

IMA REPORT

Nomenclature of the garnet supergroup

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ABSTRACT

The garnet supergroup includes all minerals isostructural with garnet regardless of what elements occupy the four atomic sites, i.e., the supergroup includes several chemical classes. There are presently 32 approved species, with an additional 5 possible species needing further study to be approved. The general formula for the garnet supergroup minerals is  $\{X_3\}[Y_2](Z_3)\varphi_{12}$ , where  $X$ ,  $Y$ , and  $Z$  refer to dodecahedral, octahedral, and tetrahedral sites, respectively, and  $\varphi$  is O, OH, or F. Most garnets are cubic, space group  $Ia\bar{3}d$  (no. 230), but two OH-bearing species (henritermierite and holstamite) have tetragonal symmetry, space group,  $I4_1/acd$  (no. 142), and their  $X$ ,  $Z$ , and  $\varphi$  sites are split into more symmetrically unique atomic positions. Total charge at the  $Z$  site and symmetry are criteria for distinguishing groups, whereas the dominant-constituent and dominant-valency rules are critical in identifying species. Twenty-nine species belong to one of five groups: the tetragonal henritermierite group and the isometric bitikleite, schorlomite, garnet, and berzeliite groups with a total charge at  $Z$  of 8 (silicate), 9 (oxide), 10 (silicate), 12 (silicate), and 15 (vanadate, arsenate), respectively. Three species are single representatives of potential groups in which  $Z$  is vacant or occupied by monovalent (halide, hydroxide) or divalent cations (oxide). We recommend that suffixes (other than Levinson modifiers) not be used in naming minerals in the garnet supergroup. Existing names with suffixes have been replaced with new root names where necessary: bitikleite-(SnAl) to bitikleite-(SnFe) to dzhuluite, bitikleite-(ZrFe) to usturite, and elbrusite-(Zr) to elbrusite. The name hibschite has been discredited in favor of grossular as Si is the dominant cation at the  $Z$  site. Twenty-one end-members have been reported as subordinate components in minerals of the garnet supergroup of which six have been reported in amounts up to 20 mol% or more, and, thus, there is potential for more species to be discovered in the garnet supergroup. The nomenclature outlined in this report has been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (Voting Proposal 11-D).

**Keywords:** Garnet group, schorlomite group, bitikleite group, berzeliite group, henritermierite group, katoite, nomenclature, crystal chemistry

INTRODUCTION

The garnets pose somewhat different nomenclature problems than other mineral supergroups recently considered for nomenclature review, i.e., sapphirine (Grew et al. 2008), apatite (Pasero et al. 2010), pyrochlore (Atencio et al. 2010), tourmaline (Henry et al. 2011), and amphibole (Hawthorne et al. 2012), where a supergroup is defined as “consisting of two or more groups that have essentially the same structure and composed of chemically similar elements” (Mills et al. 2009). Compared to the structures of the minerals in these groups, the archetypal garnet structure, cubic space group  $Ia\bar{3}d$  (no. 230) has few sites: only three cationic and one anionic (e.g., Menzer 1928; Novak and Gibbs 1971; Merli et al. 1995; Geiger 2008), and the most common garnets have relatively simple chemical compositions.

However, the garnet structure is remarkably flexible in a chemical sense: 53 elements were reported in the Inorganic Crystal Structure Database (Allmann and Hinek 2007) and five more are reported in synthetic garnets (Geller 1967; Ronniger and Mill’ 1973; Yudintsev 2003; Yudintsev et al. 2002; Utsunomiya et al. 2005). In the period 2009–2010, 10 new species of garnet, with constituents such as Sc, Y, Sn, Sb, and U, which have not been previously reported in significant quantities in natural garnet, were approved by the Commission on New Minerals, Nomenclature and Classification (CNMNC) of the International Mineralogical Association (IMA), resulting in a nearly 50% increase in the number of accepted species with the garnet structure. There are four more possible species, bringing to 26 the number of elements essential to defining existing and possible mineral species with the garnet structure.

In view of this situation, it seemed an opportune time to convene a subcommittee to review the nomenclature of garnets. The garnet group traditionally included only silicate minerals (e.g.,

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Yakovlevskaya 1972; Strunz and Nickel 2001; Back and Mandarino 2008). However, there are minerals from other classes, such as arsenates, vanadates, oxides, and even fluorides that are isostructural with the silicate garnets, and whose major constituents show chemical similarities with constituents in silicate garnets, i.e., these minerals meet the criteria for inclusion in a broader entity, the garnet supergroup (Mills et al. 2009). McConnell (1942) introduced the term “garnetoid” to “designate those substances which are not primarily silicates but have structures similar to that of true garnets,” such as “hydrogarnet,” berzeliite and the phosphate griphite (Headden 1891). It does not appear that garnetoid was discredited as a group name (Clark 1993), but our preference is to use the term garnet for the supergroup. Rinaldi (1978) showed that griphite is not isostructural with garnet, although he found that there are some structural features in common, which were also discussed by Sokolova and Hawthorne (2002), and thus griphite is not considered to be a garnet. In addition, the silicate mineral wadalite had been thought to be related to garnet because of similarities in cell dimensions and diffraction intensities (Feng et al. 1988; Tsukimura et al. 1993; Glasser 1995). Although wadalite lacks a center of symmetry, so that the single tetrahedral site found in grossular is split in wadalite into two sites, one of which is vacant, it still can be considered a derivative of grossular, but Glasser (1995) emphasized the much closer relationship of wadalite to mayenite. Recent crystal structure refinements make no mention of a relationship of wadalite or mayenite to garnet (Boysen et al. 2007; Iwata et al. 2008; Ma et al. 2011), and the structural relationship between garnet and wadalite (or mayenite) is sufficiently distant that these minerals are not included in the garnet supergroup. The so-called “tetragonal almandine-pyrope phase” (TAPP) has the stoichiometry, but not the structure of garnet (Harris et al. 1997; Finger and Conrad 2000), i.e., TAPP has edges shared between tetrahedra and octahedra, a feature not found in garnet (see below) and thus is not considered further in this report. Similarly, although some natural and synthetic arsenates of the alluaudite group, e.g., caryinite, are approximately polymorphous with the garnet supergroup mineral manganberzeliite (Ercit 1993; Khorari et al. 1995, 1997), the structures of alluaudite-group compounds are too different from garnet to warrant further consideration of the alluaudite group in this report.

Twenty-nine of the thirty-two approved species of the garnet supergroup are divided here into five groups on the basis of the total charge of cations at the tetrahedral site, leaving three ungrouped species (Table 1); four potential new species can be accommodated in two of these groups (see below). One group is also distinguished on the basis of symmetry: the tetragonal henritermierite group (Fig. 1a). The classification in Table 1 keeps the number of groups at a practical level that still reflects crystal-chemical relationships. Table 1 also gives the class for the five groups and ungrouped species to emphasize that the garnet supergroup comprises not only silicates (Figs. 1a, 1c, 1d, and 1e), but also a halide (Fig. 1b), hydroxides, oxides, vanadates, and arsenates (Fig. 1g). The groups are listed in order of increasing charge of cations that occupy the Z site of the end-members. Species within each group are listed as end-members with increasing atomic number of the Z site, followed by increasing atomic number of the Y site and last, by increasing

atomic number of the X site, whereas species with joint occupancies at the Y site are placed last. Table 2 lists the 32 species as end-members in the same order and compares formulas given in the 2009 list (updated in 2012) of minerals approved by the CNMNC with the end-member formulas approved with the classification presented here.

Subdivision of the groups into mineral subgroups or mineral series is not recommended, as these terms should be reserved for homologous or polysomatic series (Mills et al. 2009). This restriction constitutes another rationale for discouraging the traditional division of the garnet group into the “pyralspite” and “ugrandite” species (Winchell 1933) or series (Strunz and Nickel 2001), although there could be some fundamental structural differences that limit solid solution between the two groupings (e.g., Ungaretti et al. 1995; Boiocchi et al. 2012; cf. Geiger 2008).

Our procedure for distinguishing species relies heavily on the dominant-valency rule, which is an extension of the dominant-constituent rule (Hatert and Burke 2008). The latter rule states that species designation is based on the dominant constituent at a given crystallographic site, which works well when all constituents have the same valence. However, when ions at a given crystallographic site have different valences, it is essential that the dominant valence be determined first, and then species and group designation is determined by the dominant ion having this valence. Traditionally, identifying a garnet species has

**TABLE 1.** A classification of the 32 approved species in the garnet supergroup

Z charge	GROUP or species name	Class	X	Y	Z	φ
0	Katoite	Hydroxide	Ca <sub>3</sub>	Al <sub>3</sub>	□	(OH) <sub>12</sub>
3	Cryolithionite	Halide	Na <sub>3</sub>	Al <sub>2</sub>	Li <sub>3</sub>	F <sub>12</sub>
6	Yafsoanite	Oxide	Ca <sub>3</sub>	Te <sub>2</sub> <sup>2+</sup>	Zn <sub>3</sub>	O <sub>12</sub>
8	HENRITERMIERITE	Silicate				
	Holtstamite		Ca <sub>3</sub>	Al <sub>2</sub>	Si <sub>2</sub>   □	O <sub>8</sub> (OH) <sub>4</sub>
	Henritermierite		Ca <sub>3</sub>	Mn <sub>3</sub> <sup>2+</sup>	Si <sub>2</sub>   □	O <sub>8</sub> (OH) <sub>4</sub>
9	BITIKLEITE	Oxide				
	Bitikleite		Ca <sub>3</sub>	Sb <sup>5+</sup> Sn <sup>4+</sup>	Al <sub>3</sub>	O <sub>12</sub>
	Usturite		Ca <sub>3</sub>	Sb <sup>5+</sup> Zr	Fe <sub>3</sub> <sup>3+</sup>	O <sub>12</sub>
	Dzhuluite		Ca <sub>3</sub>	Sb <sup>5+</sup> Sn <sup>4+</sup>	Fe <sub>3</sub> <sup>3+</sup>	O <sub>12</sub>
	Elbrusite		Ca <sub>3</sub>	U <sub>0.5</sub> <sup>6+</sup> Zr <sub>1.5</sub>	Fe <sub>3</sub> <sup>3+</sup>	O <sub>12</sub>
10	SCHORLOMITE	Silicate				
	Kimzeyite		Ca <sub>3</sub>	Zr <sub>2</sub>	SiAl <sub>2</sub>	O <sub>12</sub>
	Irinarassite		Ca <sub>3</sub>	Sn <sub>2</sub> <sup>4+</sup>	SiAl <sub>2</sub>	O <sub>12</sub>
	Schorlomite		Ca <sub>3</sub>	Ti <sub>2</sub>	SiFe <sub>2</sub> <sup>3+</sup>	O <sub>12</sub>
	Kerimasite		Ca <sub>3</sub>	Zr <sub>2</sub>	SiFe <sub>2</sub> <sup>3+</sup>	O <sub>12</sub>
	Toturite		Ca <sub>3</sub>	Sn <sub>2</sub> <sup>4+</sup>	SiFe <sub>2</sub> <sup>3+</sup>	O <sub>12</sub>
12	GARNET	Silicate				
	Menzerite-(Y)		Y <sub>2</sub> Ca	Mg <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
	Pyrope		Mg <sub>3</sub>	Al <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
	Grossular		Ca <sub>3</sub>	Al <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
	Spessartine		Mn <sub>3</sub> <sup>2+</sup>	Al <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
	Almandine		Fe <sub>3</sub> <sup>3+</sup>	Al <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
	Eringaite		Ca <sub>3</sub>	Sc <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
	Goldmanite		Ca <sub>3</sub>	V <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
	Momoiite		Mn <sub>3</sub> <sup>2+</sup>	V <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
	Knorringtonite		Mg <sub>3</sub>	Cr <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
	Uvarovite		Ca <sub>3</sub>	Cr <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
	Andradite		Ca <sub>3</sub>	Fe <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
	Calderite		Mn <sub>3</sub> <sup>2+</sup>	Fe <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
	Majorite		Mg <sub>3</sub>	SiMg	Si <sub>3</sub>	O <sub>12</sub>
	Morimotoite		Ca <sub>3</sub>	TiFe <sub>2</sub> <sup>4+</sup>	Si <sub>3</sub>	O <sub>12</sub>
15	BERZELIITE	Vanadate, arsenate				
	Schäferite		Ca <sub>2</sub> Na	Mg <sub>2</sub>	V <sub>3</sub> <sup>5+</sup>	O <sub>12</sub>
	Palenzonaite		Ca <sub>2</sub> Na	Mn <sub>2</sub> <sup>2+</sup>	V <sub>3</sub> <sup>5+</sup>	O <sub>12</sub>
	Berzeliite		Ca <sub>2</sub> Na	Mg <sub>2</sub>	As <sub>3</sub> <sup>5+</sup>	O <sub>12</sub>
	Manganberzeliite		Ca <sub>2</sub> Na	Mn <sub>2</sub> <sup>2+</sup>	As <sub>3</sub> <sup>5+</sup>	O <sub>12</sub>

Notes: Formulas are given in the form {X<sub>3</sub>}[Y<sub>2</sub>](Z<sub>3</sub>)φ<sub>12</sub>. Group names are given in capitals.



**FIGURE 1.** Photographs of representative garnet supergroup minerals illustrating the diversity in appearance exhibited by the supergroup. **(a)** Holtstamite, formula  $\{Ca_3\}[Al,Mn^{3+}](Si_2)(\square)O_8(OH)_4$ , as a yellow brown crystal between grains of Mn- and Cu-rich vesuvianite (purplish black) and calcite (white) in the holotype specimen from Wessels Mine, South Africa. Swedish Museum of Natural History specimen no. 19960380. Photo by U. Hålenius. **(b)** Cryolithionite, end-member formula  $\{Na_3\}[Al_2](Li_3)F_{12}$ : a transparent, colorless single grain in yellowish-white fine-grained cryolite. Specimen size is  $4.5 \times 2 \times 1.7$  cm. From the type locality, Ivigtut Cryolite deposit, Ivittuut (Ivigtut), Kitaa, Greenland. Pavel M. Kartashov collection and photograph. **(c)** Grossular, end-member formula  $\{Ca_3\}[Al_2](Si_3)O_{12}$ : a trapezohedron  $\{211\}$ , 3.5 cm across on the left and crystals in a cyclic intergrowth on the right, from the type locality, Wiluy River, Sakha-Yakutia Republic, Russia. The distinctive brown color is due a 30–50  $\mu m$  zone of brown andradite a short distance under the crystal faces. Evgeny and Irina Galuskin collection and Evgeny Galuskin photograph. **(d)** Uvarovite, end-member formula  $\{Ca_3\}[Cr_3^{3+}](Si_3)O_{12}$ : green dodecahedral crystals on chromite, from the type locality, Saranovskii Mine, Permskaya Oblast, Middle Urals, Russia. Largest crystal is 4 mm across. Museum of the Faculty of Earth Sciences, University of Silesia, no. WNoZ/M/9/19. Evgeny Galuskin photograph. **(e)** Almandine, end-member formula  $\{Fe_3\}[Al_2](Si_3)O_{12}$ : a crystal group 2.5 cm across on granite, Mount Lady Franklin, Barnawartha, Victoria, Australia. Museum Victoria registration no. M34200. Frank Coffa photograph. **(f)** Schorlomite, end-member formula  $\{Ca_3\}[Ti_2](SiFe_3^{3+})O_{12}$ : an incomplete crystal from the type locality, Magnet Cove, Hot Spring County, Arkansas. E.S. Grew collection and photograph. **(g)** Manganberzeliite, end-member formula  $\{Ca_2Na\}[Mn_2^{2+}](As_3^{5+})O_{12}$ , from the type locality, Långban, Sweden. The largest crystals are 3 mm across. Swedish Museum of Natural History specimen no. 19170722. M. Cooper photograph.

relied heavily on the proportion of end-member components, and therefore depended on a specific sequence of calculating end-member proportions: garnet end-member proportions constitute an underdetermined system from the point of view of linear algebra: there are more end-members than oxides (e.g., Rickwood 1968; Locock 2008).

The purpose of this report is to present the essential elements of garnet nomenclature, to define concepts that are central to

**TABLE 2.** Former formulas and end-member formulas approved in the present report

Name	Former formula	Approved end-member formula
Katoite	$Ca_3Al_2(SiO_4)_{3-x}(OH)_{4x}$ ( $x = 1.5-3.0$ )	$\{Ca_3\}[Al_2](\square)(OH)_{12}$
Cryolithionite	$Na_3Al_2(LiF_4)_3$	$\{Na_3\}[Al_2](Li_3)F_{12}$
Yafsoanite	$Ca_3Te_2Zn_3O_{12}$	$\{Ca_3\}[Te_2^6+](Zn_3)O_{12}$
Holtstamite	$Ca_3Al_2(SiO_4)_2(OH)_4$	$\{Ca_3\}[Al_2](Si_2)(\square)O_8(OH)_4$
Henritermierite	$Ca_3(Mn^{3+})_2(SiO_4)_2(OH)_4$	$\{Ca_3\}[Mn_2^{3+}](Si_2)(\square)O_8(OH)_4$
Bitikleite*	$Ca_3SbSnAl_3O_{12}$	$\{Ca_3\}[Sb^{5+}Sn^{4+}](Al_3)O_{12}$
Usturite*	$Ca_3SbZrFe_3O_{12}$	$\{Ca_3\}[Sb^{5+}Zr](Fe_3^3+)O_{12}$
Dzhuluite*	$Ca_3(SnSb^{5+})Fe_3^3+O_{12}$	$\{Ca_3\}[Sb^{5+}Sn^{4+}](Fe_3^3+)O_{12}$
Elbrusite*	$Ca_3(U^{6+}Zr)(Fe_3^3+Fe^{2+})O_{12}$	$\{Ca_3\}[U_0.5Zr_1.5](Fe_3^3+)O_{12}$
Kimzeyite	$Ca_3(Zr,Ti)_2(Si,Al,Fe^{3+})_3O_{12}$	$\{Ca_3\}[Zr_2](SiAl_2)O_{12}$
Irinarassite	$Ca_3SnAl_2SiO_{12}$	$\{Ca_3\}[Sn^{2+}](SiAl_2)O_{12}$
Schorlomite	$Ca_3(Ti,Fe^{3+})_2(Si,FeO_4)_3O_{12}$	$\{Ca_3\}[Ti_2](SiFe_3^3+)O_{12}$
Kerimasite	$Ca_3Zr_2(Fe_3^3+Si)O_{12}$	$\{Ca_3\}[Zr_2](SiFe_3^3+)O_{12}$
Toritrite	$Ca_3Sn_2Fe_2SiO_{12}$	$\{Ca_3\}[Sn_2^{2+}](SiFe_2^3+)O_{12}$
Menzerite-(Y)	$\{CaY\}[Mg_2](Si_3)O_{12}$	$\{Y,Ca\}[Mg_2](Si_3)O_{12}$
Pyrope	$Mg_3Al_2(SiO_4)_3$	$\{Mg_3\}[Al_2](Si_3)O_{12}$
Grossular	$Ca_3Al_2(SiO_4)_3$	$\{Ca_3\}[Al_2](Si_3)O_{12}$
Spessartine	$(Mn^{2+})_3Al_2(SiO_4)_3$	$\{Mn_3^2+\}[Al_2](Si_3)O_{12}$
Almandine	$(Fe^{2+})_3Al_2(SiO_4)_3$	$\{Fe_3^2+\}[Al_2](Si_3)O_{12}$
Eringaite	$Ca_3Sc_2(SiO_4)_3$	$\{Ca_3\}[Sc_2](Si_3)O_{12}$
Goldmanite	$Ca_3(V^{3+})_2(SiO_4)_3$	$\{Ca_3\}[V_2^{3+}](Si_3)O_{12}$
Momoiite	$(Mn^{2+},Ca_3)(V^{3+},Al)_2Si_3O_{12}$	$\{Mn_3^2+\}[V_2^3+](Si_3)O_{12}$
Knorringite	$Mg_3Cr_2(SiO_4)_3$	$\{Mg_3\}[Cr_2^3+](Si_3)O_{12}$
Uvarovite	$Ca_3Cr_2(SiO_4)_3$	$\{Ca_3\}[Cr_2^3+](Si_3)O_{12}$
Andradite	$Ca_3(Fe^{3+})_2(SiO_4)_3$	$\{Ca_3\}[Fe_2^3+](Si_3)O_{12}$
Calderite	$(Mn^{2+})_3(Fe^{3+})_2(SiO_4)_3$	$\{Mn_3^2+\}[Fe_2^3+](Si_3)O_{12}$
Majorite	$Mg_3(Fe^{2+},Si)_2(SiO_4)_3$	$\{Mg_3\}[SiMg](Si_3)O_{12}$
Morimotoite	$Ca_3(Ti,Fe^{2+},Fe^{3+})_2(Si,Fe^{3+})_3O_{12}$	$\{Ca_3\}[TiFe^{2+}](Si_3)O_{12}$
Schäferite	$NaCa_2Mg_2(VO_4)_3$	$\{Ca_2Na\}[Mg_2](V_3^5+)O_{12}$
Palenzonaite	$NaCa_2(Mn^{2+})_2(VO_4)_3$	$\{Ca_2Na\}[Mn_2^{2+}](V_3^5+)O_{12}$
Berzeliite	$NaCa_2Mg_2(AsO_4)_3$	$\{Ca_2Na\}[Mg_2](As_3^5+)O_{12}$
Manganberzeliite	$NaCa_2(Mn^{2+})_2(AsO_4)_3$	$\{Ca_2Na\}[Mn_2^{2+}](As_3^5+)O_{12}$

Note: Former names from IMA-CNMC List of Mineral Names compiled in March 2009 by E.H. Nickel and M.C. Nichols and from the Official IMA list of mineral names (updated from March 2009 list) at <http://pubsites.uws.edu.au/ima-cnmc/>. Names of minerals approved after the list was published are taken from the original description.

\* Table 5 lists the names under which these four minerals were originally described.

garnet classification, and to provide practical guidelines for application of the nomenclature in distinguishing species. The nomenclature outlined in this report has been approved by the CNMC (Voting proposal 11-D, April 3, 2012).

### CRYSTALLOGRAPHIC AND CRYSTAL-CHEMICAL ASPECTS OF GARNET-SUPERGROUP MINERALS

In the structure of cubic garnets (e.g., Menzer 1928; Novak and Gibbs 1971; Hawthorne 1981; Merli et al. 1995; Geiger 2008), space group  $Ia\bar{3}d$  (no. 230), there are only four symmetrically unique atomic sites (not including hydrogen): dodecahedral  $\{X\}$ , octahedral  $[Y]$ , and tetrahedral  $(Z)$  cation sites, as well as an anionic site designated  $\varphi$  to indicate O, OH, and F, giving a generalized chemical formula for the garnet supergroup,  $\{X_3\}[Y_2](Z_3)\varphi_{12}$  (modified after Geller 1967). The three cation sites are at special positions fixed by symmetry, with the Wyckoff positions  $24c$ ,  $16a$ , and  $24d$ , respectively, whereas the anion site is located at a general position,  $96h$ . The structure consists of alternating  $Z\varphi_4$  tetrahedra and  $Y\varphi_6$  octahedra, which share corners to form a three-dimensional framework (Fig. 2). Cavities enclosed in this framework have the form of triangular dodecahedra surrounding the  $X$  site (Novak and Gibbs 1971). Each anion is coordinated by one  $Z$ , one  $Y$ , and two  $X$  cations, resulting in a high percentage of shared edges between the dodecahedra on the one hand and the octahedra and tetrahedra on the other. However, the octahedra



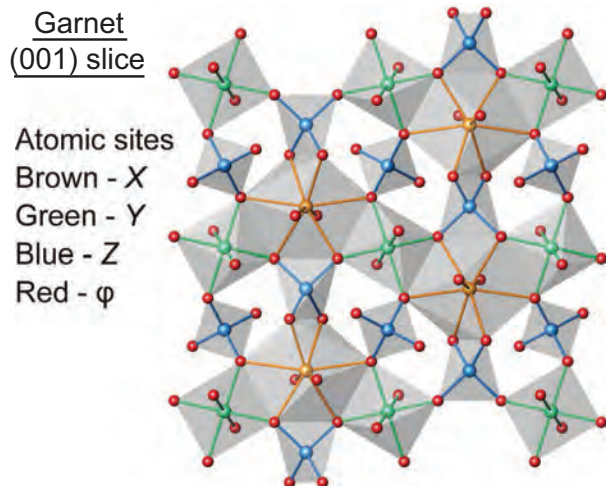


FIGURE 2. Portion of the garnet structure projected along [001].

and tetrahedra do not share edges with each other (cf. TAPP: Harris et al. 1997; Finger and Conrad 2000).

In hydrous garnets, the major mechanism of hydroxyl incorporation is by the coupled substitution  $4\text{H}^{+2}\square \rightarrow \square^{+2}\text{Si}$ , i.e., the hydrogen ions occupy a separate site of general symmetry (Wyckoff position 96*h*) coordinated to O defining the tetrahedral site, which is vacant (e.g., Ferro et al. 2003; Lager et al. 1987, 1989). The hydrogen ions lie approximately on the faces of the tetrahedron of O around a vacant center, as do the deuterium ions shown in Figure 3. The O-H and O-D distances reported for minerals or their synthetic analogues range from 0.65 Å in synthetic deuterium katoite (X-ray diffraction, Lager et al. 1987) and 0.68 Å in natural katoite (X-ray diffraction, Sacerdoti and Passaglia 1985) to 0.75 Å in henritermierite (X-ray diffraction, Armbruster et al. 2001) to 0.904–0.95 Å in synthetic katoite (neutron diffraction, Lager et al. 1987; Cohen-Addad et al. 1967). Allowing that O-H and O-D distances obtained by X-ray diffraction are shorter than those obtained by neutron diffraction, Lager et al. (1987) concluded that the reported distances are consistent with isolated OH groups (lacking H-bonding) and assumed that the residual density located near oxygen can be attributed to the displaced (bonding) electron between O and H and not to the hydrogen itself.

However, compositional data, nuclear magnetic resonance (NMR) spectra, and infrared (IR) spectra have been cited as evidence for multiple H occupancy in grossular and garnets in the hydrogrossular series. Cation vacancies at the X and Y sites calculated from electron microprobe analyses without direct determination of H<sub>2</sub>O have been cited as evidence for the presence of H in these polyhedra, either without crystallographic data (Birkett and Trzcinski 1984), or in conjunction with single-crystal refinements of Ca, Al, Fe, and Si, whereas H could be located only in a few of the crystals studied and not quantified (Basso et al. 1984a, 1984b; Basso and Cabella 1990). Kalinichenko et al. (1987) interpreted NMR spectra obtained on a grossular to indicate 2H in the octahedra and 1H in the tetrahedra. In a comprehensive IR study of the hydrogrossular series, Rossman and Aines (1991) reported that samples containing substantial

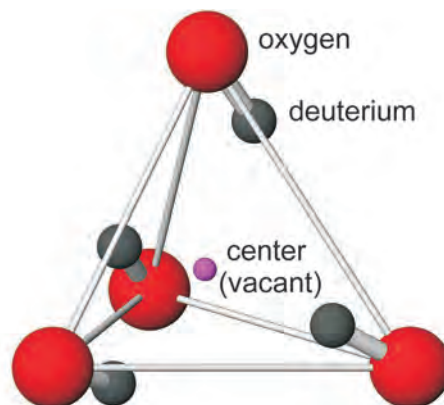


FIGURE 3. Local coordination environment of the tetrahedral position from the low-*T* (200 K) refinement of synthetic deuterated katoite (Lager et al. 1987) showing that the deuterium ions are approximately on the faces of the O tetrahedron and ~1.3 Å from the ideal tetrahedral cation position, which is vacant. O-O distances shown as thin rods, O-D bonds as thick rods.

H (>11.7 wt% H<sub>2</sub>O equivalent to >5.43 OH per formula unit) gave spectra consistent with the substitution  $4\text{H}^{+2}\square \rightarrow \square^{+2}\text{Si}$ , whereas samples with much less H (<3.6 wt% H<sub>2</sub>O, mostly <0.5 wt%) gave 7 different types of IR spectra, suggesting OH groups were present in multiple site environments, an inference supported by NMR spectra on three grossular samples (Cho and Rossman 1993). On the basis of Fourier-transform IR spectra, Eeckhout et al. (2002) concluded that there is no evidence for a multisite OH substitution in spessartine-almandine garnets from Brazilian pegmatites, leaving the hydrogrossular substitution as the only proposed mechanism for the incorporation of H. In summary, garnet samples in which concentrations of H are too low to be studied by conventional X-ray and neutron diffraction techniques give conflicting and equivocal results, whereas H-rich samples in which H can be determined by these techniques give data consistent with  $4\text{H}^{+2}\square \rightarrow \square^{+2}\text{Si}$ . Consequently, for nomenclature purposes, we have assumed that H is incorporated exclusively by  $4\text{H}^{+2}\square \rightarrow \square^{+2}\text{Si}$ .

The symmetry of garnet is predominantly isometric, space group  $Ia\bar{3}d$  (no. 230) but the two species in the henritermierite group have tetragonal symmetry  $I4_1/acd$  (no. 142), and the X, Z, and  $\varphi$  sites are split into more symmetrically unique sites, without altering the topology such that the idealized formula becomes  $\{\text{Ca}_1\} \{\text{Ca}_2\} [\text{R}^{3+}] (\text{Si}_1)_2 (\square)_1 \text{O}_4 (\text{O}_3\text{H})_4$ , where  $\text{R}^{3+} = \text{Mn}$  or Al. Armbruster et al. (2001) concluded that Jahn-Teller distortion resulting from Mn<sup>3+</sup> occupancy of Y and the arrangement of the hydroxyl tetrahedra are coupled, and together are responsible for the lowering to tetragonal symmetry in henritermierite. Moreover, stabilization of the Al-dominant analog holtstamite has been thought to require a minimum Mn<sup>3+</sup> content, which is estimated to be at least 0.2 Mn<sup>3+</sup> per formula unit (pfu), the amount reported in an isometric andradite (Armbruster 1995) and no more than 0.64 Mn<sup>3+</sup> pfu, the lowest amount found in holtstamite, i.e., between 10 and 32% of the henritermierite end-member must be present to stabilize the tetragonal form (Hålenius 2004; Hålenius et al. 2005). However, these arguments are not supported by a Si-deficient spessartine containing no Mn<sup>3+</sup>, but showing  $I4_1/acd$  symmetry attributed to (OH,F)<sub>4</sub> groups (Boiocchi et al. 2012),

implying symmetry lowering could have more than one cause.

In addition, there are numerous reports of natural garnets having orthorhombic, monoclinic, or triclinic symmetry, which have been attributed to crystal growth phenomena, multiple diffraction, strain, and/or cation ordering (e.g., Griffen et al. 1992; McAloon and Hofmeister 1993; Armbruster and Geiger 1993; Rossmann and Armbruster 1995; Hofmeister et al. 1998; Wildner and Andrut 2001; Shtukenberg et al. 2005; Frank-Kamenetskaya et al. 2007). As these structures have essentially the same topology, they are not regarded as separate species (Nickel and Grice 1998).

Table 3 gives the relative abundance of the generalized cations ( $R^{n+}$  with  $n = 1-6$ ) and anions ( $\varphi^{1-}$ ,  $\varphi^{2-}$ ) at each of the sites reported in the  $Ia\bar{3}d$  structure, and presents the major reported cation and anion substituents in natural garnets for each of the valence states of the ions. Table 4 summarizes significant heterovalent substitutions in natural garnet, as well as some chemical relations among species.

### SPECIFIC NOMENCLATURE ISSUES IN THE GARNET SUPERGROUP

Historical information on the 32 approved species of the garnet supergroup is summarized in Appendix 1. A more complete list of 715 synonyms, varietal, obsolete, and discredited names applied to minerals in the garnet supergroup since antiquity has been compiled in Appendix 2<sup>1</sup>. This list includes the synonyms

**TABLE 3.** Relative site abundances of cations and anions in garnet-supergroup minerals

Site	Relative abundance of ions	Cations and anions at each site in order of relative abundance
X	$R^{2+} \gg R^{3+} \gg R^{1+} \gg R^{4+}$	$R^{2+}$ : <b>Fe ~ Mn ~ Ca &gt; Mg</b> >> Pb $R^{3+}$ : Y > HREE > LREE $R^{1+}$ : Na $R^{4+}$ : Th
Y	$R^{3+} > R^{4+} > R^{2+} > R^{5+} > R^{6+}$	$R^{3+}$ : <b>Al ~ Fe</b> > V, Cr, Mn > Sc >> Ga $R^{4+}$ : <b>Ti &gt; Zr</b> > Si, Sn $R^{2+}$ : Mg > Fe, Mn $R^{5+}$ : Sb, Nb $R^{6+}$ : Te, U
Z	$R^{4+} > R^{3+} > R^{2+} \sim \square$ (vacancy) > $R^{2+}$ , $R^{1+}$	$R^{4+}$ : <b>Si</b> >> Ti > Ge $R^{3+}$ : <b>Fe ~ Al</b> $R^{2+}$ : As > V > P $R^{2+}$ : Zn, Fe $R^{1+}$ : Li
$\varphi$	$\varphi^{2-} \gg \varphi^{1-}$	$\varphi^{2-}$ : <b>O</b> $\varphi^{1-}$ : <b>OH</b> > F

Notes: The cations and anions shown in bold type represent the most common ions at these sites. HREE and LREE are heavy and light rare-earth elements, respectively, excluding Y.

**TABLE 4.** Significant garnet coupled heterovalent substitutions

Generalized coupled substitution	Relationship
$\square + 4\varphi^{1-} \rightarrow 2\text{Si}^{4+} + 4\text{O}^{2-}$	relates katoite, henritermierite and holtstamite to OH-free minerals in the garnet group
${}^Y R^{2+} + {}^Y R^{4+} \rightarrow 2{}^Y R^{3+}$	relates morimotoite ( <sup>60</sup> Ti) and majorite ( <sup>60</sup> Si) to other garnet-group minerals
${}^Z R^{4+} + {}^Y R^{3+} \rightarrow {}^Z R^{3+} + {}^Y R^{4+}$	relates the schorlomite group to the garnet group
${}^X(\text{Y, REE})^{3+} + {}^Z R^{3+} \rightarrow {}^X R^{2+} + {}^Z R^{4+}$	introduces Y + REE as a YAG, $\{\text{Ca}_3\}[\text{Al}_2](\text{Al}_2)\text{O}_{12}$ -type component
${}^X(\text{Y, REE})^{3+} + {}^Y \text{Na}^{1+} \rightarrow 2{}^Y R^{2+}$	introduces Y + REE into garnet-group minerals
${}^X(\text{Y, REE})^{3+} + {}^Y R^{2+} \rightarrow {}^X R^{2+} + {}^Y R^{3+}$	relates menzerite-(Y) to other garnet-group minerals
${}^Y R^{5+} + {}^Z R^{3+} \rightarrow {}^Y R^{4+} + {}^Z R^{4+}$	relates bitikleite, dzhuluite and usturite with schorlomite-group minerals
${}^Y 0.5R^{5+} + {}^Z R^{3+} \rightarrow {}^Y 0.5R^{4+} + {}^Z R^{4+}$	relates elbrusite with schorlomite-group minerals
${}^Y \text{U}^{6+} + {}^Z R^{2+} \rightarrow {}^Y R^{4+} + {}^Z R^{4+}$	observed relationship between elbrusite and schorlomite group minerals (Fig. 4)
$0.5{}^X \text{Th}^{4+} + {}^Z R^{3+} \rightarrow 0.5{}^X R^{2+} + {}^Z R^{4+}$	introduces Th into minerals of the bitikleite and schorlomite groups
${}^Y R^{4+} + 0.5{}^V \text{V}^{5+} \rightarrow 0.5{}^Y R^{3+} + {}^V \text{Sb}^{5+}$	introduces V into bitikleite
${}^Y R^{4+} + {}^V \text{V}^{5+} \rightarrow {}^Y \text{U}^{6+} + {}^Z R^{3+}$	introduces V into elbrusite
${}^X \text{Na}^{1+} + {}^Y R^{4+} \rightarrow {}^X R^{2+} + {}^Y R^{3+}$	introduces Na and <sup>60</sup> Si or <sup>60</sup> Ti into the garnet group
${}^X \text{Na}^{1+} + {}^Z R^{5+} \rightarrow {}^X R^{2+} + {}^Z R^{4+}$	relates the berzeliite group to the garnet group

Note: R represents generalized cations (see Table 3).

of current names that have been used in the mineralogical and gemological literature. In the following section, we discuss only those species in which there were problems or difficulties in their original characterization or where the name or formula has had to be significantly modified since the original description.

### Suffixes

With the exception of manganberzeliite (see below), up until 2009, garnets have been given new root names, without prefixes or suffixes. However, since 2009 five new names with suffixes have been approved by the CNMNC. For one of these, menzerite-(Y), the suffix is a Levinson modifier for the rare earth elements (Levinson 1966), whereas the suffixes for the other four garnets identified the dominant tetravalent cation at the Y site, i.e., Sn vs. Zr in two bitikleite species [formerly bitikleite-(SnFe) and bitikleite-(ZrFe)] and elbrusite [formerly elbrusite-(Zr)], and the dominant trivalent cation at the Z site, i.e., Al vs. Fe [formerly bitikleite-(SnAl) and bitikleite-(ZrFe), Table 5]. In the present report we restrict the term “rare earth elements” to the elements from La to Lu (atomic numbers 57–71) and Y (atomic number 39) as defined by Levinson (1966), rather than calling La-Lu “lanthanoids” and including Sc as well as Y in the rare earth elements as recommended by the International Union of Pure and Applied Chemistry. With the exception of the Levinson modifiers for the rare earth elements, e.g., menzerite-(Y), the application of suffixes results in unnecessary complexity in the nomenclature and could lead to confusion as further new spe-

<sup>1</sup> Deposit item AM-13-036, Appendixes 2–4. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at <http://www.minsocam.org>, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

**TABLE 5.** Former names, new names and approved end-member formulas for renamed/discredited minerals listed in this report

Former name	New name (approved by CNMNC)	Formula (approved by CNMNC)
Bitikleite-(SnAl)	Bitikleite	$\{\text{Ca}_3\}[\text{Sb}^{5+}\text{Sn}^{4+}](\text{Al}_2)\text{O}_{12}$
Bitikleite-(SnFe)	Dzuluite	$\{\text{Ca}_3\}[\text{Sb}^{5+}\text{Sn}^{4+}](\text{Fe}_3^{3+})\text{O}_{12}$
Bitikleite-(ZrFe)	Usturite	$\{\text{Ca}_3\}[\text{Sb}^{3+}\text{Zr}](\text{Fe}_3^{3+})\text{O}_{12}$
Elbrusite-(Zr)	Elbrusite	$\{\text{Ca}_3\}[\text{U}_{0.5}^{6+}\text{Zr}_{1.5}](\text{Fe}_3^{3+})\text{O}_{12}$
Hibschite*	Grossular	$\{\text{Ca}_3\}[\text{Al}_2](\text{Si}_{3-x}\square_x)\text{O}_{12-4x}(\text{OH})_{4x}$ where $x < 1.5$ †

\* Former formula:  $\text{Ca}_3\text{Al}_2(\text{SiO}_{4-x})(\text{OH})_{4x}$ , where  $x = 0.2-1.5$ .

† Includes OH-bearing grossular. Ideal anhydrous grossular has the formula:  $\{\text{Ca}_3\}[\text{Al}_2](\text{Si}_3)\text{O}_{12}$ .

cies are discovered. Consequently, we recommend that suffixes (except Levinson modifiers for the REE) not be used for names of minerals in the garnet supergroup. Moreover, as the four garnets with suffixes, which are not Levinson modifiers, have only recently been described and are not entrenched in the literature, we have given these garnets new names without suffixes. This renaming has been approved by the CNMNC as part of the overall nomenclature (Table 5). The etymology of the new names can also be found in Appendix 1.

### “Hydrogarnets”

The nomenclature of naturally occurring garnet containing substantial amounts of the hydroxyl ion has had a complex history (e.g., Pertlik 2003). Many of these garnets have compositions intermediate between grossular ( $x = 0$ ) and katoite ( $x = 3$ ), i.e.,  $\{Ca_3\}[Al_2](Si_{3-x}\square_x)O_{12-4x}(OH)_{4x}$  where  $0 < x < 3$  and  $\square$  is vacancy. For the majority of these garnets,  $x < 1.5$  (e.g., Passaglia and Rinaldi 1984). “Hibschite” was approved by the then Commission on New Minerals and Mineral Names (CNMMN, the predecessor of the CNMNC) as a name for OH-bearing grossular with  $x < 1.5$  (Dunn et al. 1985) because “hibschite” had priority (Cornu 1905, 1906) over “plazolite” (Foshag 1920) and “hydrogrossular” (Hutton 1943). However, “hibschite” is not distinct from grossular according to the dominant-constituent rule, i.e.,  $Si > \square$  at the Z site, therefore “hibschite” is discredited in favor of grossular (Table 5). Dunn et al. (1985) allowed that “the name hydrogrossular may still be applied to members of the series with appreciable OH content but undetermined  $SiO_4/(OH)_4$  ratio.”

Several names have also been used describe the OH-bearing garnets considered together, including the “grossularoid group” (Belyankin and Petrov 1941) and the “hydrogarnet series” (Flint et al. 1941). Dunn et al. (1985) implied that the term “hydrogrossular group” and “hydrogrossular series” would be acceptable for compositions along the grossular katoite join, but in our classification the binary would no longer qualify as a group, whereas the term “series” has a more restrictive meaning than a simple binary solid solution (Mills et al. 2009; see above).

The tetragonal hydroxyl-bearing garnets henritermierite and holtstamite (Fig. 1a) are considered to constitute a distinct group because of their lower symmetry and because one tetrahedral site is largely vacant, i.e.,  $\square > Si$  at one of the two sites corresponding to Z in the archetypal garnet structure (Aubry et al. 1969; Armbruster et al. 2001; Hålenius et al. 2005). Optical determinations are sufficient to distinguish this group from members of the garnet group, and crystal structure determinations are not necessary. Holtstamite is uniaxial and shows a high (0.030) birefringence. In contrast birefringent grossular garnets are normally biaxial (as a consequence of symmetry lowering to orthorhombic, monoclinic, or triclinic symmetries) and show low to moderate (0.001–0.010) birefringence (Shtukenberg et al. 2001, 2005), although birefringence as high as 0.015 has been observed for compositions with considerable andradite component. In addition, the powder XRD pattern for holtstamite and grossular are distinct because they show different  $d$ -spacings for their respective 5 strongest reflections. Henritermierite and holtstamite are distinguished from each other on the basis of the dominant cation at the Y site, respectively  $Mn^{3+}$  and Al.

### Elbrusite

Elbrusite was originally described as “elbrusite-(Zr)” with the formula  $\{Ca_3\}[U^{6+}Zr](Fe_3^{3+}Fe^{2+})O_{12}$  (Table 2 from Galuskina et al. 2010a). Determination of the site occupancies and valence states were hampered by its metamict state, which was nearly complete in elbrusite containing 24 wt%  $UO_3$  (0.62 U per formula unit) and well advanced in U-rich kerimasite (Fe-dominant analog of kimzeyite in the original description) (15–17 wt%  $UO_3$ , 0.37–0.42 U pfu); single-crystal X-ray diffraction was only practical for kerimasite containing 9 wt%  $UO_3$  (0.21 U pfu) (Galuskina et al. 2010a). The authors noted that a Raman band below  $700\text{ cm}^{-1}$  could indicate the presence of some  $Fe^{2+}$  in elbrusite, but the only evidence for U being hexavalent is the association with vorlanite,  $CaU^{+6}O_4$ , for which the hexavalent state of U could be determined (Galuskina et al. 2011a).

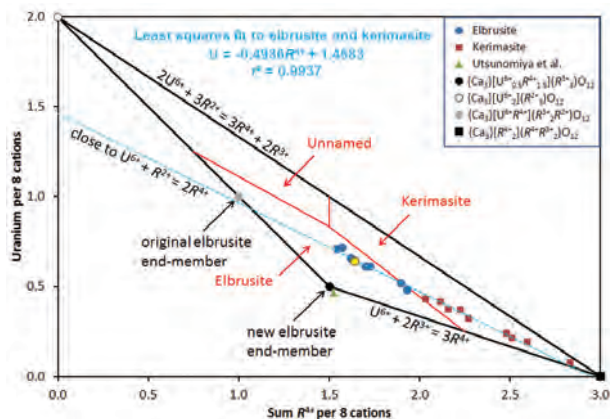
The composition  $\{Ca_3\}[U^{6+}Zr](Fe_3^{3+}Fe^{2+})O_{12}$  is not a valid end-member because more than one site has two occupants (Hawthorne 2002). Instead, it can be considered as the sum of two valid end-members,  $\frac{2}{3}\{Ca_3\}[U_{0.5}^{6+}Zr_{1.5}](Fe_3^{3+})O_{12} + \frac{1}{3}\{Ca_3\}[U_2^{6+}](Fe_3^{3+})O_{12}$  (Fig. 4). Compositions of elbrusite and U-rich kerimasite plot in a linear trend in terms of U and the sum of tetravalent cations between the composition representing kerimasite,  $\{Ca_3\}[R_2^{4+}](R^{4+}R_3^{3+})O_{12}$ , and  $\{Ca_3\}[U^{6+}R^{4+}](R_3^{3+}R^{2+})O_{12}$  (Fig. 4). The trend is very close to the substitution mechanism  $U^{6+}+R^{2+} = 2R^{4+}$ , and thus is consistent with the interpretation by Galuskina et al. (2010a) that U is hexavalent and  $Fe^{2+}$  is present. Moreover, the compositions that Galuskina et al. (2010a) identified as elbrusite and kerimasite plot in the fields for  $\{Ca_3\}[U^{6+}R^{4+}](R_3^{3+}R^{2+})O_{12}$  and  $\{Ca_3\}[R_2^{4+}](R^{4+}R_3^{3+})O_{12}$ , respectively, requiring no revision of their species identifications if  $\{Ca_3\}[U_{0.5}^{6+}Zr_{1.5}](Fe_3^{3+})O_{12}$  is considered to be the end-member of elbrusite. Therefore  $\{Ca_3\}[U_{0.5}^{6+}Zr_{1.5}](Fe_3^{3+})O_{12}$  should now be used as the elbrusite end-member formula.

Yudintsev (2001) and Yudintsev et al. (2002) reported a U-rich garnet, one of three compounds synthesized in corundum crucibles from a  $(Ca_{2.5}U_{0.5})Zr_2Fe_3O_{12}$  bulk composition at  $1400\text{ }^\circ\text{C}$  in air:  $\{Ca_{2.64}U_{0.36}\}[Zr_{1.66}Fe_{0.30}U_{0.04}](Fe_{1.85}Al_{1.15})O_{12}$ , whereas Utsunomiya et al. (2002) reported synthesis of a U-rich garnet with a slightly different composition,  $\{Ca_{2.93}U_{0.07}\}[Zr_{1.52}U_{0.47}Fe_{0.01}](Fe_{1.83}Al_{1.17})O_{12}$ , under unspecified conditions, but presumably similar. Uranium is largely tetravalent in the starting material, and despite having been heated in a relatively oxidizing environment, was assumed by Yudintsev (2001) to have remained mostly tetravalent in the garnet because of its association with cubic oxide with the fluorite structure typical of  $U^{4+}$ . However, charge balance requires that 72–81% of the U be hexavalent in the two synthetic garnets. If U is assumed to be tetravalent at the X site and hexavalent at the Y site, a distribution consistent with the relative sizes of the two U ions, the two formulas give 11.754 and 12.030 positive charges, respectively. The formula of the garnet synthesized by Utsunomiya et al. (2002) is very close to the proposed elbrusite end-member (Fig. 4), and thus provides support for use of this end-member for elbrusite.

### Ti-rich garnets: Schorlomite and morimotoite

The site occupancies of Ti-rich garnets have been the subject of considerable controversy despite being extensively studied using a diverse arsenal of spectroscopic techniques as well





**FIGURE 4.** Compositions of U-rich garnets from the Upper Chegem caldera, Northern Caucasus, Russia (Galuskina et al. 2010a; Utsunomiya et al. 2002). The red lines mark the boundaries between elbrusite, kerimasite and an unnamed species based on the relative proportions of the kerimasite end-member, new elbrusite end-member and the unnamed  $\{Ca_3\}[U_2^{6+}](R_3^{2+})O_{12}$  end-member. Yellow circle indicates the Sn-dominant analog of elbrusite, which was included in the least-squares fit.

as X-ray diffraction (e.g., Chakhmouradian and McCammon 2005). The two species currently accepted by the CNMNC are schorlomite,  $Ca_3(Ti,Fe^{3+})_2(Si,Fe)_3O_{12}$ , and morimotoite,  $Ca_3(Ti,Fe^{2+},Fe^{3+})_2(Si,Fe^{3+})_3O_{12}$  (Table 2). These formulas, which are listed as approved by the CNMNC, are too generalized to indicate what the distinction is between the two species, and clearly new formulas based on end-members are needed.

Schorlomite (Fig. 1f) was first described and named by Shepard (1846), who reported it to be a hydrous silicate containing Y, Fe, and possibly Th from Magnet Cove, Arkansas, U.S.A. However, Whitney (1849) and Rammelsberg (1850a, 1850b) showed schorlomite to be a silicate of Ca, Fe, and Ti, reporting compositions approaching those obtained by modern techniques. Chemical data obtained subsequently of Ti-bearing andradite, often called by the varietal name “melanite,” showed that  $TiO_2$  content ranged continuously from 0 to 19 wt%, whereas Labotka (1995) reported immiscibility at one locality. Grapes et al. (1979) and Laverne et al. (2006) reported up to 30 wt%  $TiO_2$  in garnets having anomalous compositions, which will be discussed separately below. Chakhmouradian and McCammon (2005) summarized the criteria proposed by various authors for distinguishing schorlomite from Ti-bearing andradite; among the most frequently used have been  ${}^7Ti > {}^6Fe^{3+}$  (Ito and Frondel 1967a; Deer et al. 1982), approximately the same as  $TiO_2 > 15$  wt% (Zedlitz 1933) and about twice the minimum Ti content suggested by Howie and Woolley (1968). Chakhmouradian and McCammon (2005) recommended that the proportion of schorlomite be determined as the amount of  ${}^7Ti$ , balanced by substitutions at the Z site, relative to the total occupancy in the Y site,  $({}^7Ti - {}^7Fe^{2+} - {}^7Mg - {}^7Na)/2$ , i.e., deducting a morimotoite component (see below) together with a contribution from a hypothetical  $\{Na_2Ca\}[Ti_2](Si_3)O_{12}$  component. Several end-member formulas have been proposed for schorlomite, e.g.,  $\{Ca_3\}[Ti_2](Fe_2^{3+}Si)O_{12}$  (Ito and Frondel 1967a) and  $\{Ca_3\}[Ti_2](Fe_2^{3+}Ti)O_{12}$  (Rickwood 1968), whereas Chakhmouradian and McCammon

(2005) argued that the crystal chemistry was too complex to be represented by a single end-member, and proposed a generalized formula instead,  $\{Ca_3\}[Ti_2](Si_{3-x})(Fe^{3+},Al,Fe^{2+})_xO_{12}$ .

Morimotoite was introduced by Henmi et al. (1995) with an end-member formula  $Ca_3TiFe^{2+}Si_3O_{12}$ , based entirely on electron-microprobe data of garnet containing nearly 20 wt%  $TiO_2$  from Fuka, Okayama Prefecture, Japan. Formulas that we recalculated assuming 8 cations and 12 O anions from three analyses in Henmi et al. (1995), including the one designated as type, gave 1–8% andradite,  $\{Ca_3\}[Fe_2^{3+}](Si_3)O_{12}$ , 27–34%  $\{Ca_3\}[Ti_2](Fe_2^{3+}Si)O_{12}$ , and 58–71%  $\{Ca_3\}[TiFe^{2+}](Si_3)O_{12}$  with minor Zr, Mg, Mn, and Al included with Ti,  $Fe^{2+}$ , Ca, and  $Fe^{3+}$  according to valence. Garnets synthesized by Henmi et al. (1995) under reducing conditions (iron-wüstite buffer) have compositions very similar to the natural material; end-member morimotoite could not be synthesized. However, no structural or spectroscopic data were obtained to confirm the assumed site occupancies and calculated Fe valence, and thus the report raised objections. Fehr and Amthauer (1996) and Rass (1997) questioned the assumption that Ti was all  $Ti^{4+}$ . The latter authors also dismissed the infrared evidence that Henmi et al. (1995) used to justify their conclusion that OH was absent, and cited experiments by Kühberger et al. (1989) that OH is likely to be present in morimotoite. Their conclusion is supported by the report by Armbruster et al. (1998) that the morimotoite substitution,  $Fe^{2+} + Ti^{4+} \rightarrow 2Fe^{3+}$  at the Y site is coupled with  $4OH^- \rightarrow SiO_4^-$  at the tetrahedral site in Ti-bearing andradite.

Despite the variety of methods deployed to locate cations in the structure of Ti-rich garnets, authors have yet to reach a consensus, which reflects not only differing interpretations of the spectroscopic and structural data, but probably also variation between samples. Nonetheless, the question confronting us is whether we can still propose a meaningful classification based on formulas calculated from a full electron microprobe analysis assuming 8 cations and 12 oxygen anions. There is little disagreement on the occupancy of the X site, which with rare exception contains at least 2.7 (Ca+Na) atoms per formula unit (apfu), to which are added sufficient Mn and Mg to bring total X site occupancy to 3, but fewer authors (e.g., Chakhmouradian and McCammon 2005) would also place  $Fe^{2+}$  at the X site. Problematic issues include the valence and location of Ti and Fe, as well as the location of Al. Locock (2008) reviewed the literature on  $Ti^{3+}$  in garnet and concluded that the oxygen fugacities required for this valence were far too low to be found in most geologic environments. This conclusion is consistent with most spectroscopic studies, for example, X-ray absorption near-edge structure spectroscopy (XANES) has revealed little or no  $Ti^{3+}$  in natural garnet (Waychunas 1987; Locock et al. 1995), whereas electron spin resonance spectroscopy revealed that  $Ti^{3+}$  is much subordinate to  $Ti^{4+}$  in pyrope synthesized under relatively reducing conditions (Rager et al. 2003; Geiger 2004). In contrast, Malitesta et al. (1995) and Schingaro et al. (2004) reported significant  $Ti^{3+}$  in Ti-bearing garnet by X-ray photoelectron spectroscopy (XPS). Since XPS examines the near-surface of a solid, i.e., to a depth of a few tens of angstroms (Hochella 1988), the discrepancy between the XPS and XANES results could be due to differences at the mineral surface not detected by XANES, and consequently we are inclined to accept the conclu-

sion that  $\text{Ti}^{3+}$  plays a negligible role in natural terrestrial garnet, although it could be significant constituent in some meteoritic garnet (e.g., Ma 2012).

As regards the location of Ti, Armbruster et al. (1998) located Ti at Z as well as Y, but most authors place Ti only at Y, which seems reasonable in the relatively Si-rich and Ti-rich garnets ( $\text{Si} > 2$  apfu) because of the rarity of  $\text{Si} = \text{Ti}$  substitution at tetrahedral sites (Hartman 1969). Nonetheless, combined low pressure and high temperature could favor Ti substitution for Si at a tetrahedral site as it does in lamproitic richterite (Oberti et al. 1992). The most robust element-specific technique, XANES, yields results consistent with the bulk of Ti occupying the octahedral site in most natural garnets (Waychunas 1987; Locock et al. 1995). Significant Ti may occupy the Z site in Si-poor garnets such as elbrusite and bitikleite (e.g., Galuskina et al. 2010a, 2010b), and its presence has been demonstrated in Si-free synthetic garnets (Povarennykh and Shabilin 1983; Cartie et al. 1992; Yamane and Kawano 2011). Another question is the possible presence of tetrahedrally coordinated  $\text{Fe}^{2+}$ . Some studies reported Mössbauer spectroscopic evidence for significant  $\text{Fe}^{2+}$  at the Z site (e.g., Locock et al. 1995; Koritnig et al. 1978), but the spectroscopic data do not always give unequivocal site assignments (Chakhmouradian and McCammon 2005). Last, there is the role of the hydroxyl ion; ignoring hydroxyl results in an underestimate of  $\text{Fe}^{2+}$  in the formulas calculated by the method of Droop (1987). However, the effect would be serious only if  $>0.4$  wt%  $\text{H}_2\text{O}$  were present, in which case at least 0.1  $\text{Fe}^{2+}$  per formula unit would not show up in the calculated formula unless OH were included in the formula calculation, i.e.,  $(\text{OH}) + \text{O} = 12$  and  $\sum\{X\} + \sum[Y] + \sum(Z) + \sum\text{O}_{(\text{OH})/4} = 8$ , or if F present,  $\text{O} + (\text{OH}) + \text{F} = 12$  and  $\sum\{X\} + \sum[Y] + \sum(Z) + \sum\text{O}_{(\text{OH})/4} + \sum\text{F}_{/4} = 8$ . The few analyses available in the recent comprehensive studies give 0.02–0.21 wt%  $\text{H}_2\text{O}$  for natural Ti-rich garnets with  $>12$  wt%  $\text{TiO}_2$  (Kühberger et al. 1989; Locock et al. 1995; Amthauer and Rossman 1998; Chakhmouradian and McCammon 2005). An exception is “hydroschorlomite” with 5 wt%  $\text{H}_2\text{O}$  (Galuskin 2005); such  $\text{H}_2\text{O}$ -rich garnets cannot be treated in the approach discussed below.

To identify end-member formulas for the two Ti-rich garnet species schorlomite and morimotoite, we should compare the results from as many studies as possible, which necessitate our relying on chemical data. Few authors have supplemented chemical data with structure refinements using X-ray diffraction and with spectroscopic methods to determine site occupancy, and thus we think that reliance on chemical data is the most consistent approach for treating compositional data from different studies. In addition, we have made the following assumptions in treating the chemical data.

(1) Ti is  $\text{Ti}^{4+}$  and preferentially occupies the Y site, which rules out the end-member  $\{\text{Ca}_3\}[\text{Ti}_2](\text{TiFe}_3^{3+})\text{O}_{12}$  proposed by Rickwood (1968).

(2)  $\text{H}_2\text{O}$  content is  $\leq 0.2$  wt%.

(3) Site occupancies are estimated using formulas calculated for 8 cations and 12 oxygen anions and the procedure outlined in the next section (see below).

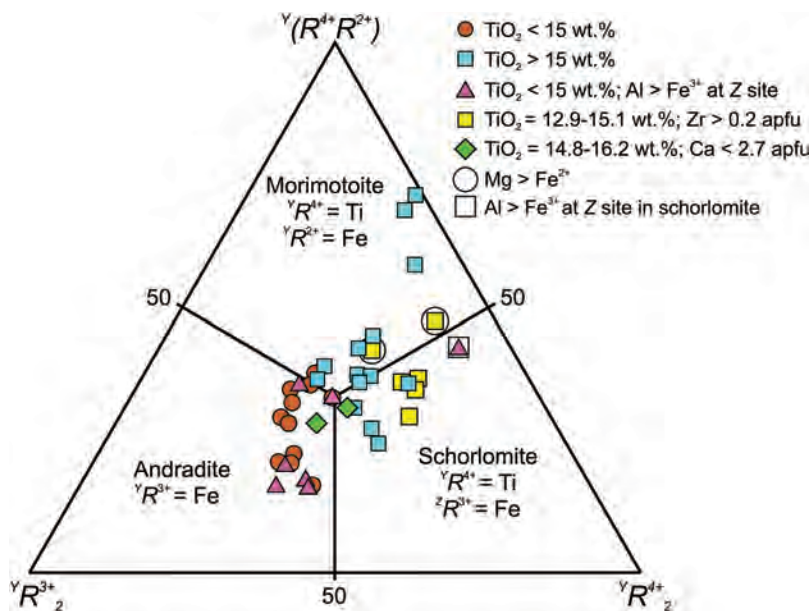
Figure 5 is a plot of Y-site compositions for garnets containing  $>12$  wt%  $\text{TiO}_2$  and  $\text{Ti} > \text{Zr}$  apfu in terms of the following

generalized end-members  $\{\text{Ca}_3\}[\text{R}_3^{3+}](\text{Si}_3)\text{O}_{12}$ ,  $\{\text{Ca}_3\}[\text{R}_2^{4+}](\text{SiR}_3^{3+})\text{O}_{12}$ , and  $\{\text{Ca}_3\}[\text{R}^{4+}\text{R}^{2+}](\text{Si}_3)\text{O}_{12}$ . For  $\text{R}^{4+} = \text{Ti}$ ,  $\text{R}^{3+} = \text{Fe}^{3+}$ , and  $\text{R}^{2+} = \text{Fe}^{2+}$ , these generalized end-members correspond, respectively, to andradite, the schorlomite end-member of Ito and Frondel (1967a), and the morimotoite end-member of Henmi et al. (1995), i.e., the same components plotted by Henmi et al. (1995, their Fig. 1). It turns out that 15 wt%  $\text{TiO}_2$ , which Zedlitz (1933) suggested as a cutoff for schorlomite, is a good estimate of the minimum  $\text{TiO}_2$  content of compositions plotting in the morimotoite and schorlomite fields unless significant Zr is present.

Three reports of garnets reported to contain over 20 wt%  $\text{TiO}_2$  have not been plotted in Figure 5 either because of their high- $\text{H}_2\text{O}$  content or because of their questionable identity as garnet. Galuskina and Galuskin (unpublished data) were able to confirm the identity of an OH-bearing schorlomite in a xenolith from the upper Chegem caldera, northern Caucasus by Raman spectroscopy. Analyses of the cores of two honey-colored crystals about 30  $\mu\text{m}$  across enclosed in grossular-katoite give 12.61–13.75 wt%  $\text{SiO}_2$ , 25.42–25.86 wt%  $\text{TiO}_2$ , 0.41–0.49 wt%  $\text{SnO}_2$ , 2.20–2.28 wt%  $\text{Al}_2\text{O}_3$ , 24.86–26.09 wt% Fe as  $\text{Fe}_2\text{O}_3$ , 31.03–31.71 wt% CaO,  $\leq 0.03$  wt% MgO, and 0.27 to 1.2 wt%  $\text{H}_2\text{O}$  (calculated); Mn, Cr, Zr, Nb, V, Ce, La, Na, F, and Cl were below the detection limit. These data correspond approximately to 73–76%  $\{\text{Ca}_3\}[\text{Ti}_2^{4+}](\text{SiFe}_3^{3+})\text{O}_{12}$ , the highest proportion of the schorlomite end-member reported in a natural garnet, 12–13%  $\{\text{Ca}_3\}[\text{Ti}_2^{4+}](\text{SiAl})\text{O}_{12}$  and 12–14% andradite plus its OH analog. Grapes et al. (1979) reported an electron microprobe analysis of a garnet from Morotu, Sakhalin Island, Russia, containing 27.38 wt%  $\text{TiO}_2$  and 33.50 wt% Fe as FeO, but deficient in Si and Ca with the formula:  $\{\text{Ca}_{1.53}\text{Fe}_{1.46}\text{Mn}_{0.01}\}[\text{Ti}_{1.28}\text{Fe}_{0.71}\text{Mg}_{0.01}](\text{Si}_{1.84}\text{Ti}_{0.60}\text{Fe}_{0.38}\text{Al}_{0.18})\text{O}_{12}$ , i.e., a morimotoite from site occupancies, but anomalous because so much Ti (or  $\text{Fe}^{2+}$ ) is forced by the formula calculation onto the Z site. A possible explanation for the high-Fe and Ti contents is X-ray fluorescence from contiguous phases (Chakhmouradian and McCammon 2005). In a study of altered basalt from the equatorial east Pacific, Laverne et al. (2006) described a “hydroschorlomite” with 22.0–28.6 wt%  $\text{TiO}_2$ , 6.2–12.9 wt% Fe as FeO and 22.5–26.5 wt% CaO. Laverne et al. (2006) tried to correct for celadonite impurities, which were manifested by the presence of  $\sim 1$  wt%  $\text{K}_2\text{O}$  in the analyses. The study included SEM and TEM, as well as micro-Raman spectra, but none provided corroborative evidence that the mineral was indeed a garnet; the reported compositions suggest the mineral could be titanite.

Three analyses, including the holotype, from the type locality of morimotoite in Fuka, Japan, plot in the morimotoite field and show that Ti and  $\text{Fe}^{2+}$  are the dominant  $\text{R}^{4+}$  and  $\text{R}^{2+}$  cations at Y if we assume that Ti and  $\text{Fe}^{2+}$  do not occupy the Z site, whereas four of the five analyses of garnet from the type locality of schorlomite at Magnet Cove, U.S.A., plot in the schorlomite field and show that Ti is the dominant  $\text{R}^{4+}$  cation, and  $\text{Fe}^{3+}$  is the dominant  $^2\text{R}^{3+}$  cation. The latter situation holds even if Al is assumed to preferentially occupy the Z site (e.g., Chakhmouradian and McCammon 2005), which is not supported by all studies (e.g., Locock et al. 1995; Armbruster et al. 1998). Thus, we recommend that  $\{\text{Ca}_3\}[\text{Ti}^{4+}\text{Fe}^{2+}](\text{Si}_3)\text{O}_{12}$  and  $\{\text{Ca}_3\}[\text{Ti}_2^{4+}](\text{SiFe}_3^{3+})\text{O}_{12}$  be the end-member formulas for morimotoite and schorlomite, respectively. Despite the assumptions and simplifications discussed above,





**FIGURE 5.** Plot of the Y-site contents of 40 natural garnets with  $\text{TiO}_2 > 12$  wt% based on formulas normalized to 8 cations and 12 O anions (excluding H); BaO and ZnO not included. Y-site contents were calculated from the relative proportions of (1) Ti+Zr ( $=R^{3+}$  at Z), (2) remaining Ti+Zr as  $R^{4+}R^{2+}$ , and (3)  $R^{3+}$ , which correspond to schorlomite, morimotoite and andradite, respectively. Sources of data: Zedlitz (1935); Lehighjärvi (1960); Gnevushev and Fedorova (1964); Howie and Woolley (1968); Dowty (1971); von Eckermann (1974); Amthauer et al. (1977); Huggins et al. (1977); Koritnig et al. (1978); Platt and Mitchell (1979); Flohr and Ross (1989); Lupini et al. (1992); Henmi et al. (1995); Labotka (1995); Locock et al. (1995); Chakhmouradian and McCammon (2005); Marks et al. (2008); Melluso et al. (2010); Saha et al. (2010). Circles for  $\text{Mg} > \text{Fe}^{2+}$  (total for analysis) have been added only for compositions plotting in the morimotoite field. The square enclosing a triangle indicates the schorlomite in which  $^{\text{Z}}\text{Al} > ^{\text{Z}}\text{Fe}^{3+}$  and 0.55 Zr pfu reported by Koritnig et al. (1978); it is a possible new species, the Al-dominant analog of schorlomite. Compositions are plotted under the assumption that Al preferentially is incorporated at the Z site (except from Fuka, see text).

we believe that Figure 5 can be used to distinguish schorlomite and morimotoite in the absence of structural and spectroscopic studies if allowance is made for the uncertainties in attempting to identify borderline cases.

Figure 5 shows that many garnets reported as schorlomite plot in the morimotoite and andradite fields; garnets plotting in the schorlomite field other than those from Magnet Cove are from Ardnamurchan, Scotland (Huggins et al. 1977), the Tamazeght complex, Morocco (Marks et al. 2008), the Polino carbonatite, Italy (Lupini et al. 1992), and Alnö Island, Sweden (von Eckermann 1974). The dominant  $^{\text{Z}}\text{R}^{3+}$  cation in these garnets is  $\text{Fe}^{3+}$ , even if Al is assumed to preferentially occupy the Z site. Using the above assumptions, garnets plotting in the morimotoite field (with  $\text{Fe}^{2+} > \text{Mg}$  at the Y site) are from Iivaara, Finland (Zedlitz 1935), Afrikanda, Russia (Chakhmouradian and McCammon 2005), Ice River, Canada (Locock et al. 1995; Peterson et al. 1995), Sung Valley, India (Melluso et al. 2010), and Rusing Island, Kenya (Howie and Woolley 1968). However, Mössbauer spectroscopy of the Ice River garnet indicates that a significant proportion of the  $\text{Fe}^{2+}$  is located at the Z site and dominance of  $[(\text{Ti},\text{Zr})_2]$  over  $[(\text{Ti},\text{Zr})\text{R}^{2+}]$  at Y, so Locock et al. (1995) and Peterson et al. (1995) had reason to call this garnet schorlomite. Two relatively Zr-rich garnets from the Marathon Dikes, Ontario, Canada (Platt and Mitchell 1979), also plot in the morimotoite field, but are unique in that total  $\text{Mg} > \text{Fe}^{2+}_{\text{total}}$  (circled in Fig. 5) suggesting the possibility of a Mg-dominant analog of morimotoite (see the section on Possible new species

and compositional variations in natural garnet).

All the analyses plotted in Figure 5 have  $\text{Si} > 2$  and total charge at Z  $> 11$ , i.e., all the garnets would be classed as garnet group, including compositions of schorlomite from the type locality (e.g., Appendix 3<sup>1</sup>). This contradiction arises because the compositions include more garnet-group components, largely andradite,  $\{\text{Ca}_3\}[\text{R}^{3+}](\text{Si}_3)\text{O}_{12}$ , and morimotoite,  $\{\text{Ca}_3\}[\text{R}^{4+}\text{R}^{2+}](\text{Si}_3)\text{O}_{12}$ , than schorlomite-group components, largely,  $\{\text{Ca}_3\}[\text{R}^{2+}](\text{Si}_3)\text{O}_{12}$ .

### Menzerite-(Y)

The validity of menzerite-(Y) has been questioned because the end-member formula proposed for menzerite-(Y),  $\{\text{Y}_2\text{Ca}\}[\text{Mg}_2](\text{Si}_3)\text{O}_{12}$ , is quite far from the measured compositions of the type and only known material, which averages much closer to  $\{\text{Y}(\text{Ca},\text{Fe}^{2+})_2\}[(\text{Mg},\text{Fe}^{2+})(\text{Fe}^{3+},\text{Al})](\text{Si}_3)\text{O}_{12}$ , an empirical formula that can be simplified to  $\{\text{YCa}_2\}[\text{MgFe}^{3+}](\text{Si}_3)\text{O}_{12}$ . This simplified formula is not a valid end-member because it has two sites with two occupants (Hawthorne 2002). Instead, it can be resolved into an equal mixture of  $\{\text{Y}_2\text{Ca}\}[\text{Mg}_2](\text{Si}_3)\text{O}_{12}$  [menzerite-(Y)] and  $\{\text{Ca}_3\}[\text{Fe}^{3+}](\text{Si}_3)\text{O}_{12}$  (andradite). Type menzerite-(Y) compositions are close to the midpoint between these two end-members, but in two grains divalent cations are dominant at the Y site and Mg is the dominant divalent cation at this site (e.g., Appendices 3 and 4), confirming that menzerite-(Y) is a valid species (Grew et al. 2010). Of course, this approach depends on the accuracy of the electron microprobe analyses and calculation of  $\text{Fe}^{3+}/\text{Fe}^{2+}$

ratio from stoichiometry (Droop 1987). The calculated  $\text{Fe}^{3+}/\text{Fe}^{2+}$  ratios are consistent with single-crystal X-ray diffraction data although not with preliminary micro-X-ray absorption near-edge spectroscopy (Grew et al. 2010).

A second argument forwarded to challenge the validity of menzerite-(Y) is that trivalent cations, i.e., Y+REE, are not dominant at the X site in any of the analyzed menzerite-(Y) grains, the maximum being 1.1 Y+REE per formula unit. Simple application of the dominant-valency rule gives  $\{\text{Ca}_3\}[\text{Mg}_2](\text{Si}_3)\text{O}_{12}$ , which is not balanced in charge. Charge balance allows only 2 (Y+REE) per formula unit, i.e., the menzerite end-member should be  $\{\text{Y}_2\text{Ca}\}[\text{Mg}_2](\text{Si}_3)\text{O}_{12}$ . The presence of >1 (Y+REE) means that  $[(\text{Y},\text{REE})_2\text{Ca}]$  exceeds 50% of the maximum possible consistent with valency-imposed double site-occupancy.

Rates of diffusion of Y and REE in garnet provide evidence for the importance of the menzerite component in garnet, i.e., mobility of Y and REE at the X site is closely linked to mobility of Al at the Y site (Carlson 2012).

### Majorite

The current list of CNMNC approved minerals (<http://pub-sites.uws.edu.au/ima-cnmnc/>) gives the formula for majorite as  $\text{Mg}_3(\text{Fe}^{2+},\text{Si})(\text{SiO}_4)_3$  (Table 2), equivalent to  $\{\text{Mg}_3\}[\text{SiFe}^{2+}](\text{Si}_3)\text{O}_{12}$ , which indeed is a good approximation of the empirical formula of the type material reported by Smith and Mason (1970),  $(\text{Mg},\text{Na})_3(\text{Fe},\text{Si},\text{Al},\text{Cr})_2\text{Si}_3\text{O}_{12}$ . It was assumed that Fe occupied the Y site, but the valence and distribution of the Fe were not determined. Recalculating a formula for 8 cations and 12 oxygen anions from the published analysis and listing cations at a given site in order of decreasing abundance gives:  $\{\text{Mg}_{2.91}\text{Na}_{0.09}\}[(\text{Si}_{0.71}\text{Fe}_{0.60}\text{Fe}_{0.41}\text{Al}_{0.22}\text{Cr}_{0.04}\text{Mg}_{0.02})(\text{Si}_3)\text{O}_{12}]$ .

However, the assumption regarding  $\text{Fe}^{2+}$  occupancy is not supported by Mössbauer spectroscopic data on synthetic majorite (Geiger et al. 1991a, 1991b; O'Neill et al. 1993a, 1993b; McCammon and Ross 2003). In a study that included samples that Geiger et al. (1991a, 1991b) and O'Neill et al. (1993a, 1993b) had investigated, McCammon and Ross (2003) reported that  $^x\text{Fe}^{2+}/\Sigma\text{Fe}^{2+} = 0.89\text{--}0.95$ , and  $\text{Fe}^{2+}/(\text{Fe}^{2+}+\text{Mg})$  at X (0.05–0.22) is three to seven times  $\text{Fe}^{2+}/(\text{Fe}^{2+}+\text{Mg})$  at Y (0.01–0.08) in 15 synthetic tetragonal majorite samples, and  $^x\text{Fe}^{2+}/\Sigma\text{Fe}^{2+} = 1.0$  in one isometric synthetic sample, demonstrating that  $\text{Fe}^{2+}$  is strongly fractionated onto the X site. Because the compositions of the type specimen and these synthetic samples are similar, we think it is reasonable to assume that Fe distribution is the same in synthetic and natural majorite, and the partial ordering at the X and Y sites in tetragonal samples does not significantly affect the Fe distribution. Assuming that  $\text{Fe}^{2+}$  occupies only the X site, the formula of the type material becomes  $\{\text{Mg}_{2.31}\text{Fe}_{0.60}\text{Na}_{0.09}\}[(\text{Si}_{0.71}\text{Mg}_{0.62}\text{Fe}_{0.41}\text{Al}_{0.22}\text{Cr}_{0.04})(\text{Si}_3)\text{O}_{12}]$ , i.e., the dominant component is  $\{\text{Mg}_3\}[\text{SiMg}](\text{Si}_3)\text{O}_{12}$ . Consequently, we recommend that  $\{\text{Mg}_3\}[\text{SiMg}](\text{Si}_3)\text{O}_{12}$  be used as the end-member formula for majorite. A natural  $^x\text{Fe}^{2+}$  analog has not been reported, and as far as we are aware, it has not been synthesized (e.g., Kato 1986).

Although synthetic majorite has tetragonal symmetry (space group  $I4_1/a$ , no. 88) resulting from a high degree of ordering of Mg and Si at the two symmetrically unique octahedral sites (e.g., Angel et al. 1989), no naturally occurring tetragonal majorite has been reported. Apparently, majorite in shocked meteorites was

quenched with sufficient rapidity to preserve cubic symmetry (Tomioka et al. 2002). The problem of preserving cubic symmetry on cooling would probably not arise in terrestrial majorite, which contains substantial Al, because incorporation of Al at the Y site is thought to stabilize the cubic structure (Hatch and Ghose 1989). Moore and Gurney (1985) confirmed isometric symmetry for garnet from the Monastery Mine kimberlite pipe, South Africa, one of which we calculated to contain 36% of a generalized majorite component,  $\{\text{R}_3^{2+}\}[\text{MgSi}](\text{Si}_3)\text{O}_{12}$ .

The term “majoritic” has found wide use in the literature on garnets included in diamond (e.g., Harte 2010; Collerson et al. 2010), i.e., garnet is described as “majoritic” if Si is incorporated at the Y site through the “majorite” substitution  $^y\text{R}^{2+}+^y\text{Si} \rightarrow 2^y\text{Al}$  (Table 4). Collerson et al. (2010) also include the contribution from the generalized component  $\{\text{R}^{2+}\text{Na}_2\}[\text{R}_2^{4+}](\text{Si}_3)\text{O}_{12}$  in their majorite substitution parameter,  $X^{\text{Mj}}$ . In contrast to majorite reported from shocked meteorites, in which the majorite component is clearly dominant (Collerson et al. 2010), none of the “majoritic” garnets occurring in diamonds are properly majorite, i.e., the majorite component  $\{\text{Mg}_3\}[\text{SiMg}](\text{Si}_3)\text{O}_{12}$  or  $(\text{R}^{2+}+\text{R}^{4+}) > 2\text{R}^{3+}$  at the Y site, is not dominant, even in sample JF-22 from the Jagersfontein kimberlite, South Africa (Tappert et al. 2005; Harte 2010), which has the highest content of Si at the Y site among terrestrial garnet as far as we are aware: a maximum 47.2%  $\{\text{R}_3^{2+}\}[\text{R}^{4+}\text{Mg}](\text{Si}_3)\text{O}_{12}$  or 44.9%  $\{\text{R}_3^{2+}\}[\text{SiMg}](\text{Si}_3)\text{O}_{12}$  (Appendix 3<sup>1</sup>, example 5). The “Ca-rich majorite” in shock veins of crustal rocks from the Ries impact crater, Germany (Stähle et al. 2011), is not majorite because  $(^y\text{Si}+^y\text{Ti}) < (^y\text{Al}+^y\text{Fe}^{3+}+^y\text{Cr})$ ; instead, the three average compositions comprise about 58–71% pyrope-grossular-almandine, 17–33%  $\{\text{R}_3^{2+}\}[\text{R}^{4+}\text{Mg}](\text{Si}_3)\text{O}_{12}$  (generalized majorite), and 10–13%  $\{\text{R}^{2+}(\text{Na},\text{K})_2\}[\text{R}_2^{4+}](\text{Si}_3)\text{O}_{12}$ , where  $^y\text{R}^{4+} = 90\text{--}93\%$  Si.

### Manganberzeliite

Manganberzeliite,  $\{\text{Ca}_2\text{Na}\}[\text{Mn}_2^{2+}](\text{As}_3^{5+})\text{O}_{12}$  (Fig. 1g) has a complicated history revolving around the use of its name, which is briefly described below. Over 40 yr after the original description of berzeliite from Långban, Filipstad district, Sweden (Kühn 1840), Igelström (1886) described a Sb-bearing, Mn-rich berzeliite-like mineral from the nearby Sjögruvan mine, and named it “pyrrhoarsenite.” On the basis of a new chemical analysis giving 28.38 wt% MnO, Igelström (1894) concluded that “pyrrhoarsenite” is a manganese-dominant variety of berzeliite and could also be referred to as “Mangan-Berzeliit.”

In summarizing his discussion of the mineral, Hintze (1922) wrote that Igelström (1894) had found no antimony and had concluded from his studies that “pyrrhoarsenite” is just a Mn-rich variety of berzeliite. Hintze (1922) cited Igelström’s (1894) conclusion that the mineral containing 28% MnO can be referred to as “Manganberzeliit,” but Hintze (1922) wrote the name in bold type and unhyphenated.

Landergren (1930) used the terms “Mg-berzeliit” and “Mn-berzeliit” for the end-members of the series. These names were later used by other mineralogists studying this series, e.g., Blix and Wickman (1959).

Moore (1972) reported powder XRD data for the type specimen of “pyrrhoarsenite” studied by Igelström (specimen NRM18870324 at the Swedish Museum of Natural History)

from Sjögruvan. He concluded that “pyrrhoarsenite” = berzeliite. However, recent energy-dispersive spectroscopic analyses (Hålenius, unpublished data) of fragments of the mineral from this specimen, as well as cell parameter refinement (Locock, unpublished data) of Moore’s powder X-ray diffraction data, show that it is in fact Mn-dominant berzeliite, i.e., manganberzeliite (or “pyrrhoarsenite”). Prior to publication, Moore in 1971 submitted to the CNMMN a proposal to discredit several of the minerals outlined in his 1972 paper. After Moore published his paper, it was subsequently abstracted by Fleischer (1973), who noted that these minerals were discredited by the CNMMN and that “pyrrhoarsenite” was equivalent to berzeliite. However, the discreditation of pyrrhoarsenite was actually not included in Moore’s proposal to the CNMMN. Therefore, the report by Fleischer (1973), which was then carried forward by Nickel and Mandarino (1987), was in error.

This raises the question whether “pyrrhoarsenite” has priority over manganberzeliite and should be reinstated, although manganberzeliite has been the preferred name since 1894 (e.g., Hintze 1922; Palache et al. 1951). Given that Igelström’s original description of the mineral was poor even by the standards of the late 19th century, e.g., he did not detect the appreciable sodium content, in contrast to his contemporary Sjögren (1894), we conclude that priority does not justify reviving “pyrrhoarsenite” at the present time and manganberzeliite should remain the name for the Mn analog of berzeliite.

#### APPLYING THE NOMENCLATURE OF THE GARNET SUPERGROUP

##### Assumed cation occupancies

A major objective of the classification is to provide a basis for identifying the species of an analyzed garnet from its chemical composition. As is the case for the tourmaline supergroup (Henry et al. 2011), chemical analyses of garnet establish which elements are present, but provide no information on which site(s) they occupy in the structure. Proper site allocation requires single-crystal or Rietveld structure refinement using X-ray or neutron diffraction methods, and spectroscopic data are often also needed for unambiguous site assignment, particularly when constituents could be present in more than one valence state, which is not rare in garnet. However, most investigators have only electron microprobe analyses, which provide no direct evidence of valence state. An added difficulty is that as a result of charge balance requirements, several garnet end-members have one site with mixed occupancy, the so-called valency-imposed double site-occupancy of Hatert and Burke (2008).

For all garnet-supergroup minerals we recommend that cations be allocated from a chemical analysis with the procedure given in the next section. This procedure is analogous to that proposed in connection with the nomenclature recommended for the tourmaline supergroup of Henry et al. (2011). It includes only constituents found in known end-members (Table 1) or some potential end-members (Tables 6–7). Examples illustrating our recommended procedure are given in Appendix 3<sup>1</sup>, and a spreadsheet is given in Appendix 4<sup>1</sup>.

As in the case of many mineral groups, some reasonable assumptions can be made concerning site assignments of specific

cations on the basis of relative abundance (Table 3). Lithium and hydrogen are the only light elements (atomic number < 8) that have been reported in major amounts in garnet supergroup minerals, e.g., cryolithionite and katoite, respectively. When common silicate garnet species are checked for light elements, generally very little is found, i.e., Li contents are reported to not exceed 121 ppm, and Be and B contents, not to exceed 20 ppm (e.g., Grew et al. 1990; Grew 2002a, 2002b; Steppan 2003; Marschall 2005). An exception are the 259–1113 ppm Li in almandine from leucocratic granulite at Horní Bory, Czech Republic, corresponding to 0.019–0.079 Li pfu, determined by laser ablation-inductively coupled plasma-mass spectroscopy (Cempírek et al. 2010 and unpublished data). According to Cempírek et al. (2010), Li could occupy either the *X* site as it does in synthetic  $\{\text{Li}_2\text{Mg}\}[\text{Si}_2](\text{Si}_3)\text{O}_{12}$  (Yang et al. 2009) or sites occupied by Li in synthetic garnets. The majority of synthetic Li garnets are compounds of Li with REE, Ta, Nb, Te, Zr, and Ba that are valued for their high-ionic conductivity (e.g., Cussen 2006, 2010; O’Callaghan and Cussen 2007; Wang and Lai 2012). Lithium occupies not only the *Z* site, but also octahedral sites that are vacant in natural garnet, resulting in Li contents up to 6.8 apfu and cation totals up to 11.8 apfu. Other exceptions involving light elements are the reports of 4.40 wt%  $\text{B}_2\text{O}_3$  determined by electron microprobe analysis (EMPA) in andradite (Galuskin et al. 1995) and 0.45–2.09 wt%  $\text{B}_2\text{O}_3$  by EMPA in OH-bearing grossular (Galuskina et al. 1998, 2001) from the Wiluy River, Yakutia, Russia. Pending studies of Li and B in silicate and hydroxyl garnet, it would be best to assume Li and B, as well as  $\text{S}^{6+}$  (up to 2.27 wt%  $\text{SO}_3$ , equivalent to 0.11 S pfu, Passaglia and Rinaldi 1984; Galuskina et al. 2001), are located at the *Z* site.

Calcium has been assumed to occupy only the *X* site in natural garnet; even in synthetic garnets there are very few reports of Ca at the *Y* site and none can be considered unequivocal (Geller 1967; Lobanov et al. 1989). Nonetheless, it should be noted that Huggins et al. (1977) and Pieper et al. (1983) concluded that a small excess of cations at *X* and a correspondingly small deficit at *Y* could be explained in some cases by small amounts of Ca at *Y*, 0.024–0.055 apfu in andradite and 0.04 apfu in grossular, respectively. Gadas et al. (2012) reported up to 3.15 Ca pfu in grossular from pegmatite at Ruda nad Moravou, Czech Republic.

Scandium is assumed to occupy only the *Y* site as in eringaitite, although its role could depend on the occupancy of *X* if synthetic garnets are any guide, where Sc preferentially occupies *Y* only in andradite, whereas in pyrope, *X* is favored and in grossular, a more even distribution (Oberti et al. 2006; Quartieri et al. 2006). Titanium is assumed to be tetravalent, and V, either pentavalent or trivalent. The last assumption received validation from Bordage et al. (2010), who reported that V was entirely  $\text{V}^{3+}$  in a grossular (variety “tsavorite” containing 0.14 V pfu) based on the *K*-edge X-ray absorption near-edge structure (XANES) spectra obtained with high-energy resolution fluorescence-detected X-ray absorption spectroscopy. In contrast, Righter et al. (2011) reported mixed valences also based on the *K*-edge X-ray absorption near-edge structure in other garnets, viz. 2.46–2.55  $\pm 0.15$  in pyrope of mantle origin and 2.56–2.67 ( $\pm 0.15$ ) for V valence in a goldmanite from the Czech Republic, i.e., 40% of the V in the goldmanite is  $\text{V}^{2+}$ , the remainder  $\text{V}^{3+}$ . However, this conclusion is in contrast to the structural and chemical data reported by these authors.



**TABLE 6.** Components and end-members reported in the literature, but not yet found to be dominant in natural garnet

Name	X	Y	Z	$\psi$	Syn?	Occurrence in natural garnet	Source
<b>"Kenogarnet" group</b>							
Fe <sup>3+</sup> analog of katoite	Ca <sub>3</sub>	Fe <sub>3</sub> <sup>2+</sup>	□ <sub>3</sub>	(OH) <sub>12</sub>	Yes	≤35 mol% in andradite	(1)
F analog of katoite	Ca <sub>3</sub>	Al <sub>2</sub>	□ <sub>3</sub>	F <sub>12</sub>	No	≤11 mol% in OH-bearing grossular	(2)
Mn <sup>2+</sup> , F analog of katoite	Mn <sub>3</sub> <sup>2+</sup>	Al <sub>2</sub>	□ <sub>3</sub>	F <sub>12</sub>	–	≤8 mol% in spessartine	(3)
<b>Unnamed group</b>							
Pb <sup>2+</sup> analog of yafsoanite	Pb <sub>3</sub>	Te <sub>3</sub> <sup>6+</sup>	Zn <sub>3</sub>	O <sub>12</sub>	–	9 mol% in yafsoanite	(4)
unnamed	Ca <sub>3</sub>	U <sub>3</sub> <sup>6+</sup>	Fe <sub>3</sub> <sup>3+</sup>	O <sub>12</sub>	–	≤24 mol% in elbrusite	(5)
<b>Henritermierite group</b>							
Mn <sup>2+</sup> analog of holtstamite	Mn <sub>3</sub> <sup>2+</sup>	Al <sub>2</sub>	Si <sub>2</sub> □	O <sub>8</sub> (OH) <sub>4</sub>	–	28 mol% in spessartine	(6)
Mn <sup>2+</sup> , F analog of holtstamite	Mn <sub>3</sub> <sup>2+</sup>	Al <sub>2</sub>	Si <sub>2</sub> □	O <sub>8</sub> F <sub>4</sub>	–	20 mol% in spessartine	(6)
<b>Bitikleite group</b>							
unnamed	Th <sub>0.5</sub> Ca <sub>2.5</sub>	R <sub>2</sub> <sup>2+</sup>	R <sup>3+</sup>	O <sub>12</sub>	Yes	≤20 mol% in kerimasite	(7)
<b>Unnamed group</b>							
Y <sub>3</sub> Al <sub>5</sub> O <sub>12</sub> , Y <sub>3</sub> Fe <sub>5</sub> O <sub>12</sub>	(Y,REE) <sub>3</sub> <sup>3+</sup>	R <sub>2</sub> <sup>2+</sup>	R <sup>3+</sup>	O <sub>12</sub>	Yes	≤8 mol% in menzerite-(Y), spessartine, andradite	(8)
<b>Garnet group</b>							
"Blythite" in part	R <sub>2</sub> <sup>2+</sup>	Mn <sub>3</sub> <sup>2+</sup>	Si <sub>3</sub>	O <sub>12</sub>	Yes	≤9 mol% in calderite-andradite±spessartine	(9)
Fe analog of menzerite-(Y)	Y <sub>2</sub> Ca	Fe <sub>3</sub> <sup>2+</sup>	Si <sub>3</sub>	O <sub>12</sub>	–	≤20 mol% in menzerite (Y)	(10)
unnamed	(Y,Yb) <sub>1.5</sub> Na <sub>1.5</sub>	R <sub>2</sub> <sup>2+</sup>	Si <sub>3</sub>	O <sub>12</sub>	–	≤7 mol% in almandine, spessartine, grossular	(11)
unnamed	R <sup>2+</sup> Na <sub>2</sub>	Si <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>	Yes	≤12 mol% in pyrope-grossular	(12)
<b>Berzeliite group</b>							
unnamed	Na <sub>3</sub>	Al <sub>2</sub>	P <sub>3</sub>	O <sub>12</sub>	Yes	<1 mol% in almandine and pyrope	(13)
unnamed	Ca <sub>2</sub> Na	Fe <sub>2</sub> <sup>2+</sup>	As <sub>3</sub> <sup>5+</sup>	O <sub>12</sub>	No	<6 mol% in berzeliite	(14)

Note: Syn? = has compound been synthesized? Yes: synthesis in which component is dominant as well as syntheses in which component constitutes 100%. No: synthesis attempted but failed. Sources for contents in natural garnets and syntheses of end-members:

(1) Armbruster (1995); Cohen-Addad (1970).

(2) Chakhmouradian et al. (2008); Takamori et al. (1987).

(3) Smyth et al. (1990).

(4) Mills et al. (2010).

(5) Galuskina et al. (2010a).

(6) Si and □ are not fully ordered at Z1 and Z2. Boiocchi et al. (2012).

(7) Ito and Frondel (1967a); Yudinsev (2003); Galuskina et al. (2010e and unpublished).

(8) Yoder and Keith (1951); Geller (1967); Jaffe (1951); Kasowski and Hogarth (1968); Grew et al. (2010).

(9) Fursenko (1982); Nishizawa and Koizuma (1975); Böhn et al. (1995); Amthauer et al. (1989); Arlt et al. (1998).

(10) Grew et al. (2010).

(11) Enami et al. (1995); Røhr et al. (2007).

(12) Ringwood and Major (1971); Stähle et al. (2011).

(13) Bishop et al. (1978); Ye et al. (2000); Breiter et al. (2005); Brunet et al. (2006).

(14) Nagashima and Armbruster (2012); Ito (1968).

### Site allocation of cations

The assumed occupancies, most importantly, <sup>7</sup>Li, <sup>4</sup>Ca, <sup>4</sup>Sc, Ti<sup>4+</sup>, V<sup>3+</sup>, and V<sup>5+</sup> in conjunction with Table 3, lead to the following procedure for recasting chemical data into idealized site occupancies for purposes of classification.

(1) Calculate formulas from the chemical analysis assuming 8 cations and 12 anions and apportion Fe<sup>2+</sup> and Fe<sup>3+</sup> or Mn<sup>2+</sup> and Mn<sup>3+</sup> if calculations give negative values for Fe<sup>2+</sup> (method of Droop 1987). If quantitative F or H data are available, assume  $Z\Box = \frac{1}{4}F + \frac{1}{4}H$ . In this case, the basis for formula calculation becomes O+(OH)+F = 12 and  $\sum\{X\} + \sum\{Y\} + \sum\{Z\} + Z\Box_{(OH)_4} + Z\Box_{F/4} = 8$ .

(2) Li, Zn, P, As<sup>5+</sup>, and V<sup>5+</sup> to Z. If Li < 1/4F, assume sufficient vacancies to make up the deficit (see step 1).

(3) Si and Ge: First to Z to a maximum of 3 apfu, including □, overflow to Y.

(4) Al: First to Z to bring total to 3 apfu, then Y.

(5) Fe<sup>3+</sup>: First to Z to bring total to 3 apfu, then Y.

(6) Ca, Na, K, Y, REE, Th, Pb to X.

(7) Al (remainder after deducting Al at Z), Sc<sup>3+</sup>, Ti<sup>4+</sup>, V<sup>3+</sup>, Cr<sup>3+</sup>, Mn<sup>3+</sup>, Fe<sup>3+</sup> (remainder after deducting Fe<sup>3+</sup> at Z), Ga, Zr<sup>4+</sup>, Hf<sup>4+</sup>, Nb<sup>5+</sup>, Sn<sup>4+</sup>, Sb<sup>5+</sup>, Te<sup>6+</sup>, and U<sup>6+</sup> to Y. If Z is still <3 apfu, then add Fe<sup>2+</sup> to bring Z total to 3 apfu. If the content of Y exceeds 2 apfu, and Z is <3 apfu, then move Ti to Z to bring Z total to 3 apfu.

(8) Mg: First to Y to bring total to 2 apfu, then to X.

(9) Fe<sup>2+</sup> (remainder after deducting Fe<sup>2+</sup> at Z): First to Y to bring total to 2 apfu, then to X.

(10) Mn<sup>2+</sup>: First to Y to bring total to 2 apfu, then to X. This should bring total X to 3 apfu, if calculations were done correctly.

If H is suspected, but no quantitative data are available, as is the case with electron microprobe analyses, then either its content must be assumed so that Fe<sup>2+</sup>/Fe<sup>3+</sup> ratio can be calculated, or the Fe<sup>2+</sup>/Fe<sup>3+</sup> ratio must be assumed so that H content can be calculated. In garnets containing significant Si, it is reasonable to assume that H is incorporated at the expense of Si, that is, H = 4\*(Z□).

The site allocation procedure above, based solely on chemical data, fails to differentiate holtstamite from grossular, which would require additional information such as optical properties or crystallographic data, although henritermierite is uniquely determined because there is no report as yet of an isometric garnet having the composition {Ca<sub>3</sub>}[Mn<sub>3</sub><sup>2+</sup>](Si<sub>2</sub><sup>2+</sup>□)O<sub>8</sub>(OH)<sub>4</sub>.

We have also prepared an Excel spreadsheet (Appendix 4) to perform the above cation allocation, species and group determination, but have omitted several elements that rarely exceed 1 wt% in natural garnets: B, S, K, Ni, Sr; or which occur in significant amounts but whose occurrence is rare: Ga, Ge, and Pb (Tables 6 and 8).

### Identifying a garnet species

Once the cations have been allocated, then the dominant valence is determined for each site by summing the ions for each valence, e.g., Ca+Mg+Mn at the X site, and then the dominant

cation identified. As species are defined in terms charge-balanced end-members (Hawthorne 2002), the possibility of valency-imposed double site-occupancy (Hatert and Burke 2008) must be considered. The dominant ion for each valence determines the species (e.g., bitikleite group, Fig. 6). Six examples are given in Appendix 3<sup>1</sup>, and a calculation procedure for species and group determination in Appendix 4<sup>1</sup>. Our discussion below is limited to the schorlomite and garnet groups because these are most likely to cause difficulties in identifying species.

### Applying the nomenclature to the schorlomite group

Characteristic of the end-member formulas in this group is Si = 1 apfu; there are no divalent and trivalent cations at the Y site and no divalent or pentavalent cations at the Z site. However, in most analyses of Ti-, Zr-, or Sn-rich garnets containing minor Sb<sup>5+</sup>, Nb<sup>5+</sup>, or U<sup>6+</sup>, Si commonly exceeds 1 apfu, e.g., all the analyses plotting in the schorlomite field in Figure 5 have Si > 2 apfu and total charge at the Z site > 11, because all contain substantial proportions of garnet group components (see above).

The primary criterion for a composition to belong to the schorlomite group is that the generalized schorlomite component  $\{R_3^{2+}\}[R_3^{4+}](R^{4+}R_3^{2+})O_{12}$  be the most abundant (Fig. 7); i.e., the spreadsheet gives this as the most abundant component possible.

In the worked example of schorlomite from the type locality, Magnet Cove, Arkansas (Example 2), the schorlomite component is dominant, with  $R^{4+} > R^{3+} > R^{2+}$  at the Y site in the empirical formula (Example 2), whereas in the garnet-group mineral morimotoite, the generalized morimotoite component,  $\{R_3^{2+}\}[R^{4+}R^{2+}](R_3^{3+})O_{12}$ , is dominant with  $R^{4+} > R^{2+} > R^{3+}$  at the Y site in the empirical formula (Example 5). Homovalent substitutions at the Y and Z sites distinguish species within the schorlomite group (Figs. 7 and 8), whereas the X site remains occupied exclusively by Ca in all end-members (Table 1).

### Applying the nomenclature to the garnet group

In contrast to the schorlomite group, heterovalent substitutions relating species within the garnet group involve only the Y site, or the X and Y sites. Figure 9 illustrates the division of the garnet group in terms of valence of the Y site cations:  $R^{2+}$  = menzerite-(Y),  $R^{3+}$  = the familiar silicate garnets, and  $R^{2+}R^{4+}$  = majorite, morimotoite, which results from valency-imposed double site-occupancy.

Figure 10 illustrates one approach to identification of species in complex garnet-group minerals. It is the same as Figure 9, but adapted specifically for compositions of menzerite-(Y) reported by Grew et al. (2010), i.e.,  $R^{4+}$  = Ti,  $R^{3+}$  = Fe<sup>3+</sup>, Al,

**TABLE 7.** Summary of specific components potentially significant in natural garnets

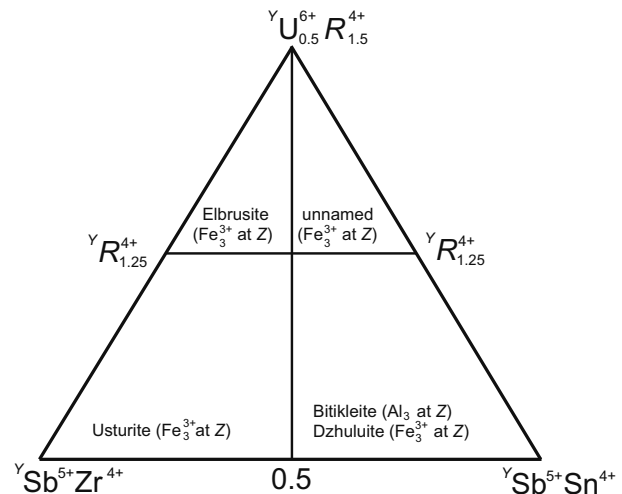
Name	Synthesis	Formula
–	62 to 90%	$\{Fe_3^{2+}\}[Al_2](\square_3)(OH)_{12}$
–	No	$\{Ca_3\}[Al_2](\square_3)F_{12}$
–	–	$\{Mn_3^{2+}\}[Al_2](\square_3)F_{12}$
–	–	$\{Fe_3^{2+}\}[Al_2](\square_3)F_{12}$
–	–	$\{Pb_3^{2+}\}[Te_2^{2+}](Zn_3)O_{12}$
–	–	$\{Ca_3\}[U_3^{6+}](Fe_3^{2+})O_{12}$
–	–	$\{Mn_3^{2+}\}[Al_2](Si_2)(\square)O_4(OH)_4$
–	–	$\{Mn_3^{2+}\}[Al_2](Si_2)(\square)O_8F_4$
–	–	$\{Th_{0.5}Ca_{2.5}\}[Zr_2](Fe_3^{2+})O_{12}$
YIG	100%	$\{Y_3\}[Al_2](Al_3)O_{12}$
YAG	100%	$\{Y_3\}[Fe_3^{2+}](Fe_3^{3+})O_{12}$
"Blythite"	100%	$\{Mn_3^{2+}\}[Mn_3^{2+}](Si_3)O_{12}$
–	100%	$\{Ca_3\}[Mn_3^{2+}](Si_3)O_{12}$
"Khoharite"	100%	$\{Mg_3\}[Fe_3^{2+}](Si_3)O_{12}$
"Skiagite"	100%	$\{Fe_3^{2+}\}[Fe_3^{2+}](Si_3)O_{12}$
–	–	$\{Y_2Ca\}[Fe_2^{2+}](Si_3)O_{12}$
–	–	$\{Y_{1.5}Na_{1.5}\}[Al_2](Si_3)O_{12}$
–	100%	$\{CaNa_3\}[Si_2](Si_3)O_{12}$
–	100%	$\{CaNa_3\}[Ti_2](Si_3)O_{12}$
–	100%	$\{Na_3\}[Al_2](P_3)O_{12}$
–	No	$\{Ca_2Na\}[Fe_2^{2+}](As_3^{3+})O_{12}$

Note: Syntheses: percentage gives the amount of the component reported in the synthesis; no = synthesis attempted but without success, dash = synthesis has not been not attempted. Sources are given in the text and Table 6.

**TABLE 8.** Possible new species in the garnet supergroup

Relationship to known species	UM no.	End-member formula	Criteria	Source
<b>Bitikleite group</b>				
Sn analog of elbrusite		$\{Ca_3\}[U_{0.5}^{6+}Sn_{1.5}^{4+}](Fe_3^{3+})O_{12}$	$Sn/(Sn + Zr) = 0.93$	(1)
Nb analog of usturite		$\{Ca_3\}[NbZr](Fe_3^{3+})O_{12}$	1.33 Zr, 0.05 Ti, 0.48 Nb pfu at Y site	(2)
<b>Schorlomite group</b>				
Al analog of schorlomite (Ti analog of kimzeyite)		$\{Ca_3\}[Ti_2](SiAl_2)O_{12}$	$Al/(Al+Fe^{3+}) = 0.65$	(3)
<b>Garnet group</b>				
Mg analog of morimotoite		$\{Ca_3\}[TiMg](Si_3)O_{12}$	$Mg/(Mg + Fe^{2+}) = 0.63-0.64$	(4)
Ga-Ge analog of grossular	UM1986-19	$\{Ca_3\}[Ga_2](Ge_3)O_{12}$	${}^ZGe > {}^ZSi; {}^YGa > {}^YFe^{3+}, {}^YAl$	(5)
Ge analog of grossular	UM1986-20	$\{Ca_3\}[Al_2](Ge_3)O_{12}$	Criterion of ${}^ZGe > {}^ZSi$ not met.	(5)

Note: UM no. refers to the list of valid unnamed minerals, update 2011-01 (Smith and Nickel 2007). Sources: (1) Galuskina et al. (2010a); (2) Zaitsev et al. (2010); (3) Koritnig et al. (1978); (4) Platt and Mitchell (1979); (5) Johan and Oudin (1986); Jambor et al. (1988b).



**FIGURE 6.** Y-site occupancy in species of the bitikleite group, including the possible unnamed Sn-dominant analog of elbrusite. Placement of the divisions is indicated.

and  $R^{2+} = \text{Mg}, \text{Fe}^{2+}$ , and differs from Figure 7a of Grew et al. (2010) in that the Ti corner is now  $\text{Ti}R^{2+}$ , representing a component in garnet, morimotoite. However, menzerite-(Y) is a four component system because of the substitution of  $R^{3+}$  for Si at the Z site, and compositions must be projected from four-component space onto the three-component plane shown in Figure 10. Appendix 3<sup>1</sup> (Example 3) gives the five possible generalized components in menzerite-(Y), of which only four are independent. We have selected the  $\{\text{Y}_3\}[\text{Al}_2](\text{Al}_3)\text{O}_{12}$ -type component to project menzerite-(Y) compositions. The  $\{\text{Y}_3\}[\text{Al}_2](\text{Al}_3)\text{O}_{12}$ -type component comprises 4–8% of the analyzed menzerite-(Y) grains. Despite the differences between Figure 10 and Figure 7a of Grew et al. (2010), the disposition of the points is very similar.

The most widespread garnet-group minerals are related by homovalent substitutions at the X and Y sites, i.e.,  $\{R_3^{3+}\}[R_2^{3+}]$

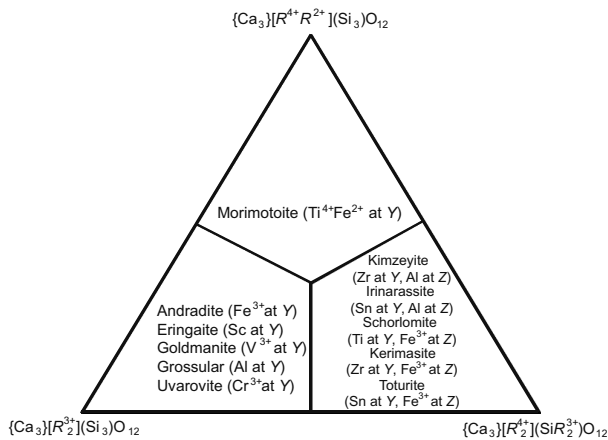


FIGURE 7. Diagram for discriminating the five species of the schorlomite group from Ca species in the garnet group.

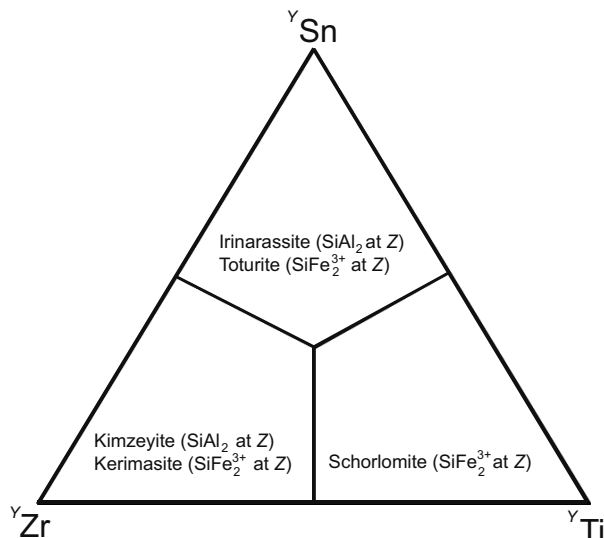


FIGURE 8. Y-site occupancy in species of the schorlomite group.

$(\text{Si}_3^+)\text{O}_{12}$ . Since only four constituents occupy the X site, the compositions can be plotted in a tetrahedron with Ca, Mg,  $\text{Mn}^{2+}$ , and  $\text{Fe}^{2+}$  as vertices (Fig. 11a). Garnets with one of these cations dominant at the X site fill a volume whose edges inside the Ca-Mg-Mn<sup>2+</sup>-Fe<sup>2+</sup> tetrahedron are shown as lines inside this tetrahedron. Figures 11b and 11c show compositions projected from the Mn and Ca vertices of the tetrahedron, respectively. These two faces of the tetrahedron suffice to illustrate the dispositions of the species. Final characterization will depend on the dominant occupancy of the Y site.

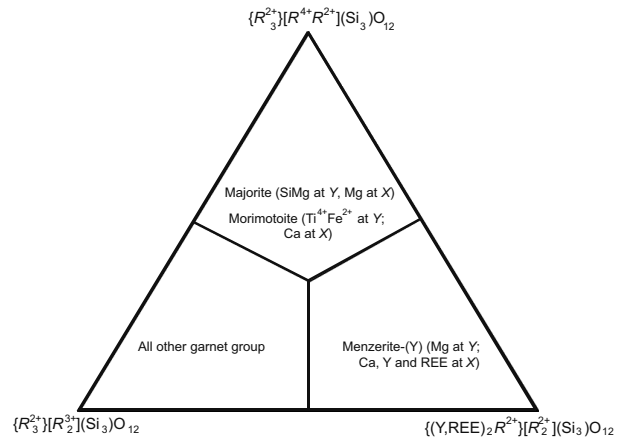


FIGURE 9. Diagram distinguishing menzerite-(Y) from species within the garnet group.

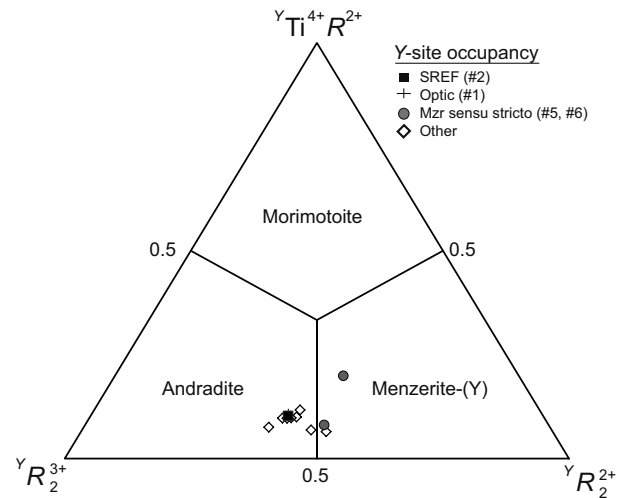


FIGURE 10. Plot of menzerite-(Y) compositions at the Y site projected from  $\{\text{Y}_3\}[\text{R}_2^{3+}](\text{R}_3^+)\text{O}_{12}$  onto the plane defined by the components  $\{\text{Ca}_3\}[\text{Ti}^{4+}\text{R}^{2+}](\text{Si}_3^+)\text{O}_{12}$ ,  $\{\text{Ca}_3\}[\text{R}_2^{3+}](\text{Si}_4^+)\text{O}_{12}$ , and  $\{(\text{REE})_2\text{Ca}\}[\text{R}_2^{2+}](\text{Si}_3^+)\text{O}_{12}$  (cf. Fig. 7a, Grew et al. 2010).  $R^{2+} = \text{Fe}$  in morimotoite, Mg in menzerite-(Y);  $R^{3+} = \text{Fe}$  in andradite. Numbers refer to grains used for the crystal-structure refinement (SREF), optical measurements, and menzerite-(Y) sensu stricto (Mzr), including grain no. 5 used as the holotype to characterize the mineral. The points for SREF and Optic are superimposed. Open diamonds indicate the other nine grains analyzed (data from Grew et al. 2010).



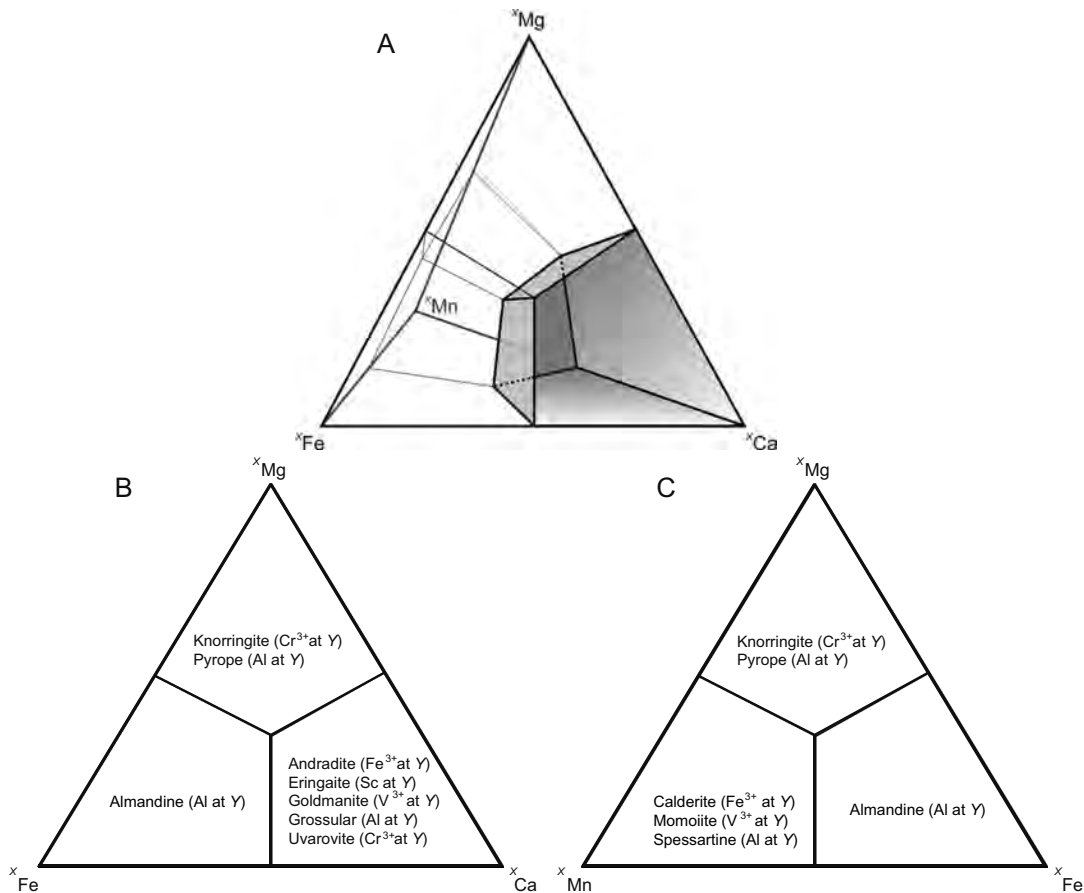
### Possible new species and compositional variations in natural garnet

The compositional variations found in the 32 approved species by no means exhaust the compositional variations observed in natural garnet, which is greatly exceeded by the very extensive variations in synthetic garnet. In the present section we will consider these variations, note compositions containing components that could be new species if they were present in larger amounts (Tables 6 and 7), and briefly describe possible new species (Table 8). Synthetic garnets will be considered only in so far that they relate to natural garnets. The components are discussed under the group to which they would belong.

### Vacancy-dominant garnets—A “kenogarnet” group?

Vacancy-dominant garnets are distinguished by  $\varphi$  being a monovalent anion such as OH or F, as well as low content of cations at the Z site. Katoite is the only known garnet that is vacancy-dominant. However, there is considerable potential to discover more species, and thus a group could be recognized following the procedures outlined in Mills et al. (2009). In anticipation, we suggest the name “kenogarnet” from the Greek *kenos*, meaning “empty,” a term introduced as a prefix in pyrochlore supergroup nomenclature (Atencio et al. 2010).

The most abundant vacancy-dominant garnets are the so-called “hydrogarnets,” an informal term (Appendix 2) introduced by Flint et al. (1941) and generally used for any garnet containing OH incorporated by the substitution of  $(\text{O}_4\text{H}_4)$  tetrahedra for  $(\text{SiO}_4)$  tetrahedra (Fig. 3). Significant incorporation of OH by this substitution is largely limited to garnet in which the X site is occupied by Ca, e.g., katoite, henritermierite, and holtstamite. Up to 10 wt%  $\text{H}_2\text{O}$  has also been reported in andradite (Peters 1965; Lager et al. 1989; Armbruster 1995; Amthauer and Rossman 1998), leading to compositions with up to 35% of the  $\text{Fe}^{3+}$  analog of katoite (Table 6) and 4.5% of its  $\text{Mn}^{3+}$  analog (H content calculated by difference from Si occupancy determined by single-crystal refinement, Armbruster 1995). Galuskina and Galuskin (2003) and Galuskin (2005) calculated OH contents of 2.6–2.9 apfu (equivalent to 4.8–5.1 wt%  $\text{H}_2\text{O}$ ) from charge balance in “hydroschorlomite” containing 13.5–14.5 wt%  $\text{TiO}_2$  from the Wiluy River, Yakutia, Russia, the highest reported in Ti-rich garnets (cf. Chegem caldera schorlomite discussed above). In contrast,  $\text{H}_2\text{O}$  contents in pyrope, almandine, and uvarovite are reported not to exceed 0.3 wt%, and, in spessartine, not above 0.64 wt% (e.g., Aines and Rossman 1984; Rossman et al. 1988; Smyth et al. 1990; Andrut and Wildner 2001; Maldener et al. 2003; Beran and Libowitzky 2006; Johnson 2006). Wilkins and Sabine (1973) reported 2.5 wt%  $\text{H}_2\text{O}$  in spessartine,



**FIGURE 11.** (a) Tetrahedron illustrating divisions in the garnet group based on occupancy of the X site. One compositional volume is shown with shading. (b) Projection from the Mn vertex onto front face of the tetrahedron to distinguish species. (c) Projection from the Ca vertex onto left face of the tetrahedron to distinguish species.

but this high content is anomalous and needs confirmation.

Only “hydrogarnets” with the large cations Ca and Sr (Ito and Frondel 1967b; Ivanov-Emin et al. 1982a, 1982b) at the *X* site have been synthesized, including katoite (Flint et al. 1941; Cohen-Addad et al. 1967). Syntheses of the hydroxyl-dominant analogues of uvarovite (Morán-Miguel et al. 1986) and eringaite (Ivanov-Emin et al. 1982a); as well as of  $\{Ca_3\}[Mn_2^{3+}](\square_3)(OH)_{12}$  (Ivanov-Emin et al. 1982b),  $\{Ca_3\}[TiFe^{3+}](Fe^{3+}\square_2)(OH)_8O_4$  (Ito and Frondel 1967b), and  $\{Ca_3\}[ZrFe^{3+}](Fe^{3+}\square_2)(OH)_8O_4$  (Ito and Frondel 1967b) have been reported. However, attempts to synthesize the end-member  $\{Ca_3\}[Fe_2^{3+}](\square_3)(OH)_{12}$  failed, although a garnet with about 90%  $\{Ca_3\}[Fe_2^{3+}](\square_3)(OH)_{12}$  and 10% andradite could be synthesized (Flint et al. 1941; Ito and Frondel 1967b). The reported compositions are based on starting materials; only the compositions of katoite and a hydroxyl-dominant analog of andradite,  $\{Ca_3\}[Fe_2^{3+}](Si_{1.15}\square_{1.85})(OH)_{7.4}O_{4.6}$ , have been confirmed independently (e.g., by structure refinement, Cohen-Addad 1970; Cohen-Addad et al. 1967). In summary, the H<sub>2</sub>O contents of natural and synthetic garnets are consistent with the conclusion reached by Lager et al. (1989) that the extent of OH substitution in garnets appears to be structurally controlled, i.e., it is greater, when the effective ionic radius (Shannon 1976) of the *X*-site cation exceeds 1.0 Å and the shared octahedral edge is longer than the unshared edge, which is the case for natural and synthetic garnets with Ca dominant at the *X* site (Novak and Gibbs 1971; Quartieri et al. 2006).

Fluorine contents up to 6 wt% F, equivalent to about 11 mol% of a  $\{R_3^{3+}\}[R_3^{3+}](\square_3)F_{12}$ , have been reported in grossular, spessartine, and andradite (Valley et al. 1983; Flohr and Ross 1989; Manning and Bird 1990; Smyth et al. 1990; Barbanson and Bastos Neto 1992; Visser 1993; Włodyka and Karwowski 2006; Chakhmouradian et al. 2008). Only Smyth et al. (1990) measured H<sub>2</sub>O content, reporting 0.64 wt% in the F-bearing spessartine (Table 6), equivalent to 3%  $\{R_3^{3+}\}[R_3^{3+}](\square_3)(OH)_{12}$ , but Flohr and Ross (1989) and Chakhmouradian et al. (2008) reported evidence for H<sub>2</sub>O in the infrared and Raman spectra. Attempts to synthesize an F-dominant analog of katoite have not been successful (Takamori et al. 1987).

Chlorine was sought in four of the studies of F-bearing garnet cited above, but no more than 0.01 wt% Cl was reported. Up to 0.2 wt% Cl was reported in OH-bearing grossular from the Wiluy River, Yakutia, Russia (Galuskina et al. 2001). Chesnokov (1996), Chesnokov and Bushmakina (1995), and Chesnokov et al. (1994, 2008) described “igumnovite,” ideally  $\{Ca_3\}[Al_2](Si_2\square)O_8Cl_4$ , and “chlorhibschite,” ideally,  $\{Ca_3\}[Al_2](Si_{3-x}\square_x)O_8Cl_{4-x}$ , from burned material in the Chelyabinsk coal basin, Urals, Russia, but these compounds are not considered to be naturally formed, and thus do not qualify as minerals (e.g., “igumnovite,” Jambor et al. 1997). The reported cell parameter of 12.008 Å for “igumnovite” is smaller than expected for a Cl-rich garnet from the relationship of Langley and Sturgeon (1979). Although the measured composition for “igumnovite,”  $Ca_{3.04}Al_{1.72}Fe_{0.13}Mg_{0.01}Si_{2.07}F_{0.03}O_{7.90}Cl_{4.07}$  approaches ideal garnet stoichiometry, it is doubtful that either “igumnovite” or “chlorhibschite” are garnets. More likely, “igumnovite” is related to mayenite, wadalite, and the new mineral eltyubuyite (Galuskin et al. 2011b), whereas “chlorhibschite” could be a mixture of grossular, wadalite, and, perhaps, chlorides.

### Yafsoanite

The 9% proportion of the component  $\{Pb_3^{2+}\}[Te_2^{6+}](Zn_3)O_{12}$  listed in Tables 6 and 7 is based on the single-crystal structure refinement of material from the type locality (Mills et al. 2010; cf. Jarosch and Zemmann 1989). Electron microprobe analyses reported in the original description gave 11–16% of the Pb analog (Kim et al. 1982), but the formulas deviate from ideal stoichiometry, possibly as a result of using sulfides, a silicate and a native element for standards. Ronniger and Mill' (1973) reported synthesis of several Pb<sup>2+</sup>-bearing vanadate garnets (berzeliite group) with Pb at the *X* site, and Mill' (1970) reported synthesis of yafsoanite and other Te-bearing garnets, but neither reported attempts to synthesize the Pb<sup>2+</sup> analog of yafsoanite.

The unnamed end-member  $\{Ca_3^{2+}\}[U_2^{6+}](Fe_3^{3+})O_{12}$  is calculated to be major constituent of elbrusite (Fig. 4; Table 6) and dzhuluite (Appendix 3'), but has not yet been synthesized.

### Henritermierite group

Boiocchi et al. (2012) reported nearly end-member spessartine containing 0.09 Fe and 0.04 Ca pfu, but only 2.52 Si pfu, the deficiency being made up by OH and F in nearly equal proportions (Table 6). The *I*<sub>41</sub>/*acd* symmetry indicates that the mineral is more closely analogous to holtstamite rather than katoite. The spessartine is the first example of a garnet showing *I*<sub>41</sub>/*acd* symmetry but containing no Mn<sup>3+</sup>, and thus Boiocchi et al. (2012) attribute the lower symmetry to (OH, F)<sub>4</sub> groups. Si is partially ordered, preferentially occupying the Z1 site (93.0%) vs. the Z2 site (73.8%).

### Bitikleite group

Given the large number of elements found in analyses of garnets of the bitikleite group, the potential for new species is great. For example, analysis 10 of elbrusite in Table 2 of Galuskina et al. (2010a) corresponds to the Sn-dominant analog of elbrusite (Fig. 4), and is possibly a new species (Table 8). Zaitsev et al. (2010) reported a zone with up to 10.1 wt% Nb<sub>2</sub>O<sub>5</sub> in a kerimasite crystal, this amount corresponds to 0.48 Nb per formula unit, or nearly 50% of a  $\{Ca_3\}[NbZr](R_3^{3+})O_{12}$  component, which implies the possibility of new species for  $R^{3+} = Fe$  and Al, the Nb analog of usturite (Table 8).

Up to 4 wt% ThO<sub>2</sub> (0.1 Th pfu) has been reported in bitikleite and schorlomite-group minerals (Lupini et al. 1992; Galuskina et al. 2010a, 2010e), which would correspond to 20 mol% of a  $\{Th_{0.5}Ca_{2.5}\}[R_2^{4+}](R_3^{3+})O_{12}$  component. The end-member with Zr and Fe, i.e.,  $\{Th_{0.5}Ca_{2.5}\}[Zr_2^{4+}](Fe_3^{3+})O_{12}$ , has been synthesized (Ito and Frondel 1967a; Yuditsev 2003; Utsunomiya et al. 2005).

### Yttrium-aluminum (YAG) and yttrium-iron (YIG) garnets

The rare earth elements can form a large number of synthetic compounds having general formulas of the type  $\{R_3^{3+}\}[R_2^{3+}](R_3^{3+})O_{12}$  and isostructural with garnet (e.g., Yoder and Keith 1951; Geller 1967), of which  $\{Y_3\}[Al_2](Al_3)O_{12}$  (yttrium aluminum garnet or YAG) and  $\{Y_3\}[Fe_2^{3+}](Fe_3^{3+})O_{12}$  (yttrium iron garnet or YIG) are the most relevant to minerals (Tables 6 and 7). Although the total charge at Z is 9, the garnet end-members YAG and YIG have not been placed in the bitikleite group because of the very different occupancies at *Y* and *X*. Up to 5 mol% of the YAG component has been reported in spessartine and almandine (e.g.,

Jaffe 1951; Røhr et al. 2007), and 5 mol% of the YIG component has been reported in andradite (Kasowski and Hogarth 1968), but the maximum proportion of a generalized  $\{(Y, \text{REE})_3\}[(\text{Fe}^{3+}, \text{Al})_2](\text{Al}_3)\text{O}_{12}$  component in a natural garnet is 8% in menzerite-(Y)-andradite solid solution (Grew et al. 2010).

### Schorlomite group

Koritnig et al. (1978) reported Zr-rich schorlomite from calc-silicate inclusions in gabbro of Radautal, Harz Mountains, Germany. Analyses of three samples gave 6.2–6.8 wt%  $\text{Al}_2\text{O}_3$  and 23.1–25.6 wt%  $\text{SiO}_2$  contents; the sample giving the highest ZrO<sub>2</sub> content (Zr = 0.55 apfu) is plotted in Figure 5. Our calculations for this sample give 48.9–49.0%  $\{\text{Ca}_3\}[\text{R}_3^{3+}](\text{SiR}_3^{3+})\text{O}_{12}$  with Ti > Zr at Y and Al > Fe<sup>3+</sup> at Z, i.e., a possible Al analog of schorlomite or Ti analog of kimzeyite. Using Mössbauer spectroscopic data, Koritnig et al. (1978) gave the Z site composition as  $(\text{Si}_{2.00}\text{Al}_{0.56}\text{Fe}_{0.24}^{2+}\text{Ti}_{0.16}\text{Fe}_{0.03}^{3+})$ . Ito and Frondel (1967a) synthesized end-member schorlomite and kimzeyite, but we are not aware of a successful synthesis of the end-member  $\{\text{Ca}_3\}[\text{Ti}_2](\text{SiAl}_2)\text{O}_{12}$ .

### Garnet group

Formulas calculated from the two analyses richest in Ti from garnets of the Marathon dikes, Ontario (Platt and Mitchell 1979), plot in the morimotoite field (Fig. 5) and have total Mg/(Mg+Fe<sup>2+</sup>) = 0.63–0.64, i.e., the end-member  $\{\text{Ca}_3\}[\text{TiMg}](\text{Si}_3)\text{O}_{12}$ , the Mg analog of morimotoite, is dominant (Table 8). However, the Marathon dike compositions plot close to the boundary with schorlomite and calculation of Fe<sup>2+</sup>/Fe<sup>3+</sup> ratio from stoichiometry has a large uncertainty (Giaramita and Day 1990); thus a clear dominance of  $\{\text{Ca}_3\}[\text{TiMg}](\text{Si}_3)\text{O}_{12}$  in a natural garnet remains to be demonstrated.

Gallium and germanium can form a large number of synthetic compounds isostructural with garnet (Geller 1967), but only  $\{\text{Ca}_3\}[\text{Ga}_2](\text{Ge}_3)\text{O}_{12}$  might have a natural analog. Johan and Oudin (1986) reported from the Pyrenees of France equant, six-sided crystals up to 10 μm across of a Ca-Ga-Ge mineral having compositions consistent with garnet stoichiometry (abstract in Jambor et al. 1988b). Cores of the highly zoned grains are close to  $\{\text{Ca}_3\}[\text{Ga}_2](\text{Ge}_3)\text{O}_{12}$  in composition, whereas the rims have compositions approximately intermediate between this composition and grossular. The list of valid unnamed minerals (Smith and Nickel 2007) also gave  $\{\text{Ca}_3\}[\text{Al}_2](\text{Ge}_3)\text{O}_{12}$  as a possible new species (Table 8), but our recalculation of formulas from the two compositions closest to this end-member (Johan and Oudin 1986) gave Si > Ge at the Z site and minor Ge at the Y site assuming Si is preferentially incorporated at the Z site. The crystals were too small to confirm the identification as a garnet by the technologies available at the time.

Fermor (1926, 1938) introduced three hypothetical garnet end-members (Tables 6–7; Appendix 2): “blythite,”  $\{\text{Mn}_3^{2+}\}[\text{Mn}_2^{3+}](\text{Si}_3)\text{O}_{12}$ , as a subordinate component in a garnet from Cargoon, Nagpur, India; “khoharite,”  $\{\text{Mg}_3^{3+}\}[\text{Fe}_2^{3+}](\text{Si}_3)\text{O}_{12}$ , as the precursor to enstatitic chondrules in the Khohar meteorite and as a subordinate component in a pyrope from a “garnet-diopside” xenolith (eclogite?) in kimberlite from South Africa; and “skiaigite,”  $\{\text{Fe}_3^{2+}\}[\text{Fe}_2^{3+}](\text{Si}_3)\text{O}_{12}$ , as a component in almandine from Glen Skiag, Scotland. Although later studies have reported up to nearly 9 mol% “blythite” based on measurement or stoichiometric

calculation of Mn<sup>3+</sup> in andradite from manganese formations, Otjosondou, Namibia (Amthauer et al. 1989; Bühn et al. 1995), “khoharite” and “skiaigite” have been elusive, e.g., Virgo and Yoder (1974) failed to find “skiaigite” in spessartine-almandine from the type locality at Glen Skiag, Scotland. The main problem in identifying these components in complex natural garnets is that the calculation depends on the sequence of calculation (Rickwood 1968; Locock 2008), i.e., Fe<sup>3+</sup> is first assumed to be present as the andradite component; only leftover Fe<sup>3+</sup> would be combined with Fe<sup>2+</sup> or Mg in the “skiaigite” or “khoharite” components, respectively, and Mn<sup>3+</sup> could be present as  $\{\text{Ca}_3\}[\text{Mn}_3^{2+}](\text{Si}_3)\text{O}_{12}$  as well as  $\{\text{Mn}_3^{2+}\}[\text{Mn}_2^{3+}](\text{Si}_3)\text{O}_{12}$  in the Otjosondou garnet (Table 6). Garnets containing a significant proportion of the  $\{\text{Ca}_3\}[\text{Mn}_2^{3+}](\text{Si}_3)\text{O}_{12}$ , “blythite,” “khoharite,” and “skiaigite” end-members have been synthesized at relatively high pressures, i.e., above 30 kbar (Coes 1955; Nishizawa and Koizumi 1975; Karpinskaya et al. 1982; Fursenko 1983; Woodland and O’Neill 1993, 1995; Arlt et al. 1998), and could become more abundant under mantle pressures.

Rudashevskii and Mochalov (1984) reported a Mn-Cr-Si mineral thought to be a garnet in heavy concentrates from eluvium of Pt-bearing serpentinite in the Far East of Russia (summary in Jambor et al. 1988a). The mineral forms highly zoned grains 1–30 μm across enclosed in Cr-Ni-bearing γ-Fe. The formula (with cations grouped by valence) for the analysis with the highest Cr content is  $\{\text{Mn}_{2.99}^{2+}\}[(\text{Cr}_{1.14}^{3+}\text{Mn}_{0.51}^{3+})\text{Ti}_{0.35}](\text{Si}_{2.22}\text{Ti}_{0.35})(\text{Al}_{0.28}\text{Fe}_{0.08}^{3+})\text{O}_{12}$ , i.e., a  $\{\text{Mn}_3^{2+}\}[\text{Cr}_2^{3+}](\text{Si}_3)\text{O}_{12}$  component can be considered dominant, whereas that for the lowest Cr content is  $\{\text{Mn}_3^{2+}\}[(\text{Mn}_{0.79}^{3+}\text{Cr}_{0.60}^{3+}\text{Al}_{0.09}\text{Fe}_{0.08}^{3+})\text{Ti}_{0.22}\text{Mn}_{0.22}^{2+}](\text{Si}_{3.01})\text{O}_{12}$ , i.e., with “blythite” dominant. The presence of significant Mn<sup>3+</sup> in association with Fe<sup>0</sup> is unexpected, as is the preservation of metallic Fe in eluvium. In the absence of X-ray or electron diffraction patterns and clearer evidence for the natural origin of the concentrates, the natural occurrence of a  $\{\text{Mn}_3^{2+}\}[\text{Cr}_2^{3+}](\text{Si}_3)\text{O}_{12}$ -dominant or  $\{\text{Mn}_3^{2+}\}[\text{Mn}_2^{3+}](\text{Si}_3)\text{O}_{12}$ -dominant garnet remains to be demonstrated.

Three components have been proposed for incorporation of Na in garnet-group minerals (Tables 4 and 6), all of which have been inferred to be favored by increasing pressure,  $^{\text{X}}\text{Na}+^{\text{Y}}(\text{Y}, \text{Yb}) = 2^{\text{X}}\text{R}^{2+}$  (Enami et al. 1995; Røhr et al. 2007) and  $^{\text{X}}\text{Na}+^{\text{Y}}\text{Si} = ^{\text{X}}\text{R}^{2+}+^{\text{Y}}\text{Al}$  or  $^{\text{X}}\text{Na}+^{\text{Y}}\text{Ti} = ^{\text{X}}\text{R}^{2+}+^{\text{Y}}\text{Al}$  (Ringwood and Major 1971; Sobolev and Lavrent’ev 1971; Bobrov et al. 2008; Harte 2010; Collerson et al. 2010).

### Berzeliite group

Phosphorus contents generally do not exceed 1 wt% P<sub>2</sub>O<sub>5</sub> in pyrope, almandine, and spessartine, both in wet chemical (e.g., Koritnig 1965; Deer et al. 1982) and in electron microprobe analyses (e.g., Bishop et al. 1978; Hiroi et al. 1997; Breiter et al. 2005; Kawakami and Hokada 2010). Mason and Berggren (1942) reported 4.1 wt% P<sub>2</sub>O<sub>5</sub> in spessartine from Wodgina, Australia (sample no. NRM 884695, Swedish Museum of Natural History), but Breiter et al. (2005) found only 0.24–0.27 wt% with the electron microprobe. An energy-dispersive spectroscopic analysis of the spessartine in this specimen (normalized to 100%) with an SEM gave P contents closer to the amounts reported by Breiter et al. (2005): SiO<sub>2</sub> 35.78, Al<sub>2</sub>O<sub>3</sub> 20.52, FeO 3.91, MnO 39.15, CaO 0.20, P<sub>2</sub>O<sub>5</sub> 0.42 (±0.12) (Hålenius, unpublished data). The spessartine grains are cut by microfissures ranging



from <1  $\mu\text{m}$  to ca. 10  $\mu\text{m}$  thick filled with Ca-Mn-phosphates. In some grains, the microfissures are sufficiently abundant to form networks, whereas in other grains they occurred singly up to 100  $\mu\text{m}$  apart. It would have been nearly impossible to obtain a pure spessartine concentrate suitable for wet chemical analyses from this specimen.

Thompson (1975) reported experimental evidence for increased incorporation of P and Na with increasing pressure, a relationship consistent with the presence of up to 0.25 wt%  $\text{P}_2\text{O}_5$  in pyrope associated with coesite at Dora Maira, Italy (Brunet and Lecocq 1999), exsolved apatite in garnet from mantle eclogite (Haggerty et al. 1994) and with the synthesis of  $\{\text{Na}_3\}[\text{Al}_2](\text{P}_3)\text{O}_{12}$  at 150–170 kbar by Brunet et al. (2006). Thilo (1941) reported synthesis of  $\{\text{Na}_3\}[\text{Al}_2](\text{P}_3)\text{O}_{12}$  at atmospheric pressure, but subsequent attempts to reproduce such syntheses failed (Schwarz and Schmidt 1971). On the basis of a large number of analyses yielding up to 1.21 wt%  $\text{P}_2\text{O}_5$  (equivalent to 0.086 P pfu) in almandine and spessartine from granitic rocks, Breiter et al. (2005) showed that: (1) P content varies inversely with Si; (2) Na/P ratio to be approximately 1/5; and (3) Al is relatively constant, consistent with the substitutions  $^X\text{Al}^{3+} + 2^Z\text{P} = ^X\text{R}^{2+} + 2^Z\text{Si}$  and much subordinate  $^X\text{Na}^{+} + ^Z\text{P} = ^X\text{R}^{2+} + ^Z\text{Si}$ . There was no evidence in their data for the substitution  $^Z(\text{Al}, \text{Fe}^{3+}) + ^Z\text{P} = 2^Z\text{Si}$  reported in an almandine-spessartine containing up to 2.1 wt%  $\text{P}_2\text{O}_5$  from rhyolite, Tanzawa Mountainland, Japan (Arima and Yamashita 1994). Breiter et al. (2005) also concluded that the main control on incorporation of P seems to be the P contents in melt or post-magmatic fluid instead of pressure.

The maximum FeO content reported in a berzeliite-group mineral is 1.52 wt% in berzeliite from Montaldo mine, Italy, equivalent to 6% of the  $\{\text{Ca}_2\text{Na}\}[\text{Fe}_2^{2+}](\text{As}_3^{5+})\text{O}_{12}$  end-member (Nagashima and Armbruster 2012). Attempts to synthesize the  $\text{Fe}^{2+}$  analog of berzeliite have not been successful (Ito 1968; Schwarz and Schmidt 1971).

#### SUMMARY OF CONCLUSIONS, ACTIONS, AND RECOMMENDATIONS

- The garnet supergroup comprises 32 approved species, with an additional 5 possible species needing further study to be approved.
- The supergroup includes all minerals isostructural with garnet regardless of what elements occupy specific cation or anion sites.
- We have subdivided the supergroup into groups based on symmetry and total charge at the tetrahedral Z site. Twenty-nine species belong to one of five groups, one tetragonal (henritermierite), and four isometric—bitikleite, schorlomite, garnet, and berzeliite, in which the total Z charge is 8, 9, 10, 12, and 15, respectively. Three species are single representatives of potential groups in which total charge at Z is 0 (katoite), 3 (cryolithionite), and 6 (yafsoanite).
- Species are identified on the basis of the dominant-constituent and dominant-valency rules, and in some cases, by valency-imposed double site-occupancy.
- We recommend that suffixes (other than Levinson modifiers) not be used in naming minerals in the garnet supergroup. We have discredited existing names that have suffixes and replaced them with new root names where

necessary, specifically, bitikleite-(SnAl) with bitikleite, bitikleite-(SnFe) with dzhuluite, bitikleite-(ZrFe) with usturite, and elbrusite-(Zr) with elbrusite.

- We have discredited the name hibschite in favor of grossular, as Si is the dominant cation at the Z site.
- Twenty-one end-members have been reported as subordinate components in minerals of the garnet supergroup of which six have been reported in amounts up to 20 mol% or more, whereas several others have been synthesized, which implies the potential for more species in the garnet supergroup.

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## APPENDIX 1. LIST OF GARNET SPECIES, END-MEMBER FORMULAS, MODIFICATIONS, ETYMOLOGY, TYPE LOCALITIES; CRYSTAL STRUCTURE REFINEMENTS

The following garnet species either have been previously accepted by the IMA-CNMNC or have been modified by the current garnet subcommittee. Modifications to the original garnet species descriptions are noted except for grandfathered species. One or two references are given for the crystal structure, either of natural material (when available) or of synthetic material, or both.

### Almandine

End-member formula:  $\{\text{Fe}^{2+}\}[\text{Al}_2](\text{Si}_3)\text{O}_{12}$

Group: Garnet

IMA number: Grandfathered

Modifications: None

Etymology: The “Alabandic carbuncles” of Pliny were so named as they were cut and polished in Alabanda (Dana 1837, 1892), an ancient city in what is presently Aydin Province, Turkey.

Type locality: Not known

Crystal system, space group and structure refinement: Isometric,  $\bar{3}a$ . Novak and Gibbs (1971); synthetic material: Armbruster et al. (1992).

Original or oldest description: Known in ancient times. Name first used by D.L.G. Karsten in 1800 (Dana 1892).

### Andradite

End-member formula:  $\{\text{Ca}_3\}[\text{Fe}^{2+}](\text{Si}_3)\text{O}_{12}$

Group: Garnet

IMA number: Grandfathered

Modifications: None

Etymology: For José Bonifácio de Andrada e Silva (1763–1838), the Brazilian mineralogist who described a variety under the name “allochroite” in 1800 (Dana 1892; Clark 1993).

Type locality: Not known

Crystal system, space group and structure refinement: Isometric,  $\bar{3}a$ . Armbruster and Geiger (1993). Original or oldest description: “allochroite” of de Andrada in 1800 and “melanite” of Werner in 1800 (Dana 1892).

### Berzeliite

End-member formula:  $\{\text{Ca}_2\text{Na}\}[\text{Mg}_2](\text{As}^{5+})\text{O}_{12}$

Group: Berzeliite

IMA number: Grandfathered

Modifications: None

Etymology: For Jacob Berzelius (1799–1848), a Swedish chemist.

Type locality: Långban, Filipstad district, Värmland, Sweden.

Crystal system and structure refinement: Isometric,  $la\bar{3}d$ . Hawthorne (1976); Nagashima and Armbruster (2012).

Original or oldest description: Kühn (1840)

### Bitikleite

End-member formula:  $\{\text{Ca}_3\}[\text{Sb}^{5+}\text{Sn}^{4+}](\text{Al}_3)\text{O}_{12}$

Group: Bitikleite

IMA number: 2009-052

Modifications: Originally described as bitikleite-(SnAl) with the same formula.

Etymology: From Bitikle, the name of an old fortification near the type locality.

Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia. Crystal system, space group and structure refinement: Isometric,  $la\bar{3}d$ . Galuskina et al. (2010b)

Original or oldest description: Galuskina et al. (2010b)

### Calderite

End-member formula:  $\{\text{Mn}^{2+}\}[\text{Fe}^{2+}](\text{Si}_3)\text{O}_{12}$

Group: Garnet

IMA number: Grandfathered

Modifications: None

Etymology: For James Calder, a member of the Asiatic Society of Bengal, originally applied to the rock containing the mineral (Piddington 1850).

Type locality: Either in Burdwan (Bardhaman) district, West Bengal State, or near Hazaribagh, Jharkhand State, India.

Crystal system, space group and structure report: Isometric,  $\bar{3}a$ . No structure refinement; structure optimization by distance least-squares refinement (Otonello et al. 1996).

Original or oldest description: Fermor (1909, 1926)

### Cryolithionite

End-member formula:  $\{\text{Na}_3\}[\text{Al}_2](\text{Li}_3)\text{F}_{12}$

Group: ungrouped

IMA number: Grandfathered

Modifications: None

Etymology: From the presence of Li and its relation to cryolite

Type locality: The Ivigtut cryolite deposit, Ivittuut (Ivigtut), Arsuk, Kitaa Province, Greenland.

Crystal system, space group and structure refinement: Isometric,  $\bar{3}a$ . Geller (1971).

Original or oldest description: Ussing (1904)

### Dzhuluite

End-member formula:  $\{\text{Ca}_3\}[\text{Sb}^{5+}\text{Sn}^{4+}](\text{Fe}^{3+})\text{O}_{12}$

Group: Bitikleite

IMA number: 2010-64

Modifications: Originally described as bitikleite-(SnFe) with the same formula.

Etymology: After Dzhulu Mountain near the type locality.

Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia.

Crystal system and space group: Isometric,  $la\bar{3}d$ . Structure not yet refined.

Original or oldest description: Galuskina et al. (2011a)

### Elbrusite

End-member formula:  $\{\text{Ca}_3\}[\text{U}_6^{6+}\text{Zr}_{1.5}](\text{Fe}^{3+})\text{O}_{12}$

Group: Bitikleite

IMA number: 2009-051

Modifications: Originally described as elbrusite-(Zr) with a formula  $\{\text{Ca}_3\}[\text{U}^{6+}\text{Zr}](\text{Fe}^{3+}\text{Fe}^{2+})\text{O}_{12}$ .

Etymology: From the highest peak in Europe - Mount Elbrus (5642 m).

Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia.

Crystal system, space group and structure refinement: Isometric,  $la\bar{3}d$ . The structure of elbrusite has not yet been refined, but that of U-rich kerimasite has been refined [under the name “Fe-dominant analog of kimzeyite”, Galuskina et al. (2010a)].

Original or oldest description: Galuskina et al. (2010a)

### Eringaite

End-member formula:  $\{\text{Ca}_3\}[\text{Sc}_2](\text{Si}_3)\text{O}_{12}$

Group: Garnet

IMA number: 2009-054

Modifications: None

Etymology: From the Eringa River, a tributary of the Wiluy River.

Type locality: Wiluy River, Sakha-Yakutia Republic, Russia. (63.0°N, 112.3°E).

Crystal system, space group and structure refinement: Isometric,  $la\bar{3}d$ .

Synthetic material: Mill' et al. (1977), Quartieri et al. (2006)

Original or oldest description: Galuskina et al. (2010d)

### Goldmanite

End-member formula:  $\{\text{Ca}_3\}[\text{V}^{3+}](\text{Si}_3)\text{O}_{12}$



Group: Garnet  
 IMA number: 1963-003  
 Modifications: None  
 Etymology: For Marcus I. Goldman (1881–1965), a sedimentary petrologist with the U.S. Geological Survey.  
 Type locality: Sandy (or South Laguna) mine area, Laguna, New Mexico, U.S.A.  
 Crystal system, space group and structure refinement: Isometric, *Ia3d*. Novak and Gibbs (1971); Righter et al. (2011).  
 Original or oldest description: Moench and Meyrowitz (1964)

#### Grossular

End-member formula:  $\{Ca_3\}[Al_2](Si_3)O_{12}$   
 Group: Garnet  
 IMA number: Grandfathered  
 Modifications: None  
 Etymology: From the color resembling gooseberry, *Ribes grossularia* (Dana 1892; Clark 1993).  
 Type locality: Wiluy River, Sakha-Yakutia Republic, Russia.  
 Crystal system, space group and structure refinement: Isometric, *Ia3d*. Novak and Gibbs (1971).  
 Synthetic material: Geiger and Armbruster (1997).  
 Original or oldest description: A.G. Werner in 1808–1809. However, grossular was described earlier under other names, viz. as “Cinnamon Stone” (Kanelstein) from Sri Lanka by Werner in 1803–1804 and as “Granat” by Pallas in 1793 (Dana (1892).

#### Henritermierite

End-member formula:  $\{Ca_3\}[Mn^{3+}](Si_2)(\square)O_8(OH)_4$   
 Group: Henritermierite  
 IMA number: 1968-029  
 Modifications: None  
 Etymology: For Henri-François-Émile Termier (1897–1989), a French geologist.  
 Type locality: Tachgagal mine, Morocco.  
 Crystal system, space group and structure refinement: Tetragonal, *I4<sub>1</sub>/acd*. Armbruster et al. (2001).  
 Original or oldest description: Gaudefroy et al. (1969)

#### Holtstamite

Formula:  $\{Ca_3\}[Al, Mn^{3+}](Si_2)(\square)O_8(OH)_4$   
 Group: Henritermierite  
 IMA number: 2003-047  
 Modifications: None  
 Etymology: For Dan Holtstam (b. 1963), a Swedish mineralogist.  
 Type locality: Wessels Mine, Kalahari manganese field, South Africa.  
 Crystal system, space group and structure refinement: Tetragonal, *I4<sub>1</sub>/acd*. Hålenius et al. (2005)  
 Original or oldest description: Hålenius (2004), Hålenius et al. (2005)

#### Irinarassite

End-member formula:  $\{Ca_3\}[Sn^{4+}](SiAl_2)O_{12}$   
 Group: Schorlomite  
 IMA number: 2010-73  
 Modifications: None  
 Etymology: For Irina Rass (b. 1940), a Russian mineralogist.  
 Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia.  
 Crystal system and space group: Isometric, *Ia3d*. Structure not yet refined.  
 Original or oldest description: Galuskina et al. (2011b)

#### Katoite

End-member formula:  $\{Ca_3\}[Al_2](\square_3)(OH)_{12}$   
 Group: ungrouped  
 IMA number: 1982-080  
 Modifications: None  
 Etymology: For Akira Kato (b. 1931), a Japanese mineralogist.  
 Type locality: Campomorto quarry, Pietra Massa, Viterbo, Lazio, Italy.  
 Crystal system, space group and structure refinement: Isometric, *Ia3d*. Sacerdoti and Passaglia (1985); synthetic material (Lager et al. 1987).  
 Original or oldest description: Passaglia and Rinaldi (1984)

#### Kerimasite

End-member formula:  $\{Ca_3\}[Zr_2](SiF_6^{2-})O_{12}$   
 Group: Schorlomite  
 IMA number: 2009-29  
 Modifications: None  
 Etymology: For the Kerimasi volcano.  
 Type locality: Kerimasi volcano, Gregory Rift, northern Tanzania.  
 Crystal system, space group and structure refinement: Isometric, *Ia3d*. Zaitsev et al. (2010), and under the name kimzeyite, Schingaro et al. (2001); synthetic material under the name kimzeyite (Whittle et al. 2007).

Original or oldest description: Zaitsev et al. (2010). Under the name kimzeyite: Schingaro et al. (2001) and Galuskina et al. (2005); under the name “Fe-dominant analog of kimzeyite” (Galuskina et al. 2010a, 2010b, 2010c).

#### Kimzeyite

End-member formula:  $\{Ca_3\}[Zr_2](SiAl_2)O_{12}$   
 Group: Schorlomite  
 IMA number: Not recorded  
 Modifications: None  
 Etymology: For members of the Kimzey family, who were instrumental in obtaining and preserving mineral specimens from Magnet Cove.  
 Type locality: Kimzey quarry, Magnet Cove, Arkansas, U.S.A.  
 Crystal system, space group and structure refinement: Isometric, *Ia3d*. Munno et al. (1980)  
 Original or oldest description: Milton and Blade (1958), Milton et al. (1961)

#### Knorringite

End-member formula:  $\{Mg_3\}[Cr^{3+}](Si_3)O_{12}$   
 Group: Garnet  
 IMA number: 1968-010  
 Modifications: None  
 Etymology: For Oleg von Knorring (1915–1994), a Russian mineralogist who worked in Finland and the United Kingdom.  
 Type locality: Kao kimberlite pipe, Butha-Butha, Lesotho.  
 Crystal system, space group and structure refinement: Isometric, *Ia3d*. Synthetic material: Juhin et al. (2010).  
 Original or oldest description: Nixon and Hornung (1968)

#### Majorite

End-member formula:  $\{Mg_3\}[SiMg](Si_3)O_{12}$   
 Group: Garnet  
 IMA number: 1969-018. Modifications: Formula originally given as  $\{(Mg, Na)_3\}[(Fe, Si, Al, Cr)_2](Si_3)O_{12}$ .  
 Etymology: For Alan Major, who assisted A.E. Ringwood in experiments.  
 Type locality: Coorara L6 chondrite (recovered in Western Australia).  
 Crystal system, space group and structure refinement: Isometric, *Ia3d*.  
 Synthetic material: Hazen et al. (1994)  
 Original or oldest description: Smith and Mason (1970)

#### Manganberzeliite

End-member formula:  $\{Ca_2Na\}[Mn^{2+}](As^{5+})O_{12}$   
 Group: Berzeliite  
 IMA number: Grandfathered  
 Modifications: See text.  
 Etymology: The manganese analog of berzeliite.  
 Type locality: Långban, Filipstad district, Värmland, Sweden.  
 Crystal system, space group and structure refinement: Isometric, *Ia3d*.  
 Qualitative description of the structure: Bubeck and Machatschki (1935); Nagashima and Armbruster (2012)  
 Original or oldest description: Igelström (1886, 1894)

#### Menzerite-(Y)

End-member formula:  $\{Y_2Ca\}[Mg_2](Si_3)O_{12}$   
 Group: Garnet  
 IMA number: 2009-050  
 Modifications: None  
 Etymology: For Georg Menzer (1897–1989), the German crystallographer who was the first to solve the structure of garnet (Menzer 1928); the suffix Y is a Levinson modifier that indicates that Y is dominant among the sum of Y and the rare-earth elements.  
 Type locality: Bonnet Island in Georgian Bay, near Parry Sound, Ontario, Canada.  
 Crystal system, space group and structure refinement: Isometric, *Ia3d*. Grew et al. (2010)  
 Original or oldest description: Grew et al. (2010)

#### Momoite

End-member formula:  $\{Mn^{2+}\}[V^{3+}](Si_3)O_{12}$   
 Group: Garnet  
 IMA number: 2009-026.  
 Modifications: None; see the “yamatoite” of Momoi (1964), which was not approved because this component was not dominant in the material that they investigated (Fleischer 1965).  
 Etymology: For Hitoshi Momoi (1930–2002), the Japanese mineralogist who was the first to recognize  $\{Mn^{2+}\}[V^{3+}](Si_3)O_{12}$  as a component in garnet.  
 Type locality: Kurase mine, Ehime Prefecture, Japan.  
 Crystal system and space group: Isometric, *Ia3d*. Structure not yet refined, but the atomic coordinates were predicted by Novak and Gibbs (1971).  
 Original or oldest description: Tanaka et al. (2010)

**Morimotoite**

End-member formula:  $\{\text{Ca}_3\}[\text{TiFe}^{2+}](\text{Si}_3)\text{O}_{12}$   
 Group: Garnet  
 IMA number: 1992-017  
 Modifications: None  
 Etymology: For Nobuo Morimoto (b. 1925), a Japanese mineralogist.  
 Type locality: Fuku, Bitchu-Cho, Okayama Prefecture, Japan.  
 Crystal system and space group: Isometric,  $Ia\bar{3}d$ . Structure not yet refined.  
 Original or oldest description: Henmi et al. (1995)

**Palenzonaite**

End-member formula:  $\{\text{Ca}_2\text{Na}\}[\text{Mn}_2^{2+}](\text{V}_3^{5+})\text{O}_{12}$   
 Group: Berzeliite  
 IMA number: 1986-011  
 Modifications: None  
 Etymology: For Andrea Palenzona (b. 1935), an Italian chemist.  
 Type locality: Molinello mine, Ne, Val Graveglia, Liguria, Italy.  
 Crystal system, space group and structure refinement: Isometric,  $Ia\bar{3}d$ . Basso (1987); Nagashima and Armbruster (2012)  
 Original or oldest description: Basso (1987)

**Pyrope**

End-member formula:  $\{\text{Mg}_3\}[\text{Al}_2](\text{Si}_3)\text{O}_{12}$   
 Group: Garnet  
 IMA number: Grandfathered  
 Modifications: None  
 Etymology: From the Greek πυροπός (pyropos) – firelike for its deep-red color.  
 Type locality: Bohemia (Czech Republic).  
 Crystal system, space group and structure refinement: Isometric,  $Ia\bar{3}d$ . Novak and Gibbs (1971)  
 Synthetic material: Armbruster et al. (1992)  
 Original or oldest description: Recognized by Georgius Agricola (1546), but the name pyrope was introduced by A.G. Werner in 1800 (Dana 1892; Clark 1993).

**Schäferite**

End-member formula:  $\{\text{Ca}_2\text{Na}\}[\text{Mg}_2](\text{V}_3^{5+})\text{O}_{12}$   
 Group: Berzeliite  
 IMA number: 1997-048  
 Modifications: None  
 Etymology: For Helmut Schäfer (b. 1931), an amateur German mineralogist who discovered the mineral.  
 Type locality: Bellberg volcano near Mayen, Eifel, Germany.  
 Crystal system, space group and structure refinement: Isometric,  $Ia\bar{3}d$ . Krause et al. (1999)  
 Original or oldest description: Krause et al. (1999)

**Schorlomite**

End-member formula:  $\{\text{Ca}_3\}[\text{Ti}_2](\text{SiFe}_2^{3+})\text{O}_{12}$   
 Group: Schorlomite  
 IMA number: Grandfathered  
 Modifications: Extensive; see main text.  
 Etymology: For its resemblance to schorl.  
 Type locality: Magnet Cove, Hot Springs County, Arkansas, U.S.A.  
 Crystal system, space group and structure refinement: Isometric,  $Ia\bar{3}d$ . Chakhmouradian and McCammon (2005)  
 Original or oldest description: Shepard (1846), Whitney (1849), and Rammelsberg (1850a, 1850b)

**Spessartine**

End-member formula:  $\{\text{Mn}_3^{2+}\}[\text{Al}_2](\text{Si}_3)\text{O}_{12}$   
 Group: Garnet  
 IMA number: Grandfathered  
 Modifications: None  
 Etymology: From the Spessart Mountains, Germany.  
 Type locality: Sommer quarry, Wendelberg Mt., Spessart Mountains, Bavaria, Germany.  
 Crystal system, space group and structure refinement: Isometric,  $Ia\bar{3}d$ . Novak and Gibbs (1971); for F-bearing, Smyth et al. (1990).  
 Synthetic material: Geiger and Armbruster (1997)  
 Original or oldest description: Recognized by M.H. Klaproth (1797), but the name spessartine was introduced by F.S. Beudant (1832) according to Dana (1892) and Clark (1993).

**Toturite**

End-member formula:  $\{\text{Ca}_3\}[\text{Sn}_2^{4+}](\text{SiFe}_3^{3+})\text{O}_{12}$   
 Group: Schorlomite  
 IMA number: 2009-033  
 Modifications: None  
 Etymology: From both the Totur River situated in Eltybyu village near the type locality and the name of a Balkarian deity and ancient warrior.  
 Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia.  
 Crystal system and space group: Isometric,  $Ia\bar{3}d$ . Structure not yet refined.  
 Original or oldest description: Galuskina et al. (2010c)

**Usturite**

End-member formula:  $\{\text{Ca}_3\}[\text{Sb}^{5+}\text{Zr}](\text{Fe}_3^{3+})\text{O}_{12}$   
 Group: Bitikleite  
 IMA number: 2009-053  
 Modifications: Originally described as bitikleite-(ZrFe) with the same formula.  
 Etymology: From the Ustur Mountain near the type locality.  
 Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia.  
 Crystal system and space group: Isometric,  $Ia\bar{3}d$ . Structure not yet refined.  
 Original or oldest description: Galuskina et al. (2010b)

**Uvarovite**

End-member formula:  $\{\text{Ca}_3\}[\text{Cr}_2^{3+}](\text{Si}_3)\text{O}_{12}$   
 Group: Garnet  
 IMA number: Grandfathered  
 Modifications: None  
 Etymology: For Count Sergei Semenovich Uvarov (1786–1855), a Russian historian.  
 Type locality: Saranovskiy mine Biserskoye chromite deposit, Perm district, Urals, Russia (Pekov 1998).  
 Crystal system, space group and structure refinement: Isometric,  $Ia\bar{3}d$ . Novak and Gibbs (1971)  
 For birefringent uvarovite: Wildner and Andrut (2001)  
 Original or oldest description: Hess (1832)

**Yafsoanite**

End-member formula:  $\{\text{Ca}_3\}[\text{Te}_2^{6+}](\text{Zn}_3)\text{O}_{12}$   
 Group: ungrouped  
 IMA number: 1981-022  
 Modifications: Introduced with the idealized formula  $(\text{Zn}_{1.38}\text{Ca}_{1.36}\text{Pb}_{0.26})_{2=3.00}\text{TeO}_6$ ; current formula from Jarosch and Zemann (1989) and Mills et al. (2010).  
 Etymology: From the acronym Yafskiy Filial Sibirskogo Otdeleniya Akademii Nauk (Yafskiy Filial of the Siberian Branch of the Academy of Sciences).  
 Type locality: Kuranakh gold deposit, near Aldan, Yakutia, Russia (Pekov 1998).  
 Crystal system, space group and structure refinement: Isometric,  $Ia\bar{3}d$ . Mills et al. (2010)  
 Original or oldest description: Kim et al. (1982)