#### **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  $Ia\overline{3}d$  (no. 230), but two OH-bearing species (henritermierite and holtstamite) 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 Zof 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, 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  $Ia\overline{3}d$  (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.

species with the garnet structure.

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

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 endmembers 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 dominantconstituent 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

	supergroup					
Z charge	GROUP or species name	e Class	Χ	Y	Ζ	φ
0	Katoite	Hydroxide	Ca₃	$AI_2$		(OH) <sub>12</sub>
3	Cryolithionite	Halide	Na₃	$AI_2$	Li₃	F <sub>12</sub>
6	Yafsoanite	Oxide	Ca₃	Te <sub>2</sub> <sup>6+</sup>	Zn₃	O <sub>12</sub>
8	HENRITERMIERITE	Silicate				
	Holtstamite		Ca₃	$AI_2$	$Si_2   \square$	$O_8(OH)_4$
	Henritermierite		Ca₃	Mn <sub>2</sub> <sup>3+</sup>		$O_8(OH)_4$
9	BITIKLEITE	Oxide				
	Bitikleite		Ca₃	Sb <sup>5+</sup> Sn <sup>4+</sup>	Al₃	O <sub>12</sub>
	Usturite		Ca₃	Sb⁵⁺Zr	Fe <sub>3</sub> <sup>3+</sup>	O <sub>12</sub>
	Dzhuluite		Ca₃	Sb <sup>5+</sup> Sn <sup>4+</sup>	Fe <sub>3</sub> <sup>3+</sup>	O <sub>12</sub>
	Elbrusite		Ca₃	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		Ca₃	Zr <sub>2</sub>	SiAl <sub>2</sub>	O <sub>12</sub>
	Irinarassite		Ca₃	Sn <sub>2</sub> <sup>4+</sup>	SiAl <sub>2</sub>	O <sub>12</sub>
	Schorlomite		Ca₃	Ti <sub>2</sub>	SiFe <sub>2</sub> <sup>3+</sup>	O <sub>12</sub>
	Kerimasite		Ca₃	Zr <sub>2</sub>	SiFe <sub>2</sub> <sup>3+</sup>	O <sub>12</sub>
	Toturite		Ca₃	Sn <sub>2</sub> <sup>4+</sup>	SiFe <sub>2</sub> <sup>3+</sup>	O <sub>12</sub>
12	GARNET	Silicate				
	Menzerite-(Y)		Y₂Ca	Mg <sub>2</sub>	Si₃	O <sub>12</sub>
	Pyrope		Mg₃	$A\bar{l}_2$	Si₃	O <sub>12</sub>
	Grossular		Ca₃	$AI_2$	Si₃	O <sub>12</sub>
	Spessartine		$Mn_3^{2+}$	$AI_2$	Si₃	O <sub>12</sub>
	Almandine		Fe <sub>3</sub> <sup>2+</sup>	$AI_2$	Si₃	O <sub>12</sub>
	Eringaite		Ca₃	Sc <sub>2</sub>	Si₃	O <sub>12</sub>
	Goldmanite		Ca₃	V <sub>2</sub> <sup>3+</sup>	Si₃	O <sub>12</sub>
	Momoiite		$Mn_3^{2+}$	V <sub>2</sub> <sup>3+</sup>	Si₃	O <sub>12</sub>
	Knorringite		Mg₃	Cr <sub>2</sub> <sup>3+</sup>	Si₃	O <sub>12</sub>
	Uvarovite		Ca₃	Cr <sub>2</sub> <sup>3+</sup>	Si₃	O <sub>12</sub>
	Andradite		Ca₃	Fe <sub>2</sub> <sup>3+</sup>	Si₃	O <sub>12</sub>
	Calderite		$Mn_3^{2+}$	Fe <sub>2</sub> <sup>3+</sup>	Si₃	O <sub>12</sub>
	Majorite		Mg₃	SiMg	Si₃	O <sub>12</sub>
	Morimotoite		Ca₃	TiFe <sup>2+</sup>	Si₃	O <sub>12</sub>
15	BERZELIITE V	anadate, arser	nate			
	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 <sup>2+</sup>	V <sub>3</sub> <sup>5+</sup>	O <sub>12</sub>
	Berzeliite		Ca₂Na	Mg <sub>2</sub>	As 3+	O <sub>12</sub>
	Manganberzeliite		Ca₂Na	Mn <sub>2</sub> <sup>+</sup>	As3+	O <sub>12</sub>
Notes: For	rmulas are given in the	e form $\{X_3\}[Y_2]$	(Z <sub>3</sub> )φ <sub>12</sub> .	Group n	ames a	

*Notes*: Formulas are given in the form  $\{X_3\}[Y_2](Z_3)\phi_{12}$ . Group names are given in capitals.

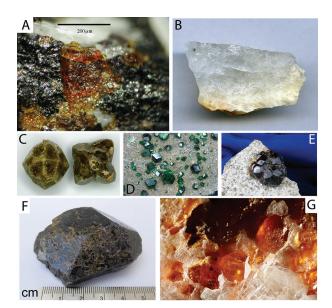


FIGURE 1. Photographs of representative garnet supergroup minerals illustrating the diversity in appearance exhibited by the supergroup. (a) Holtstamite, formula {Ca<sub>3</sub>}[Al,Mn<sub>2</sub><sup>3+</sup>](Si<sub>2</sub>)(□)O<sub>8</sub>(OH)<sub>4</sub>, as a yellow brown crystal between grains 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<sub>3</sub>} [Al<sub>2</sub>](Li<sub>3</sub>)F<sub>12</sub>: 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, endmember formula {Ca<sub>3</sub>}[Al<sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>: 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 µm 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  $\{Ca_3\}[Cr_2^{3+}](Si_3)O_{12}$ : 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<sub>3</sub>}[Al<sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>: 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  $\{Ca_3\}[Ti_2]$  $(SiFe_2^{3+})O_{12}$ : 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

the	present report	
Name	Former formula	Approved
		end-member formula
Katoite	Ca <sub>3</sub> Al <sub>2</sub> (SiO <sub>4</sub> ) <sub>3-x</sub> (OH) <sub>4x</sub> (x = 1.5-3.0)	{Ca <sub>3</sub> }[Al <sub>2</sub> ](□ <sub>3</sub> )(OH) <sub>12</sub>
Cryolithionite	$Na_3Al_2(LiF_4)_3$	$\{Na_3\}[Al_2](Li_3)F_{12}$
Yafsoanite	Ca <sub>3</sub> Te <sup>6+</sup> Zn <sub>3</sub> O <sub>12</sub>	$\{Ca_3\}[Te_2^{6+}](Zn_3)O_{12}$
Holtstamite	$Ca_3AI_2(SiO_4)_2(OH)_4$	${Ca_3}[AI_2](Si_2)(\Box)O_8(OH)_4$
Henritermierite	Ca <sub>3</sub> (Mn <sup>3+</sup> ) <sub>2</sub> (SiO <sub>4</sub> ) <sub>2</sub> (OH) <sub>4</sub>	$\{Ca_3\}[Mn_2^{3+}](Si_2)(\Box)O_8(OH)_4$
Bitikleite*	Ca <sub>3</sub> SbSnAl <sub>3</sub> O <sub>12</sub>	${Ca_3}[Sb^{5+}Sn^{4+}](Al_3)O_{12}$
Usturite*	Ca <sub>3</sub> SbZrFe <sub>3</sub> O <sub>12</sub>	{Ca <sub>3</sub> }[Sb <sup>5+</sup> Zr](Fe <sup>3+</sup> <sub>3</sub> )O <sub>12</sub>
Dzhuluite*	Ca <sub>3</sub> (SnSb <sup>5+</sup> )Fe <sup>3+</sup> O <sub>12</sub>	{Ca <sub>3</sub> }[Sb <sup>5+</sup> Sn <sup>4+</sup> ](Fe <sup>3+</sup> <sub>3</sub> )O <sub>12</sub>
Elbrusite*	Ca <sub>3</sub> (U <sup>6+</sup> Zr)(Fe <sub>2</sub> <sup>3+</sup> Fe <sup>2+</sup> )O <sub>12</sub>	${Ca_{3}}[U_{0.5}^{6+}Zr_{1.5}](Fe_{3}^{3+})O_{12}$
Kimzeyite	Ca <sub>3</sub> (Zr,Ti) <sub>2</sub> (Si,Al,Fe <sup>3+</sup> ) <sub>3</sub> O <sub>12</sub>	${Ca_3}[Zr_2](SiAl_2)O_{12}$
Irinarassite	$Ca_3Sn_2Al_2SiO_{12}$	$\{Ca_3\}[Sn_2^{4+}](SiAl_2)O_{12}$
Schorlomite	Ca <sub>3</sub> (Ti,Fe <sup>3+</sup> ) <sub>2</sub> [(Si,Fe)O <sub>4</sub> ] <sub>3</sub> O <sub>12</sub>	${Ca_3}[Ti_2](SiFe_2^{3+})O_{12}$
Kerimasite	$Ca_{3}Zr_{2}(Fe_{2}^{3+}Si)O_{12}$	${Ca_3}[Zr_2](SiFe_2^{3+})O_{12}$
Toturite	$Ca_3Sn_2Fe_2SiO_{12}$	$Ca_{3}[Sn_{2}^{4+}](SiFe_{2}^{3+})O_{12}$
Menzerite-(Y)	${CaY_2}[Mg_2](Si_3)O_{12}$	${Y_2Ca}[Mg_2](Si_3)O_{12}$
Pyrope	Mg <sub>3</sub> Al <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	${Mg_3}[AI_2](Si_3)O_{12}$
Grossular	$Ca_3Al_2(SiO_4)_3$	$\{Ca_3\}[Al_2](Si_3)O_{12}$
Spessartine	(Mn <sup>2+</sup> ) <sub>3</sub> Al <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	{Mn <sub>3</sub> <sup>2+</sup> }[Al <sub>2</sub> ](Si <sub>3</sub> )O <sub>12</sub>
Almandine	(Fe <sup>2+</sup> ) <sub>3</sub> Al <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	${Fe_3^{2+}}[AI_2](Si_3)O_{12}$
Eringaite	$Ca_3Sc_2(SiO_4)_3$	${Ca_3}[Sc_2](Si_3)O_{12}$
Goldmanite	Ca <sub>3</sub> (V <sup>3+</sup> ) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	{Ca <sub>3</sub> }[V <sub>2</sub> <sup>3+</sup> ](Si <sub>3</sub> )O <sub>12</sub>
Momoiite	(Mn <sup>2+</sup> ,Ca) <sub>3</sub> (V <sup>3+</sup> ,Al) <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>	${Mn_3^{2+}}[V_2^{3+}](Si_3)O_{12}$
Knorringite	Mg <sub>3</sub> Cr <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	${Mg_3}[Cr_2^{3+}](Si_3)O_{12}$
Uvarovite	Ca <sub>3</sub> Cr <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	${Ca_3}[Cr_2^{3+}](Si_3)O_{12}$
Andradite	Ca <sub>3</sub> (Fe <sup>3+</sup> ) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	${Ca_3}[Fe_2^{3+}](Si_3)O_{12}$
Calderite	(Mn <sup>2+</sup> ) <sub>3</sub> (Fe <sup>3+</sup> ) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	{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> (Fe <sup>2+</sup> ,Si) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	$\{Mg_3\}[SiMg](Si_3)O_{12}$
Morimotoite	Ca <sub>3</sub> (Ti,Fe <sup>2+</sup> ,Fe <sup>3+</sup> ) <sub>2</sub> (Si,Fe <sup>3+</sup> ) <sub>3</sub> O <sub>12</sub>	${Ca_3}[TiFe^{2+}](Si_3)O_{12}$
Schäferite	NaCa <sub>2</sub> Mg <sub>2</sub> (VO <sub>4</sub> ) <sub>3</sub>	${Ca_2Na}[Mg_2](V_3^{5+})O_{12}$
Palenzonaite	NaCa <sub>2</sub> (Mn <sup>2+</sup> ) <sub>2</sub> (VO <sub>4</sub> ) <sub>3</sub>	$Ca_2Na$ [Mn <sub>2</sub> <sup>2+</sup> ](V <sub>3</sub> <sup>5+</sup> )O <sub>12</sub>
Berzeliite	NaCa <sub>2</sub> Mg <sub>2</sub> (AsO <sub>4</sub> ) <sub>3</sub>	$Ca_2Na$ [Mg <sub>2</sub> ] $As_3^{5+}O_{12}$
Manganberzeliite	$hacha_2(Mn^{2+})_2(AsO_4)_3$	${Ca_2Na}[Mn_2^{2+}](As_3^{5+})O_{12}$

Note: Former names from IMA-CNMNC 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-cnmnc/. 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 CNMNC (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  $Ia\overline{3}d$  (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

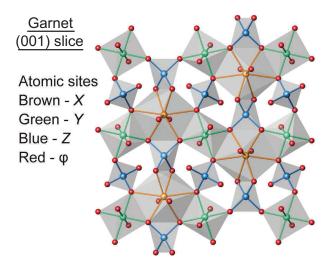


FIGURE 2. Portion of the garnet structure projected along [001].

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  $4H^{+Z} \rightarrow \Box^{+Z}S_{i}$ , i.e., the hydrogen ions occupy a separate site of general symmetry (Wyckoff position 96h) 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 Trzcienski 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

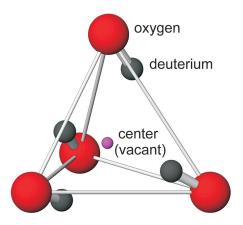


FIGURE 3. Local coordination environment of the tetrahedral position from the low-T (200 K) refinement of synthetic deuterated katoite (Lager et al. 1987) showing that the deuterium ions are approximately on the faces of the O tetrahedron and ~1.3 Å from the ideal tetrahedral cation position, which is 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  $4H^{+Z} \square \rightarrow \square^{+Z}Si$ , 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 hydrogarnet 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 Hrich samples in which H can be determined by these techniques give data consistent with  $4H^{+Z} \rightarrow \Box^{+Z}Si$ . Consequently, for nomenclature purposes, we have assumed that H is incorporated exclusively by  $4H^{+Z} \square \rightarrow \square^{+Z}Si$ .

The symmetry of garnet is predominantly isometric, space group  $Ia\overline{3}d$  (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  $\{Ca1_2\} \{Ca2\} [R_2^{3+}] (Si1_2) (\Box 2) O1_4 O2_4 (O3H)_4$ , where  $R^{3+} = Mn$  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 Mn3+ 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<sub>1</sub>/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; Rossmanith 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  $Ia\overline{3}d$  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 garnetsupergroup minerals

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

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 for-
	mulas for renamed/discredited minerals listed in this report

	is for renarrea, alsereare	
Former name	New name	Formula (approved by CNMNC)
	(approved by CNMNC)	
Bitikleite-(SnAl)	Bitikleite	${Ca_3}[Sb^{5+}Sn^{4+}](Al_3)O_{12}$
Bitikleite-(SnFe)	Dzhuluite	{Ca <sub>3</sub> }[Sb <sup>5+</sup> Sn <sup>4+</sup> ](Fe <sup>3+</sup> <sub>3</sub> )O <sub>12</sub>
Bitikleite-(ZrFe)	Usturite	{Ca <sub>3</sub> }[Sb <sup>5+</sup> Zr](Fe <sup>3+</sup> <sub>3</sub> )O <sub>12</sub>
Elbrusite-(Zr)	Elbrusite	$\{Ca_3\}[U_{0.5}^{6+}Zr_{1.5}](Fe_3^{3+})O_{12}$
Hibschite* Grossular		$\{Ca_3\}[Al_2](Si_{3-x}\Box_x)O_{12-4x}(OH)_{4x}$
		where x < 1.5†

\* Former formula:  $Ca_3Al_2(SiO_4)_{3,*}(OH)_{4,*}$  where x = 0.2-1.5. † Includes OH-bearing grossular. Ideal anhydrous grossular has the formula:  $\{Ca_3\}[Al_2](Si_3)O_{12}$ .

Generalized coupled substitution	Relationship
$\overline{Z\Box} + 4\varphi^{1-} \rightarrow \overline{Z}Si^{4+} + 4O^{2-}$	relates katoite, henritermierite and holtstamite to OH-free minerals in the garnet group
${}^{\gamma}R^{2+} + {}^{\gamma}R^{4+} \rightarrow 2^{\gamma}R^{3+}$	relates morimotoite ( <sup>(6)</sup> Ti) and majorite ( <sup>(6)</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
$X(Y, REE)^{3+} + {}^{Z}R^{3+} \rightarrow {}^{X}R^{2+} + {}^{Z}R^{4+}$	introduces Y + REE as a YAG, $\{Y_3\}$ [Al_2](Al_3)O <sub>12</sub> -type component
$^{X}$ (Y, REE) <sup>3+</sup> + $^{X}$ Na <sup>1+</sup> $\rightarrow$ 2 $^{X}R^{2+}$	introduces Y + REE into garnet-group minerals
$X(Y, REE)^{3+} + {}^{Y}R^{2+} \rightarrow {}^{X}R^{2+} + {}^{Y}R^{3+}$	relates menzerite-(Y) to other garnet-group minerals
${}^{\gamma}R^{5+} + {}^{Z}R^{3+} \longrightarrow {}^{\gamma}R^{4+} + {}^{Z}R^{4+}$	relates bitikleite, dzhuluite and usturite with schorlomite-group minerals
$^{9}0.5R^{6+} + ^{Z}R^{3+} \rightarrow ^{9}0.5R^{4+} + ^{Z}R^{4+}$	relates elbrusite with schorlomite-group minerals
${}^{Y}U^{6+} + {}^{Z}R^{2+} \longrightarrow {}^{Y}R^{4+} + {}^{Z}R^{4+}$	observed relationship between elbrusite and schorlomite group minerals (Fig. 4)
$0.5^{X}$ Th <sup>4+</sup> + $^{Z}R^{3} \rightarrow 0.5^{X}R^{2+} + {}^{Z}R^{4+}$	introduces Th into minerals of the bitikleite and schorlomite groups
${}^{\gamma}R^{4+} + 0.5{}^{z}V^{5+} \rightarrow 0.5{}^{z}R^{3+} + {}^{\gamma}Sb^{5+}$	introduces V into bitikleite
${}^{\gamma}R^{4+} + {}^{z}V^{5+} \longrightarrow {}^{\gamma}U^{6+} + {}^{z}R^{3+}$	introduces V into elbrusite
${}^{X}Na^{1+} + {}^{Y}R^{4+} \rightarrow {}^{X}R^{2+} + {}^{Y}R^{3+}$	introduces Na and <sup>[6]</sup> Si or <sup>[6]</sup> Ti into the garnet group
${}^{X}\mathrm{Na}^{1+} + {}^{Z}R^{5+} \rightarrow {}^{X}R^{2+} + {}^{Z}R^{4+}$	relates the berzeliite group to the garnet group
<i>Note: R</i> represents generalized cations (see Table 3).	

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.,  $\{Ca_3\}[Al_2](Si_{3-x}\Box_x)O_{12-4x}(OH)_{4x}$  where 0 < x < 3and  $\Box$  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.,  $Si > \Box$  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<sub>4</sub>/(OH)<sub>4</sub> 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.,  $\Box > Si$  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

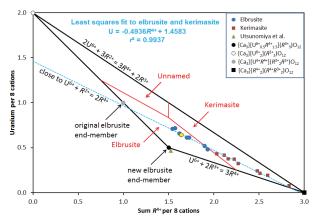
Elbrusite was originally described as "elbrusite-(Zr)" with the formula {Ca<sub>3</sub>}[U<sup>6+</sup>Zr](Fe<sub>2</sub><sup>3+</sup>Fe<sup>2+</sup>)O<sub>12</sub> (Table 2 from Galuskina et al. 2010a). Determination of the site occupancies and valence states were hampered by its metamict state, which was nearly complete in elbrusite containing 24 wt% UO<sub>3</sub> (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<sub>3</sub>, 0.37–0.42 U pfu); single-crystal X-ray diffraction was only practical for kerimasite containing 9 wt% UO<sub>3</sub> (0.21 U pfu) (Galuskina et al. 2010a). The authors noted that a Raman band below 700 cm<sup>-1</sup> could indicate the presence of some Fe<sup>2+</sup> in elbrusite, but the only evidence for U being hexavalent is the association with vorlanite, CaU<sup>+6</sup>O<sub>4</sub>, for which the hexavalent state of U could be determined (Galuskin et al. 2011a).

The composition  $\{Ca_3\}[U^{6+}Zr](Fe_2^{3+}Fe^{2+})O_{12}$  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<sub>3</sub>}  $[U_{0.5}^{6+}Zr_{1.5}]$  (Fe<sup>3+</sup>)O<sub>12</sub> +  $\frac{1}{3}$  {Ca<sub>3</sub>}  $[U_2^{6+}]$  (Fe<sup>2+</sup>)O<sub>12</sub> (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,  $\{Ca_3\}[R_2^{4+}](R^{4+}R_2^{3+})O_{12}$ , and  $\{Ca_3\}[U^{6+}R^{4+}](R_2^{3+}R^{2+})O_{12}$ (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<sup>2+</sup> is present. Moreover, the compositions that Galuskina et al. (2010a) identified as elbrusite and kerimasite plot in the fields for  $\{Ca_3\}[U^{6+}R^{4+}]$  $(R_2^{3+}R^{2+})O_{12}$  and  $\{Ca_3\}[R_2^{4+}](R^{4+}R_2^{3+})O_{12}$ , respectively, requiring no revision of their species identifications if  $\{Ca_3\}[U_{0,5}^{6+}Zr_{1,5}](Fe_3^{3+})$ O12 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<sub>2.5</sub>U<sub>0.5</sub>)Zr<sub>2</sub>Fe<sub>3</sub>O<sub>12</sub> bulk composition at 1400 °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<sub>1.83</sub>Al<sub>1.17</sub>)O<sub>12</sub>, 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<sup>4+</sup>. 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<sub>2</sub> 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  ${}^{y}Ti > {}^{y}Fe^{3+}$  (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 <sup>y</sup>Ti, balanced by substitutions at the Z site, relative to the total occupancy in the Y site,  $({}^{y}\text{Ti}-{}^{y}\text{Fe}^{2+}-{}^{y}\text{Mg}-{}^{x}\text{Na})/2$ , i.e., deducting a morimotoite component (see below) together with a contribution from a hypothetical {Na<sub>2</sub>Ca}[Ti<sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub> 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 Ca3TiFe2+Si3O12, based entirely on electron-microprobe data of garnet containing nearly 20 wt% TiO<sub>2</sub> 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% and radite,  $\{Ca_3\}[Fe_2^{3+}](Si_3)O_{12}, 27-34\% \{Ca_3\}$ [Ti<sub>2</sub>](Fe<sub>2</sub><sup>3+</sup>Si)O<sub>12</sub>, and 58-71% {Ca<sub>3</sub>}[TiFe<sup>2+</sup>](Si<sub>3</sub>)O<sub>12</sub> with minor Zr, Mg, Mn, and Al included with Ti, Fe<sup>2+</sup>, Ca, and Fe<sup>3+</sup> 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 Ti4+. 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<sup>3+</sup> 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<sup>3+</sup> in natural garnet (Waychunas 1987; Locock et al. 1995), whereas electron spin resonance spectroscopy revealed that Ti<sup>3+</sup> is much subordinate to Ti<sup>4+</sup> 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 Ti3+ 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 conclusion that Ti<sup>3+</sup> 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 (Si > 2 apfu) because of the rarity of Si = 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 Sifree synthetic garnets (Povarennykh and Shabilin 1983; Cartie et al. 1992; Yamane and Kawano 2011). Another question is the possible presence of tetrahedrally coordinated Fe<sup>2+</sup>. Some studies reported Mössbauer spectroscopic evidence for significant Fe2+ 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 Fe<sup>2+</sup> in the formulas calculated by the method of Droop (1987). However, the effect would be serious only if >0.4 wt% H<sub>2</sub>O were present, in which case at least 0.1 Fe<sup>2+</sup> per formula unit would not show up in the calculated formula unless OH were included in the formula calculation, i.e., (OH)+O=12and  $\Sigma \{X\} + \Sigma [Y] + \Sigma (Z) + Z \square_{(OH)/4} = 8$ , or if F present, O+(OH)+F = 12 and  $\Sigma \{X\} + \Sigma [Y] + \Sigma (Z) + Z \square_{(OH)/4} + Z \square_{F/4} = 8$ . The few analyses available in the recent comprehensive studies give 0.02-0.21 wt% H<sub>2</sub>O for natural Ti-rich garnets with >12 wt% TiO<sub>2</sub> (Kühberger et al. 1989; Locock et al. 1995; Amthauer and Rossman 1998; Chakhmouradian and McCammon 2005). An exception is "hydroschorlomite" with 5 wt% H<sub>2</sub>O (Galuskin 2005); such H<sub>2</sub>Orich 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 Ti<sup>4+</sup> and preferentially occupies the *Y* site, which rules out the end-member  $\{Ca_3\}[Ti_2](TiFe_2^{3+})O_{12}$  proposed by Rickwood (1968).

(2)  $H_2O$  content is  $\leq 0.2$  wt%.

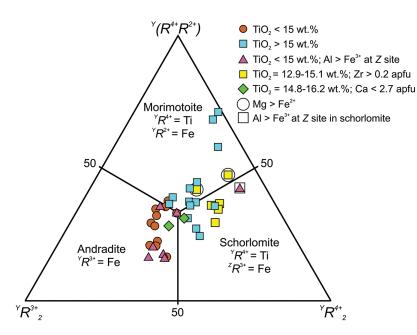
(3) Site occupancies are estimated using formulas calculated for 8 cations and 12 oxygen anions and the procedure outlined in the next section (see below).

Figure 5 is a plot of *Y*-site compositions for garnets containing >12 wt% TiO<sub>2</sub> and Ti > Zr apfu in terms of the following

generalized end-members {Ca<sub>3</sub>}[ $R_{2}^{3+}$ ](Si<sub>3</sub>)O<sub>12</sub>, {Ca<sub>3</sub>}[ $R_{2}^{4+}$ ](Si $R_{2}^{3+}$ ) O<sub>12</sub>, and {Ca<sub>3</sub>}[ $R^{4+}R^{2+}$ ](Si<sub>3</sub>)O<sub>12</sub>. For  $R^{4+}$  = Ti,  $R^{3+}$  = Fe<sup>3+</sup>, and  $R^{2+}$ = Fe<sup>2+</sup>, 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% TiO<sub>2</sub>, which Zedlitz (1933) suggested as a cutoff for schorlomite, is a good estimate of the minimum TiO<sub>2</sub> 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%  $TiO_2$  have not been plotted in Figure 5 either because of their high-H<sub>2</sub>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 µm across enclosed in grossular-katoite give 12.61-13.75 wt% SiO<sub>2</sub>, 25.42-25.86 wt% TiO<sub>2</sub>, 0.41-0.49 wt% SnO<sub>2</sub>, 2.20–2.28 wt% Al<sub>2</sub>O<sub>3</sub>, 24.86–26.09 wt% Fe as Fe<sub>2</sub>O<sub>3</sub>,  $31.03-31.71 \text{ wt\% CaO} \le 0.03 \text{ wt\% MgO}$ , and 0.27 to 1.2 wt% H<sub>2</sub>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% {Ca<sub>3</sub>}[Ti<sub>2</sub><sup>4+</sup>](SiFe<sub>2</sub><sup>3+</sup>)O<sub>12</sub>, the highest proportion of the schorlomite end-member reported in a natural garnet, 12-13%  $\{Ca_3\}$  [Ti<sub>2</sub><sup>+</sup>](SiAl<sub>2</sub>)O<sub>12</sub> and 12–14% and radite 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% TiO<sub>2</sub> and 33.50 wt% Fe as FeO, but deficient in Si and Ca with the formula:  $\{Ca_{1.53}Fe_{1.46}^{2+}Mn_{0.01}\}[Ti_{1.28}Fe_{0.71}^{2+}Mg_{0.01}]$  $(Si_{1.84}Ti_{0.60}Fe_{0.38}^{3+}Al_{0.18})O_{12}$ , i.e., a morimotoite from site occupancies, but anomalous because so much Ti (or Fe<sup>2+</sup>) 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% TiO<sub>2</sub>, 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 ~1 wt% K<sub>2</sub>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 Fe<sup>2+</sup> are the dominant  $R^{4+}$  and  $R^{2+}$  cations at Y if we assume that Ti and Fe<sup>2+</sup> 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  $R^{4+}$  cation, and Fe<sup>3+</sup> is the dominant  $ZR^{3+}$ 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 {Ca<sub>3</sub>}[Ti<sup>4+</sup>Fe<sup>2+</sup>](Si<sub>3</sub>)O<sub>12</sub> and {Ca<sub>3</sub>}[Ti<sup>4+</sup>\_2](SiFe<sup>3+</sup><sub>2</sub>)O<sub>12</sub> be the endmember 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  $TiO_2 > 12$  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); Lehijärvi (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 Mg > Fe<sup>2+</sup> (total for analysis) have been added only for compositions plotting in the morimotoite field. The square enclosing a triangle indicates the schorlomite in which <sup>Z</sup>Al > <sup>Z</sup>Fe<sup>3+</sup> 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  ${}^{Z}R^{3+}$  cation in these garnets is Fe<sup>3+</sup>, even if Al is assumed to preferentially occupy the Z site. Using the above assumptions, garnets plotting in the morimotoite field (with  $Fe^{2+}$  > 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  $Fe^{2+}$  is located at the Z site and dominance of  $[(Ti,Zr)_2]$  over  $[(Ti,Zr)R^{2+}]$  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  $Mg > Fe_{total}^{2+}$ (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 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, {Ca<sub>3</sub>}[ $R_{2}^{3+}$ ](Si<sub>3</sub>)O<sub>12</sub>, and morimotoite, {Ca<sub>3</sub>}[ $R_{2}^{4+}R^{2+}$ ] (Si<sub>3</sub>)O<sub>12</sub>, than schorlomite-group components, largely, {Ca<sub>3</sub>}[ $R_{2}^{4+}$ ](Si<sub>8</sub><sup>3+</sup>)O<sub>12</sub>.

#### Menzerite-(Y)

The validity of menzerite-(Y) has been questioned because the end-member formula proposed for menzerite-(Y),  $\{Y_2Ca\}$  $[Mg_2](Si_3)O_{12}$ , is quite far from the measured compositions of the type and only known material, which averages much closer to  ${Y(Ca, Fe^{2+})_2}[(Mg, Fe^{2+})(Fe^{3+}, Al)](Si_3)O_{12}$ , an empirical formula that can be simplified to {YCa<sub>2</sub>}[MgFe<sup>3+</sup>](Si<sub>3</sub>)O<sub>12</sub>. 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  $\{Y_2Ca\}[Mg_2](Si_3)O_{12}$  [menzerite-(Y)] and  $\{Ca_3\}[Fe_2^{3+}](Si_3)O_{12}$  (and radite). 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 Fe3+/Fe2+

ratio from stoichiometry (Droop 1987). The calculated  $Fe^{3+}/Fe^{2+}$  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  $\{Ca_3\}[Mg_2](Si_3)$  O<sub>12</sub>, which is not balanced in charge. Charge balance allows only 2 (Y+REE) per formula unit, i.e., the menzerite end-member should be  $\{Y_2Ca\}[Mg_2](Si_3)O_{12}$ . The presence of >1 (Y+REE) means that [(Y,REE)<sub>2</sub>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://pubsites.uws.edu.au/ima-cnmnc/) gives the formula for majorite as Mg<sub>3</sub>(Fe<sup>2+</sup>,Si)(SiO<sub>4</sub>)<sub>3</sub> (Table 2), equivalent to {Mg<sub>3</sub>}[SiFe<sup>2+</sup>](Si<sub>3</sub>) O<sub>12</sub>, which indeed is a good approximation of the empirical formula of the type material reported by Smith and Mason (1970), (Mg,Na)<sub>3</sub>(Fe,Si,Al,Cr)<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>. 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: {Mg<sub>2.91</sub>Na<sub>0.09</sub>} [(Si<sub>0.71</sub>Fe<sup>2+</sup><sub>0.60</sub>Fe<sup>3+</sup><sub>0.41</sub>Al<sub>0.22</sub>Cr<sub>0.04</sub> Mg<sub>0.02</sub>](Si<sub>3</sub>)O<sub>12</sub>.

However, the assumption regarding Fe<sup>2+</sup> occupancy is not supported by Mössbauer spectroscopic data on synthetic majorite (Geiger et al. 1991a, 1991b; O'Neill et al. 1993a, 1993b; Mc-Cammon 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  ${}^{X}Fe^{2+}/\Sigma Fe^{2+} = 0.89-0.95$ , and  $Fe^{2+}/(Fe^{2+}+Mg)$  at X (0.05-0.22) is three to seven times  $Fe^{2+}/(Fe^{2+}+Mg)$  at Y (0.01-0.08) in 15 synthetic tetragonal majorite samples, and  ${}^{X}Fe^{2+}/\Sigma Fe^{2+} = 1.0$ in one isometric synthetic sample, demonstrating that Fe<sup>2+</sup> 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  $Fe^{2+}$  occupies only the X site, the formula of the type material becomes  $\{Mg_{2,31}Fe_{0,60}^{2+}Na_{0,09}\}$ [(Si<sub>0.71</sub>Mg<sub>0.62</sub>Fe<sup>3+</sup><sub>0.41</sub>Al<sub>0.22</sub>Cr<sub>0.04</sub>](Si<sub>3</sub>)O<sub>12</sub>, i.e., the dominant component is  $\{Mg_3\}[SiMg](Si_3)O_{12}$ . Consequently, we recommend that  $\{Mg_3\}[SiMg](Si_3)O_{12}$  be used as the end-member formula for majorite. A natural XFe2+ 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,  $\{R_3^{2+}\}$ [MgSi](Si<sub>3</sub>)O<sub>12</sub>.

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  ${}^{Y}R^{2+}+{}^{Y}Si \rightarrow 2{}^{Y}A1$ (Table 4). Collerson et al. (2010) also include the contribution from the generalized component  $\{R^{2+}Na_2\}[R_2^{4+}](Si_3)O_{12}$  in their majorite substitution parameter, X<sup>cat</sup>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  $\{Mg_3\}[SiMg](Si_3)O_{12}$  or  $(R^{2+}+R^{4+})$  $> 2R^{3+}$  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%  $\{R_3^{2+}\}[R^{4+}Mg](Si_3)O_{12}$  or 44.9%  $\{R_3^{2+}\}[SiMg](Si_3)O_{12}$ (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 ( ${}^{y}Si+{}^{y}Ti$ ) < ( ${}^{y}Al+{}^{y}Fe^{3+}+{}^{y}Cr$ ); instead, the three average compositions comprise about 58-71% pyrope-grossular-almandine,  $17-33\% \{R_3^{2+}\}[R^{4+}Mg](Si_3)O_{12}$ (generalized majorite), and 10–13%  $\{R^{2+}(Na,K)_2\}[R_2^{4+}](Si_3)O_{12}$ , where  ${}^{Y}R^{4+} = 90-93\%$  Si.

#### Manganberzeliite

Manganberzeliite,  $\{Ca_2Na\}[Mn_2^{2+}](As_3^{4+})O_{12}$  (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, Mnrich 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 "Mnberzeliit" 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  $\{Li_2Mg\}[Si_2](Si_3)$ O<sub>12</sub> (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 11.8 apfu. Other exceptions involving light elements are the reports of 4.40 wt% B<sub>2</sub>O<sub>3</sub> determined by electron microprobe analysis (EMPA) in andradite (Galuskin et al. 1995) and 0.45-2.09 wt% B<sub>2</sub>O<sub>3</sub> 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 S6+ (up to 2.27 wt% SO3, 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 eringaite, 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 V3+ 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 ±0.15 in pyrope of mantle origin and 2.56-2.67 (±0.15) for V valence in a goldmanite from the Czech Republic, i.e., 40% of the V in the goldmanite is  $V^{2+}$ , the remainder V3+. However, this conclusion is in contrast to the structural and chemical data reported by these authors.

Name	Х	Y	Ζ	φ	Syn?	Occurrence in natural garnet	Source
			"Keno	garnet" group	<b>b</b>		
Fe <sup>3+</sup> analog of katoite	Ca₃	Fe <sub>2</sub> <sup>3+</sup>	$\square_3$	(OH) <sub>12</sub>	Yes	≤35 mol% in andradite	(1)
F analog of katoite	Ca3	Al <sub>2</sub>	$\Box_3$	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>		F <sub>12</sub>	-	≤8 mol% in spessartine	(3)
	-	-	Unn	amed group			
Pb <sup>2+</sup> analog of yafsoanite	Pb₃	Te <sub>2</sub> <sup>6+</sup>	Zn₃	0 <sub>12</sub>	-	9 mol% in yafsoanite	(4)
unnamed	Ca	U <sup>6+</sup>	Fe <sub>3</sub> <sup>2+</sup>	O <sub>12</sub>	-	≤24 mol% in elbrusite	(5)
			Henrite	ermierite grou	р		
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>	Alz	Si <sub>2</sub> □	O <sub>8</sub> F <sub>4</sub>	-	20 mol% in spessartine	(6)
-			Biti	kleite group			
unnamed	Th <sub>0.5</sub> Ca <sub>2.5</sub>	$R_{2}^{4+}$	R <sup>3+</sup>	0 <sub>12</sub>	Yes	≤20 mol% in kerimasite	(7)
		-	Unn	amed group			
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)3+	$R_{2}^{3+}$	R <sup>3+</sup>	O <sub>12</sub>	Yes	≤8 mol% in menzerite-(Y), spessartine, andradite	(8)
			Ga	rnet group			
"Blythite" in part	$R_{3}^{2+}$	Mn <sub>2</sub> <sup>3+</sup>	Si₃	O <sub>12</sub>	Yes	≤9 mol% in calderite-andradite±spessartine	(9)
Fe analog of menzerite-(Y)	Y <sub>2</sub> Ca	Fe <sub>2</sub> <sup>2+</sup>	Si₃	O <sub>12</sub>	-	≤20 mol% in menzerite (Y)	(10)
unnamed	(Y,Yb)15Na15	$R_{2}^{3+}$	Si3	O <sub>12</sub>	-	≤7 mol% in almandine, spessartine, grossular	(11)
unnamed	$R^{2+}Na_2$	Si <sub>2</sub>	Si	O <sub>12</sub>	Yes	≤12 mol% in pyrope-grossular	(12)
	-	-	Berz	zeliite group			
unnamed	Na₃	Al <sub>2</sub>	P3	0 <sub>12</sub>	Yes	<1 mol% in almandine and pyrope	(13)
unnamed	Ca₂Na	Fe <sup>2+</sup>	As35+	O <sub>12</sub>	No	<6 mol% in berzeliite	(14)

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

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  $\Box$  are not fully ordered at Z1 and Z2. Boiocchi et al. (2012).

(7) Ito and Frondel (1967a); Yudintsev (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); Bühn 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>z</sup>Li, <sup>x</sup>Ca, <sup>y</sup>Sc,  $Ti^{4+}$ ,  ${}^{y}V^{3+}$ , and  ${}^{Z}V^{5+}$  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  $\Sigma \{X\} + \Sigma [Y] + \Sigma (Z) + Z \Box_{(OH)/4} + Z \Box_{F/4} = 8$ .

(2) Li, Zn, P, As<sup>5+</sup>, and V<sup>5+</sup> to Z. If Li  $< \frac{1}{4}$ F, 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  $\Box$ , 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),  $Sc^{3+}$ ,  $Ti^{4+}$ ,  $V^{3+}$ ,  $Cr^{3+}$ , 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  $\leq$ 3 apfu, then add  $Fe^{2+}$  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)  $Fe^{2+}$  (remainder after deducting  $Fe^{2+}$  at Z): First to Y to bring total to 2 apfu, then to X.

(10)  $Mn^{2+}$ : 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  $Fe^{2+}/Fe^{3+}$  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,  $H = 4^*(^{\mathbb{Z}}\square).$ 

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  $\{Ca_3\}[Mn_2^{3+}](Si_2^{4+}\Box)O_8(OH)_4$ .

We have also prepared an Excel spreadsheet (Appendix 4<sup>1</sup>) 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 valencyimposed 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 Sb5+, Nb5+, or U6+, 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  ${R_{3}^{2+}}[R_{2}^{4+}](R^{4+}R_{2}^{3+})O_{12}$  be the most abundant (Fig. 7); i.e., the spreadsheet gives this as the most abundant component possible.

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

Name	Synthesis	Formula
-	62 to 90%	${Fe_{3}^{2+}}[AI_{2}](\Box_{3})(OH)_{12}$
-	No	$\{Ca_3\}[AI_2](\Box_3)F_{12}$
-	-	$\{Mn_3^{2+}\}[Al_2](\square_3)F_{12}$
-	-	$\{Fe_{3}^{2+}\}[Al_{2}](\Box_{3})F_{12}$
-	-	{Pb <sub>3</sub> <sup>2+</sup> }[Te <sub>2</sub> <sup>6+</sup> ](Zn <sub>3</sub> )O <sub>12</sub>
-	-	${Ca_3}[U_2^{6+}](Fe_3^{2+})O_{12}$
-	-	$\{Mn_3^{2+}\}[Al_2](Si_2)(\Box)O_8(OH)_4$
-	-	$\{Mn_{3}^{2+}\}[Al_{2}](Si_{2})(\Box)O_{8}F_{4}$
-	100%	${Th_{0.5}Ca_{2.5}}[Zr_2](Fe_2^{3+})O_{12}$
YIG	100%	{Y <sub>3</sub> }[Al <sub>2</sub> ](Al <sub>3</sub> )O <sub>12</sub>
YAG	100%	{Y <sub>3</sub> }[Fe <sub>2</sub> <sup>3+</sup> ](Fe <sub>3</sub> <sup>3+</sup> )O <sub>12</sub>
"Blythite"	100%	{Mn <sub>3</sub> <sup>2+</sup> }[Mn <sub>2</sub> <sup>3+</sup> ](Si <sub>3</sub> )O <sub>12</sub>
-	100%	{Ca <sub>3</sub> }[Mn <sub>2</sub> <sup>3+</sup> ](Si <sub>3</sub> )O <sub>12</sub>
"Khoharite"	100%	{Mg <sub>3</sub> }[Fe <sub>2</sub> <sup>3+</sup> ](Si <sub>3</sub> )O <sub>12</sub>
"Skiagite"	100%	{Fe <sub>3</sub> <sup>2+</sup> }[Fe <sub>2</sub> <sup>3+</sup> ](Si <sub>3</sub> )O <sub>12</sub>
-	-	{Y <sub>2</sub> Ca}[Fe <sup>2+</sup> ](Si <sub>3</sub> )O <sub>12</sub>
-	-	{Y <sub>15</sub> Na <sub>15</sub> }[Al <sub>2</sub> ](Si <sub>3</sub> )O <sub>12</sub>
-	100%	{CaNa <sub>2</sub> }[Si <sub>2</sub> ](Si <sub>3</sub> )O <sub>12</sub>
-	100%	{CaNa <sub>2</sub> }[Ti <sub>2</sub> ](Si <sub>3</sub> )O <sub>12</sub>
-	100%	{Na <sub>3</sub> }[Al <sub>2</sub> ](P <sub>3</sub> )O <sub>12</sub>
-	No	${Ca_2Na}{Fe_2^{2+}}(As_3^{5+})O_{12}$

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 supergrou
I ADLE O.	FOSSIBLE HEW	species in the	yamet supergro

TABLE 8. Possible new species	in the garnet supergr	oup		
Relationship to known species	UM no.	End-member formula	Criteria	Source
		Bitikleite group		
Sn analog of elbrusite		{Ca <sub>3</sub> }[U <sup>6+</sup> <sub>0.5</sub> Sn <sup>4+</sup> <sub>1.5</sub> ](Fe <sup>3+</sup> <sub>3</sub> )O <sub>12</sub>	Sn/(Sn + Zr) = 0.93	(1)
Nb analog of usturite		{Ca <sub>3</sub> }[NbZr](Fe <sup>3+</sup> )O <sub>12</sub>	1.33 Zr, 0.05 Ti, 0.48 Nb pfu at Y site	(2)
-		Schorlomite group		
Al analog of schorlomite		{Ca <sub>3</sub> }[Ti <sub>2</sub> ](SiAl <sub>2</sub> )O <sub>12</sub>	$AI/(AI+Fe^{3+}) = 0.65$	(3)
(Ti analog of kimzeyite)				
		Garnet group		
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 <sub>3</sub> }[Ga <sub>2</sub> ](Ge <sub>3</sub> )O <sub>12</sub>	$^{z}$ Ge > $^{z}$ Si; $^{\gamma}$ Ga > $^{\gamma}$ Fe <sup>3+</sup> , $^{\gamma}$ Al	(5)
Ge analog of grossular	UM1986-20	${Ca_3}[AI_2](Ge_3)O_{12}$	Criterion of <sup><i>z</i></sup> Ge > <sup><i>z</i></sup> Si not met.	(5)
Note: LIM po, refers to the list of valie	lunnamod minorals und	to 2011 01 (Smith and Nickol 2007)	Sourcos: (1) Calusking of al. (2010a): (2) Zaitsou	ot al (2010). (2)

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).

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,  $\{R_3^{2+}\}$  $R^{2+}$ ] $(R^{4+}_3)O_{12}$ , 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.,  $R^{4+} = \text{Ti}$ ,  $R^{3+} = \text{Fe}^{3+}$ , Al,

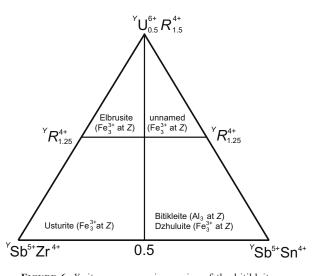
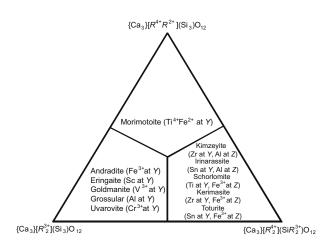


FIGURE 6. Y-site occupancy in species of the bitikleite group, including the possible unnamed Sn-dominant analog of elbrusite. Placement of the divisions is indicated.

and  $R^{2+} = Mg$ ,  $Fe^{2+}$ , and differs from Figure 7a of Grew et al. (2010) in that the Ti corner is now  $TiR^{2+}$ , 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 {Y<sub>3</sub>}[Al<sub>2</sub>](Al<sub>3</sub>)O<sub>12</sub>-type component to project menzerite-(Y) compositions. The {Y<sub>3</sub>} [Al<sub>2</sub>](Al<sub>3</sub>)O<sub>12</sub>-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.,  $\{R_3^{3+}\}\{R_3^{3+}\}$ 



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

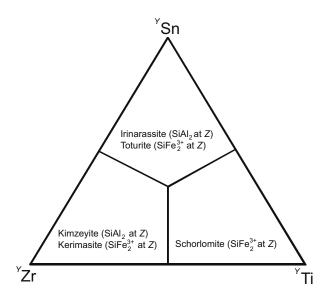
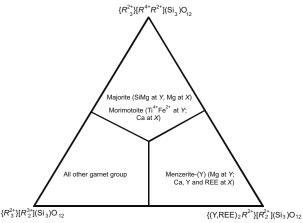
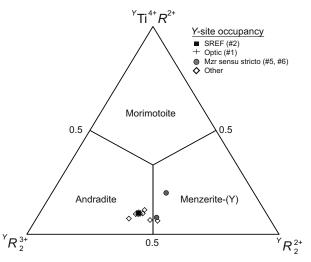


FIGURE 8. Y-site occupancy in species of the schorlomite group.

 $(Si_3^{++})O_{12}$ . Since only four constituents occupy the *X* site, the compositions can be plotted in a tetrahedron with Ca, Mg, Mn<sup>2+</sup>, and Fe<sup>2+</sup> 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 {Y<sub>3</sub>}[ $R_{2}^{3+}$ ]( $R_{3}^{3+}$ )O<sub>12</sub> onto the plane defined by the components {Ca<sub>3</sub>}[Ti<sup>4+</sup> $R^{2+}$ ](Si<sub>3</sub><sup>4+</sup>)O<sub>12</sub>, {Ca<sub>3</sub>}[ $R_{2}^{3+}$ ](Si<sub>4</sub><sup>4+</sup>)O<sub>12</sub>, and {(REE)<sub>2</sub>Ca}[ $R_{2}^{2+}$ ] (Si<sub>4</sub><sup>4+</sup>)O<sub>12</sub> (cf. Fig. 7a, Grew et al. 2010).  $R^{2+}$  = Fe in morimotoite, Mg in menzerite-(Y);  $R^{3+}$  = 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).

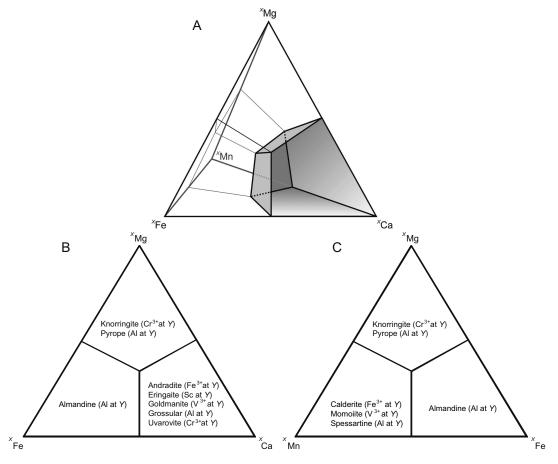
# Possible new species and compositional variations in natural garnet

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 vacancydominant. 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  $(O_4H_4)$  tetrahedra for  $(SiO_4)$ 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% H<sub>2</sub>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 Fe<sup>3+</sup> analog of katoite (Table 6) and 4.5% of its Mn<sup>3+</sup> 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% H<sub>2</sub>O) from charge balance in "hydroschorlomite" containing 13.5-14.5 wt% TiO<sub>2</sub> from the Wiluy River, Yakutia, Russia, the highest reported in Ti-rich garnets (cf. Chegem caldera schorlomite discussed above). In contrast, H<sub>2</sub>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% H<sub>2</sub>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-Miguélez 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),  $\{Ca_3\}[TiFe^{3+}](Fe^{3+}\Box_2)(OH)_8O_4$  (Ito and Frondel 1967b), and {Ca<sub>3</sub>}[ZrFe<sup>3+</sup>](Fe<sup>3+</sup>□<sub>2</sub>)(OH)<sub>8</sub>O<sub>4</sub> (Ito and Frondel 1967b) have been reported. However, attempts to synthesize the end-member  $\{Ca_3\}[Fe_2^{3+}](\Box_3)(OH)_{12}$  failed, although a garnet with about 90% {Ca<sub>3</sub>} [Fe<sub>2</sub><sup>3+</sup>]( $\square_3$ )(OH)<sub>12</sub> and 10% and radite 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<sub>3</sub>}[Fe<sub>2</sub><sup>3+</sup>](Si<sub>1.15</sub>□<sub>1.85</sub>)(OH)<sub>7.4</sub>O<sub>4.6</sub>, 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  $\{R_3^{2+}\}[R_2^{4+}](\Box_3)F_{12}$ , 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%  $\{R_3^{2+}\}[R_2^{3+}](\Box_3)(OH)_{12}$ , 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 Bushmakin (1995), and Chesnokov et al. (1994, 2008) described "igumnovite," ideally {Ca<sub>3</sub>}[Al<sub>2</sub>]  $(Si_2\Box)O_8Cl_4$ , and "chlorhibschite," ideally,  $\{Ca_3\}[Al_2](Si_{3-x}\Box_x)$ O<sub>8</sub>Cl<sub>4-x</sub>, 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<sub>3.04</sub>Al<sub>1.72</sub>Fe<sub>0.13</sub>Mg<sub>0.01</sub> Si<sub>2.07</sub>F<sub>0.03</sub>O<sub>7.90</sub>Cl<sub>4.07</sub> 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 eltyubyuite (Galuskin et al. 2011b), whereas "chlorhibschite" could be a mixture of grossular, wadalite, and, perhaps, chlorides.

#### Yafsoanite

The 9% proportion of the component  $\{Pb_3^{++}\}[Te_2^{++}](Zn_3)O_{12}$ 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 Zemann 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  $\{Ca_3^{2+}\}[U_2^{6+}](Fe_3^{2+})O_{12}$  is calculated to be major constituent of elbrusite (Fig. 4; Table 6) and dzhuluite (Appendix 3<sup>1</sup>), 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  $I4_1/acd$  symmetry indicates that the mineral is more closely analogous to holtstamite rather than katoite. The spessartine is the first example of a garnet showing  $I4_1/acd$  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<sub>3</sub>}[NbZr]( $R_3^{3+}$ )O<sub>12</sub> 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; Yudintsev 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  $\{R_3^{3+}\}[R_3^{3+}](R_3^{3+})$ O<sub>12</sub> 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  $\{(Y,REE)_3\}[(Fe^{3+},AI)_2]$ (Al<sub>3</sub>)O<sub>12</sub> 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% Al<sub>2</sub>O<sub>3</sub> and 23.1–25.6 wt% SiO<sub>2</sub> 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% {Ca<sub>3</sub>} [R<sub>2</sub><sup>4+</sup>](SiR<sub>2</sub><sup>3+</sup>)O<sub>12</sub> 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 (Si<sub>2.00</sub>Al<sub>0.56</sub>Fe<sup>2+</sup><sub>0.24</sub> Ti<sub>0.16</sub>Fe<sup>3+</sup><sub>0.03</sub>). Ito and Frondel (1967a) synthesized end-member schorlomite and kimzeyite, but we are not aware of a successful synthesis of the end-member {Ca<sub>3</sub>}[Ti<sub>2</sub>](SiAl<sub>2</sub>)O<sub>12</sub>.

#### 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 {Ca<sub>3</sub>}[TiMg] (Si<sub>3</sub>)O<sub>12</sub>, 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 {Ca<sub>3</sub>}[TiMg](Si<sub>3</sub>)O<sub>12</sub> 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  $\{Ca_3\}[Ga_2](Ge_3)O_{12}$  might have a natural analog. Johan and Oudin (1986) reported from the Pyrenees of France equant, sixsided 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  $\{Ca_3\}[Ga_2](Ge_3)O_{12}$  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  $\{Ca_3\}[Al_2](Ge_3)O_{12}$  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 endmembers (Tables 6–7; Appendix 2): "blythite,"  $\{Mn_3^{2+}\}[Mn_2^{2-}](Si_3)$ O<sub>12</sub>, as a subordinate component in a garnet from Cargoan, Nagpur, India; "khoharite,"  $\{Mg_3^{2+}\}[Fe_2^{3+}](Si_3)O_{12}$ , 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 "skiagite,"  $\{Fe_3^{2+}\}[Fe_2^{2+}](Si_3)O_{12}$ , 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, Otjosondu, Namibia (Amthauer et al. 1989; Bühn et al. 1995), "khoharite" and "skiagite" have been elusive, e.g., Virgo and Yoder (1974) failed to find "skiagite" 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 "skiagite" or "khoharite" components, respectively, and  $Mn^{3+}$  could be present as {Ca<sub>3</sub>}  $[Mn_2^{3+}](Si_3)O_{12}$  as well as  $\{Mn_3^{2+}\}[Mn_2^{3+}](Si_3)O_{12}$  in the Otjosondu garnet (Table 6). Garnets containing a significant proportion of the {Ca<sub>3</sub>}[Mn<sub>2</sub><sup>3+</sup>](Si<sub>3</sub>)O<sub>12</sub>,"blythite," "khoharite," and "skiagite" 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 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  $\{Mn_{2.99}^{2+}\}[(Cr_{1.14}^{3+}Mn_{0.51}^{3+})Ti_{0.35}]\{(Si_{2.22}Ti_{0.35})(Al_{0.28}Fe_{0.08}^{3+})\}$  $O_{12}$ , i.e., a { $Mn_3^{2+}$ }[ $Cr_2^{3+}$ ]( $Si_3$ ) $O_{12}$  component can be considered dominant, whereas that for the lowest Cr content is  $\{Mn_3^{2+}\}$  $[(Mn_{0.79}^{3+}Cr_{0.60}^{3+}Al_{0.09}Fe_{0.08}^{3+})Ti_{0.22}Mn_{0.22}^{2+}](Si_{3.01})O_{12}$ , i.e., with "blythite" dominant. The presence of significant Mn3+ 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  $\{Mn_3^{2+}\}$   $[Cr_2^{3+}](Si_3)O_{12}$ -dominant or  $\{Mn_3^{2+}\}$  $[Mn_2^{3+}](Si_3)O_{12}$ -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,  ${}^{x}Na+{}^{x}(Y, Yb) = 2{}^{x}R^{2+}$  (Enami et al. 1995; Røhr et al. 2007) and  ${}^{x}Na+{}^{y}Si = {}^{x}R^{2+}$  (Al or  ${}^{x}Na+{}^{y}Ti = {}^{x}R^{2+}{}^{y}Al$  (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%  $P_2O_5$  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%  $P_2O_5$  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,  $P_2O_5$  0.42 (±0.12) (Hålenius, unpublished data). The spessartine grains are cut by microfissures ranging from <1  $\mu$ m to ca. 10  $\mu$ 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  $\mu$ 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% P2O5 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 {Na<sub>3</sub>}[Al<sub>2</sub>] (P<sub>3</sub>)O<sub>12</sub> at 150–170 kbar by Brunet et al. (2006). Thilo (1941) reported synthesis of  $\{Na_3\}[Al_2](P_3)O_{12}$  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% P<sub>2</sub>O<sub>5</sub> (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  ${}^{X}\Box + 2{}^{Z}P = {}^{X}R^{2+}+2{}^{Z}Si$ and much subordinate  ${}^{X}Na+{}^{Z}P = {}^{X}R^{2+}+{}^{Z}Si$ . There was no evidence in their data for the substitution  ${}^{Z}(A1,Fe^{3+})+{}^{Z}P = 2{}^{Z}Si$  reported in an almandine-spessartine containing up to 2.1 wt% P2O5 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 postmagmatic 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  $\{Ca_2Na\}[Fe_2^{2+}](As_3^{5+})O_{12}$  end-member (Nagashima and Armbruster 2012). Attempts to synthesize the Fe<sup>2+</sup> 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. Twentynine 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: {Fe<sub>3</sub><sup>2+</sup>}[Al<sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>

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, Ia3d. 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:  ${Ca_3}[Fe_2^{3+}](Si_3)O_{12}$ 

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, *Ia3d*. 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: {Ca<sub>2</sub>Na}[Mg<sub>2</sub>](As $_3^{5+}$ )O<sub>12</sub> 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, *Ia3d*. Hawthorne (1976); Nagashima and Armbruster (2012).

Original or oldest description: Kühn (1840)

#### Bitikleite

End-member formula: {Ca<sub>3</sub>}[Sb<sup>5+</sup>Sn<sup>4+</sup>](Al<sub>3</sub>)O<sub>12</sub>

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, *Ia*3d. Galuskina et al. (2010b)

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

#### Calderite

End-member formula:  $\{Mn_3^{2+}\}[Fe_2^{3+}](Si_3)O_{12}$ 

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, *Ia*, *d*. No structure refinement; structure optimization by distance least-squares refinement (Ottonello et al. 1996). Original or oldest description: Fermor (1909, 1926)

Original of oldest description. Fernior (1909, 1

#### Cryolithionite

End-member formula: {Na<sub>3</sub>}[Al<sub>2</sub>](Li<sub>3</sub>)F<sub>12</sub>

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, *Ia3d*. Geller (1971). Original or oldest description: Ussing (1904)

#### Dzhuluite

End-member formula: {Ca<sub>3</sub>}[Sb<sup>5+</sup>Sn<sup>4+</sup>](Fe<sub>3</sub><sup>3+</sup>)O<sub>12</sub>

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, *Ia3d*. Structure not yet refined.

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

### Elbrusite

End-member formula:  $\{Ca_3\}[U_{0.5}^{6+}Zr_{1.5}](Fe_3^{3+})O_{12}$ 

Group: Bitikleite

IMA number: 2009-051

Modifications: Originally described as elbrusite-(Zr) with a formula  $\{Ca_3\}[U^{6+}Zr]$   $(Fe_2^{3+}Fe^{2+})O_{12}$ 

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, *Ia3d*. 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: {Ca<sub>3</sub>}[Sc<sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>

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, *Ia3d*.

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

Synthetic material. Will et al. (1977), Quartien et al. (200

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

#### Goldmanite

End-member formula:  ${Ca_3}[V_2^{3+}](Si_3)O_{12}$ 

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<sub>3</sub>}[Mn<sub>2</sub><sup>3+</sup>](Si<sub>2</sub>)(□)O<sub>8</sub>(OH)<sub>4</sub>

Group: Henritermierite

IMA number: 1968-029

Modifications: None

Etymology: For Henri-François-Émile Termier (1897–1989), a French geologist. Type locality: Tachgagalt mine, Morocco.

Crystal system, space group and structure refinement: Tetragonal, 141/acd. Armbruster et al. (2001).

Original or oldest description: Gaudefroy et al. (1969)

#### Holtstamite

Formula: {Ca<sub>3</sub>}[Al,Mn<sub>2</sub><sup>2+</sup>](Si<sub>2</sub>)(□)O<sub>8</sub>(OH)<sub>4</sub> 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, *I*4<sub>1</sub>/*acd*. Hålenius et al. (2005)

Original or oldest description: Hålenius (2004), Hålenius et al. (2005)

#### Irinarassite

End-member formula:  ${Ca_3}[Sn_2^{4+}](SiAl_2)O_{12}$ 

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<sub>3</sub>}[Al<sub>2</sub>](□<sub>3</sub>)(OH)<sub>12</sub> 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:  $\{Ca_3\}[Zr_2](SiFe_2^{3+})O_{12}$  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).

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#### Kimzeyite

End-member formula: {Ca<sub>3</sub>}[Zr<sub>2</sub>](SiAl<sub>2</sub>)O<sub>12</sub>

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<sub>3</sub>}[Cr<sub>2</sub><sup>3+</sup>](Si<sub>3</sub>)O<sub>12</sub>

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-Buthe, Lesotho.

Crystal system, space group and structure refinement: Isometric, *Ia3d*. Synthetic material: Juhin et al. (2010).

Original or oldest description: Nixon and Hornung (1968)

#### Maiorite

End-member formula: {Mg<sub>3</sub>}[SiMg](Si<sub>3</sub>)O<sub>12</sub>

Group: Garnet

IMA number: 1969-018. Modifications: Formula originally given as {(Mg,Na)<sub>3</sub>} [(Fe,Si,ALCr)<sub>2</sub>](Si<sub>2</sub>)O<sub>12</sub>.

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:  $\{Ca_2Na\}[Mn_2^{2+}](As_3^{5+})O_{12}$ 

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<sub>2</sub>Ca}[Mg<sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>

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, *Ia*3*d*. Grew et al. (2010)

Original or oldest description: Grew et al. (2010)

#### Momoiite

End-member formula:  $\{Mn_3^{2+}\}[V_2^{3+}](Si_3)O_{12}$ 

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  $\{Mn_3^{2+}\}[V_2^{3+}](Si_3)O_{12}$  as a component in garnet

Type locality: Kurase mine, Ehime Prefecture, Japan.

Crystal system and space group: Isometric, *Ia*3*d*. 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: {Ca<sub>3</sub>}[TiFe<sup>2+</sup>](Si<sub>3</sub>)O<sub>12</sub> 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, Ia3d. Structure not yet refined. Original or oldest description: Henmi et al. (1995)

#### Palenzonaite

End-member formula:  $\{Ca_2Na\}[Mn_2^{2+}](V_3^{5+})O_{12}$ 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, Ia3d. Basso (1987); Nagashima and Armbruster (2012)

Original or oldest description: Basso (1987)

#### Pyrope

End-member formula: {Mg<sub>3</sub>}[Al<sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>

Group: Garnet

IMA number: Grandfathered

Modifications: None

Etymology: From the Greek πνρωπός (pyropos) - firelike for its deep-red color. Type locality: Bohemia (Czech Republic).

Crystal system, space group and structure refinement: Isometric, Ia3d. 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:  $\{Ca_2Na\}[Mg_2](V_3^{5+})O_{12}$ 

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, Ia3d. Krause et al. (1999)

Original or oldest description: Krause et al. (1999)

#### Schorlomite

End-member formula: {Ca<sub>3</sub>}[Ti<sub>2</sub>](SiFe<sub>2</sub><sup>3+</sup>)O<sub>12</sub>

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, Ia3d. Chakhmouradian and McCammon (2005)

Original or oldest description: Shepard (1846), Whitney (1849), and Rammelsberg (1850a 1850b)

#### Spessartine

End-member formula: {Mn3+}[Al2](Si3)O12

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, Ia3d. 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:  ${Ca_3}[Sn_2^{4+}](SiFe_2^{3+})O_{12}$ 

Group: Schorlomite

IMA number: 2009-033

Modifications: None

Etymology: From both the Totur River situated in Eltyubyu 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, Ia3d. Structure not yet refined. Original or oldest description: Galuskina et al. (2010c)

#### Usturite

End-member formula: {Ca<sub>3</sub>}[Sb<sup>5+</sup>Zr](Fe<sub>3</sub><sup>3+</sup>)O<sub>12</sub>

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, Ia3d. Structure not yet refined. Original or oldest description: Galuskina et al. (2010b)

#### Uvarovite

End-member formula:  $\{Ca_3\}[Cr_2^{3+}](Si_3)O_{12}$ 

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, Ia3d. Novak and Gibbs (1971)

For birefringent uvarovite: Wildner and Andrut (2001)

Original or oldest description: Hess (1832)

#### Yafsoanite

End-member formula:  ${Ca_3}[Te_2^{6+}](Zn_3)O_{12}$ 

Group: ungrouped

IMA number: 1981-022

Modifications: Introduced with the idealized formula (Zn1.38Ca1.36Pb0.26)2=3.00TeO6;

current formula from Jarosch and Zemann (1989) and Mills et al. (2010). Etymology: From the acronym Yakytskii Filial Sibirskogo Otdeleniya Akademii

Nauk (Yakyt 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, Ia3d. Mills et al. (2010)

Original or oldest description: Kim et al. (1982)

## Appendix 2. List of synonyms, obsolete, varietal, and discredited names for garnet supergroup minerals

This list is necessarily incomplete as it was assembled mostly from secondary sources and compilations. In general, the identifications and attributions of those references have been accepted here. As many of the attributions are themselves secondary sources or compilations, they often do not refer to the first use or origin of the name.

Although some of the names are also synonymous with other minerals, or other materials (alloy, glass, etc.), these other meanings are not compiled here. The present terms are largely restricted to mineral species, solid-solution series, and groups of the garnet supergroup.

Name (n = 715)	Present Term (species, solid- solution series, or group)	Attribution	Reference				
achtaragdit <sup>*</sup>	grossular-katoite	Ernst Friedrich Glocker	Chester (1896)	alamandina	almandine		Simpson (1989)
achtaragdite*	grossular-katoite	Ernst Friedrich Glocker	Clark (1993)	alamandine	almandine	Dietrich Ludwig Gustav	Clark (1993)
achtarandit*	grossular-katoite	Johann Friedrich August Breithaupt	Clark (1993)	alexandrite garnet	garnet	Karsten Robert Webster, Basil	Bayliss (2000)
achtarandite*	grossular-katoite	I	Chester (1896)			William Anderson	
achtaryndit*	grossular-katoite	J. Auerbach	Clark (1993)	Al-garnet	almandine-	Masaki <b>Enami</b>	Bayliss (2000)
Adelaide ruby	almandine	Peter G. Read	Bayliss (2000)		spessartine- grossular		
African jade	grossular	Peter G. Read	Bayliss (2000)	Al-grandite	grossular-andradite	Michael J. Holdaway	Bayliss (2000)
Afrikanischer jade	grossular	Johann Georg Haditsch, H.	Bayliss (2000)	allochite	andradite	Thomas Allison Readwin	Chester (1896)
Alabandic carbuncles	almandine	Maus Pliny (Gaius Plinius Secundus)	Dana and Brush (1868)	allochroite	andradite	José Bonifácio de <b>Andrada</b> e Silva	Dana and Brush (1868)
alabandicus	almandine	Pliny (Gaius Plinius	Dana and Brush	allochroïte	andradite	José Bonifácio de <b>Andrada</b> e Silva	Allan (1814)
		Secundus)	(1868)	allocroita	andradite	Jeffrey de Fourestier	Bayliss (2000)
alabandina	almandine		Simpson (1989)	almandin	garnet	Georgius Agricola	Egleston (1892)
alabandine	garnet		Chester (1896)	almandina	almandine	Sande H. Zirlin	Bayliss (2000)
alabandine ruby	almandine	Peter G. Read	Bayliss (2000)	almandino	almandine	Centro Informazione e	Bayliss (2000)
alabandite (of Chester)	garnet		Chester (1896)	almandite	almandine	Servizi Gemmologici (CISGEM) James Dwight Dana	Dana and Brush
alabaunderryne	almandine		Simpson (1989)			-	(1868)
alabraundyne	almandine		Simpson (1989)	almendine	almandine	Jeffrey de Fourestier	Bayliss (2000)
alamandin	almandine	Dietrich Ludwig Gustav Karsten	Dana and Brush (1868)	almond stone	almandine		Manutchehr- Danai (2009)

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almondine amandine	almandine almandine		Simpson (1989) Simpson (1989)	berzelit	berzeliite	William Haidinger	Dana and Brush (1868)
American ruby	almandine	Peter G. Read	Bayliss (2000)	berzelite	berzeliite	William Haidinger	Clark (1993)
amethystizontes	garnet	<b>Pliny</b> (Gaius Plinius Secundus)	Dana and Brush (1868)	bijazi	almandine	Abū al-Rayhān Muhammad ibn Ahmad <b>al-Bīrūnī</b>	Lemmlein (1963)
anthill garnet	pyrope		Manutchehr-	bitikleite-(SnAl)	bitikleite	Irina O. Galuskina	this work
			Danai (2009)	bitikleite-(SnFe)	dzhuluite	Irina O. Galuskina	this work
anthracitis	garnet (?)	Pliny (Gaius Plinius	Dana and Brush	bitikleite-(ZrFe)	usturite	Irina O. Galuskina	this work
		Secundus)	(1868)	black garnet	andradite		Dana and Brush
anthrax, $\dot{\alpha}\nu\theta\rho\alpha\xi$	garnet	Theophrastus	Moore (1859),				(1868)
(of Theophrastus) aplome	andradite	René Just <b>Haüy</b>	Caley and Richards (1956) Jameson (1816)	black garnet of Frascati	andradite		Egleston (1892)
apricotine	garnet	icele sust many	Manutchehr- Danai (2009)	black garnet of the Pyrenees	andradite		Allan (1814)
Arizona rubin	pyrope	Johann Georg <b>Haditsch</b> , H.	Bayliss (2000)	blythite	hypothetical component:	Lewis Leigh Fermor	Clark (1993)
Arizona ruby	pyrope	<b>Maus</b> William Alexander <b>Deer</b> , Robert Andrew <b>Howie</b> ,	Bayliss (2000)	Bobrovka garnet	Mn <sub>3</sub> Mn <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> andradite		Simpson (1989)
Arizona spinel	almandine	Jack <b>Zussman</b> Robert <b>Webster</b> , Basil William <b>Anderson</b>	Bayliss (2000)	Bobrovska garnet	andradite		Manutchehr- Danai (2009)
Arizona-spinell	almandine	Johann Georg Haditsch, H.	Bayliss (2000)	Bobrowka garnet	andradite	Peter G. Read	Bayliss (2000)
Alizona-spinen	annanume	Maus	Bay1188 (2000)	bodenbenderite	spessartine and	Eberhard Rimann	Bayliss (2000)
asterias garnet	garnet		Hertz (1839)	Bohemian garnet	fluorite <b>pyrope-almandine</b>	Abraham Gottlob Werner	Dana and Brush
Australian ruby	garnet	Peter G. Read	Bayliss (2000)	Doneman gamer	pyrope-annanume	Abraham Gottioo Weiner	(1868)
azbazashtt	grossular	Ahmad ibn Yusuf <b>Al</b> Tifaschi	Huda (1998)	Bohemian ruby	pyrope	Robert Webster, Basil	Bayliss (2000)
azbazashtti	grossular	Ahmad ibn Yusuf Al	Huda (1998)			William Anderson	
bahandji	garnet	Tifaschi Ahmad ibn Yusuf Al Tifaschi	Huda (1998)	Böhmischer granat	pyrope-almandine	Abraham Gottlob Werner	Dana and Brush (1868)
bahdji	garnet	Ahmad ibn Yusuf Al Tifaschi	Huda (1998)	Böhmischer rubin	pyrope	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)
banafsh	garnet	Ahmad ibn Yusuf Al	Huda (1998)	bombita	andradite	Edward Salisbury Dana	Bayliss (2000)
bechet	garnet	Tifaschi	Lemmlein	brandãosite	spessartine	A. Mario de Jesus	Clark (1993)
	8		(1963),	braunstein kiesel	spessartine	Franz Ambrosius Reuss	Allan (1814)
becheta	garnet		Akhmetov (1990) Akhmetov	braunsteinkiesel	spessartine	Dietrich Ludwig Gustav Karsten	Dana and Brush (1868)
berzeliit	berzeliite	Otto B. Kühn	(1990) Dana and Brush (1868)	bredbergite	andradite	James Dwight Dana	Dana and Brush (1868)

Broddbo granat Broddbogranat	spessartine spessartine	Jöns Jacob <b>Berzelius</b> Jöns Jacob <b>Berzelius</b>	Egleston (1892) Dana and Brush	calderite (of Piddington)	andradite-bearing rock	Henry <b>Piddington</b>	Clark (1993)
	-		(1868)	California ruby	garnet	Richard M. Pearl	Bayliss (2000)
Ca(Al,Fe) garnet	grossular	William Alexander Deer,	Bayliss (2000)	Californian ruby	garnet	Peter G. Read	Bayliss (2000)
	1 1 2	Robert Andrew Howie, Jack Zussman		californite	grossular-katoite		Manutchehr- Danai (2009)
cacoclase	grossular, calcite and prehnite	Henry Carvill Lewis	Clark (1993)	canelhstein	grossular		Egleston (1892)
cacoclasite	l	U	$C_{1}$ (1002)	Cape garnet	pyrope		Manutchehr-
cacociasite	<b>grossular</b> , calcite and prehnite	Henry Carvill Lewis	Clark (1993)	Cupe guillet	pyrope		Danai (2009)
Ca-Fe garnet	andradite	William Alexander <b>Deer</b> , Robert Andrew <b>Howie</b> , Jack <b>Zussman</b>	Bayliss (2000)	Cape ruby	ругоре	William Alexander <b>Deer</b> , Robert Andrew <b>Howie</b> , Jack <b>Zussman</b>	Bayliss (2000)
Ca-Fe-spessartine	spessartine	Toyohumi Yosimura	Bayliss (2000)	caprubin	pyrope	Karl Franz Johann	Bayliss (2000)
Ca-garnet	grossular	William Alexander Deer,	Bayliss (2000)	carbocle	garnet	Chudoba	Simpson (1989)
		Robert Andrew <b>Howie</b> , Jack <b>Zussman</b>		carbokyl	garnet		Simpson (1989)
calcareo-aluminous	grossular	Edward John Chapman	Chapman (1843)	carbonchio	garnet		Simpson (1989)
garnet				carboncla	garnet		Simpson (1989)
calciospessartine	spessartine	Lewis Leigh Fermor	Clark (1993)	carboncle	garnet		Simpson (1989)
calcio-spessartite	spessartine	Leonard James Spencer	Bayliss (2000)	carbonclo	garnet		Simpson (1989)
calcium fer	spessartine	Madeleine Aballain	Bayliss (2000)	carbonkel	garnet		Simpson (1989)
spessartine				carboucle	garnet		Simpson (1989)
calcium-aluminum	grossular	Edward Salisbury Dana	Bayliss (2000)	carbuccle	garnet		Simpson (1989)
garnet				carbuckle	garnet		Simpson (1989)
calcium-chromium	uvarovite	Edward Salisbury Dana	Bayliss (2000)	carbuckyl	garnet		Simpson (1989)
garnet				carbucle	garnet		Simpson (1989)
calcium-	spessartine	Karl Franz Johann	Clark (1993)	carbucul	garnet		Simpson (1989)
eisenspessartine		Chudoba		carbunacle	garnet		Simpson (1989)
calcium-ferrigranat	andradite	Cornelio August Severius <b>Doelter</b> Cisterich y de la	Clark (1993)	carbunckle	garnet		Simpson (1989)
		Torre		carbuncle	garnet		Egleston (1892)
calcium-iron garnet	andradite	Edward Salisbury Dana	Bayliss (2000)	carbunclo	garnet		Simpson (1989)
calcium-zirconium	kimzeyite		Manutchehr-	carbunco	garnet		Simpson (1989)
garnet			Danai (2009)	carbuncul	garnet		Simpson (1989)
calc-pyralmandite	almandine	Lewis Leigh Fermor	Clark (1993)	carbuncules	garnet		Simpson (1989)
calc-spessartine	spessartine	Peter G. <b>Embrey</b> , John P. <b>Fuller</b> Lewis Leigh <b>Fermor</b>	Bayliss (2000) Clark (1993)	carbunculi charcedonii	ругоре	Georgius Agricola	Dana and Brush (1868)
calc-spessartite	spessartine	LEWIS LEIGH FERMOR	Claik (1993)	carbúnculo	garnet		Simpson (1989)
				carbunculum	garnet		Simpson (1989)

carbunculus	garnet		Dana and Brush (1868)	Ceylon garnet	pyrope		Egleston (1892)
			(1000)	Ceylon ruby	garnet		Manutchehr-
carbunculus Alabandicus	almandine	Pliny (Gaius Plinius Secundus)	Egleston (1892)	Cevlonhyacinth	gragerian	Jahann Caara <b>Haditaa</b> h H	Danai (2009)
<b>.</b>		,	E-lastar (1902)	Ceylonnyacının	grossular	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)
carbunculus Carchedonius	garnet		Egleston (1892)	Ceylonspinell	garnet	Johann Georg Haditsch, H. Maus	Bayliss (2000)
carbunculus	garnet	James Dwight Dana	Dana (1837)	chairbunkle	garnet		Simpson (1989)
dodecahedrus				charbocle	garnet		Simpson (1989)
carbunculus	garnet		Egleston (1892)	charbokel	garnet		Simpson (1989)
Garamanticus				charbokele	garnet		Simpson (1989)
carbunculus of Pliny	garnet	John Kidd	Allan (1814)	charbokell	garnet		Simpson (1989)
carbunculus	garnet		Egleston (1892)	charbokelle	garnet		Simpson (1989)
Troezenius	0			charbokil	garnet		Simpson (1989)
carbunkel	garnet		Simpson (1989)	charbokill	garnet		Simpson (1989)
carbunkile	garnet		Simpson (1989)	charbokle	garnet		Simpson (1989)
carbunkill	garnet		Simpson (1989)	charbokull	garnet		Simpson (1989)
carbunkle	garnet		Simpson (1989)	charbokyll	garnet		Simpson (1989)
carbunkulle	garnet		Simpson (1989)	charboncle	garnet		Simpson (1989)
carbunkyl	garnet		Simpson (1989)	charbonkkel	garnet		Simpson (1989)
carcbuncle	garnet		Simpson (1989)	charboukel	garnet		Simpson (1989)
carcedony	garnet	Edward Phillips	Simpson (1989)	charbouncle	garnet		Simpson (1989)
carchedonii in	pyrope	Georgius Agricola	Egleston (1892)	charbuche	garnet		Simpson (1989)
Boëmorum agris		6 8	6 ( )	charbuchle	garnet		Simpson (1989)
carchedonius	garnet	Edward Salisbury Dana	Bayliss (2000)	charbuckle	garnet		Simpson (1989)
carchedony	garnet	N. Bailey	Simpson (1989)	charbucle	garnet		Simpson (1989)
carfunkel	garnet	Johann Georg Haditsch, H.	Bayliss (2000)	charbugle	garnet		Simpson (1989)
~	0	Maus	• • •	charbukel	garnet		Simpson (1989)
Carthagenian carbuncle	garnet		Egleston (1892)	charbukelle	garnet		Simpson (1989)
				charbukill	garnet		Simpson (1989)
Carthaginian carbuncle	garnet	James Dwight Dana	Dana and Brush (1868)	charbukkill	garnet		Simpson (1989)
				charbukle	garnet		Simpson (1989)
Ca-spessartite	spessartine	Sylvie <b>Parc</b> , Daniel <b>Nahon</b> , Yves <b>Tardy</b> ,	Bayliss (2000)	charbunckell	garnet		Simpson (1989)
		Philippe Viellard		charbunckile	garnet		Simpson (1989)
caswellite	andradite-	Albert Huntington Chester	Clark (1993)	charbunckle	garnet		Simpson (1989)
ceraunio	spessartine pyrope	Solinus	Manutchehr-	charbuncle	garnet		Simpson (1989)
	+		Danai (2009)	charbuncul	garnet		Simpson (1989)

charbunkel	garnet		Simpson (1989)
charbunkil	garnet		Simpson (1989)
charbunkill	garnet		Simpson (1989)
charbunkle	garnet		Simpson (1989)
charbunkylle	garnet		Simpson (1989)
charebocle	garnet		Simpson (1989)
charebokyll	garnet		Simpson (1989)
chareboncle	garnet		Simpson (1989)
chaux arseniatée anhydre	berzeliite	Ours Pierre Armand Petit <b>Dufrénoy</b>	Dana and Brush (1868)
cherbukkill	garnet		Simpson (1989)
cherbukle	garnet		Simpson (1989)
chlorhibschite	not a mineral species: Ca <sub>3</sub> Al <sub>2</sub> Si <sub>3-x</sub> o <sub>x</sub> O <sub>8</sub> Cl <sub>4-x</sub>	Boris Valentinovich Chesnokov	Jambor et al. (1997)
chornomita	andradite	Jeffrey de Fourestier	Bayliss (2000)
chrom grossular	grossular	Jeffrey de Fourestier	Bayliss (2000)
chrome garnet	pyrope	Edward John Chapman	Chapman (1843)
chrome garnet	uvarovite		Egleston (1892)
chrome pyrope	ругоре	William Alexander <b>Deer</b> , Robert Andrew <b>Howie</b> , Jack <b>Zussman</b>	Bayliss (2000)
chromgranat	uvarovite	Karl Franz Johann	Bayliss (2000)
chromium garnet	uvarovite	Chudoba Jeffrey de Fourestier	Bayliss (2000)
chromium pyrope	pyrope or	Peter H. Nixon, George	Bayliss (2000)
cinnamite	knorringite grossular	Hornung G. Poggi	Allan (1814)
cinnamon garnet	grossular	Edward Salisbury Dana	Bayliss (2000)
cinnamon granat	grossular	Andrew M. Clark	Bayliss (2000)
cinnamon stone	grossular	Robert Jameson	Allan (1814)
cirolite	synthetic compound: Y <sub>3</sub> Al <sub>2</sub> Al <sub>3</sub> O <sub>12</sub>		Manutchehr- Danai (2009)
colofonite	andradite-grossular	Sande H. Zirlin	Bayliss (2000)
colophonit	andradite	Franz Ambrosius Reuss	Allan (1814)
colophonite	andradite	Dietrich Ludwig Gustav	Chester (1896)
Colorado ruby	pyrope	Karsten Peter G. Read	Bayliss (2000)
common garnet	garnet	Robert Jameson	Allan (1814)
coticule	garnet-bearing		Brongniart

	schist		(1807)
Cr-pyrope	pyrope or	Gary A. Novak, Gerald V.	Bayliss (2000)
dchanrasit	knorringite pyrope-almandine	Gibbs Karl Franz Johann Chudoba	Bayliss (2000)
dél-afrikaijade	grossular	Jeffrey de Fourestier	Bayliss (2000)
demantoid	andradite	Nils Adolf Erik	Chester (1896)
demantoiet	andradite	Nordenskiöld Sande H. Zirlin	Bayliss (2000)
dhanrasite	pyrope-almandine	S.R.N. Murthy	Bayliss (2000)
diamanite	synthetic compound: Y <sub>3</sub> Al <sub>2</sub> Al <sub>3</sub> O <sub>12</sub>		Manutchehr- Danai (2009)
diamantoid	andradite	Max Hutchinson Hey	Bayliss (2000)
diamantoïde	andradite	Sande H. Zirlin	Bayliss (2000)
diamite	synthetic compound: $Y_3Al_2Al_3O_{12}$		Manutchehr- Danai (2009)
diamonaite	synthetic compound: Y <sub>3</sub> Al <sub>2</sub> Al <sub>3</sub> O <sub>12</sub>		Manutchehr- Danai (2009)
diemlite	synthetic compound: Y <sub>3</sub> Al <sub>2</sub> Al <sub>3</sub> O <sub>12</sub>		Manutchehr- Danai (2009)
dimanthoid	garnet	Henry William Bristow	Egleston (1892)
dodecahedral garnet	garnet	Carl Friedrich Christian	Egleston (1892)
dodekaedrischer granat	garnet	Mohs Johann Georg Haditsch, H. Maus	Bayliss (2000)
dshonstonotit	spessartine	Karl Franz Johann <b>Chudoba</b>	Bayliss (2000)
Dubbelbrytande berzeliit	berzeliite	Edward Salisbury <b>Dana</b>	Bayliss (2000)
edler granat	garnet	Abraham Gottlob Werner	Allan (1814)
eisenandradit	hypothetical component: Fe <sub>3</sub> Fe <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>	Carl Walther Fischer (?)	Clark (1993)
eisen-calcium- spessartin	spessartine	Max Hutchinson Hey	Bayliss (2000)
eisenthongranat	almandine	Edward Salisbury Dana	Bayliss (2000)
eisentongranat	almandine	Karl Franz Johann <b>Chudoba</b>	Bayliss (2000)
elbrusite-(Zr)	elbrusite	Irina O. Galuskina	this work
Elie ruby	pyrope		Egleston (1892)

### Appendix 2

Ely ruby emaldine émeraude de oural	pyrope spessartine andradite spessartine	J. Stephen van der Lingen	Manutchehr- Danai (2009) Clark (1993)	feketegranat felsinrubin Fe-Mn-garnet	andradite pyrope-almandine	Jeffrey <b>de Fourestier</b> Max Hutchinson <b>Hey</b>	Bayliss (2000) Bayliss (2000)
	andradite	J. Stephen van der Lingen	Clark (1993)		10 1	·	5
	andradite	J. Stephen van der Lingen		Fe-Mn-garnet			
émeraude de oural				•	calderite	William Alexander Deer,	Bayliss (2000)
	anogantina		Manutchehr- Danai (2009)	Fe-pyrope	pyrope	Robert Andrew <b>Howie</b> , Jack <b>Zussman</b> Gary A. <b>Novak</b> , Gerald V.	Bayliss (2000)
emildine		J. Stephen van der Lingen	Clark (1993)	ге-руюре	pyrope	Gibbs	Bayliss (2000)
emilite	spessartine	J. Stephen van der Lingen	Clark (1993)	ferric kimzeyite	kerimasite	Peter C. Rickwood	Rickwood (1968)
erinadine	spessartine	J. Stephen van der Lingen	Clark (1993)	ferro-calderite	calderite	Lewis Leigh Fermor	(1908) Bayliss (2000)
erinite	spessartine	J. Stephen van der Lingen	Clark (1993)	ferrospessartine	spessartine	Karl Franz Johann	Clark (1993)
ernita	grossular	<b>Frank</b> (Franck or Francke?)	Clark (1993)	ferro-spessartite	spessartine	<b>Chudoba</b> Lewis Leigh <b>Fermor</b>	Clark (1993)
ernite	grossular	Frank (Franck or Francke?)	Clark (1993)	ferrotitanite	schorlomite	Josiah Dwight Whitney	Dana and Brush (1868)
escarboucle	garnet		Simpson (1989)	ferrugino-aluminous	almandine	Edward John Chapman	Chapman (1843)
escarbuncle	garnet		Simpson (1989)	garnet	annanunic	Edward John Chapman	Chapman (1045)
espartita	spessartine	Andrew M. Clark	Bayliss (2000)	ferrugino-calcareous	andradite	Edward John Chapman	Chapman (1843)
espesartita	spessartine	Edward Salisbury Dana	Bayliss (2000)	garnet	anurautte	Edward John Chapman	Chapman (1045)
espessartita	spessartine	Madeleine Aballain	Bayliss (2000)	Fe-Ti garnet	andradite-	Kenneth B. Schwartz,	Bayliss (2000)
essonit essonite	grossular grossular	Hauy René Just <b>Haüy</b>	Simpson (1989) Dana and Brush	re-riganici	schorlomite	Daniel A. Nolet, Roger George Burns	Day1133 (2000)
essonite	grossulai	Refic Just Hauy	(1868)	fire garnet	pyrope	George Durins	Egleston (1892)
Fahlungranat	almandine	Jöns Jacob Berzelius	Dana and Brush (1868)	flower of Jove	garnet	<b>Pliny</b> (Gaius Plinius Secundus)	Manutchehr- Danai (2009)
falscher hyacinth	grossular	Johann Georg <b>Haditsch</b> , H.	Bayliss (2000)	garamantic carbuncle	garnet		Egleston (1892)
,	0	Maus	,	garamantious	garnet	<b>Pliny</b> (Gaius Plinius	Clark (1993)
false hyacinth	garnet	Jeffrey de Fourestier	Bayliss (2000)	garnat	garnet	Secundus) Sande H. <b>Zirlin</b>	Bayliss (2000)
false ruby	garnet		Manutchehr- Danai (2009)	garnate	garnet		Simpson (1989)
C 1 1 4				garnetite	garnet		Chester (1896)
fashoda garnet	pyrope	Peter G. Read	Bayliss (2000)	garnet-jade	grossular	Leonard James Spencer	Clark (1993)
fashoda ruby	ругоре		Manutchehr- Danai (2009)	garnetoid	mineral(s) with the	Duncan McConnell	Clark (1993)
$(\mathbf{F}_{\mathbf{a}}^{2+}\mathbf{C}_{\mathbf{a}})$ correct	almandine-	Debart C. Newton, Demand	Davidas (2000)	-	garnet structure		
(Fe <sup>2+</sup> ,Ca) garnet	grossular	Robert C. Newton, Bernard J. Wood	Bayliss (2000)	garnette	garnet		Simpson (1989)
Fe <sup>3+</sup> -garnet	andradite- spessartine	Masaki Enami	Bayliss (2000)	garvi	garnet (pyrope?)	Abū al-Rayhān Muhammad ibn Ahmad <b>al-Bīrūnī</b>	Lemmlein (1963)
Fe-Ca-spessartine	spessartine	Toyohumi Yosimura	Bayliss (2000)	gemeiner granat	garnet	Abraham Gottlob Werner	Allan (1814)
Fe-garnet	almandine	William Alexander <b>Deer</b> , Robert Andrew <b>Howie</b> ,	Bayliss (2000)	geminaite	synthetic compound: Y <sub>3</sub> Al <sub>2</sub> Al <sub>3</sub> O <sub>12</sub>	Abraham Cothou Weiner	Manutchehr- Danai (2009)
Fe-grandite	andradite	Jack <b>Zussman</b> Michael J. <b>Holdaway</b>	Bayliss (2000)				

#### Manutchehrgemolyte synthetic compound: grenat almandin almandine Egleston (1892) Y<sub>3</sub>Al<sub>2</sub>Al<sub>3</sub>O<sub>12</sub> Danai (2009) René Just Haüy Allan (1814) grenat brun garnet grenat chromifère uvarovite Egleston (1892) Simpson (1989) gernat garnet Egleston (1892) grenat de chaux grossular gernate Simpson (1989) garnet Dana and Brush grenat du chaux grossular Francois Sulpice Beudant Simpson (1989) gernet garnet (1868)Leonard James Spencer Clark (1993) gibbsite (of Spencer) grossular grenat émarginé noir René Just Haüy Allan (1814) Clark (1993) andradite gibschite Leonard James Spencer grossular René Just Haüy Allan (1814) grenat granuliforme pyrope gooseberry-garnet grossular Chester (1896) Egleston (1892) grenat grossulaire Sande H. Zirlin Bayliss (2000) grossular graanat garnet André-Jean-François-Marie grenat manganèse spessartine Egleston (1892) gralmandite Lewis Leigh Fermor Clark (1993) grossular-Brochant de Villiers almandine Sande H. Zirlin Bayliss (2000) granada garnet grenat manganesié spessartine Alexandre Brongniart Allan (1814) granat garnet Johan Gottschalk Dana and Brush Egleston (1892) grenat manganesien spessartine (1868)Wallerius grenat mélanite andradite André-Jean-Francois-Marie Egleston (1892) granat von Longban andradite Emanuel Rothoff Dana and Brush Brochant de Villiers (1868)grenat noble garnet Egleston (1892) granat von Longbau andradite Emanuel Rothoff Egleston (1892) René Just Haüy Egleston (1892) grenat noir andradite Johann Georg Haditsch, H. Bayliss (2000) granatbord garnet grenat noir de Frescati andradite Allan (1814) Maus Sande H. Zirlin granate garnet Bayliss (2000) grenat ordinaire Allan (1814) garnet granatförmiges Martin Heinrich Klaproth Dana and Brush Alexandre Brongniart Allan (1814) spessartine grenat pyrop pyrope (1868)braunsteinerz René Just Haüy Allan (1814) grenat resinite andradite Seifert and Dana and Brush granati Bohemici A.B. De Boot René Just Haüv pyrope grenat résinite andradite Vrána (2005) (1868)granat-jade grossular Reinhard Anton Brauns Clark (1993) grenat rouge de feu René Just Haüv Egleston (1892) pyrope granuliforme granato Centro Informazione e Bayliss (2000) garnet Servizi Gemmologici René Just Haüy Allan (1814) grenat rougeâtre garnet (CISGEM) grenat Siriam Manutchehr-Max Hutchinson Hey Bayliss (2000) garnet granatoid garnet Danai (2009) granatus garnet Albertus Magnus Dana and Brush (1868)grenat Syrian garnet Dana and Brush (1868)grandite grossular-andradite Lewis Leigh Fermor Clark (1993) grenat Syrien garnet Egleston (1892) granular garnet Allan (1814) garnet Egleston (1892) grenat titanifère andradite green amorphous Allan (1814) garnet garnet René Just Haüy Allan (1814) grenat verdâtre garnet Allan (1814) grenat vert olive garnet René Just Haüy Martin Heinrich Klaproth Chester (1896) greenlandite garnet Egleston (1892) André-Jean-François-Marie Allan (1814) grenat yttrifère andradite grenat garnet

Madeleine Aballain

Bayliss (2000)

grenat-asterie

almandine

Brochant de Villiers

### Appendix 2

grenate	garnet		Manutchehr- Danai (2009)	hyacinth	grossular		Dana and Brush (1868)
grenatus	garnet		Egleston (1892)	hyacinthe de Ceylon	grossular		Egleston (1892)
grenaz	garnet (plural)		Simpson (1989)	hyacinthe la bella	garnet		Egleston (1892)
grönlandit (of Klaproth)	garnet	Martin Heinrich Klaproth	Bayliss (2000)	hyacinth-garnet	garnet		Dana and Brush (1868)
gronlandite	garnet	Madeleine Aballain	Bayliss (2000)	hyacinthoide	grossular	Jean-Claude Delamétherie	Chester (1896)
groslarita	grossular	Sande H. Zirlin	Bayliss (2000)	hyazinthe	pyrope	Carl Friedrich Christian	Egleston (1892)
grossulaar	grossular	Sande H. Zirlin	Bayliss (2000)	hudroon drodito	anduadita	Mohs W. Żabiński	Doutlile (2002)
grossulaire	grossular	François Sulpice Beudant	Dana and Brush (1868)	hydroandradite hydrogarnet	andradite grossular-katoite	W. Zabinski Einar P. Flint, Howard F. McMurdie, Lansing S.	Pertlik (2003) Clark (1993)
grossulare grossularia	grossular grossular	R. Jameson Abraham Gottlob <b>Werner</b>	Simpson (1989) Allan (1814)	hydrogranat	grossular-katoite	Wells Karl Franz Johann Chudoba	Clark (1993)
grossularite	grossular	Abraham Gottlob Werner	Dana and Brush (1868)	hydrograndit	grossular- andradite-katoite	Hugo Strunz	Clark (1993)
grossularoid	grossular	Dmitry Stepanovich Belyankin,	Clark (1993)	hydrograndite	grossular- andradite-katoite	H.G. <b>Huckenholz</b> , W. Lindhuber, K.T. Fehr	Pertlik (2003)
groszular	grossular	Valeriy Petrovich Petrov	Egleston (1892)	hydrogrenat	grossular-katoite	Madeleine Aballain	Bayliss (2000)
guarnaccine garnet	garnet		Manutchehr-	hydrogrossulaire	grossular-katoite	Madeleine Aballain	Bayliss (2000)
0 0	8		Danai (2009)	hydrogrossular	grossular-katoite	Colin Osborne Hutton	Clark (1993)
guarnaccino	garnet		Dana and Brush (1868)	hydrogrossularite	grossular-katoite	Shigeki <b>Iwamoto</b> , Toshio <b>Sudo</b>	Bayliss (2000)
hanléite	uvarovite	Lewis Leigh Fermor	Clark (1993)	hydromelanite	andradite	William Alexander Deer, Robert Andrew Howie,	Bayliss (2000)
haplome	andradite	René Just Haüy	Chester (1896)			Jack Zussman	
hematite garnet	garnet	Peter G. <b>Read</b>	Bayliss (2000)	hydropyralspite	hydroxyl-bearing <b>pyrope-almandine-</b>	Franz <b>Pertlik</b>	Pertlik (2003)
hessonite	grossular	Karl Cäsar Ritter von Leonhard	Dana and Brush (1868)	hydropyrope	<b>spessartine</b> hypothetical	Olav H.J. Christie	Bayliss (2000)
H-garnet	grossular-katoite	Jun Ito, Joel E. Arem	Bayliss (2000)		component: Mg <sub>3</sub> Al <sub>2</sub> (OH) <sub>12</sub>		
hibschit	grossular	Felix Cornu	Clark (1993)	hydroschorlomite	schorlomite;	Franz <b>Pertlik</b>	Pertlik (2003),
hibschite	grossular	Felix Cornu	Clark (1993)		titanite?		Laverne et al. (2006)
hibshite	grossular	JF. Parrot, C. Guernet	Parrot and Guernet (1972)	hydroshorlomite	titanite?	Christine Laverne, Olivier Grauby, Jeffrey C. Alt, Marcel Bohn	Laverne et al. (2006)
hidrogrossular	grossular	R. Dixon	Bayliss (2000)			Marcer Donn	
hollandine garnet	spessartine	Thomas Lind, Hermann	Lind et al.	hydrougrandite	andradite	Tsao Yung Lung	Bayliss (2000)
-	-	Bank, Ulrich Henn	(1993)	hydrouvarovite	uvarovite	Franz <b>Pertlik</b>	Pertlik (2003)
				hydroxygarnet	hydroxyl-bearing garnet	Hugo <b>Strunz</b> , Ernest H. <b>Nickel</b>	Pertlik (2003)

### Appendix 2

(1990)

idrogrossularia	grossular-katoite	Centro Informazione e Servizi Gemmologici (CISGEM)	Bayliss (2000)	jellettite	andradite		Manutchehr- Danai (2009)
igumnovite	not a mineral	Boris Valentinovich	Jambor et al.	jellitite	andradite	Jeffrey de Fourestier	Bayliss (2000)
	species:	Chesnokov	(1997)	jivaarit	schorlomite	Max Hutchinson Hey	Bayliss (2000)
iivaarite	Ca <sub>3</sub> Al <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> Cl <sub>4</sub> schorlomite	William Alexander Deer,	Bayliss (2000)	jiwaarit	schorlomite	Stepan Semyonovich	Clark (1993)
		Robert Andrew Howie, Jack Zussman		johnstonotite	spessartine- grossular	Kutorga W.A. Macleod, O.E. White	Clark (1993)
iiwaarit	schorlomite	Stepan Semyonovich Kutorga	Clark (1993)	jonstonotit	garnet	Johann Georg Haditsch, H.	Bayliss (2000)
iiwaarite	schorlomite	Stepan Semyonovich Kutorga	Clark (1993)	kakoklas	grossular, calcite	Maus Carl Adolf Ferdinand	Clark (1993)
imanite	synthetic compound: $Ca_3Ti^{3+}_2Si_3O_{12}$	A.V. Rudneva	Fleischer (1959), Valldor	kakoklasit	and prehnite grossular, calcite	Hintze Rudolf <b>Koechlin</b>	Clark (1993)
Indian compt			et al. (2011) Manutahahr	Kakokiash	and prehnite	Rudon Kotennii	Clark (1995)
Indian garnet	almandine		Manutchehr- Danai (2009)	Kalifornischer rubin	garnet	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)
iron alumina garnet	almandine	Thomas Egleston	Egleston (1892)	kalkchromgranat	uvarovite	Edward Salisbury Dana	Bayliss (2000)
iron-aluminagarnet	almandine	James Dwight Dana	Dana and Brush (1868)	kalkeisengranat	andradite	Carl Adolf Ferdinand Hintze	Clark (1993)
iron-andradite	hypothetical component:	Carl Walther Fischer	Clark (1993)	kalkeisentongranat	andradite	Cornelio August Severius <b>Doelter</b> Cisterich y de la Torre	Clark (1993)
iron-lime-garnet	Fe <sub>3</sub> Fe <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> andradite	Albert Huntington Chester	Chester (1896)	kalkgranat	andradite	Jöns Jacob Berzelius	Dana and Brush (1868)
ispid-chashma	garnet	Abū al-Rayhān Muhammad ibn Ahmad <b>al-Bīrūnī</b>	Lemmlein (1963)	kalkspessartit	spessartine	Max Hutchinson Hey	Bayliss (2000)
ivaarite	schorlomite	Stepan Semyonovich	Dana and Brush	kalkthongranat	grossular	Edward Salisbury Dana	Bayliss (2000)
		Kutorga	(1868)	kalktongranat	grossular	Max Hutchinson Hey	Bayliss (2000)
iwaarit	schorlomite	Stepan Semyonovich	Dana and Brush	kalophonit	andradite		Egleston (1892)
		Kutorga	(1868)	kameelstein	grossular	Max Hutchinson Hey	Bayliss (2000)
iwaarite	schorlomite		Egleston (1892)	kandy spinel	almandine	Peter G. Read	Bayliss (2000)
jacinta la bella	garnet		Dana and Brush	kandyspinell	almandine	Johann Georg Haditsch, H. Maus	Bayliss (2000)
·	5		(1868)	kaneelstein	garnet	Abraham Gottlob Werner	Allan (1814)
jacinth	garnet		Manutchehr- Danai (2009)	kanelstein	grossular	Abraham Gottlob Werner	Dana and Brush (1868)
jafszoanit	yafsoanite	Jeffrey de Fourestier	Bayliss (2000)	kapgranat	pyrope	Johann Georg Haditsch, H.	Bayliss (2000)
jellelite	andradite		Egleston (1892)	kaprubin	pyrope	Maus Max Hutchinson Hey	Bayliss (2000)
jellesite	andradite		Egleston (1892)	karbokle	garnet	·	Simpson (1989)
jelletite	andradite	James Apjohn	Dana and Brush	karboncle	garnet		Simpson (1989)
			(1868)	karbun	garnet		Akhmetov (1990)

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karbuncle	garnet		Simpson (1989)	lime-chromegarnet	uvarovite	James Dwight Dana	Dana and Brush (1868)
karbunkul	garnet		Akhmetov (1990)				
karbunkulus	almandine or	Jeffrey de Fourestier	Bayliss (2000)	lime-iron garnet	andradite	Thomas Egleston	Egleston (1892)
karfamukolos	pyrope		Akhmetov	lime-irongarnet	andradite	James Dwight Dana	Dana and Brush (1868)
kartaillukoios	garnet		(1990)	<b>.</b>			
karfunckel	pyrope	Franz Ambrosius Reuss	Allan (1814)	lime-magnesia-iron garnet	andradite	Thomas Egleston	Egleston (1892)
karfunfel	pyrope	Madeleine Aballain	Bayliss (2000)	0			E 1 ( (190 <b>2</b> )
karfunkel	pyrope		Dana and Brush	magnesia garnet	pyrope		Egleston (1892)
			(1868)	magnesia-alumina garnet	pyrope	Thomas Egleston	Egleston (1892)
karfunkel-stein	pyrope	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)	magnasia		James Dwight Dana	Dana and Brush
karmakaul	garnet	iviaus	Akhmetov (1990)	magnesia- aluminagarnet	ругоре	James Dwight Dana	(1868)
khoharite	hypothetical	Lewis Leigh Fermor	Clark (1993)	magnesia-blythite	pyrope-blythite	Lewis Leigh Fermor	Clark (1993)
	component: Mg <sub>3</sub> Fe <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>			magnesia-gralmandite	grossular-	Lewis Leigh Fermor	Clark (1993)
kimseyite	kimzeyite	Madeleine Aballain	Bayliss (2000)	magnesian calcium-	almandine andradite	Jeffrey de Fourestier	Bayliss (2000)
kirpuk	garnet	Afanasii Nikitin	Lemmlein	iron garnet			
			(1963), Akhmetov (1990)	magnesian pharmacolite	berzeliite	James Dwight Dana	Dana and Brush (1868)
Kollen garnet	almandine		Manutchehr-	magnesiathongranat	pyrope	Edward Salisbury Dana	Bayliss (2000)
			Danai (2009)	magnesiatongranat	pyrope	John Sinkankas	Bayliss (2000)
Kollin garnet	almandine	Peter G. Read	Bayliss (2000)	magnesio-blythite	pyrope-blythite	Lewis Leigh Fermor	Clark (1993)
kollophonit	andradite	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)	magnesium-aluminum	pyrope	Edward Salisbury Dana	Bayliss (2000)
kolofonit	andradite-grossular	Madeleine Aballain	Bayliss (2000)	garnet			
kolophonit	garnet	Dietrich Ludwig Gustav	Chester (1896)	magnesium-berzeliit	berzeliite	Wolfgang Bubeck	Bayliss (2000)
Kolorado-rubin	pyrope	Karsten Johann Georg Haditsch, H.	Bayliss (2000)	magnesiumtongranat	pyrope	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)
kryolithionit	cryolithionite	Maus Carl Adolf Ferdinand	Clark (1993)	malaia	pyrope-spessartine	Carol M. Stockton, D.	Stockton and
Kryontinoint	ci yontinomite	Hintze	Clark (1995)			Vincent <b>Manson</b> (personal communication from	Manson (1985)
kühnite	berzeliite	Henry James <b>Brooke</b> , William Hallows <b>Miller</b>	Dana and Brush (1868)			Campbell R. Bridges)	
				malaya	pyrope-spessartine		Stockton and Manson (1985)
landerite	grossular	Manuel M. Villada	Clark (1993)				× /
leucogarnet	grossular		Egleston (1892)	Mali garnet	grossular-andradite		Johnson et al. (1995)
leukogranat	grossular		Egleston (1892)	mandarin garnet	spessartine	Thomas Lind, Hermann	Lind et al.
lime-alumina garnet	grossular	Thomas Egleston	Egleston (1892)			Bank, Ulrich Henn	(1993)
lime-aluminagarnet	grossular	James Dwight Dana	Dana and Brush (1868)	mangan-almandine	almandine- spessartine	John Palmgren	Clark (1993)
lime-chrome garnet	uvarovite	Thomas Egleston	Egleston (1892)	mangan-almandite	almandine-	Lewis Leigh Fermor	Clark (1993)

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	spessartine			melanit	andradite	Abraham Gottlob Werner	Dana and Brush (1868)
mangan-berzeliit	manganberzeliite	Lars Johann Igelström	Igelström (1894)				(1808)
manganberziliit	manganberzeliite	Karl Franz Johann	Bayliss (2000)	melanite	andradite	Robert Jameson	Allan (1814)
manganese alumina garnet	spessartine	<b>Chudoba</b> Thomas <b>Egleston</b>	Egleston (1892)	(Mg,Ca) garnet	pyrope-grossular	Robert C. Newton, Bernard J. Wood	Bayliss (2000)
manganese berzeliite	manganberzeliite	Jun <b>Ito</b>	Bayliss (2000)	Mg-berzeliit	berzeliite	Sture Landergren	Landergren
manganese berzelite	manganberzeliite	Jun Ito	Bayliss (2000) Bayliss (2000)	Mn-berzeliit	manganberzeliite	Sture Landergren	(1930) Landergren
•	8		Allan (1814)	win-berzenn	manganberzennte	Sture Lander gren	(1930)
manganèse granatiforme	spessartine	André-Jean-François-Marie Brochant de Villiers	Allali (1814)	Mn-garnet	spessartine	Martin P. <b>Whitworth</b> , Martin <b>Feely</b>	Bayliss (2000)
manganese-	spessartine	James Dwight Dana	Dana and Brush	Mn-grossular	grossular	Gary A. Novak, Gerald V. Gibbs	Bayliss (2000)
aluminagarnet			(1868)	Mont Blanc ruby	garnet	GIDDS	Manutchehr-
manganese-aluminum	spessartine	Edward Salisbury Dana	Bayliss (2000)	5	<b>9</b>		Danai (2009)
garnet				Montana rubin	garnet	Johann Georg <b>Haditsch</b> , H.	Bayliss (2000)
manganese-garnet	spessartine	Mervyn H. Maskelyne	Clark (1993)	Wohunu ruom	garnet	Maus	Buy 155 (2000)
manganese-	grossular-	Lewis Leigh Fermor	Clark (1993)	Montana ruby	garnet	Peter G. Read	Bayliss (2000)
gralmandite	almandine			mother-of-ruby	garnet		Manutchehr-
manganesian garnet	spessartine	Henry Seybert	Dana and Brush				Danai (2009)
mungunosiun gurnet	spessurence	field y seybere	(1868)	mountain ruby	garnet	Peter G. Read	Bayliss (2000)
mangangralmandit	grossular-	Karl Franz Johann	Clark (1993)	mursinskite	andradite	Nikolai Ivanovich von	Bayliss (2000)
mangangrannanun	almandine-	Chudoba	Clark (1995)	4 1 1 1	1 1,	Koksharov	CL 1 (1002)
	spessartine			natronberzeliite	berzeliite	Helge Mattias Backstrom	Clark (1993)
mangangranat	spessartine		Dana and Brush (1868)	noble garnet	almandine		Egleston (1892)
			(1888)	nophak	garnet		Manutchehr- Danai (2009)
mangan-grandite	grossular-	Lewis Leigh Fermor	Clark (1993)				Danai (2009)
	andradite- almandine-			nophech	garnet		Manutchehr- Danai (2009)
	spessartine		D 1: (2000)			ndine F t N t N t N dine F ndine N	
manganthongranat	spessartine	Edward Salisbury Dana	Bayliss (2000)	nophek	almandine		Kunz (1913)
mangantongranat	spessartine	Max Hutchinson Hey	Bayliss (2000)	olivene	andradite		Manutchehr-
Manila garnet	pyrope-spessartine		Manutchehr- Danai (2009)				Danai (2009)
			Dallal (2009)	olivine garnet	andradite		Manutchehr-
mazenbi	pyrope	Ahmad ibn Yusuf Al	Huda (1998)				Danai (2009)
mazendi	almandine	<b>Tifaschi</b> Ahmad ibn Yusuf <b>Al</b>	Huda (1998)	olyntholite	grossular	Johann Gotthelf Fischer	Egleston (1892)
		Tifaschi				von Waldheim	
mazinadj	garnet	Mukhammed ibn Mansur	Lemmlein	olyntholith	grossular	Johann Gotthelf Fischer	Allan (1814)
medshorit	majorite or	Karl Franz Johann	(1963) Bayliss (2000)			von Waldheim	
	khoharite	Chudoba		olyntholyth	grossular	Edward John Chapman	Chapman (1843)
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oolongolite	synthetic compound	Dominique <b>Robert</b>	Manutchehr- Danai (2009)	polyadephite	andradite	Thomas <b>Thomson</b>	Dana and Brush (1868)
Oregon jade	grossular		Manutchehr-	precious garnet	garnet	Robert Jameson	Allan (1814)
			Danai (2009)	pseudoberzeliite	berzeliite	Valdemar Lindgren	Clark (1993)
oriental garnet	almandine		Dana and Brush	pyralmandin	pyrope-almandine	Max Hutchinson Hey	Bayliss (2000)
			(1868)	pyralmandite	pyrope-almandine	Lewis Leigh Fermor	Clark (1993)
oriental garnet of the lapidary	pyrope		Allan (1814)	pyralspite	pyrope-almandine- spessartine	Alexander Newton Winchell	Clark (1993)
orientalischer granat	almandine	Martin Heinrich Klaproth	Dana and Brush	pyramandite	pyrope-almandine	Basil William Anderson	Clark (1993)
			(1868)	pyramidal garnet	vesuvianite		Manutchehr-
orletz	pyrope	Peter G. Read	Bayliss (2000)				Danai (2009)
ouvarovite	uvarovite		Dana and Brush	pyrandine	pyrope-almandine	Basil William Anderson	Clark (1993)
			(1868)	pyrenäit	andradite	Abraham Gottlob Werner	Allan (1814)
ouwarowite	uvarovite	Germain Henri Hess	Dana (1837)	pyrenaite	andradite	Thomas Thomson	Clark (1993)
owarowite	uvarovite	Max Hutchinson Hey	Bayliss (2000)	pyreneit	andradite	Abraham Gottlob Werner	Dana and Brush
partschin	spessartine	William Haidinger	Chester (1896)				(1868)
partschinite	spessartine	William Haidinger	Larsen (1917)	pyreneite	andradite	Abraham Gottlob Werner	Chester (1896)
pearl garnet	andradite		Manutchehr-	ругоор	pyrope	Sande H. Zirlin	Bayliss (2000)
			Danai (2009)	pyrop	pyrope	Abraham Gottlob Werner	Dana and Brush
pech granat	andradite	Dietrich Ludwig Gustav	Allan (1814)				(1868)
piedra de grosella	grossular	Karsten	Manutchehr-	pyropi	pyrope (plural)		Simpson (1989)
prodia de grosoria	g. 000 <b></b>		Danai (2009)	ругоро	pyrope		Simpson (1989)
piedra miel	andradite		Manutchehr-	pyropus	pyrope		Simpson (1989)
r			Danai (2009)	pyrrharsenite	manganberzeliite	Edward Salisbury Dana	Clark (1993)
piroop	pyrope	E.K. Macintosh	Bayliss (2000)	pyrrhoarsenite	manganberzeliite	Lars Johann <b>Igelström</b>	Chester (1896)
pirop	pyrope		Egleston (1892)	pytenäit	andradite	Karl Franz Johann	Bayliss (2000)
pirope	pyrope		Simpson (1989)	ransätit	spessartine with	Chudoba Lars Johann Igelström	Bayliss (2000)
piropo	pyrope	Centro Informazione e	Bayliss (2000)		quartz, hematite,		
1 1	r, r	Servizi Gemmologici	5 ( )	ransatite	pyroxene spessartine with	Madeleine Aballain	Bayliss (2000)
piropus	pyrope	(CISGEM)	Simpson (1989)	Tunbullo	quartz, hematite,		<i>Duy1150</i> (2000)
pitch garnet	andradite		Manutchehr-	rathoffit	pyroxene andradite	Albert Huntington Chester	Pavilias (2000)
Price Burnet			Danai (2009)	rhodolite		Albert Huntington Chester William Earl Hidden,	Bayliss (2000) Clark (1993)
plazolite	grossular	William Frederick Foshag	Clark (1993)	mouonic	pyrope	Joseph Hyde <b>Pratt</b>	Claix (1995)
polyadelphine	andradite	Thomas <b>Thomson</b>	Chester (1896)	rhodomacon	nurono	Ian C.C. <b>Campbell</b>	Clark (1993)
polyadelphite	andradite	Thomas <b>Thomson</b>	Egleston (1892)	rhotofita	pyrope andradite	Jeffrey de Fourestier	Bayliss (2000)
Polladolpinto	undiaute	inoniuo inomioon	25.05001 (10)2)	rock-ruby		Jonney de Fourestier	Chester (1896)
				TOCK-TUDY	garnet		Chester (1890)

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Rocky Mountain ruby	pyrope	Robert <b>Webster</b> , Basil William <b>Anderson</b>	Bayliss (2000)	schorlemmite	schorlomite	Dorothy Lavelle <b>Bailey</b> , Kenneth Claude <b>Bailey</b>	Clark (1993)
rodolite	pyrope	Centro Informazione e	Bayliss (2000)	Siberian chrisolite	andradite	Peter G. Read	Bayliss (2000)
		Servizi Gemmologici (CISGEM)		Siberian chrysolite	andradite		Manutchehr-
rodomakon	pyrope	Karl Franz Johann	Bayliss (2000)				Danai (2009)
romanzovit	grossular	<b>Chudoba</b> Nils Adolf Erik	Dana and Brush	Siberian garnet	almandine		Manutchehr-
Tomanzovit	Grossular	Nordenskiöld	(1868)				Danai (2009)
romanzovite	garnet	Nils Adolf Erik <b>Nordenskiöld</b>	Dana (1837)	Siberian olivine	andradite		Manutchehr- Danai (2009)
romazowit	grossular		Egleston (1892)	Sibirischer chrysolith	andradite	Johann Georg Haditsch, H.	Bayliss (2000)
rose garnet	almandine		Egleston (1892)	Sibirischer granat	almandine	<b>Maus</b> Johann Georg <b>Haditsch</b> , H.	Bayliss (2000)
rose garnet	grossular or pyrope	George Letchworth	Bayliss (2000)	Sibilisence granat	annanume	Maus	Bay1133 (2000)
rose garnet	pyrope	<b>English</b> William Earl <b>Hidden</b> ,	Clark (1993)	Sibirischer olivin	andradite	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)
C		Joseph Hyde Pratt		silicamanganberzeliite	berzeliite	Michael Fleischer	Bayliss (2000)
roselite (of Webster)	grossular	Robert Webster	Clark (1993)	silicomanganberzeliite	berzeliite	M.M. Kaupova	Clark (1993)
rosolite	grossular	George Frederick Kunz	Clark (1993)	Singhalese garnet	almandine		Manutchehr-
rothoffit	andradite	Jöns Jacob Berzelius	Egleston (1892)		(pyrope?)		Danai (2009)
rothoffite	andradite	Jöns Jacob Berzelius	Dana and Brush (1868)	Sirianischer granat	almandine	Martin Heinrich Klaproth	Dana and Brush (1868)
rubinco di rocca	garnet		Egleston (1892)	skiagite	hypothetical	Lewis Leigh Fermor	Clark (1993)
rubino-di-rocca	garnet		Dana and Brush		component: $Fe_3Fe_2Si_3O_{12}$		
			(1868)	smeraldo degli Urali	andradite		Manutchehr-
rumanzowit	grossular	Stepan Semyonovich	Clark (1993)				Danai (2009)
rumjanzowit	grossular	Kutorga Stepan Semyonovich	Clark (1993)	Sn-andradite	andradite	I.R. Mulholland	Bayliss (2000)
5	8	Kutorga		soda berzeliite	manganberzeliite	Sten Anders Hjalmar	Sjögren (1894)
Russian chrysolite	andradite		Manutchehr- Danai (2009)	South African jade	grossular	<b>Sjögren</b> Arthur Lewis <b>Hall</b>	Clark (1993)
scandium-andradite	eringaite	Jun Ito and Clifford	Bayliss (2000)	South African ruby	pyrope		Manutchehr-
scandrum andraute	eringane	Frondel	Buyiiss (2000)				Danai (2009)
Sc-garnet	eringaite	Jun <b>Ito</b>	Bayliss (2000)	spalmandite	spessartine-	Lewis Leigh Fermor	Clark (1993)
schlackiger granat	andradite	Dietrich Ludwig Gustav Karsten	Allan (1814)	spandite	almandine spessartine-	Lewis Leigh Fermor	Clark (1993)
schorlamite	schorlomite	Karl Friedrich August	Rammelsberg	1	andradite	e	
		Rammelsberg	(1850)	spessartite	spessartine	François Sulpice Beudant	Chester (1896)
schorlemite	schorlomite		Manutchehr-	splintery garnet	andradite	District Links 1 C +	Egleston (1892)
			Danai (2009)	splittriger granat	andradite	Dietrich Ludwig Gustav Karsten	Allan (1814)

stachelbeerstein

grossular

Rudolf Koechlin

Clark (1993)

star garnet	almandine	Max Hutchinson Hey	Bayliss (2000)
succingranat	grossular	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)
succinite (of Bonvoisin)	garnet	Costanzo Benedetto Bonvicino ( <b>Bonvoisin</b> )	Allan (1814)
succnite	grossular	Costanzo Benedetto Bonvicino ( <b>Bonvoisin</b> )	Clark (1993)
Südafrikanische jade	grossular	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)
Suriam garnet	almandine	Robert Webster, Basil William Anderson	Bayliss (2000)
Syriam garnet	almandine	Robert <b>Webster</b> , Basil William <b>Anderson</b>	Bayliss (2000)
Syrian garnet	garnet		Egleston (1892)
Syrian garnet of the lapidary	garnet		Allan (1814)
talkgranat	andradite	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)
Tanga garnet	pyrope-almandine	Maus	Seifert and Hyrsl (1999)
Tanganyika rubies	garnet		Manutchehr- Danai (2009)
tellemarkite	grossular	Julius Albin Weisbach	Clark (1993)
Ti-andradite	andradite- schorlomite	William Alexander <b>Deer</b> , Robert Andrew <b>Howie</b> , Jack <b>Zussman</b>	Bayliss (2000)
Ti-garnet	schorlomite	Glenn A. Waychunas	Bayliss (2000)
titangarnet	garnet	Wilhelm Kunitz	Clark (1993)
titangranat	andradite	Karl Friedrich August <b>Rammelsberg</b>	Bayliss (2000)
titanmelanite	andradite- schorlomite	Adolf Knop	Clark (1993)
titanomelanite	andradite- schorlomite	Franz <b>Pertlik</b>	Pertlik (2003)
titano-melanite	andradite- schorlomite	William T. Pecora	Pecora (1942)
tonkalkgranat	grossular	John Sinkankas	Bayliss (2000)
tonmangangranat	spessartine	John <b>Sinkankas</b>	Bayliss (2000)
tontalkgranat	ругоре	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)

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topazolite	andradite	Costanzo Benedetto Bonvicino ( <b>Bonvoisin</b> )	Dana and Brush (1868)
topazolith	andradite	Costanzo Benedetto Bonvicino ( <b>Bonvoisin</b> )	Egleston (1892)
Transvaal garnet	grossular		Manutchehr- Danai (2009)
Transvaal jade	grossular	Reinhard Anton Brauns	Clark (1993)
Transvaalnephrit	grossular	Johann Georg Haditsch, H.	Bayliss (2000)
Transvaalsejade	grossular	Maus E.K. Macintosh	Bayliss (2000)
trautwineite	uvarovite	Edward Goldsmith	Goldsmith
trautwinite	uvarovite	Edward Goldsmith	(1873) Chester (1896)
tsavolite	grossular	Hermann Bank	Clark (1993)
tsavolith	grossular	Hermann Bank	Bayliss (2000)
tsavorite	grossular	Campbell R. Bridges and	Stockton and
ugrandite	uvarovite- grossular-andradite	Henry B. <b>Platt</b> Alexander Newton <b>Winchell</b>	Manson (1985) Clark (1993)
umbalite	pyrope-spessartine	Edward Joseph Gübelin (?)	Shigley et al. (1990)
Ural chrysolite	andradite	Robert <b>Webster</b> , Basil William <b>Anderson</b>	Bayliss (2000)
Ural emerald	andradite	Robert <b>Webster</b> , Basil William <b>Anderson</b>	Bayliss (2000)
Uralian emerald	andradite	Edward Salisbury Dana	Bayliss (2000)
Uralian olivine	andradite		Manutchehr- Danai (2009)
Uralischer smaragd	andradite	Johann Georg Haditsch, H.	Bayliss (2000)
Uralolivin	andradite	Maus Johann Georg Haditsch, H. Maus	Bayliss (2000)
uvarowit	uvarovite	Germain Henri Hess	Chester (1896)
uwarowit	uvarovite	Germain Henri <b>Hess</b>	Dana and Brush (1868)
uwarowite	uvarovite	Gustav Adolf Kenngott	Egleston (1892)
vanadium-garnet	grossular	S.T. Badalov	Clark (1993)
vanadiumgranat	grossular	S.T. Badalov	Clark (1993)
venisa	garnet		Akhmetov (1990)

vermeil	garnet	Peter G. Read	Bayliss (2000)
vermeille	garnet		Dana and Brush (1868)
vermeillegranat	<b>pyrope</b> or almandine	Johann Georg <b>Haditsch</b> , H. <b>Maus</b>	Bayliss (2000)
V-grossularite	grossular	Kurt Nassau	Bayliss (2000)
viluit	grossular	Vasilij Mikhailovich <b>Severgin</b>	Dana and Brush (1868)
viluite	grossular	Edward Salisbury Dana	Clark (1993)
vinisa	garnet		Hellie (1999)
vogesit	pyrope	Julius Albin Weisbach	Bayliss (2000)
vogesite	pyrope	Julius Albin Weisbach	Clark (1993)
white garnet	garnet		Egleston (1892)
white jade	grossular		Manutchehr- Danai (2009)
wilouite	grossular		Chester (1896)
wilouithe	grossular	Vasilij Mikhailovich	Clark (1993)
wiluit	grossular	Severgin Vasilij Mikhailovich Severgin	Dana and Brush (1868)
wiluite (of Severgin)	grossular	Vasilij Mikhailovich Severgin	Egleston (1892)
xalostocite	grossular	Sever gin	Clark (1993)
xantholite	andradite	Thomas Nuttall	Clark (1993)
yamatoite	momoiite	Toyofumi <b>Yoshimura</b> , Hitoshi <b>Momoi</b>	Clark (1993)
ytriogranate	andradite	Jeffrey de Fourestier	Bayliss (2000)
ytter-garnet	andradite	Carl Wilhelm Bergemann	Chester (1896)
yttergranat	andradite	Carl Wilhelm Bergemann	Dana and Brush (1868)
yttria garnet	andradite		Egleston (1892)
yttriferous lime-iron garnet	andradite	James Dwight Dana	Dana and Brush (1868)
yttriogarnet	andradite	Leonard James Spencer	Bayliss (2000)
yttrium-garnet	andradite	Max Hutchinson Hey	Bayliss (2000)
yttrium-granat	andradite	Hugo Strunz	Bayliss (2000)
yttrogarnet	synthetic compound: Y <sub>3</sub> Al <sub>2</sub> Al <sub>3</sub> O <sub>12</sub>	Hatten Schuyler <b>Yoder</b> , Jr., Mackenzie Lawrence <b>Keith</b>	Yoder and Keith (1951)
zimtstein	grossular	Johann Georg Haditsch, H.	Bayliss (2000)

		Maus	
Zr-schorlomite	schorlomite	Rosalba <b>Munno</b> , Giuseppe <b>Rossi</b> , Carla <b>Tadini</b>	Bayliss (2000)

\*Achtaragdit and its variant spellings (achtaragdite, achtarandit, actarandite, achtaryndit) indicate a pseudomorph (Koksharov 1866) in which garnets of the grossular-katoite series are major constituents (e.g., Clark et al. 1993; Galuskin et al. 1995; Galuskina et al. 1998).

The mineralogical nomenclature proposed by Povarennykh (1972) has been ignored in the present compilation, as have any "aluminia" and "aluminium" variants given by Bayliss (2000).

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### Appendix 2

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### Appendix 3. Six worked examples to illustrate the procedure to identify a garnet

OUTLINE OF RECOMMENDED PROCEDURE

Step 1. Calculate a formula on the basis of 12 anions and 8 cations (e.g., Appendix Table 1).

Step 2. Allocate cations (see section Site allocation of cations, e.g., Appendix Table 2).

Step 3. Identify dominant valences at each site, and dominant cation for each valence, being mindful of valencyimposed double site-occupancy (e.g., Appendix Table 3). This will identify the garnet by group and species.

Step 4. Write an empirical formula, ordering the cations first by valence and then by abundance.

Step 5. Calculate the maximum proportions of generalized components using the spreadsheet in Appendix 4 (e.g., Appendix Table 4).

Step 6. It may be necessary to factor in the results from step 4 before finalizing species identification (see notes).

Step 7. In some cases the maximum proportions of generalized components total 100% (examples 2, 6), in which case the components are all independent variables and can be used for plotting in Figures 6-9, 11. In most cases, the maximum proportions will total above 100%, and a subset of independent generalized components must be selected and recalculated to 100% for plotting, which is done for the other four examples.

Note: Discrepancies in the last decimal place are the result of rounding of tabulated values.

EXAMPLE 1. URANIAN DZHULUITE FROM THE NORTHERN CAUCASUS (GALUSKINA AND GALUSKIN, UNPUBLISHED DATA)

analysis w	ith calculated l	Fe <sup>2+</sup> /Fe <sup>3+</sup> rati	0
	wt.%		ı per 12
0			
UO <sub>3</sub>	11.15	$U^{6+}$	0.282
$Nb_2O_5$	0.87	Nb <sup>5+</sup>	0.047
$Sb_2O_5$	14.79	$\mathrm{Sb}^{5+}$	0.661
SiO <sub>2</sub>	0.15	Si	0.018
TiO <sub>2</sub>	1.32	Ti	0.120
ZrO <sub>2</sub>	3.48	Zr	0.204
$SnO_2$	16.20	Sn	0.777
$Al_2O_3$	4.26	Al	0.604
$Sc_2O_3$	0.13	Sc	0.014
$Fe_2O_3$	20.96	Fe <sup>3+</sup>	1.897
MgO	0.03	Mg	0.005
CaO	22.79	Ca	2.936
FeO	4.35	Fe <sup>2+</sup>	0.437
Sum	100.48		8.000

Appendix Table 1. Electron microprobe analysis with calculated  $Fe^{2^+}/Fe^{3^+}$  ratio

Appendix Table 2. Site Allocation				
		Ζ		
Fe <sup>2+</sup>	0.437	0.379		
$Al^{3+}$	0.604	0.604		
Fe <sup>3+</sup>	1.897	1.897		
Si <sup>4+</sup>	0.018	0.018		
Ti <sup>4+</sup>	0.044	0.103		
Sum	3.000	3.000		
charge	8.625	8.793		
		Y		
$Sc^{3+}$	0.014	0.014		
Ti <sup>4+</sup>	0.075	0.016		
$\mathrm{Sn}^{4+}$	0.777	0.777		
$Zr^{4+}$	0.204	0.204		
Nb <sup>5+</sup>	0.047	0.047		
$\mathrm{Sb}^{5+}$	0.661	0.661		
$U^{6+}$	0.282	0.282		
Sum	2.060	2.000		
		X		
Ca	2.936	2.936		
Mg	0.005	0.005		
Fe <sup>2+</sup>	0.000	0.059		
Sum	2.941	3.000		

1. Si, Al,  $Fe^{3+}$ ,  $Fe^{2+}$  and sufficient Ti to fill Z

2. Sc, remaining Ti, Sn, Nb, Sb and U to Y.

3. Ca and Mg to X

Column 1 gives allocation from Appendix 4. Because of the assignment of  $Fe^{2+}$  to the Z site in advance of Ti, calculated Y site occupancy exceeds 2 apfu, and X site occupancy is less than 3 apfu. Column 2 allocation with distribution of  $Fe^{2+}$  to achieve stoichiometry.

Appendix Table 3. Dominant valences, constituents and percent o	of
homovalent cations (from column 1 of Table 1)	

noniov	noniovalent cations (noni column 1 of 1 able 1)					
Site	Valence	Constituent	%	Identification		
Ζ	+3	Fe	76	Bitikleite group		
Y	+5	Sb	93	Dzhuluite		
Y	+4	Sn	74	Dzhuluite		
X	+2	Ca	99.8	Dzhuluite		

Note: *Y* is constrained to have two occupants because of valency-imposed double site-occupancy.

$$\label{eq:constraint} \begin{split} & \text{Empirical formula from Table 2, column 1 (dominant cation for dominant valence in bold):} \\ & \{ \textbf{Ca}_{2.936} Mg_{0.005} \} [(\textbf{Sn}_{0.777} Zr_{0.204} Ti_{0.075})(\textbf{Sb}_{0.661} Nb_{0.047}) U_{0.282} Sc_{0.014}] ((\textbf{Fe}^{3+}_{1.897} Al_{0.604}) Fe^{2+}_{0.437} (Ti_{0.044} Si_{0.018})) O_{12} \} \end{split}$$

Appendix	Table 4.1	Proportions	s of ger	eralized	components

	Maximum	Proportion	Group or
Component	Proportion <sup>*</sup>	as independent	formula type
$(n^{2+})$ ( $n^{2+}$ )	14.000/	variable <sup>#</sup>	0
$\{R^{2+}_{3}\}[R^{6+}_{2}](R^{2+}_{3})O_{12}$	14.08%	12.62%	yafsoanite-type
$\{R_{3}^{2+3}\}[R_{1.5}^{4+1}R_{0.5}^{6+0}](R_{3}^{3+3})O_{12}$	56.32%	5.85%	Bitikleite: elbrusite-type
${R^{2+}_{3}}[R^{5+}R^{4+}](R^{3+}_{3})O_{12}$	70.78%	70.78%	Bitikleite: dzhuluite-type
$\{R^{2+3}\}[R^{4+2}](R^{4+}R^{3+2})O_{12}$	6.24%	10.07%	Schorlomite
${R^{2+}_{3}}[R^{3+}_{2}](R^{4+}_{3})O_{12}$	0.68%	0.68%	Garnet: eringaite-type
Total	141.11%	100.00%	

Note: \*From column 1. <sup>#</sup>From column 2. The five generalized components are independent variables, but proportions as independent variables can only be calculated from a formula for ideal stoichiometry.

Comment: Uranium is split between two components (bitikleite and yafsoanite-type), both of which are subordinate, and thus Table 4 (either column 2 or column 3) and the empirical formulae give the same identification, dzhuluite, which has the generalized formula,  $\{R^{2+}\}[R^{5+}R^{4+}](R^{3+})O_{12}$ .

EXAMPLE 2. GARNET MCO4, HIGH TI, SCHORLOMITE FROM MAGNET COVE, ARKANSAS (CHAKHMOURADIAN AND MCCAMMON 2005)

Appendix Table 5. Electron microprobe analysis with calculated  $Fe^{2+}/Fe^{3+}$  ratio

anaryon	in this value and the	/1.0	iune
	Wt%		apfu per 12 O
SiO <sub>2</sub>	26.16	Si	2.250
TiO <sub>2</sub>	16.52	Ti	1.069
$ZrO_2$	1.31	Zr	0.055
$Al_2O_3$	1.60	Al	0.162
Fe <sub>2</sub> O <sub>3</sub>	17.07	Fe <sup>3+</sup>	1.105
FeO	3.44	Fe <sup>2+</sup>	0.247
MnO	0.48	Mn	0.035
MgO	1.21	Mg	0.155
CaO	31.54	Ca	2.907
Na <sub>2</sub> O	0.09	Na	0.015
Sum	99.42	Sum	8.000

Appendix Tal	ole 6. Sit	e Allocation
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	Ζ
Si	2.250
Al	0.162
Fe <sup>3+</sup>	0.588
Sum	3.000
Charge	11.250
U	Y
Ti	1.069
Zr	0.055
Fe <sup>3+</sup>	0.517
Mg	0.155
Fe <sup>2+</sup>	0.204
Sum	2.000
	X
Fe <sup>2+</sup>	0.043
Ca	2.907
Mn	0.035
Na	0.015
Sum	3.000

- 1. Si to Z
- 2. Al to Z
- 3. Fe<sup>3+</sup> to Z to bring total to 3 apfu, then Y
- 4. Ca and Na to X
- 5.  $Ti^{4+}$ , remaining Fe<sup>3+</sup>, and Zr to Y.
- 6. Mg: First to Y
- 7.  $\text{Fe}^{2+}$  First to *Y* to bring total to 2 apfu, then to *X* 8.  $\text{Mn}^{2+}$  to *X*, which brings total *X* to 3 apfu

Appendix Table 7. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%	Identification
Ζ	+4	Si	100	Garnet group*
Y	+4	Ti	95	Schorlomite
X	+2	Ca	97	Schorlomite
NT /	* 0.0 1	TT 1 1 0 1 1 1	• • • •	

Note: \*Cf. Appendix Table 8, which gives schorlomite group

Empirical formula (dominant cation for dominant valence in bold):

 $\{(\mathbf{\hat{Ca}}_{2.907}Fe^{2+}_{0.043}Mn_{0.035})Na_{0.015}\}[(\mathbf{Ti}_{1.069}Zr_{0.055})Fe^{3+}_{0.517}(Fe^{2+}_{0.204}Mg_{0.155})](\mathbf{Si}_{2.250}(Fe^{3+}_{0.588}Al_{0.162}))O_{12}]$ 

Appendix Table 8. Maximum proportions of generalized components

Component	Proportion	Group and type
${R^{2+}_{3}}[R^{4+}_{2}](R^{4+}R^{3+}_{2})O_{12}$	37.5%	Schorlomite
${R^{2+}_{3}}[R^{3+}_{2}](R^{4+}_{3})O_{12}$	25.9%	Garnet: andradite-type
${R^{2+}_{3}}[R^{4+}R^{2+}](R^{4+}_{3})O_{12}$	35.9%	Garnet: morimotoite-type
${R^{+}_{2}R^{2+}}[R^{4+}_{2}](R^{4+}_{3})O_{12}$	0.8%	Garnet: {Na <sub>2</sub> Ca}[Ti <sub>2</sub> ](Si <sub>3</sub> )O <sub>12</sub> -type
Total	100.00%	

Note: The four generalized components are independent variables.

Comment: The empirical formula gives  $R^{4+}$  the dominant valence at *Z* and *Y*, but the identification is clear only from Table 8, which gives,  $\{R^{2+}_{3}\}[R^{4+}_{2}](R^{4+}R^{3+}_{2})O_{12}$ , schorlomite, as the dominant component. The contradiction results from garnet-group components together being dominant, whereas schorlomite is more abundant than any one of the garnet components.

EXAMPLE 3. HOLOTYPE MENZERITE, PARRY SOUND, ONTARIO, CANADA-(Y) (GRAIN NO. 1-5, GREW ET AL. 2010)

Appendix Table 9. Electron microprobe	
analysis with calculated Fe <sup>2+</sup> /Fe <sup>3+</sup> ratio	

anaryon			1000
	Wt%		apfu per 12 O
SiO <sub>2</sub>	30.64	Si	2.820
TiO <sub>2</sub>	1.10	Ti	0.076
$Al_2O_3$	4.87	Al	0.528
$Sc_2O_3$	0.17	Sc	0.014
$V_2O_3$	0.17	V	0.013
$Cr_2O_3$	0.04	Cr	0.003
$Fe_2O_3$	8.36	Fe <sup>3+</sup>	0.579
$Y_2O_3$	16.93	Y	0.829
$La_2O_3$	0.00	La	0.000
$Ce_2O_3$	0.01	Ce	0.000
$Pr_2O_3$	0.00	Pr	0.000
$Nd_2O_3$	0.12	Nd	0.004
$Sm_2O_3$	0.15	Sm	0.005
$Eu_2O_3$	0.01	Eu	0.000
$Gd_2O_3$	0.36	Gd	0.011
$Tb_2O_3$	0.11	Tb	0.003
$Dy_2O_3$	1.52	Dy	0.045
Ho <sub>2</sub> O <sub>3</sub>	0.63	Но	0.018
$Er_2O_3$	2.40	Er	0.069
$Tm_2O_3$	0.38	Tm	0.011
$Yb_2O_3$	2.03	Yb	0.057
$Lu_2O_3$	0.68	Lu	0.019
MgO	3.98	Mg	0.546
CaO	13.92	Ca	1.372
MnO	0.85	Mn	0.066
FeO	11.84	$\mathrm{Fe}^{2+}$	0.911
Sum	101.26	Sum	8.000

Z	
Si	2.820
Al	0.180
Sum	3.000
Charge	11.820
Y	
Ti	0.076
Al	0.348
Sc	0.014
V	0.013
Cr	0.003
Fe <sup>3+</sup>	0.580
Mg	0.546
Fe <sup>2+</sup>	0.422
Sum	2.000
X	
Y + REE	1.072
Ca	1.372
Mn	0.066
Fe <sup>2+</sup>	0.489
Sum	3.000

- 1. Si: First to Z
- 2. Al to Z to bring total to 3 apfu, then Y
- 3. Fe<sup>3+</sup> to *Y*
- 4. Ca, Y, REE to X
- 5. Al (after deducting Al at Z),  $Sc^{3+}$ ,  $Ti^{4+}$ ,  $V^{3+}$ ,  $Cr^{3+}$ ,  $Fe^{3+}$  to Y.
- 6. Mg: First to Y
- 7. Fe<sup>2+</sup> First to *Y* to bring total to 2 apfu, then to *X* 8. Mn<sup>2+</sup> to *X*, which brings total *X* to 3 apfu

Appendix Table 11. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%	Identification
Ζ	+4	Si	100	Garnet group
Y	+2	Mg	56	Menzerite-(Y)
X	+3	Y	77	Menzerite-(Y)
X	+2	Ca	71	Menzerite-(Y)

Note: X is constrained to have two occupants because of valency-imposed double site-occupancy.

Empirical formula (dominant cation for dominant valence in bold):  $\{(\mathbf{Ca}_{1,372}Fe^{2+}_{0,489}Mn_{0.066})(\mathbf{Y}_{0,829}REE_{0.243})\}[(\mathbf{Mg}_{0.546}Fe^{2+}_{0.422})(Fe^{3+}_{0.579}Al_{0.348}Sc_{0.014}V_{0.013}Cr_{0.003})Ti_{0.076}](\mathbf{Si}_{2.820}Al_{0.180})O_{12}]$ 

Appendix Table 12. Proportions of generalized components

Component	Maximum Proportion <sup>*</sup>	Proportion as independent variable <sup>#</sup>	Group and type
$\{R_{3}^{3+}\}[R_{2}^{3+}](R_{3}^{3+})O_{12}$	6.02%	6.02%	${Y_3}[Al_2](Al_3)O_{12}$ -type
${R^{2+3}}[R^{4+2}](R^{4+}R^{3+2})O_{12}$	3.81%	-	Schorlomite
${R^{2+}_{3}}[R^{4+}R^{2+}](R^{4+}_{3})O_{12}$	7.61%	7.61%	Garnet: morimotoite-type
${R^{3+}_{2}R^{2+}}[R^{2+}_{2}](R^{4+}_{3})O_{12}$	48.42%	44.61%	Garnet: menzerite-(Y)-type
$ \{ R^{3+}_{2} R^{2+} \} [ R^{2+}_{2} ] (R^{4+}_{3}) O_{12}  \{ R^{2+}_{3} \} [ R^{3+}_{2} ] (R^{4+}_{3}) O_{12} $	47.77%	41.75%	Garnet: andradite-type
Total	113.64	100.00%	

Note: Y represents Y and REE. \*From Appendix 4. Only four of these generalized components are independent. <sup>#</sup>One of two sets of independent variables

EXAMPLE 4. FLUORINE-BEARING SPESSARTINE FROM CLEAR CREEK COUNTY, COLORADO (SMYTH ET AL. 1990)

Appendix Table 13. Electron microprobe analysis with calculated  $Fe^{2+}/Fe^{3+}$  ratio

	Wt%	apfu	per 12 O
SiO <sub>2</sub>	32.55	Si	2.681
TiO <sub>2</sub>	0.06	Ti	0.004
$Al_2O_3$	20.13	Al	1.954
$Fe_2O_3$	0.33	Fe <sup>3+</sup>	0.020
FeO	4.50	Fe <sup>2+</sup>	0.310
MnO	37.98	$Mn^{2+}$	2.650
CaO	0.60	Ca	0.053
		Sum	7.672
$H_2O+$	0.64	OH	0.352
F	3.68	F	0.959
O=F	-1.55	0	10.690
Total	98.92	Sum	12.000

Note: H<sub>2</sub>O content by IR spectroscopy.

	Ζ
Si	2.672
vacancies	0.328
Sum	3.000
Charge	10.690
	Y
Al	1.954
Fe <sup>3+</sup>	0.020
Fe <sup>2+</sup>	0.013
Si	0.009
Ti	0.004
Sum	2.000
	X
$Mn^{2+}$	2.650
Fe <sup>2+</sup>	0.297
Ca	0.053
Sum	3.000

1. Vacancies equal to  $\frac{1}{4}$  F plus  $\frac{1}{4}$  (OH) to Z

- 2. Si to Z to bring total of Si and vacancies to 3
- 3. Remaining Si to *Y*
- 4. Al, Ti to  $\tilde{Y}$

5.  $Fe^{2+}$  to *Y* to bring total to 2 apfu

6. Mn, Ca and remaining  $Fe^{2+}$  to X

Appendix Table 15. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%	Identification
Ζ	+4	Si	100	Garnet group
Y	+3	Al	99	Garnet group
X	+2	Mn	88	Spessartine

Empirical formula (dominant cation for dominant valence in bold):  $(\mathbf{M}_{\mathbf{T}} = \mathbf{E}_{2} - \mathbf{C}_{2} \rightarrow) \mathbf{f}(\mathbf{A}_{\mathbf{L}} = \mathbf{E}_{2}^{3+}) \mathbf{E}_{2}^{2+} - (\mathbf{S}_{1}^{2} = \mathbf{T}_{1}^{2}) \mathbf{I}(\mathbf{S}_{1}^{2} = \mathbf{T}_{2}^{2})$ 

 $\{Mn_{2.650}Fe_{0.297}Ca_{0.053}\}[(Al_{1.954}Fe^{3+}_{0.020})Fe^{2+}_{0.013}(Si_{0.009}Ti_{0.004})](Si_{2.672}\square_{0.328})O_{10.690}F_{0.959}(OH)_{0.352}]$ 

Generalized Component	Maximum proportion <sup>*</sup>	Proportion as independent variable <sup>#</sup>	Group or formula type
$\{R^{2+}_{3}\}[R^{3+}_{2}](\Box)_{3}(OH)_{12}$	2.93%	2.93%	katoite-type
$\{R^{2+}_{3}\}[R^{3+}_{2}](\Box)_{3}F_{12}$	7.99%	7.99%	$\{Mn_3\}[Al_2](\Box)_3F_{12}$ -type
${R^{2+}_{3}}[R^{3+}_{2}](R^{4+}_{2}\square)(OH)_{4}$	8.79%	_	Henritermierite-type
${R^{2+}_{3}}[R^{4+}_{2}](R^{4+}R^{3+}_{2})O_{12}$	0.02%	_	Schorlomite-type
${R^{2+}_{3}}[R^{4+}R^{2+}](R^{4+}_{3})O_{12}$	1.27%	1.27%	Garnet: morimotoite-type
${R^{2+}_{3}}[R^{3+}_{2}](R^{4+}_{3})O_{12}$	89.08%	87.81%	Garnet: spessartine-type
Total	110.06%	100.00%	
Note: *From Appendix 4.			

Appendix Table 16. Proportions of generalized components

EXAMPLE 5. GARNET JF22. "MAJORITIC" GARNET INCLUDED IN DIAMOND, JAGERSFONTEIN KIMBERLITE, SOUTH AFRICA (TAPPERT ET AL. 2005)

Appendix Table 17. Electron microprobe analysis with calculated  $Fe^{2+}/Fe^{3+}$  ratio

analysis with calculated Fe /Fe ratio					
Wt%		apfu	per 12 O		
$P_2O_5$	0.09	Р	0.006		
SiO <sub>2</sub>	48.70	Si	3.525		
TiO <sub>2</sub>	0.50	Ti	0.027		
$Al_2O_3$	9.65	Al	0.823		
$Cr_2O_3$	0.22	Cr	0.013		
$Fe_2O_3$	2.49	Fe <sup>3+</sup>	0.135		
MgO	21.70	Mg	2.341		
CaO	5.73	Ca	0.444		
MnO	0.36	Mn	0.022		
FeO	9.46	Fe <sup>2+</sup>	0.573		
Na <sub>2</sub> O	0.65	Na	0.091		
Sum	99.55	Sum	8.000		

Appendix Table 18. Site Allocation				
Z				
Р	0.006			
Si	2.994			
Sum	3.000			
Charge	12.006			
Ŭ Y				
Si	0.530			
Ti	0.027			
Al	0.823			
Cr	0.013			
Fe <sup>3+</sup>	0.135			
Mg	0.472			
Sum	2.000			
X				
Na	0.091			
Ca	0.444			
Mn	0.022			
Fe	0.573			
Mg	1.870			
Sum	3.000			

- 1. Si and P to Z to a maximum of 3 apfu, overflow of Si to Y
- 2. Ca and Na to X
- Ti<sup>4+</sup>, Cr<sup>3+</sup>, Fe<sup>3+</sup> to *Y* Mg: First to *Y* to bring total to 2 apfu, then to *X*
- 5. Fe<sup> $\bar{2}^+$ </sup> to *X*
- 6.  $Mn^{2+}$  to *X*, which brings total to 3 apfu

Appendix Table 19. Dominant valences, constituents and	ł
percent of homovalent cations	

Site	Valence	Constituent	%	Identification
Ζ	+4	Si	100	Garnet group
Y	+3	Al	85	Pyrope
X	+2	Mg	64	Pyrope

Note: Because of valency-imposed double site-occupancy at Y,  $R^{4+}$ Mg is considered as a unit, which is still subordinate to  $2R^{3+}$  (Table 8).

Empirical formula (dominant cation for dominant valence in bold):  $\{(\mathbf{Mg_{1.870}}Fe^{2^{+}}_{0.573}Ca_{0.444}Mn_{0.022})Na_{0.091}\}[(\mathbf{Al_{0.823}}Fe^{3^{+}}_{0.135}Cr_{0.013})(Si_{0.530}Ti_{0.027})Mg_{0.472}](Si_{2.994}P_{0.006})O_{12}]$ 

Appendix Table 20. Proportions of generalized components

Component	Maximum Proportion <sup>*</sup>	Proportion as independent variable <sup>#</sup>	Group and type
${R^{1+}_{3}}[R^{3+}_{2}](R^{5+}_{3})O_{12}$	0.18%	0.18%	Berzeliite: {Na <sub>3</sub> }[Al <sub>2</sub> ](P <sub>3</sub> )O <sub>12</sub> -type
${R^{2+}_{2}R^{1+}}{R^{2+}_{2}}{R^{5+}_{3}}O_{12}$	0.18%	_	Berzeliite-type
${R^{+}_{2}R^{2+}}[R^{4+}_{2}](R^{4+}_{3})O_{12}$	4.56%	4.28%	Garnet: {Na <sub>2</sub> Ca}[Ti <sub>2</sub> ](Si <sub>3</sub> )O <sub>12</sub> -type
${R^{2+}_{3}}[R^{3+}_{2}](R^{4+}_{3})O_{12}$	48.55%	48.37%	Garnet: pyrope-type
${R^{2+}_{3}}[R^{4+}R^{2+}](R^{4+}_{3})O_{12}$	47.16%	47.16%	Garnet: majorite-type
Total	100.64%	100.00%	

Note: \*From Appendix 4. Only four of these generalized components are independent. \*One of two sets of independent variables.

Comment: No matter which set of independent components is chosen, the generalized component,  ${R^{2+}_{3}}[R^{3+}_{2}](Si_{3})O_{12}$ , pyrope, is dominant.

EXAMPLE 6. HOLOTYPE MORIMOTOITE, FUKA, OKAYAMA PREFECTURE, JAPAN (HENMI ET AL. 1995)

Appendix Table 21. Electron microprobe	
analysis with calculated $Fe^{2+}/Fe^{3+}$ ratio	

			-
	Wt%		12 O
SiO <sub>2</sub>	26.93	Si	2.319
TiO <sub>2</sub>	18.51	Ti	1.199
$ZrO_2$	1.48	Zr	0.062
$Al_2O_3$	0.97	Al	0.098
$Fe_2O_3$	11.44	Fe <sup>3+</sup>	0.741
FeO	7.77	Fe <sup>2+</sup>	0.559
MnO	0.23	Mn	0.017
MgO	0.87	Mg	0.112
CaO	31.35	Ca	2.893
Sum	99.54	Sum	8.000

Appendix Table 22. Site Allocation

	Ζ	
Si		2.319
Al		0.098
Fe <sup>3+</sup>		0.583
Sum		3.000
Charge		11.319
	Y	
Ti		1.199
Zr		0.062
Fe <sup>3+</sup>		0.158
Mg		0.112
Fe <sup>2+</sup>		0.469
Sum		2.000
	X	
Fe <sup>2+</sup>		0.091
Ca		2.893
Mn		0.017
Sum		3.000

- 1. Si to Z
- 2. Al to Z
- 3. Fe<sup>3+</sup> to Z to bring total to 3 apfu, then Y
- 4. Ca to *X*

- 5. Ti<sup>4+</sup>, remaining Fe<sup>3+</sup>, and Zr to Y.
   6. Mg: to Y
   7. Fe<sup>2+</sup> First to Y to bring total to 2 apfu, then to X
- 8.  $Mn^{2+}$  to X, which brings total X to 3 apfu

Appendix Table 23. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%	Identification
Ζ	+4	Si	100	Garnet group
Y	+4	Ti	95	Morimotoite
Y	+2	Fe	81	Morimotoite
X	+2	Ca	96	Morimotoite

Note: Y is constrained to have two occupants because of valency-imposed double site-occupancy.

Empirical formula (dominant cation for dominant valence in bold):  $\{\mathbf{Ca_{2.892}}Fe^{2^{+}}_{0.091}Mn_{0.017}\}[(\mathbf{Ti_{1.199}}Zr_{0.062})(\mathbf{Fe^{2^{+}}}_{0.468}Mg_{0.112})Fe^{3^{+}}_{0.159}](\mathbf{Si_{2.319}}(Fe^{3^{+}}_{0.583}Al_{0.098}))O_{12})$ 

Appendix Table 24. Maximum proportions of generalized components

<u>- ippenant i uote = it ituatinium proportione of Senerumeta componente</u>				
Component	Proportion	Group		
${R^{2+}_{3}}[R^{4+}_{2}](R^{4+}R^{3+}_{2})O_{12}$	34.05%	Schorlomite		
${R^{2+}_{3}}[R^{3+}_{2}](R^{4+}_{3})O_{12}$	7.93%	Garnet: andradite-type		
${R^{2+}_{3}}[R^{4+}R^{2+}](R^{4+}_{3})O_{12}$	58.01%	Garnet: morimotoite type		
Total	100.00%			

Note: The three generalized components are independent variables.

Comment: The empirical formula gives  $R^{4+}$  the dominant valence at Z and Y, with  $R^{2+}$  second at Y, but the identification is clear from Table 20, which gives  $\{R^{2+3}\}[R^{4+}R^{2+}](R^{4+}_{3})O_{12}$ , morimotoite, as the dominant component.

### Appendix 4. Description of the Excel spreadsheet

#### Purpose

Appendix 4 is intended to determine the dominant species present from a chemical analysis of a natural garnet. This appendix consists of an Excel spreadsheet that can accept up to 50 analyses at a time, and yields for each analysis its group and species, as well as an empirical formula.

#### Input

The data from a chemical analysis are entered into the Data\_Report worksheet as oxides in percent by weight, with the exception of fluorine, which is entered as the element in percent by weight. Mathematical operations are undertaken on the linked Calculation worksheet; data should not be input directly into this latter worksheet. The list of inputs for the Data\_Report worksheet in percent by weight includes: SiO<sub>2</sub>, TiO<sub>2</sub>, ZrO<sub>2</sub>, SnO<sub>2</sub>, HfO<sub>2</sub>, ThO<sub>2</sub>, UO<sub>3</sub>, TeO<sub>3</sub>, Sb<sub>2</sub>O<sub>5</sub>, As<sub>2</sub>O<sub>5</sub>, V<sub>2</sub>O<sub>5</sub>, Nb<sub>2</sub>O<sub>5</sub>, P<sub>2</sub>O<sub>5</sub>, Y<sub>2</sub>O<sub>3</sub> (include REE<sub>2</sub>O<sub>3</sub> as the equivalent proportion of Y<sub>2</sub>O<sub>3</sub> along with the measured Y<sub>2</sub>O<sub>3</sub> content), Al<sub>2</sub>O<sub>3</sub>, Sc<sub>2</sub>O<sub>3</sub>, Cr<sub>2</sub>O<sub>3</sub>, V<sub>2</sub>O<sub>3</sub>, FeO, Fe<sub>2</sub>O<sub>3</sub> (but see below), ZnO, MnO, MgO, CaO, Na<sub>2</sub>O, Li<sub>2</sub>O, H<sub>2</sub>O<sup>+</sup> (water of crystallization), and F. Any correction needed for the oxygen equivalence of fluorine is calculated by the spreadsheet. The user must decide whether any vanadium content is expressed as V<sub>2</sub>O<sub>3</sub> or V<sub>2</sub>O<sub>5</sub>.

If the total iron content of the analysis is entered as FeO (wt.%), then the method of Droop (1987) is used to calculate the proportions of  $Fe^{2+}$  and  $Fe^{3+}$  and  $Mn^{2+}$  and  $Mn^{3+}$  (this latter constituent only in the absence of  $Fe^{2+}$ ) on the basis of 12 anions, where the anions are the sum of  $O^{2-}$ , (OH)<sup>-</sup>, and F<sup>-</sup>. If the user inputs some or all of the iron content as  $Fe_2O_3$  (wt.%), then this calculation of  $Fe^{2+}$  and  $Fe^{3+}$ , and  $Mn^{2+}$  and  $Mn^{3+}$ , is not performed. In any case, the user should not input  $Mn_2O_3$ , but rather allow the spreadsheet to calculate this quantity as necessary.

The cation proportions are calculated on the basis of 12 anions, with charge-balance used (as described above) to attempt to obtain a total of 8 non-H cations. The elements or valences B, S, K,  $V^{2+}$ , Ni, Ga, Ge, Sr, Ba, Pb, and  $U^{4+}$  are not included in the spreadsheet.

For analyses suspected to be of the tetragonal-symmetry minerals henritermierite or holtstamite, the entry FALSE should be given in the cells that query "cubic? (true / false)", whereas for other hydrous garnets, TRUE should be entered. For convenience, the lower symmetry and distinct structures of the tetragonal garnets are otherwise ignored in this spreadsheet.

### Site allocation of cations

Appendix 4 allocates the cations to the three distinct structural sites using an inflexible set of assumptions. It need hardly be stated that structural and/or spectroscopic data are preferable to using such an algorithm, but such information is not commonly available for large data sets, in contrast to the abundant chemical data obtained from electron microprobe analyses.

The site allocation assumptions follow those of Table 3 of the manuscript. The priority of filling each cation site is summarized here as follows:

Z > Y > X;  $Z = (As, V^{5+}, P, Li, Zn) > Si > Al > Fe^{3+} > Fe^{2+}, Ti;$   $Y = (Zr, Sn, Hf, U, Te, Sb, Nb, Sc, Cr, V^{3+}) > (Si, Ti, Al, Mn^{3+}, Fe^{3+}) > Mg > Fe^{2+} > Mn;$  $X = (Y, Ca, Na, Mn, Fe^{2+}, Th) > Mg.$  As per the manuscript, hydrogen is incorporated via the "hydrogarnet substitution":  $4H + {}^{Z}\Box \rightarrow \Box + {}^{Z}Si$ , and tetrahedral vacancies are also assumed if fluorine is present in the absence of corresponding quantities of lithium.

#### Extended dominant-constituent rule

Hatert and Burke (2008) defined "the *rule of the dominant constituent*: a mineral is a distinct species if the set of dominant constituents at the sites in the crystal structure is distinct from that of any other mineral with the same structural arrangement." Because of "cases of coupled heterovalent–homovalent substitutions", it was necessary for the rule to be "extended with the dominant-valency rule by considering a group of atoms with the same valency state as a single constituent." And therefore, "the extension [of the dominant-constituent rule] with the dominant-valency rule is necessary to establish charge-balanced end-member formulae for solid-solution series with complex mechanisms of substitution" (Hatert and Burke 2008).

In the garnet supergroup, in which the approved species (manuscript Table 1) are formulated as end-members, following Hawthorne (2002), the effect of the *extended dominant-constituent rule* is to arrange the end-members into general charge-balanced formulae. This is reflected in the classification of the approved species, in which the end-members are classified into groups by the effective charge of the Z site.

The spreadsheet determines group and species in accord with the extended dominant-constituent rule. For each cation site, the spreadsheet sums the homovalent cations that occupy that site. For example, for the *X* site, Ca+Mg+Mn+Fe yields the sum of the divalent ions, the sodium content gives the value for monovalent ions, and yttrium yields the value for trivalent ions. From the proportions of the dominant valences, the <u>maximum content</u> of each type of charge-balanced end-member formula is then calculated. These maxima are calculated separately from each other. However, in several cases, the proportions of different end-member formulae may be limited by the same minimum quantity of a valence state, e.g.,  $Na^+$ , present in the analysis. In such cases, the maximum contents of the end-member formulae are not independent, and their sum will therefore exceed 100%.

Having found the most abundant charge-balanced formula, the group to which it belongs is assigned (manuscript Table 1). From the assignment of the group, and from the site allocations of the cations, the principal cations that occupy the charge-balanced formula of that group are determined, and thus the dominant species is assigned. A set of hypothetical end-members is included in the calculations of the spreadsheet to assist in the rare cases in which an approved species is not found for an analysis.

### **Results and empirical formula**

From the allocation of the cations, and the anions determined from the chemical analysis, a preliminary empirical formula is given, with the quantities rounded to a maximum of three decimal places. The constituents of the empirical formula are ordered by atomic site, and organized in each site by decreasing abundance. The results, including group, dominant species, and empirical formula, are given below each corresponding original analysis on the Data\_Report worksheet.

Because of the limitations of text formats for calculated cells in Excel, the cations  $Fe^{2+}$  and  $Fe^{3+}$  are given respectively as Feii and FeIII in the *Y* and/or *Z* sites of an empirical formula. Similarly,  $Mn^{2+}$  and  $Mn^{3+}$  are reported on the *Y* site of an empirical formula as Mnii and MnIII. In contrast, cations whose occurrence is restricted to a given site, e.g.,  $V^{3+}$  on the *Y* site, are expressed without any charge designation, as there should be no ambiguity as to their identities. Cation vacancies on the *Z* site are not shown explicitly in the formulae yielded by the Excel spreadsheet, but are established by difference from the ideal proportions, and from the presence of F and/or OH.