be rewritten as  $\text{Ca}_2\text{Ba}_3(\text{AsO}_4)_3\text{Cl}$ , instead of  $\text{Ba}_5(\text{AsO}_4)_3\text{Cl}$ .

(2) Deloneite. The following charge-balanced formula better reflects the nature of deloneite, in which there are no REE-dominant sites:  $(\text{Na}_{0.5}\text{REE}_{0.25}\text{Ca}_{0.25})(\text{Ca}_{0.75}\text{REE}_{0.25})\text{Sr}_{1.5}(\text{CaNa}_{0.25}\text{REE}_{0.25})(\text{PO}_4)_3\text{F}_{0.5}(\text{OH})_{0.5}$ . This is in keeping with the approved removal of the Levinson suffix from its name.

**Acknowledgements:** We are grateful to all the members of the IMA Commission on New Minerals, Nomenclature and Classification who provided with suggestion and criticism, and to the CNMNC secretary, Stuart Mills, for handling the whole procedure.

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Received 25 January 2010

Accepted 25 January 2010