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Nomenclature of the Garnet Supergroup

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16 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 in order to be approved. The general formula for the garnet supergroup minerals is $\{X_3\}[Y_2](Z_3)\phi_{12}$, where X, Y and Z refer to dodecahedral, octahedral and tetrahedral sites, respectively, and φ is O, OH or F. Most garnets are cubic, space group *Ia-3d* (no. 230), but two OH-bearing species (henritermierite and holtstamite) have tetragonal symmetry, space group, I4₁/acd (no. 142), and their X, Z and φ sites are split into more symmetrically-unique atomic positions. Total charge at the Z site and symmetry are criteria for distinguishing groups, whereas the dominant-constituent and dominant-valency rules are critical in identifying species. Twenty-nine species belong to one of five groups: the tetragonal henritermierite group and the isometric bitikleite, schorlomite, garnet and berzeliite groups with a total charge at Z of 8 (silicate), 9 (oxide), 10 (silicate), 12 (silicate) and 15 (vanadate, arsenate), respectively. Three species are single representatives of potential groups in which Z is vacant or occupied by monovalent (halide, hydroxide) or divalent cations (oxide). We recommend that suffixes (other than Levinson modifiers) not be used in naming minerals in the garnet supergroup. Existing names with suffixes have been replaced with new root names where necessary: bitikleite-(SnAl) to bitikleite, 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.

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

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43 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. in press), 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-3d (no. 230) has few sites: only three cationic and one anionic (e.g., Menzer 1928; Novak and Gibbs 1971; Merli et al. 1995; Geiger 2008), and the most common garnets have relatively simple chemical compositions. However, the garnet structure is remarkably flexible in a chemical sense: 53 elements were reported in the Inorganic Crystal Structure Database (Allmann and Hinek 2007) and five more are reported in synthetic garnets (Geller 1967; Ronniger and Mill' 1973; Yudintsev 2003; Yudintsev et al. 2002; Utsunomiya et al. 2005). In the period 2009-2010, 10 new species of garnet, with constituents such as Sc, Y, Sn, Sb and U, which have not been previously reported in significant quantities in natural garnet, were approved by the Commission on New Minerals, Nomenclature and Classification (CNMNC) of the International Mineralogical Association (IMA), resulting in a nearly 50% increase in the number of accepted species with the garnet structure. There are four more possible species, bringing to 26 the number of elements essential to defining existing and possible mineral species with the garnet structure.

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

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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; Khohari 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 32 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 in order to emphasize that the garnet supergroup comprises not only silicates (Fig. 1a, c-e), but also a halide (Fig. 1b), hydroxides, oxides, vanadates and arsenates (Fig. 1g). The groups are listed in order of increasing charge of cations that occupy the *Z* site of the end-members. Species within each group are listed as end-members with increasing atomic number of the *Z* site, followed by increasing atomic number of the *Y* site and lastly, 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 formulae given in the 2009 list (updated in 2012) of minerals approved by the CNMNC with the end-member formulae approved with the classification presented here.

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

Our procedure for distinguishing species relies heavily on the dominant-valency rule, which is an extension of the dominant-constituent rule (Hatert and Burke 2008). The latter rule states that species designation is based on the dominant constituent at a given crystallographic site, which works well when all constituents have the same valence. However, when ions at a given crystallographic site have different valences, it is essential that the dominant valence be determined first, and then species and group designation is determined by the dominant ion having this valence. Traditionally, identifying a garnet species has 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 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-3d (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 φ 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 $Z\phi_4$ tetrahedra and $Y\phi_6$ octahedra, which share corners to form a three-dimensional 136 137 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 138 X cations, resulting in a high percentage of shared edges between the dodecahedra on the one hand 139 and the octahedra and tetrahedra on the other. However, the octahedra and tetrahedra do not share 140 edges with each other (cf. TAPP: Harris et al. 1997; Finger and Conrad 2000). 141 In hydrous garnets, the major mechanism of hydroxyl incorporation is by the coupled 142 substitution $4H + {}^{Z}\Box \rightarrow \Box + {}^{Z}Si$, i.e., the hydrogen ions occupy a separate site of general symmetry 143 (Wyckoff position 96h) coordinated to O defining the tetrahedral site, which is vacant (e.g., Ferro et 144 al. 2003; Lager et al. 1987, 1989). The hydrogen ions lie approximately on the faces of the 145 146 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 147 148 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, 149 Armbruster et al. 2001) to 0.904 0.95 Å in synthetic katoite (neutron diffraction, Lager et al. 1987; 150 Cohen-Addad et al. 1967). Allowing that O H and O D distances obtained by X-ray diffraction 151 are shorter than those obtained by neutron diffraction, Lager et al. (1987) concluded that the 152 153 reported distances are consistent with isolated OH groups (lacking H-bonding) and assumed that the 154 residual density located near oxygen can be attributed to the displaced (bonding) electron between O and H and not to the hydrogen itself. 155 However, compositional data, nuclear magnetic resonance (NMR) spectra and infrared (IR) 156 spectra have been cited as evidence for multiple H occupancy in grossular and garnets in the 157 158 hydrogrossular series. Cation vacancies at the X and Y sites calculated from electron microprobe analyses without direct determination of H₂O have been cited as evidence for the presence of H in 159 these polyhedra, either without crystallographic data (Birkett and Trzcienski 1984), or in 160 conjunction with single-crystal refinements of Ca, Al, Fe and Si, whereas H could be located only 161 in a few of the crystals studied and not quantified (Basso et al. 1984a,b; Basso and Cabella 1990). 162 Kalinichenko et al. (1987) interpreted NMR spectra obtained on a grossular to indicate 2H in the 163 octahedra and 1H in the tetrahedra. In a comprehensive IR study of the hydrogrossular series, 164 Rossman and Aines (1991) reported that samples containing substantial H (>11.7 wt.% H₂O 165 equivalent to >5.43 OH per formula unit) gave spectra consistent with the substitution $4H + {}^{Z}\Box \rightarrow$ 166 \Box + ^ZSi, whereas samples with much less H (<3.6 wt.% H₂O, mostly <0.5 wt.%) gave 7 different 167 168 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 169 Fourier-transform IR spectra, Eeckhout et al. (2002) concluded that there is no evidence for a 170

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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 H-rich samples in which H can be determined by these techniques give data consistent with $4H + {}^{Z}\Box \rightarrow \Box + {}^{Z}Si$. 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-3d* (no. 230) but the two species in the henritermierite group have tetragonal symmetry $I4_1/acd$ (no. 142), and the X, Z and φ sites are split into more symmetrically-unique sites, without altering the topology such that the idealized formula becomes $\{Ca1_2\}\{Ca2\}[R^{3+}_2](Si1_2)(\square 2)O1_4O2_4(O3H)_4$, where $R^{3+}=Mn$ or Al. Armbruster et al. (2001) concluded that Jahn-Teller distortion resulting from Mn^{3+} 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 analogue holtstamite has been thought to require a minimum Mn³⁺ content, which is estimated to be at least 0.2 Mn³⁺ per formula unit (pfu), the amount reported in an isometric andradite (Armbruster 1995) and no more than 0.64 Mn³⁺ 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 Sideficient spessartine containing no Mn³⁺, but showing I4₁/acd symmetry attributed to (OH,F)₄ 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-3d* 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 2¹. This list includes the synonyms 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

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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 species 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"

¹For copies of Appendices 2 and 4, Document item AM-YR-XXX, contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. Deposit items may also be available on the American Mineralogist web site at http://www.minsocam.org.

The nomenclature of naturally-occurring garnet containing substantial amounts of the 235 236 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., $\{Ca_3\}[Al_2](Si_3$ 237 $_{x}\square_{x}$)O_{12-4x}(OH)_{4x} where 0 < x < 3 and \square is vacancy. For the majority of these garnets, x < 1.5 (e.g., 238 Passaglia and Rinaldi 1984), "Hibschite" was approved by the then Commission on New Minerals 239 and Mineral Names (CNMMN, the predecessor of the CNMNC) as a name for OH-bearing 240 grossular with x < 1.5 (Dunn et al. 1985) because "hibschite" had priority (Cornu 1905, 1906) over 241 242 "plazolite" (Foshag 1920) and "hydrogrossular" (Hutton 1943). However, "hibschite" is not distinct from grossular according to the dominant-constituent rule, i.e., $Si > \square$ at the Z site, therefore 243 "hibschite" is discredited in favor of grossular (Table 5). Dunn et al. (1985) allowed that "the name 244 hydrogrossular may still be applied to members of the series with appreciable OH content but 245 undetermined SiO₄/(OH)₄ ratio." 246 247 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 248 et al. 1941). Dunn et al. (1985) implied that the term "hydrogrossular group" and "hydrogrossular 249 series" would be acceptable for compositions along the grossular katoite join, but in our 250 classification the binary would no longer qualify as a group, whereas the term "series" has a more 251 restrictive meaning than a simple binary solid solution (Mills et al. 2009; see above). 252 The tetragonal hydroxyl-bearing garnets henritermierite and holtstamite (Fig. 1a) are 253 considered to constitute a distinct group because of their lower symmetry and because one 254 tetrahedral site is largely vacant, i.e., $\square > \text{Si}$ at one of the two sites corresponding to Z in the 255 archetypal garnet structure (Aubry et al. 1969; Armbruster et al. 2001; Hålenius et al. 2005). Optical 256 257 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) 258 birefringence. In contrast birefringent grossular garnets are normally biaxial (as a consequence of 259 symmetry lowering to orthorhombic, monoclinic or triclinic symmetries) and show low to moderate 260 (0.001- 0.010) birefringence (Shtukenberg et al. 2001, 2005), although birefringence as high as 261 0.015 has been observed for compositions with considerable andradite component. In addition, the 262 powder XRD pattern for holtstamite and grossular are distinct because they show different d-263 spacings for their respective 5 strongest reflections. Henritermierite and holtstamite are 264 distinguished from each other on the basis of the dominant cation at the Y site, respectively Mn³⁺ 265 266 and Al.

Elbrusite

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Elbrusite was originally described as "elbrusite-(Zr)" with the formula

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{Ca₃}[U⁶⁺Zr](Fe³⁺₂Fe²⁺)O₁₂ (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.% UO₃ (0.62 U per formula unit) and well advanced in U-rich kerimasite (Fe-dominant analogue of kimzevite in the original description) (15 17 wt.% UO₃, 0.37 0.42 U pfu); single-crystal X-ray diffraction was only practical for kerimasite containing 9 wt.% UO₃ (0.21 U pfu) (Galuskina et al. 2010a). The authors noted that a Raman band below 700 cm⁻¹ could indicate the presence of some Fe²⁺ in elbrusite, but the only evidence for U being hexavalent is the association with vorlanite, CaU⁺⁶O₄, for which the hexavalent state of U could be determined (Galuskin et al. 2011a). The composition $\{Ca_3\}[U^{6+}Zr](Fe^{3+}{}_{2}Fe^{2+})O_{12}$ is not a valid end-member because more than one site has two occupants (Hawthorne 2002). Instead, it can be considered as the sum of two valid end-members, $\frac{2}{3}\{Ca_3\}[U^{6+}_{0.5}Zr_{1.5}](Fe^{3+}_{3})O_{12} + \frac{1}{3}\{Ca_3\}[U^{6+}_{2}](Fe^{2+}_{3})O_{12}$ (Fig. 4). Compositions of elbrusite and U-rich kerimasite plot in a linear trend in terms of U and the sum of tetravalent cations between the composition representing kerimasite, $\{Ca_3\}[R^{4+}_2](R^{4+}R^{3+}_2)O_{12}$, and $\{Ca_3\}[U^{6+}R^{4+}](R^{3+}R^{2+})O_{12}$ (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 Fe²⁺ is present. Moreover, the compositions that Galuskina et al. (2010a) identified as elbrusite and kerimasite plot in the fields for $\{Ca_3\}[U^{6+}R^{4+}](R^{3+}_2R^{2+})O_{12}$ and $\{Ca_3\}[R^{4+}_2](R^{4+}R^{3+}_2)O_{12}$, respectively, requiring no revision of their species identifications if $\{Ca_3\}[U^{6+}_{0.5}Zr_{1.5}](Fe^{3+}_{3})O_{12}$ is considered to be the end-member of elbrusite. Therefore $\{Ca_3\}[U^{6+}_{0.5}Zr_{1.5}](Fe^{3+}_{3})O_{12}$ should now be used as the elbrusite end-member formula. Yudintsev (2001) and Yudintsev et al. (2002) reported a U-rich garnet, one of three compounds synthesized in corundum crucibles from a (Ca_{2.5}U_{0.5})Zr₂Fe₃O₁₂ 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, $\{Ca_{2}, g_{3}U_{0,07}\}[Zr_{1,52}U_{0,47}Fe_{0,01}](Fe_{1,83}Al_{1,17})O_{12}$, under unspecified conditions, but presumably similar. Uranium is largely tetravalent in the starting material, and despite having been heated in a relatively oxidizing environment, was assumed by Yudintsev (2001) to have remained mostly tetravalent in the garnet because of its association with cubic oxide with the fluorite structure typical of U⁴⁺. 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 formulae 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.

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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 as Xray diffraction (e.g., Chakhmouradian and McCammon 2005). The two species currently accepted by the CNMNC are schorlomite, Ca₃(Ti, Fe³⁺)₂(Si,Fe)₃O₁₂, and morimotoite, Ca₃(Ti, Fe²⁺, Fe^{3+})₂(Si, Fe^{3+})₃O₁₂ (Table 2). These formulae, which are listed as approved by the CNMNC, are too generalized to indicate what the distinction is between the two species, and clearly new formulae 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, b) 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 TiO₂ 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.% TiO₂ 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 $^{Y}\text{Ti} > ^{Y}\text{Fe}^{3+}$ (Ito and Frondel 1967a; Deer et al. 1982), approximately the same as TiO₂ > 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 ^YTi, 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 {Na₂Ca}[Ti₂](Si₃)O₁₂ component. Several end-member formulae have been proposed for schorlomite, e.g., {Ca₃}[Ti₂](Fe³⁺₂Si)O₁₂ (Ito and Frondel 1967a) and {Ca₃}[Ti₂](Fe³⁺₂Ti)O₁₂ (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, {Ca₃}[Ti₂](Si_{3-x})(Fe³⁺ Al, Fe²⁺)_xO₁₂. 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.% TiO₂ from Fuka, Okayama Prefecture, Japan. Formulae that we recalculated assuming 8 cations and

12 oxygen anions from three analyses in Henmi et al. (1995), including the one designated as type, 337 gave 1 8% and radite, $\{Ca_3\}[Fe^{3+}_2](Si_3)O_{12}$, 27 34% $\{Ca_3\}[Ti_2](Fe^{3+}_2Si)O_{12}$ and 58 71% 338 {Ca₃}[TiFe²⁺](Si₃)O₁₂ with minor Zr, Mg, Mn and Al included with Ti, Fe²⁺, Ca and Fe³⁺ according 339 to valence. Garnets synthesized by Henmi et al. (1995) under reducing conditions (iron-wüstite 340 buffer) have compositions very similar to the natural material; end-member morimotoite could not 341 be synthesized. However, no structural or spectroscopic data were obtained to confirm the assumed 342 site occupancies and calculated Fe valence, and thus the report raised objections. Fehr and 343 Amthauer (1996) and Rass (1997) questioned the assumption that Ti was all Ti⁴⁺. The latter authors 344 also dismissed the infra-red evidence that Henmi et al. (1995) used to justify their conclusion that 345 OH was absent, and cited experiments by Kühberger et al. (1989) that OH is likely to be present in 346 morimotoite. Their conclusion is supported by the report by Armbruster et al. (1998) that the 347 morimotoite substitution, $Fe^{2+} + Ti^{4+} \rightarrow 2Fe^{3+}$ at the Y site is coupled with $4OH^{-} \rightarrow SiO_4^{4-}$ at the 348 tetrahedral site in Ti-bearing andradite. 349 Despite the variety of methods deployed to locate cations in the structure of Ti-rich garnets, 350 authors have yet to reach a consensus, which reflects not only differing interpretations of the 351 spectroscopic and structural data, but probably also variation between samples. Nonetheless, the 352 question confronting us is whether we can still propose a meaningful classification based on 353 formulae calculated from a full electron microprobe analysis assuming 8 cations and 12 oxygen 354 anions. There is little disagreement on the occupancy of the X site, which with rare exception 355 contains at least 2.7 (Ca + Na) atoms per formula unit (apfu), to which are added sufficient Mn and 356 Mg to bring total X site occupancy to 3, but fewer authors (e.g., Chakhmouradian and McCammon 357 2005) would also place Fe^{2+} at the X site. Problematic issues include the valence and location of Ti 358 and Fe, as well as the location of Al. Locock (2008) reviewed the literature on Ti³⁺ in garnet and 359 concluded that the oxygen fugacities required for this valence were far too low to be found in most 360 geologic environments. This conclusion is consistent with most spectroscopic studies, for example, 361 X-ray absorption near-edge structure spectroscopy (XANES) has revealed little or no Ti³⁺ in natural 362 garnet (Waychunas 1987; Locock et al. 1995), whereas electron spin resonance spectroscopy 363 revealed that Ti³⁺ is much subordinate to Ti⁴⁺ in pyrope synthesized under relatively reducing 364 conditions (Rager et al. 2003; Geiger 2004). In contrast, Malitesta et al. (1995) and Schingaro et al. 365 (2004) reported significant Ti³⁺ in Ti-bearing garnet by X-ray photoelectron spectroscopy (XPS). 366 Since XPS examines the near-surface of a solid (top 10 50 Å, Hochella 1988), the discrepancy 367 between the XPS and XANES results could be due to differences at the mineral surface not detected 368 by XANES, and consequently we are inclined to accept the conclusion that Ti³⁺ plays a negligible 369 role in natural terrestrial garnet, although it could be significant constituent in some meteoritic 370 371 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 372 373 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, 374 combined low pressure and high temperature could favor Ti substitution for Si at a tetrahedral site 375 as it does in lamproitic richterite (Oberti et al. 1992). The most robust element-specific technique, 376 XANES, yields results consistent with the bulk of Ti occupying the octahedral site in most natural 377 garnets (Waychunas 1987; Locock et al. 1995). Significant Ti may occupy the Z site in Si-poor 378 379 garnets such as elbrusite and bitikleite (e.g., Galuskina et al. 2010a, b), and its presence has been demonstrated in Si-free synthetic garnets (Povarennykh and Shabilin 1983; Cartie et al. 1992; 380 Yamane and Kawano 2011). Another question is the possible presence of tetrahedrally coordinated 381 Fe^{2+} . Some studies reported Mössbauer spectroscopic evidence for significant Fe^{2+} at the Z site 382 (e.g., Locock et al. 1995; Koritnig et al. 1978), but the spectroscopic data do not always give 383 384 unequivocal site assignments (Chakhmouradian and McCammon 2005). Lastly, there is the role of the hydroxyl ion: ignoring hydroxyl results in an underestimate of Fe²⁺ in the formulae calculated 385 by the method of Droop (1987). However, the effect would be serious only if >0.4 wt.% H₂O were 386 present, in which case nearly 0.1 Fe²⁺ per formula unit (5 10% of the total Fe) would not show up 387 in the calculated formula unless OH were included in the formula calculation, i.e., (OH) + O = 12388 and $\Sigma\{X\} + \Sigma[Y] + \Sigma(Z) + {}^{Z}\square_{(OH)/4} = 8$, or if F present, O + (OH) + F = 12 and $\Sigma\{X\} + \Sigma[Y] + \Sigma(Z)$ 389 $+ {}^{Z}\Box_{(OH)/4} + {}^{Z}\Box_{F/4} = 8$. The few analyses available in the recent comprehensive studies give 390 0.02 0.21 wt.% H₂O for natural Ti-rich garnets with >12 wt.% TiO₂ (Kühberger et al. 1989; 391 Locock et al. 1995: Amthauer and Rossman 1998: Chakhmouradian and McCammon 2005). An 392 exception is "hydroschorlomite" with 5 wt.% H₂O (Galuskin 2005); such H₂O-rich garnets cannot 393 394 be treated in the approach discussed below. In order to identify end-member formulae for the two Ti-rich garnet species schorlomite and 395 morimotoite, we should compare the results from as many studies as possible, which necessitate our 396 relying on chemical data. Few authors have supplemented chemical data with structure refinements 397 using X-ray diffraction and with spectroscopic methods to determine site occupancy, and thus we 398 think that relying on chemical data is the most consistent approach for treating compositional data 399

1. Ti is Ti⁴⁺ and preferentially occupies the *Y* site, which rules out the end-member {Ca₃}[Ti₂](TiFe³⁺₂)O₁₂ proposed by Rickwood (1968)

2. H_2O content is ≤ 0.2 wt.%

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chemical data:

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

from different studies. In addition, we have made the following assumptions in treating the

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Figure 5 is a plot of Y-site compositions for garnets containing >12 wt.% TiO<sub>2</sub> and Ti > Zr
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       apfu in terms of the following generalized end-members \{Ca_3\}[R^{3+}_2](Si_3)O_{12},
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        \{Ca_3\}[R^{4+}_2](SiR^{3+}_2)O_{12}, and \{Ca_3\}[R^{4+}R^{2+}](Si_3)O_{12} For R^{4+}=Ti, R^{3+}=Fe^{3+}, and R^{2+}=Fe^{2+}, these
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        generalized end-members correspond, respectively, to andradite, the schorlomite end-member of Ito
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       and Frondel (1967a), and the morimotoite end-member of Henmi et al. (1995), i.e., the same
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       components plotted by Henmi et al. (1995, their Fig. 1). It turns out that 15 wt.% TiO<sub>2</sub>, which
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       Zedlitz (1933) suggested as a cutoff for schorlomite, is a good estimate of the minimum TiO<sub>2</sub>
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       content of compositions plotting in the morimotoite and schorlomite fields unless significant Zr is
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       present.
              Three reports of garnets reported to contain over 20 wt.% TiO<sub>2</sub> have not been plotted in
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       Figure 5 either because of their high H<sub>2</sub>O content or because of their questionable identity as garnet.
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       Galuskina and Galuskin (unpublished data) were able to confirm the identity of an OH-bearing
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       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
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       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>,
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       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 wt.% CaO, \leq 0.03 wt.%
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       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
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       the detection limit. These data correspond approximately to 73-76% {Ca<sub>3</sub>}[Ti<sup>4+</sup><sub>2</sub>](SiFe<sup>3+</sup><sub>2</sub>)O<sub>12</sub>, the
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       highest proportion of the schorlomite end-member reported in a natural garnet, 12-13%
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        {Ca<sub>3</sub>}[Ti<sup>4+</sup><sub>2</sub>](SiAl<sub>2</sub>)O<sub>12</sub> and 12-14% andradite plus its OH analogue. Grapes et al. (1979) reported
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       an electron microprobe analysis of a garnet from Morotu, Sakhalin Island, Russia, containing 27.38
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       wt.% TiO<sub>2</sub> and 33.50 wt.% Fe as FeO, but deficient in Si and Ca with the formula:
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        \{Ca_{1.53}Fe^{2^{+}}_{1.46}Mn_{0.01}\}[Ti_{1.28}Fe^{2^{+}}_{0.71}Mg_{0.01}](Si_{1.84}Ti_{0.60}Fe^{3^{+}}_{0.38}Al_{0.18})O_{12}, i.e., a morimotoite from site
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       occupancies, but anomalous because so much Ti (or Fe<sup>2+</sup>) is forced by the formula calculation onto
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       the Z site. A possible explanation for the high Fe and Ti contents is X-ray fluorescence from
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       contiguous phases (Chakhmouradian and McCammon 2005). In a study of altered basalt from the
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       equatorial east Pacific, Laverne et al. (2006) described a "hydroschorlomite" with 22.0 28.6 wt.%
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       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
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       for celadonite impurities, which were manifested by the presence of \sim 1 wt.% K_2O in the analyses.
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       The study included SEM and TEM, as well as micro-Raman spectra, but none provided
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       corroborative evidence that the mineral was indeed a garnet; the reported compositions suggest the
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       mineral could be titanite.
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              Three analyses, including the holotype, from the type locality of morimotoite in Fuka, Japan,
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       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
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we assume that Ti and Fe^{2+} do not occupy the Z site, whereas four of the five analyses of garnet

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from the type locality of schorlomite at Magnet Cove, U.S.A., plot in the schorlomite field and 442 show that Ti is the dominant R^{4+} cation, and Fe³⁺ is the dominant R^{2+} cation. The latter situation 443 holds even if Al is assumed to preferentially occupy the Z site (e.g. Chakhmouradian and 444 McCammon 2005), which is not supported by all studies (e.g. Locock et al. 1995; Armbruster et al. 445 1998). Thus, we recommend that $\{Ca_3\}[Ti^{4+}Fe^{2+}](Si_3)O_{12}$ and $\{Ca_3\}[Ti^{4+}2](SiFe^{3+}2)O_{12}$ be the end-446 member formulae for morimotoite and schorlomite, respectively. Despite the assumptions and 447 simplifications discussed above, we believe that Figure 5 can be used to distinguish schorlomite and 448 morimotoite in the absence of structural and spectroscopic studies if allowance is made for the 449 uncertainties in attempting to identify borderline cases. 450 Figure 5 shows that many garnets reported as schorlomite plot in the morimotoite and 451 andradite fields; garnets plotting in the schorlomite field other than those from Magnet Cove are 452 from Ardnamurchan, Scotland (Huggins et al. 1977), the Tamazeght complex, Morocco (Marks et 453 454 al. 2008), the Polino carbonatite, Italy (Lupini et al. 1992) and Alnö Island, Sweden (Eckermann 1974). The dominant ${}^{Z}R^{3+}$ cation in these garnets is Fe³⁺, even if Al is assumed to preferentially 455 occupy the Z site. Using the above assumptions, garnets plotting in the morimotoite field (with Fe^{2+} 456 > Mg at the Y site) are from Iivaara, Finland (Zedlitz 1935), Afrikanda, Russia (Chakhmouradian 457 and McCammon 2005), Ice River, Canada (Locock et al. 1995; Peterson et al. 1995), Sung Valley, 458 India (Melluso et al. 2010) and Rusing Island, Kenya (Howie and Woolley 1968). However, 459 460 Mössbauer spectroscopy of the Ice River garnet indicates that a significant proportion of the Fe²⁺ 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 461 Peterson et al. (1995) had reason to call this garnet schorlomite. Two relatively Zr-rich garnets from 462 the Marathon Dikes, Ontario, Canada (Platt and Mitchell 1979) also plot in the morimotoite field, 463 but are unique in that total Mg > Fe $^{2+}_{total}$ (circled in Figure 5) suggesting the possibility of a Mg-464

dominant analogue 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). This contradiction arises because the compositions include more garnet-group components, largely andradite, $\{Ca_3\}[R^{3+}_2](Si_3)O_{12}$, and morimotoite, $\{Ca_3\}[R^{4+}R^{2+}](Si_3)O_{12}$, than schorlomite-group components, largely, $\{Ca_3\}[R^{4+}_2](SiR^{3+}_2)O_{12}$.

Menzerite-(Y)

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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 {YCa₂}[MgFe³⁺](Si₃)O₁₂. 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 $\{Ca_3\}[Fe^{3+}_2](Si_3)O_{12}$ (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 Fe³⁺/Fe²⁺ 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 $\{Ca_3\}[Mg_2](Si_3)O_{12}$, which is not balanced in charge. Charge balance allows only 2 (Y+REE) per formula unit, i.e., the menzerite end-member should be $\{Y_2Ca\}[Mg_2](Si_3)O_{12}$. The presence of (Y+REE) means that $\{(Y,REE)_2Ca\}$ 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 $Mg_3(Fe^{2+},Si)(SiO_4)_3$ (Table 2), equivalent to $\{Mg_3\}[SiFe^{2+}](Si_3)O_{12}$, which indeed is a good approximation of the empirical formula of the type material reported by Smith and Mason (1970), $(Mg,Na)_3(Fe,Si,Al,Cr)_2Si_3O_{12}$. It was assumed that Fe occupied the Y site, but the valence and distribution of the Fe were not determined. Recalculating a formula for 8 cations and 12 oxygen anions from the published analysis and listing cations at a given site in order of decreasing abundance gives: $\{Mg_{2.91}Na_{0.09}\}[(Si_{0.71}Fe^{2+}_{0.60}Fe^{3+}_{0.41}Al_{0.22}Cr_{0.04}Mg_{0.02}](Si_3)O_{12}$.

However, the assumption regarding Fe²⁺ occupancy is not supported by Mössbauer spectroscopic data on synthetic majorite (Geiger et al. 1991a, b; O'Neill et al. 1993a, b; McCammon and Ross 2003). In a study that included samples that Geiger et al. (1991a, b) and O'Neill et al. (1993a, b) had investigated, McCammon and Ross (2003) reported that ${}^{X}\text{Fe}^{2+}/\Sigma \text{ Fe}^{2+} = \frac{1}{2} (1993a)$

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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 = \frac{1}{2} (Fe^{2+} + Mg)
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       (0.01 0.08) in 15 synthetic tetragonal majorite samples, and {}^{X}\text{Fe}^{2+}/\Sigma\text{Fe}^{2+} = 1.0 in one isometric
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       synthetic sample, demonstrating that Fe^{2+} is strongly fractionated onto the X site. Because the
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       compositions of the type specimen and these synthetic samples are similar, we think it is reasonable
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       to assume that Fe distribution is the same in synthetic and natural majorite, and the partial ordering
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       at the X and Y sites in tetragonal samples does not significantly affect the Fe distribution. Assuming
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       that Fe^{2+} occupies only the X site, the formula of the type material becomes
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        \{Mg_{2,31}Fe^{2+}_{0,60}Na_{0,09}\}\{(Si_{0,71}Mg_{0,62}Fe^{3+}_{0,41}Al_{0,22}Cr_{0,04}\}(Si_3)O_{12}, i.e., the dominant component is
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        \{Mg_3\}\{SiMg\}(Si_3)O_{12}. Consequently, we recommend that \{Mg_3\}\{SiMg\}(Si_3)O_{12} be used as the end-
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       member formula for majorite. A natural <sup>X</sup>Fe<sup>2+</sup> analogue has not been reported, and as far as we are
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       aware, it has not been synthesized (e.g., Kato 1986).
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              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.,
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       Angel et al. 1989), no naturally occurring tetragonal majorite has been reported. Apparently,
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       majorite in shocked meteorites was quenched with sufficient rapidity to preserve cubic symmetry
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       (Tomioka et al. 2002). The problem of preserving cubic symmetry on cooling would probably not
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       arise in terrestrial majorite, which contains substantial Al, because incorporation of Al at the Y site
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       is thought to stabilize the cubic structure (Hatch and Ghose 1989). Moore and Gurney (1985)
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       confirmed isometric symmetry for garnet from the Monastery Mine kimberlite pipe, South Africa,
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       one of which we calculated to contain 36% of a generalized majorite component,
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        \{R^{2+}_{3}\} [MgSi](Si<sub>3</sub>)O<sub>12</sub>.
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              The term "majoritic" has found wide use in the literature on garnets included in diamond
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       (e.g., Harte 2010; Collerson et al. 2010), i.e., garnet is described as "majoritic" if Si is incorporated
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       at the Y site through the "majorite" substitution {}^{Y}R^{2+} + {}^{Y}Si \rightarrow 2{}^{Y}Al (Table 4). Collerson et al. (2010)
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       also include the contribution from the generalized component \{R^{2+}\text{Na}_2\}[R^{4+}_2](\text{Si}_3)\text{O}_{12} in their
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       majorite substitution parameter, X<sup>cat</sup>Mj. In contrast to majorite reported from shocked meteorites, in
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       which the majorite component is clearly dominant (Collerson et al. 2010), none of the "majoritic"
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       garnets occurring in diamonds are properly majorite, i.e., the majorite component
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       \{Mg_3\}[SiMg](Si_3)O_{12} \text{ or } (R^{2^+} + R^{4^+}) > 2R^{3^+} \text{ at the } Y \text{ site, is not dominant, even in sample JF-22}
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       from the Jagersfontein kimberlite, South Africa (Tappert et al. 2005; Harte 2010), which has the
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       highest content of Si at the Y site among terrestrial garnet as far as we are aware: a maximum 47.2%
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       \{R^{2+}_3\}[R^{4+}Mg](Si_3)O_{12} \text{ or } 44.9\% \{R^{2+}_3\}[SiMg](Si_3)O_{12} \text{ (Appendix 3, example 5). The "Ca-rich"}
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       majorite" in shock veins of crustal rocks from the Ries impact crater, Germany (Stähle et al. 2011)
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       is not majorite because ({}^{Y}Si + {}^{Y}Ti) < ({}^{Y}Al + {}^{Y}Fe^{3+} + {}^{Y}Cr); instead, the three average compositions
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comprise about 58 71% pyrope grossular almandine, 17-33 % $\{R^{2+}_3\}[R^{4+}Mg](Si_3)O_{12}$ (generalized majorite), and 10-13% $\{R^{2+}(Na,K)_2\}[R^{4+}_2](Si_3)O_{12}$, where ${}^{Y}R^{4+} = 90-93\%$ Si.

Manganberzeliite

Manganberzeliite, {Ca₂Na}[Mn²⁺₂](As⁵⁺₃)O₁₂ (Fig. 1g) has a complicated history revolving around the use of its name, which is briefly described below. Over 40 years after the original description of berzeliite from Långban, Filipstad district, Sweden (Kühn 1840), Igelström (1886) described a Sb-bearing, Mn-rich berzeliite-like mineral from the nearby Sjögruvan mine, and named it "pyrrhoarsenite". On the basis of a new chemical analysis giving 28.38 wt.% MnO Igelström (1894) concluded that "pyrrhoarsenite" is a manganese dominant variety of berzeliite and could also be referred to as "Mangan-Berzeliit."

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

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

Moore (1972) reported powder XRD data for the type specimen of "pyrrhoarsenite" studied by Igelström (specimen NRM18870324 at the Swedish Museum of Natural History) from Sjögruvan. He concluded that "pyrrhoarsenite" = berzeliite. However, recent energy-dispersive spectroscopic analyses (Hålenius, unpublished data) of fragments of the mineral from this specimen, as well as cell parameter refinement (Locock, unpublished data) of Moore's powder X-ray diffraction data, show that it is in fact Mn-dominant berzeliite, i.e. manganberzeliite (or "pyrrhoarsenite"). Prior to publication, Moore in 1971 submitted to the CNMMN a proposal to discredit several of the minerals outlined in his 1972 paper. After Moore published his paper, it was subsequently abstracted by Fleischer (1973), who noted that these minerals were discredited by the CNMMN and that "pyrrhoarsenite" was equivalent to berzeliite. However, the discreditation of pyrrhoarsenite was actually not included in Moore's proposal to the CNMMN. Therefore, the report by Fleischer (1973), which was then carried forward by Nickel and Mandarino (1987), was in error.

This raises the question whether "pyrrhoarsenite" has priority over manganberzeliite and should be reinstated, although manganberzeliite has been the preferred name since 1894 (e.g., Hintze 1922; Palache et al. 1951). Given that Igelström's original description of the mineral was

poor even by the standards of the late 19th century, e.g., he did not detect the appreciable sodium content, in contrast to his contemporary Sjögren (1894), we conclude that priority does not justify reviving "pyrrhoarsenite" at the present time and manganberzeliite should remain the name for the Mn analogue 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 tournaline 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, and a spreadsheet is given in Appendix 4.

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 H are the only light elements (atomic number less than 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, b; 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.

511	2010 and unpublished data). According to Cempírek et al. (2010), Li could occupy either the X site
512	as it does in synthetic $\{Li_2Mg\}[Si_2](Si_3)O_{12}$ (Yang et al. 2009) or sites occupied by Li in synthetic
513	garnets. The majority of synthetic Li garnets are compounds of REE, Ta, Nb, Te, Zr, Ba that are
514	valued for their high ionic conductivity (e.g., Cussen 2006, 2010; O'Callaghan and Cussen 2007;
515	Wang and Lai 2012). Lithium occupies not only the Z site, but also octahedral sites that are vacant
516	in natural garnet, resulting in Li contents up to 6.8 apfu and cation totals up 11.8 apfu. Other
517	exceptions involving light elements are the reports of 4.40 wt.% B ₂ O ₃ determined by electron
518	microprobe analysis (EMPA) in andradite (Galuskin et al. 1995) and 0.45 2.09 wt.% B_2O_3 by
519	EMPA in OH-bearing grossular (Galuskina et al. 1998, 2001) from the Wiluy River, Yakutia,
520	Russia. Pending studies of Li and B in silicate and hydroxyl garnet, it would be best to assume Li
521	and B, as well as S ⁶⁺ (up to 2.27 wt.% SO ₃ , equivalent to 0.11 S pfu, Passaglia and Rinaldi 1984;
622	Galuskina et al. 2001), are located at the Z site.
5 2 3	Calcium has been assumed to occupy only the X site in natural garnet; even in synthetic
624	garnets there are very few reports of Ca at the Y site and none can be considered unequivocal
625	(Geller 1967; Lobanov et al. 1989). Nonetheless, it should be noted that Huggins et al. (1977) and
526	Pieper et al. (1983) concluded that a small excess of cations at X and a correspondingly small deficit
627	at Y could be explained in some cases by small amounts of Ca at Y, 0.024-0.055 apfu in andradite
528	and 0.04 apfu in grossular, respectively. Gadas et al. (in press) suggested incorporation of Ca at the
529	Y site by the substitution of ${}^{Y}Ca + (OH,F)$ for ${}^{Y}Al + O$ to explain Ca contents up to 3.08 apfu and
530	deficiency at Y in grossular from pegmatite at Ruda nad Moravou, Czech Republic.
531	Scandium is assumed to occupy only the Y site as in eringaite, although its role could depend
532	on the occupancy of X if synthetic garnets are any guide, where Sc preferentially occupies Y only in
533	and radite, whereas in pyrope, X is favored and in grossular, a more even distribution (Oberti et al.
534	2006; Quartieri et al. 2006). Titanium is assumed to be tetravalent, and V, either pentavalent or
535	trivalent. The last assumption received validation from Bordage et al. (2010), who reported that V
536	was entirely V^{3+} in a grossular (variety "tsavorite" containing 0.14 V pfu) based on the K-edge
537	X-ray absorption near-edge structure (XANES) spectra obtained with high-energy resolution
538	fluorescence-detected X-ray absorption spectroscopy. In contrast, Righter et al. (2011) reported
539	mixed valences also based on the K-edge X-ray absorption near-edge structure in other garnets,
640	viz., $2.46 2.55 \pm 0.15$ in pyrope of mantle origin and $2.56 2.67 \ (\pm 0.15)$ for V valence in a
641	goldmanite from the Czech Republic, i.e., 40% of the V in the goldmanite is V^{2+} , the remainder V^{3+}
642	However, this conclusion is in contrast to the structural and chemical data reported by these authors.

Site allocation of cations

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- The assumed occupancies, most importantly, ^ZLi, ^XCa, ^YSc, Ti⁴⁺, ^YV³⁺, and ^ZV⁵⁺) in conjunction with Table 3, lead to the following procedure for recasting chemical data into idealized site occupancies for purposes of classification:
- Calculate formulae from the chemical analysis assuming 8 cations and 12 anions and apportion Fe²⁺ and Fe³⁺ or Mn²⁺ and Mn³⁺ if calculations give negative values for Fe²⁺ (method of Droop 1987). If quantitative F or H data are available, assume ^Z□ = ½F + ¼H.
 In this case, the basis for formula calculation becomes O + (OH) + F = 12 and Σ{X} + Σ[Y] + Σ(Z) + ^Z□_{(OH)/4} + ^Z□_{F/4} = 8
- 2. Li, Zn, P, As⁵⁺ and V⁵⁺ to Z. If Li < ½F, 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 \square , overflow to Y
- 4. Al: First to Z to bring total to 3 apfu, then Y
- 5. Fe³⁺: First to Z to bring total to 3 apfu, then Y
- 6. Ca, Na, K, Y, REE, Th, Pb to *X*.

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- 7. Al (remainder after deducting Al at *Z*), Sc³⁺, Ti⁴⁺, V³⁺, Cr³⁺, Mn³⁺, Fe³⁺ (remainder after deducting Fe³⁺ at *Z*), Ga, Zr⁴⁺, Nb⁵⁺, Sn⁴⁺, Sb⁵⁺, Te⁶⁺ and U⁶⁺ to *Y*. If *Z* is still less than 3 apfu, then add Fe²⁺ to bring *Z* total to 3 apfu. If the content of *Y* exceeds 2 apfu, and *Z* is less than 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. Fe²⁺ (remainder after deducting Fe²⁺ at Z): First to Y to bring total to 2 apfu, then to X
- 10. Mn²⁺: 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^{2^+}/Fe^{3^+} ratio must be assumed so that H content can be calculated. In garnets containing significant Si, it is reasonable to assume that H is incorporated at the expense of Si, that is, $H = 4*(^{Z}\Box)$.
- 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 {Ca₃}[Mn³⁺₂](Si⁴⁺₂□)O₈(OH)₄.
- We have also prepared an Excel spreadsheet (Appendix 4) to perform the above cation allocation, species and group determination, but have omitted several elements that rarely exceed 1 wt.% in natural garnets: B, S, K, Ni, Sr; or which occur in significant amounts but whose occurrence is rare: Ga, Ge, Pb and Th (Tables 6, 8).

Identifying a garnet species

Once the cations have been allocated, then the dominant valence is determined for each site by summing the ions for each valence, e.g., Ca + Mg + Mn at the *X* site, and then the dominant cation identified. As species are defined in terms charge-balanced end-members (Hawthorne 2002), the possibility of valency-imposed double site-occupancy (Hatert and Burke 2008) must be considered. The dominant ion for each valence determines the species (e.g., bitikleite group, Fig. 6). Five examples are given in Appendix 3, and a calculation procedure for species and group determination in Appendix 4. 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 formulae in this group is Si = 1 apfu; there are no divalent and trivalent cations at the Y site and no divalent or pentavalent cations at the Z site. However, in most analyses of Ti-, Zr- or Sn-rich garnets containing minor Sb^{5+} , Nb^{5+} , or U^{6+} , 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 $\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)O_{12}$ be the most abundant (Fig. 7); i.e., the spreadsheet gives this as the most abundant component possible. In the worked example of schorlomite from the type locality, Magnet Cove, Arkansas (Example 2), the schorlomite component is dominant, with $R^{4+} > R^{3+} > R^{2+}$ at the *Y* site in the empirical formula (Example 2), whereas in the garnet-group mineral morimotoite, the generalized morimotoite component, $\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)O_{12}$, 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, 8), whereas the *X* site remains occupied exclusively by Ca in all endmembers (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 and $R^{2+} = \text{Mg}$, Fe^{2+} , and differs from Figure 7a of Grew et al. (2010) in that the Ti corner is now $\text{Ti}R^{2+}$, representing a component in garnet, morimotoite. However, menzerite-(Y) is a four component system because of the substitution of R^{3+} for Si at the Z site, and compositions must be projected from four-component space onto the three-component plane shown in Figure 10. Appendix 3 (Example 3) gives the five possible generalized components in menzerite-(Y), of which only four are independent. We have selected the $\{Y_3\}[Al_2](Al_3)O_{12}$ -type component to project menzerite-(Y) compositions. The $\{Y_3\}[Al_2](Al_3)O_{12}$ -type component comprises 4 8% of the analyzed menzerite-(Y) grains. Despite the differences between Figure 10 and Figure 7a of Grew et al. (2010), the disposition of the points is very similar.

The most widespread garnet-group minerals are related by homovalent substitutions at the X and Y sites, i.e., $\{R^{2+}_3\}[R^{3+}_2](\mathrm{Si}^{4+}_3)\mathrm{O}_{12}$. Since only four constituents occupy the X site, the compositions can be plotted in a tetrahedron with Ca, Mg, Mn^{2+} and Fe^{2+} as vertices (Fig. 11a). Garnets with one of these cations dominant at the X site fill a volume whose edges inside the Ca Mg Mn^{2+} Fe $^{2+}$ 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.

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 (Table 6, 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?

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Vacancy-dominant garnets are distinguished by φ 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.% H₂O 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 Fe³⁺ analogue of katoite (Table 6) and 4.5% of its Mn³⁺ analogue (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.% H₂O) from charge balance in "hydroschorlomite" containing 13.5 14.5 wt.% TiO₂ from the Wiluy River, Yakutia, Russia, the highest reported in Ti-rich garnets (cf. Chegem caldera schorlomite discussed above). In contrast, H₂O 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.% H₂O in spessartine, 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,b) 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 $\{Ca_3\}[Mn^{3+}_2](\square_3)(OH)_{12}$ (Ivanov-Emin et al. 1982b), $\{Ca_3\}[TiFe^{3+}](Fe^{3+}\Box_2)(OH)_8O_4$ (Ito and Frondel 1967b) and $\{Ca_3\}[ZrFe^{3+}](Fe^{3+}\Box_2)(OH)_8O_4$ (Ito and Frondel 1967b) have been reported. However, attempts to synthesize the end-member $\{Ca_3\}[Fe^{3+}_2](\square_3)(OH)_{12}$ failed, although a garnet with about 90% $\{Ca_3\}[Fe^{3+}_2](\square_3)(OH)_{12}$ and 10% and and addite 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 analogue of andradite, $\{Ca_3\}[Fe^{3+}_2](Si_{1.15}\square_{1.85})(OH)_{7.4}O_{4.6}$, have been confirmed independently (e.g., by structure refinement, Cohen-Addad 1970; Cohen-Addad et al. 1967). In summary, the H₂O 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 cation at X 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 $\{R^{2+}\}$ $[R^{3+}]$ $[R^{3+}]$ $[R^{3+}]$ 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 H₂O content, reporting 0.64 wt.% in the F-bearing spessartine (Table 6), equivalent to 3% $\{R^{2+}_3\}[R^{3+}_2](\square_3)(OH)_{12}$, but Flohr and Ross (1989) and Chakhmouradian et al. (2008) reported evidence for H₂O in the infrared and Raman spectra. Attempts to synthesize an F-dominant analogue 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 1994, and Chesnokov et al. (1994, 2008) described "igumnovite", ideally $\{Ca_3\}[Al_2](Si_2\square)O_8Cl_4$, and "chlorhibschite", ideally, $\{Ca_3\}[Al_2](Si_{3-x}\square_x)O_8Cl_{4-x}$, from burned material in the Chelyabinsk coal basin, Urals, Russia, but these compounds are not considered to be naturally formed, and thus do not qualify as minerals (e.g., "igumnovite", Jambor et al. 1997). The reported cell parameter of 12.008 Å for "igumnovite" is smaller than expected for a Cl-rich garnet from the relationship of Langley and Sturgeon (1979). Although the measured composition for "igumnovite," Ca_{3.04}Al_{1.72}Fe_{0.13}Mg_{0.01}Si_{2.07}F_{0.03}O_{7.90}Cl_{4.07} approaches ideal garnet stoichiometry, it is doubtful that either "igumnovite" or "chlorhibschite" are garnets. More likely, "igumnovite" is related to mayenite, wadalite and the new mineral eltyubyuite (Galuskin et al. 2011b), whereas "chlorhibschite" could be a mixture of grossular, wadalite and, perhaps, chlorides.

Yafsoanite

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The 9% proportion of the component {Pb²⁺₃}[Te⁶⁺₂](Zn₃)O₁₂ 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 analogue (Kim et al. 1982), but the formulae 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 Pb²⁺-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 Pb²⁺ analogue of yafsoanite.

The unnamed end-member $\{Ca^{2+}_3\}[U^{6+}_2](Fe^{2+}_3)O_{12}$ is calculated to be major constituent of elbrusite (Fig. 4; Table 6) and dzhuluite (Appendix 3), but has not yet been synthesized.

Henritermierite group

 Boiocchi et al. (2012) reported nearly end-member spessartine containing 0.09 Fe and 0.04 Ca pfu, but only 2.52 Si pfu, the deficiency being made up by OH and F in nearly equal proportions (Table 6). The $I4_1/acd$ 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 Mn³⁺, and thus Boiocchi et al. (2012) attribute the lower symmetry to (OH, F)₄ 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 analogue 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.% Nb₂O₅ in a kerimasite crystal, this amount corresponds to 0.48 Nb per formula unit, or nearly 50% of a $\{Ca_3\}[NbZr](R^{3+}_3)O_{12}$ component, which implies the possibility of new species for R^{3+} = Fe and Al, the Nb analogue of usturite (Table 8).

Up to 4 wt.% ThO₂ (0.1 Th pfu) has been reported in bitikleite and schorlomite-group minerals (Lupini et al. 1992; Galuskina et al. 2010a; Galuskina et al. 2010e), which would correspond to 20 mol.% of a $\{Th_{0.5}Ca_{2.5}\}[R^{4+}_2](R^{3+}_3)O_{12}$ component. The end-member with Zr and Fe, i.e., $\{Th_{0.5}Ca_{2.5}\}[Zr^{4+}_2](Fe^{3+}_3)O_{12}$, 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 formulae of the type $\{R^{3+}_3\}[R^{3+}_2](R^{3+}_3)O_{12}$ and isostructural with garnet (e.g., Yoder and Keith 1951; Geller 1967), of which $\{Y_3\}[Al_2](Al_3)O_{12}$ (yttrium aluminum garnet or YAG) and $\{Y_3\}[Fe^{3+}_2](Fe^{3+}_3)O_{12}$ (yttrium iron garnet or YIG) are the most relevant to minerals (Tables 6, 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}[(Fe³⁺,Al)₂](Al₃)O₁₂ 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.% Al₂O₃ and 23.1-25.6 wt.% SiO₂ contents; the sample giving the highest ZrO₂ content (Zr = 0.55 apfu) is plotted in Figure 5. Our calculations for this sample give 48.9-49.0 % {Ca₃}[R⁴⁺₂](SiR³⁺₂)O₁₂ with Ti > Zr at *Y* and Al > Fe³⁺ at Z, i.e., a possible Al analogue of schorlomite or Ti analogue of kimzeyite. Using Mössbauer spectroscopic data, Koritnig et al. (1978) gave the Z site composition as (Si_{2.00}Al_{0.56}Fe²⁺_{0.24}Ti_{0.16}Fe³⁺_{0.03}). Ito and Frondel (1967a) synthesized end-member schorlomite and kimzeyite, but we are not aware of a successful synthesis of the end-member {Ca₃}[Ti₂](SiAl₂)O₁₂.

Garnet group

Formulae 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^{2+}) = 0.63 0.64, i.e., the end-member {Ca₃}[TiMg](Si₃)O₁₂, the Mg analogue of morimotoite, is dominant (Table 8). However, the Marathon dike compositions plot close to the boundary with schorlomite and calculation of Fe^{2+}/Fe^{3+} ratio from stoichiometry has a large uncertainty (Giaramita and Day 1990); thus a clear dominance of {Ca₃}[TiMg](Si₃)O₁₂ in a natural garnet remains to be demonstrated.

Gallium and Ge 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 analogue. Johan and Oudin (1986) reported from the Pyrenees of France equant, six-sided crystals up to 10 μ m 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 formulae from the two compositions closest to this endmember (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.

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Fermor (1926; 1938) introduced three hypothetical garnet end-members (Tables 6, 7;
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        Appendix 2): "blythite," {Mn<sup>2+</sup><sub>3</sub>}[Mn<sup>3+</sup><sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>, as a subordinate component in a garnet from
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        Cargoan, Nagpur, India; "khoharite," {Mg<sup>2+</sup><sub>3</sub>}[Fe<sup>3+</sup><sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>, as the precursor to enstatitic
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        chondrules in the Khohar meteorite and as a subordinate component in a pyrope from a
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        "garnet diopside" xenolith (eclogite?) in kimberlite from South Africa; and "skiagite,"
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        {Fe<sup>2+</sup><sub>3</sub>}[Fe<sup>3+</sup><sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>, as a component in almandine from Glen Skiag, Scotland. Although later
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        studies have reported up to nearly 9 mol.% "blythite" based on measurement or stoichiometric
885
        calculation of Mn<sup>3+</sup> in andradite from manganese formations, Otjosondu, Namibia (Amthauer et al.
886
        1989; Bühn et al. 1995), "khoharite" and "skiagite" have been elusive, e.g., Virgo and Yoder (1974)
887
        failed to find "skiagite" in spessartine almandine from the type locality at Glen Skiag, Scotland.
888
        The main problem in identifying these components in complex natural garnets is that the calculation
889
        depends on the sequence of calculation (Rickwood 1968; Locock 2008), i.e., Fe<sup>3+</sup> is first assumed to
890
        be present as the andradite component; only leftover Fe<sup>3+</sup> would be combined with Fe<sup>2+</sup> or Mg in
891
        the "skiagite" or "khoharite" components, respectively, and Mn<sup>3+</sup> could be present as
892
        \{Ca_3\}[Mn^{3+}_2](Si_3)O_{12} as well as \{Mn^{2+}_3\}[Mn^{3+}_2](Si_3)O_{12} in the Otjosondu garnet (Table 6). Garnets
893
        containing a significant proportion of the {Ca<sub>3</sub>}[Mn<sup>3+</sup><sub>2</sub>](Si<sub>3</sub>)O<sub>12</sub>, "blythite", "khoharite" and
894
        "skiagite" end-members have been synthesized at relatively high pressures, i.e., above 30 kbar
895
        (Coes 1955; Nishizawa and Koizumi 1975; Karpinskaya et al. 1982; Fursenko 1983; Woodland and
896
        O'Neill 1993, 1995; Arlt et al. 1998), and could become more abundant under mantle pressures.
897
               Rudashevskii and Mochalov (1984) reported a Mn Cr Si mineral thought be a garnet in
898
        heavy concentrates from eluvium of Pt-bearing serpentinite in the Far East of Russia (summary in
899
        Jambor et al. 1988a). The mineral forms highly zoned grains 1-30 µm across enclosed in Cr-Ni-
900
        bearing y-Fe. The formula (with cations grouped by valence) for the analysis with the highest Cr
901
        content is \{Mn^{2+}_{299}\}[(Cr^{3+}_{1,14}Mn^{3+}_{0,51})Ti_{0,35}]((Si_{2,22}Ti_{0,35})(Al_{0,28}Fe^{3+}_{0,08}))O_{12}, i.e., a
902
        \{Mn^{2+}\}\{Cr^{3+}\}\{Cr^{3+}\}\{Si_3\}O_{12} component can be considered dominant, whereas that for the lowest Cr
903
        content is \{Mn^{2+}_{3}\}\{(Mn^{3+}_{0.79}Cr^{3+}_{0.60}Al_{0.09}Fe^{3+}_{0.08})Ti_{0.22}Mn^{2+}_{0.22}\}(Si_{3.01})O_{12}, i.e., with "blythite"
904
        dominant. The presence of significant Mn<sup>3+</sup> in association with Fe<sup>0</sup> is unexpected, as is the
905
        preservation of metallic Fe in eluvium. In the absence of X-ray or electron diffraction patterns and
906
        clearer evidence for the natural origin of the concentrates, the natural occurrence of a
907
        \{Mn^{2+}_{3}\}[Cr^{3+}_{2}](Si_{3})O_{12}-dominant or \{Mn^{2+}_{3}\}[Mn^{3+}_{2}](Si_{3})O_{12}-dominant garnet remains to be
908
        demonstrated.
909
               Three components have been proposed for incorporation of Na in garnet-group minerals
910
        (Tables 4 and 6), all of which have been inferred to be favored by increasing pressure, {}^{X}Na + {}^{X}(Y, X)
911
        Yb) = 2^{X}R^{2+} (Enami et al., 1995; Røhr et al. 2007) and {}^{X}Na + {}^{Y}Si = {}^{X}R^{2+} + {}^{Y}Al or {}^{X}Na + {}^{Y}Ti = {}^{X}R^{2+} + {}^{Y}Al
912
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^YAl (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): SiO₂ 35.78, Al₂O₃ 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 μ m to ca. 10 μ 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 μ 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.% P_2O_5 in pyrope associated with coesite at Dora Maira, Italy (Brunet and Lecocq 1999), exsolved apatite in garnet from mantle eclogite (Haggerty et al. 1994) and with the synthesis of $\{Na_3\}[Al_2](P_3)O_{12}$ 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_2O_5 (equivalent to 0.086 P pfu) in almandine and spessartine from granitic rocks, Breiter et al. (2005) showed that: (1) P content varies inversely with Si, (2) Na/P ratio to be approximately 1/5 and (3) Al is relatively constant, consistent with the substitutions $^{x}\Box + 2^{z}P = ^{x}R^{2+} + 2^{z}Si$ and much subordinate $^{x}Na + ^{z}P = ^{x}R^{2+} + ^{z}Si$. There was no evidence in their data for the substitution $^{z}(Al,Fe^{3+}) + ^{z}P = 2^{z}Si$ reported in an almandine-spessartine containing up to 2.1 wt.% P_2O_5 from rhyolite, Tanzawa Mountainland, Japan (Arima and Yamashita 1994). Breiter et al. (2005) also concluded that the main control on incorporation of P seems to be the P contents in melt or post-magmatic fluid instead of pressure.

The maximum FeO content reported in a berzeliite-group mineral is 1.52 wt% in berzeliite from Montaldo mine, Italy, equivalent to 6% of the $\{Ca_2Na\}[Fe^{2+}_2](As^{5+}_3)O_{12}$ end-member

(Nagashima and Armbruster 2012). Attempts to synthesize the Fe²⁺ analogue 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 in order to be approved.
- The supergroup includes all minerals isostructural with garnet regardless of what elements occupy specific cation or anion sites.
- We have subdivided the supergroup into groups based on symmetry and total charge at the tetrahedral Z site. Twenty-nine species belong to one of five groups, one tetragonal henritermierite, and four isometric bitikleite, schorlomite, garnet and berzeliite, in which the total Z charge is 8, 9, 10, 12 and 15, respectively. Three species are single representatives of potential groups in which total charge at Z is 0 (katoite), 3 (cryolithionite) and 6 (yafsoanite).
- Species are identified on the basis of the dominant-constituent and dominant-valency rules, and in some cases, by valency-imposed double site-occupancy.
- We recommend that suffixes (other than Levinson modifiers) not be used in naming minerals in the garnet supergroup. We have discredited existing names that have suffixes and replaced them with new root names where necessary, specifically, bitikleite-(SnAl) with bitikleite, bitikleite-(SnFe) with dzhuluite, bitikleite-(ZrFe) with usturite and elbrusite-(Zr) with elbrusite.
- We have discredited the name hibschite in favor of grossular, as Si is the dominant cation at the *Z* site.
- 21 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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Table 1. A classification of the 32 approved species in the garnet supergroup

1722	\overline{Z} charge	GROUP or species name	Class	X	Y	Z	φ
1723	0	Katoite	Hydroxide	Ca ₃	Al ₂		(OH) ₁₂
1724	3	Cryolithionite	Halide	Na ₃	Al_2	Li ₃	F_{12}
1725	6	Yafsoanite	Oxide	Ca ₃	$Te^{\overline{6}^+}_{2}$	Zn_3	O_{12}
1726	8	HENRITERMIERITE	Silicate				
1727		Holtstamite		Ca_3	Al_2	$Si_2 \mid \square$	$O_8(OH)_4$
1728		Henritermierite		Ca_3	Mn^{3+}_{2}	$Si_2 \mid \square$	$O_8(OH)_4$
1729	9	BITIKLEITE	Oxide				
1730		Bitikleite		Ca_3	$Sb_{2}^{5+}Sn^{4+}$	Al_3	O_{12}
1731		Usturite		Ca_3	$Sb^{5+}Zr$	Fe_{3}^{3+}	O_{12}
1732		Dzhuluite		Ca_3	$Sb^{5+}Sn^{4+}$	Fe_{33}^{3+}	O_{12}
1733		Elbrusite		Ca ₃	$U^{6+}_{0.5}Zr_{1.5}$	Fe^{3+}_{3}	O_{12}
1734	10	SCHORLOMITE	Silicate				
1735		Kimzeyite		Ca_3	Zr_2	$SiAl_2$	O_{12}
1736		Irinarassite		Ca_3	$\operatorname{Sn}^{4+}_{2}$	$SiAl_2$	O_{12}
1737		Schorlomite		Ca_3	Ti_2	$SiFe_{3+}^{3+}$	O_{12}
1738		Kerimasite		Ca ₃	Zr_2	SiFe ³ ₂	O_{12}
1739		Toturite	~	Ca_3	$\operatorname{Sn}^{4+}_{2}$	SiFe ³⁺ ₂	O_{12}
1740	12	GARNET	Silicate				
1741		Menzerite-(Y)		Y ₂ Ca	Mg_2	Si ₃	O_{12}
1742		Pyrope		Mg_3	Al_2	Si ₃	O_{12}
1743		Grossular		Ca_3	Al_2	Si ₃	O_{12}
1744		Spessartine		Mn_{3}^{2+}	Al_2	Si ₃	O_{12}
1745		Almandine		Fe^{2+}_3	Al_2	Si ₃	O_{12}
1746		Eringaite		Ca ₃	Sc_2	Si ₃	O_{12}
1747		Goldmanite		Ca_{3}	V_{2}^{3+} V_{2}^{3+} Cr_{2}^{3+}	Si ₃	O_{12}
1748		Momoiite		Mn^{2+}_{3}	$\frac{V_2}{2}$	Si ₃	O_{12}
1749		Knorringite		Mg_3	$\operatorname{Cr}_{2}^{2}$	Si ₃	O_{12}
1750		Uvarovite		Ca ₃	Cr_{2}^{3+}	Si ₃	O_{12}
1751		Andradite		Ca_3	Fe ³⁺ ₂ Fe ³⁺ ₂	Si ₃	O_{12}
1752		Calderite Majorite		Mn^{2+}_{3}	re ₂	Si ₃	O_{12}
1753		Majorite		Mg_3	SiMg	Si ₃	O_{12}
1754	15	Morimotoite	Vana 1-4-	Ca ₃	TiFe ²⁺	Si ₃	O_{12}
1755	15	BERZELIITE	Vanadate, a		Ma	V_{3}^{5+}	0
1756		Schäferite Palanzanaita		Ca ₂ Na	$\mathrm{Mg_2} \mathrm{Mn}^{2+}$	V_{3}^{5+}	O_{12}
1757		Palenzonaite Berzeliite		Ca ₂ Na		V 3 A 3 ⁵⁺	O_{12}
1758				Ca ₂ Na	$\mathrm{Mg_2} \mathrm{Mn}^{2+}$	AS_{5+}	O_{12}
1759		Manganberzeliite		Ca_2Na	1 VIII 2	As^{5+}_{3}	O_{12}

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

Table 2. Former formulae and end-member formulae approved in the present report

1762	Name	Former formula	Approved end-member formula
1763	Katoite	$Ca_3Al_2(SiO_4)_{3-x}(OH)_{4x} (x=1.5-3.0)$	$\{Ca_3\}[Al_2](\square_3)(OH)_{12}$
1764	Cryolithionite	$Na_3Al_2(LiF_4)_3$	${Na_3}[Al_2](Li_3)F_{12}$
1765	Yafsoanite	$Ca_{3}Te^{6+}_{2}Zn_{3}O_{12}$	${Ca_3}[Te^{6}_2](Zn_3)O_{12}$
1766	Holtstamite	$Ca_3Al_2(SiO_4)_2(OH)_4$	${Ca_3}[Al_2](Si_2)(\square)O_8(OH)_4$
1767	Henritermierite	$Ca_3(Mn^{3+})_2(SiO_4)_2(OH)_4$	${Ca_3}[Mn^{3+}_2](Si_2)(\square)O_8(OH)_4$
1768	Bitikleite*	$Ca_3SbSnAl_3O_{12}$	${Ca_3}[Sb^{5+}Sn^{4+}](Al_3)O_{12}$
1769	Usturite*	Ca ₃ SbZrFe ₃ O ₁₂	${Ca_3}[Sb^{5+}Zr](Fe^{3+}_3)O_{12}$
1770	Dzhuluite*	$Ca_3(SnSb^{5+})Fe^{3+}_3O12$	${Ca_3}[Sb^{5+}Sn^{4+}](Fe^{3+}_{3})O_{12}$
1771	Elbrusite*	$Ca_3(U^{6+}Zr)(Fe^{3+}_2Fe^{2+})O_{12}$	${Ca_3}[U^{6+}_{0.5}Zr_{1.5}](Fe^{3+}_{3})O_{12}$
1772	Kimzeyite	$Ca_3(Zr,Ti)_2(Si,Al,Fe^{3+})_3O_{12}$	${Ca_3}[Zr_2](SiAl_2)O_{12}$
1773	Irinarassite	$Ca_3Sn_2Al_2SiO_{12}$	${Ca_3}[Sn_2^{4+}](SiAl_2)O_{12}$
1774	Schorlomite	$Ca_3(Ti,Fe^{3+})_2[(Si,Fe)O_4]_3O_{12}$	${Ca_3}[Ti_2](SiFe^{3+}_{2})O_{12}$
1775	Kerimasite	$Ca_3Zr_2(Fe^{34}_2Si)O_{12}$	${Ca_3}[Zr_2](SiFe^{3+}_2)O_{12}$
1776	Toturite	$Ca_3Sn_2Fe_2SiO_{12}$	${Ca_3}[Sn^{4+}_2](SiFe^{3+}_2)O_{12}$
1777	Menzerite-(Y)	${CaY_2}[Mg_2](Si_3)O_{12}$	${Y_2Ca}[Mg_2](Si_3)O_{12}$
1778	Pyrope	$Mg_3Al_2(SiO_4)_3$	${Mg_3}[Al_2](Si_3)O_{12}$
1779	Grossular	$Ca_3Al_2(SiO_4)_3$	${Ca_3}[Al_2](Si_3)O_{12}$
1780	Spessartine	$(Mn^{2+})_3Al_2(SiO_4)_3$	$\{Mn_{2}^{2+3}\}[Al_2](Si_3)O_{12}$
1781	Almandine	$(Fe^{2+})_3Al_2(SiO_4)_3$	${Fe^{2^{+}}_{3}}[Al_{2}](Si_{3})O_{12}$
1782	Eringaite	$Ca_3Sc_2(SiO_4)_3$	$\{Ca_3\}[Sc_2](Si_3)O_{12}$
1783	Goldmanite	$Ca_3(V^{3+})_2(SiO_4)_3$	${Ca_3}[V^{3+}_2](Si_3)O_{12}$
1784	Momoiite	$(Mn^{2+},Ca)_3(V^{3+},Al)_2Si_3O_{12}$	$\{Mn^{2+}_{3}\}[V_{2+2}^{3+}](Si_{3})O_{12}$
1785	Knorringite	$Mg_3Cr_2(SiO_4)_3$	${Mg_3}[Cr_{2}^{3+}2](Si_3)O_{12}$
1786	Uvarovite	$Ca_3Cr_2(SiO_4)_3$	${Ca_3}[Cr_{2}^{3+}](Si_3)O_{12}$
1787	Andradite	$Ca_3(Fe^{3+})_2(SiO_4)_3$	${Ca_3}[Fe^{3+}_2](Si_3)O_{12}$
1788	Calderite	$(Mn^{2+})_3(Fe^{3+})_2(SiO_4)_3$	${Mn^{2+}_{3}}[Fe^{3+}_{2}](Si_{3})O_{12}$
1789	Majorite	$Mg_3(Fe^{2+},Si)_2(SiO_4)_3$	${Mg_3}[SiMg](Si_3)O_{12}$
1790	Morimotoite	$Ca_3(Ti,Fe^{2+},Fe^{3+})_2(Si,Fe^{3+})_3O_{12}$	${Ca_3}[TiFe^{2+}](Si_3)O_{12}$
1791	Schäferite	$NaCa_2Mg_2(VO_4)_3$	${Ca_2Na}[Mg_2](V^{5+}_3)O_{12}$
1792	Palenzonaite	$NaCa_2(Mn^{2+})_2(VO_4)_3$	${Ca_2Na}[Mn^{2+}_{2}](V_{5+}^{5+}_{3})O_{12}$
1793	Berzeliite	$NaCa_2Mg_2(AsO_4)_3$	${Ca_2Na}[Mg_2](As^{5+}_3)O_{12}$
1794	Manganberzeliite	$NaCa_2(Mn^{2+})_2(AsO_4)_3$	${Ca_2Na}[Mn^{2+}_{2}](As^{5+}_{3})O_{12}$

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.

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

1802	Site	Relative abundance of ions	Cations and anions at each site in order of relative abundance
1803	\overline{X}	$R^{2+} >> R^{3+} >> R^{1+} >> R^{4+}$	
1804			R^{2+} : $\mathbf{Fe} \sim \mathbf{Mn} \sim \mathbf{Ca} > \mathbf{Mg} >> \mathbf{Pb}$
1805			R^{3+} : Y > HREE > LREE
1806			R^{1+} : Na
1807			<i>R</i> ⁴⁺ : Th
1808	Y	$R^{3+} > R^{4+} > R^{2+} > R^{5+} > R^{6+}$	
1809			R^{3+} : Al ~ Fe > V, Cr, Mn > Sc >> Ga
1810			R^{4+} : Ti $>$ Zr $>$ Si, Sn
1811			R^{2+} : Mg > Fe, Mn
1812			<i>R</i> ⁵⁺ : Sb, Nb
1813			<i>R</i> ⁶⁺ : Te, U
1814	Z	$R^{4+} > R^{3+} > R^{5+} \sim \square$ (vacancy	$(r) > R^{2+}, R^{1+}$
1815			R^{4+} : Si >> Ti > Ge
1816			R^{3+} : Fe \sim Al
1817			R^{5+} : As $>$ V $>$ P
1818			<i>R</i> ²⁺ : Zn, Fe
1819			R^{1+} : Li
1820	φ	$\varphi^{2-} >> \varphi^{1-}$	
1821			φ^{2-} : \mathbf{O}
1822			φ^{1-} : $\mathbf{OH} > F$
	> T /	TD1 .: 1 : 1	. 1 11,

Note: 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.

1826	Generalized coupled substitution	Relationship
1827	$^{Z}\Box + 4\phi^{1-} \rightarrow ^{Z}Si^{4+} + 4O^{2-}$	relates katoite, henritermierite and holtstamite to OH-free minerals in the garnet group
1828	${}^{Y}R^{2+} + {}^{Y}R^{4+} \rightarrow 2{}^{Y}R^{3+}$	relates morimotoite ([6]Ti) and majorite ([6]Si) to other garnet-group minerals
1829	${}^{Z}R^{4+} + {}^{Y}R^{3+} \rightarrow {}^{Z}R^{3+} + {}^{Y}R^{4+}$	relates the schorlomite group to the garnet group
1830	${}^{X}(Y, REE)^{3+} + {}^{Z}R^{3+} \longrightarrow {}^{X}R^{2+} + {}^{Z}R^{4+}$	introduces $Y + REE$ as a YAG , $\{Y_3\}[Al_2](Al_3)O_{12}$ -type component
1831	${}^{X}(Y, REE)^{3+} + {}^{X}Na^{1+} \rightarrow 2{}^{X}R^{2+}$	introduces Y + REE into garnet-group minerals
1832	${}^{X}(Y, REE)^{3+} + {}^{Y}R^{2+} \rightarrow {}^{X}R^{2+} + {}^{Y}R^{3+}$	relates menzerite-(Y) to other garnet-group minerals
1833	${}^{Y}R^{5+} + {}^{Z}R^{3+} \longrightarrow {}^{Y}R^{4+} + {}^{Z}R^{4+}$	relates bitikleite, dzhuluite and usturite with schorlomite-group minerals
1834	${}^{Y}0.5R^{6+} + {}^{Z}R^{3+} \rightarrow {}^{Y}0.5R^{4+} + {}^{Z}R^{4+}$	relates elbrusite with schorlomite-group minerals
1835	${}^{Y}U^{6+} + {}^{Z}R^{2+} \rightarrow {}^{Y}R^{4+} + {}^{Z}R^{4+}$	observed relationship between elbrusite and schorlomite group minerals (Fig. 4)
1836	0.5^{X} Th ⁴⁺ + Z $R^{3} \rightarrow 0.5^{X}$ R^{2+} + Z R^{4+}	introduces Th into minerals of the bitikleite and schorlomite groups
1837	${}^{Y}R^{4+} + 0.5{}^{Z}V^{5+} \rightarrow 0.5{}^{Z}R^{3+} + {}^{Y}Sb^{5+}$	introduces V into bitikleite
1838	${}^{Y}R^{4+} + {}^{Z}V^{5+} \rightarrow {}^{Y}U^{6+} + {}^{Z}R^{3+}$	introduces V into elbrusite
1839	${}^{X}\text{Na}^{1+} + {}^{Y}R^{4+} \rightarrow {}^{X}R^{2+} + {}^{Y}R^{3+}$	introduces Na and ^[6] Si or ^[6] Ti into the garnet group
1840	${}^{X}\text{Na}^{1+} + {}^{Z}R^{5+} \longrightarrow {}^{X}R^{2+} + {}^{Z}R^{4+}$	relates the berzeliite group to the garnet group
1841	Note: <i>R</i> represents generalized cations	(see Table 3)

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

1843 1844	Former name	New name (approved by CN	Formula (approved by CNMNC) MNC)
1845	Bitikleite-(SnAl)	Bitikleite	${Ca_3}[Sb^{5+}Sn^{4+}](Al_3)O_{12}$
1846	Bitikleite-(SnFe)	Dzhuluite	$\{Ca_3\}[Sb^{5+}Sn^{4+}](Fe^{3+}_3)O_{12}$
1847	Bitikleite-(ZrFe)	Usturite	${Ca_3}[Sb^{5+}Zr](Fe^{3+}_3)O_{12}$
1848	Elbrusite-(Zr)	Elbrusite	$\{Ca_3\}[U^{6+}_{0.5}Zr_{1.5}](Fe^{3+}_3)O_{12}$
1849	Hibschite*	Grossular	${Ca_3}[Al_2](Si_{3-x}\square_x)O_{12-4x}(OH)_{4x}$ where $x < 1.5^{\#}$
1850	Note: *Former formula	a: Ca ₃ Al ₂ (SiO ₄) _{3-x} (OH)	$_{4x}$, where x = 0.2-1.5. *Includes OH-bearing grossular.
1851	Ideal anhydrous gross	ular has the formula: {(Ca_3 {[Al ₂](Si ₃)O ₁₂ .
1852			

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

1855	Name	X	Y	Z	φ	Syn?	Occurrence in natural garnet (sou	urces)
1856				"Keno	garnet" gro	up		
1857	Fe ³⁺ analogue of katoite	Ca ₃	Fe^{3+}_{2}	\square_3	$(OH)_{12}$	Yes	≤ 35 mol.% in andradite	(1)
1858	F analogue of katoite	Ca ₃	Al_2	\square_3	F_{12}	No	≤ 11 mol.% in OH-bearing grossular	(2)
1859	Mn ²⁺ , F analogue of katoite	Mn^{2+}_{3}	Al_2	\square_3	F_{12}		≤ 8 mol.% in spessartine	(3)
1860	<u>-</u>			Unna	amed group)	•	
1861	Pb ²⁺ analogue of yafsoanite	Pb ₃	Te^{6+}_{2}	Zn_3	O_{12}		9 mol.% in yafsoanite	(4)
1862	unnamed	Ca ₃	U_{2}^{6+}	Fe^{2+}_3	O_{12}		≤24 mol.% in elbrusite	(5)
1863				Henrite	rmierite gro	oup		. ,
1864	Mn ²⁺ analogue of holtstamite	Mn^{2+}_{3}	Al_2	$Si_2 \mid \square$	$O_8(OH)_4$		28 mol.% in spessartine	(6)
1865	Mn ²⁺ , F analogue of holtstamite	Mn^{2+}_{3}	Al_2	$Si_2 \mid \square$	O_8F_4		20 mol.% in spessartine	(6)
1866	,				kleite group		•	. ,
1867	unnamed	$Th_{0.5}Ca_{2.5}$	R^{4+}_{2}	R^{3+}_{3}	O_{12}	Yes	≤ 20 mol.% in kerimasite	(7)
1868				Unna	amed group)		. ,
1869	$Y_3Al_5O_{12}, Y_3Fe_5O_{12}$	$(Y,REE)^{3+}_{3}$	R^{3+}_{2}	R^{3+}_{3}	O_{12}	Yes	\leq 8 mol.% in menzerite-(Y), spessartine, and adite	(8)
1870			_	Gai	rnet group		\ \ // 1	. ,
1871	"Blythite" in part	R^{2+}_{3}	Mn^{3+}_{2}	Si_3	O_{12}	Yes	≤ 9 mol.% in calderite-andradite±spessartine	(9)
1872	Fe analogue of menzerite-(Y)	Y ₂ Ca	Fe^{2+}_{2}	Si_3	O_{12}		$\leq 20 \text{ mol.}\%$ in menzerite (Y)	(10)
1873	unnamed	$(Y,Yb)_{1.5}Na_{1.5}$	$R^{3+}_{2}^{-}$	Si_3	O_{12}		≤ 7 mol.% in almandine, spessartine, grossular	(11)
1874	unnamed	R^{2+} Na ₂	Si_2	Si_3	O_{12}	Yes	≤ 12 mol.% in pyrope-grossular	(12)
1875		-	-	-	eliite group			` /
1876	unnamed	Na ₃	Al_2	P_3	O_{12}	Yes	< 1 mol.% in almandine and pyrope	(13)
1877	unnamed	Ca ₂ Na	$\mathrm{Fe}^{\mathbf{\tilde{2}}_{+}}$	As^{5+}_3	O_{12}	No	< 6 mol.% in berzeliite	(14)

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

- 1880 (1) Armbruster (1995); Cohen-Addad (1970)
- 1881 (2) Chakhmouradian et al. (2008); Takamori et al. (1987)
- 1882 (3) Smyth et al. (1990).
- 1883 (4) Mills et al. (2010).

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1884 (5) Galuskina et al. (2010a).

- 1885 (6) Si and \square are not fully ordered at Z1 and Z2. Boiocchi et al. (2012).
- 1886 (7) Ito and Frondel (1967a); Yudintsev (2003); Galuskina et al. (2010e and unpublished).
- 1887 (8) Yoder and Keith (1951); Geller (1967); Jaffe (1951); Kasowski and Hogarth (1968); Grew et al. (2010).
- 1888 (9) Fursenko (1982); Nishizawa and Koizuma (1975); Bühn et al. (1995); Amthauer et al. (1989); Arlt et al. (1998).
- 1889 (10) Grew et al. (2010).
- 1890 (11) Enami et al. (1995); Røhr et al. (2007).
- 1891 (12) Ringwood and Major (1971); Stähle et al. (2011).
- 1892 (13) Bishop et al. (1978); Ye et al. (2000); Breiter et al. (2005); Brunet et al. (2006).
- 1893 (14) Nagashima and Armbruster (2012); Ito (1968)

Table 7. Summary of specific components potentially significant in

natural garnets

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1921 1922

1896	Name	Synthesis	Formula
1897	_	62 to 90%	${Fe^{2+}_{3}}[Al_{2}](\square_{3})(OH)_{12}$
1898	_	No	${Ca_3}[Al_2](\square_3)F_{12}$
1899	_	_	$\{Mn^{2+}_{3}\}[Al_{2}](\square_{3})F_{12}$
1900	_	_	${Fe}^{2+}_{3}{Al_{2}(\square_{3})F_{12}$
1901	_	_	$\{Pb^{2+}_{3}\}[Te^{6+}_{2}](Zn_{3})O_{12}$
1902	_	_	${Ca_3}[U_2^{6+}](Fe_2^{2+})O_{12}$
1903	_	_	$\{Mn_{2}^{2+}\}\{Al_{2}\}(Si_{2})(\square)O_{8}(OH)_{4}$
1904	_	_	$\{Mn^{2+}_{3}\}[Al_{2}](Si_{2})(\square)O_{8}F_{4}$
1905	_	100%	${Th_{0.5}Ca_{2.5}}[Zr_2](Fe^{3+}_2)O_{12}$
1906	YIG	100%	${Y_3}[Al_2](Al_3)O_{12}$
1907	YAG	100%	${Y_3}[Fe^{3+}_{2}](Fe^{3+}_{3})O_{12}$
1908	"Blythite"	100%	${Mn}^{2+}_{3}{Mn}^{3+}_{2}(Si_{3})O_{12}$
1909	_	100%	${Ca_3}[Mn^{3+}_{2}](Si_3)O_{12}$
1910	"Khoharite"	100%	${Mg_3}[Fe^{3+}_2](Si_3)O_{12}$
1911	"Skiagite"	100%	${Fe^{2+}_{3}}[Fe^{3+}_{2}](Si_{3})O_{12}$
1912	_	_	${Y_2Ca}[Fe^{2+}_2](Si_3)O_{12}$
1913	_	_	${Y_{1.5}Na_{1.5}}[Al_2](Si_3)O_{12}$
1914	_	100%	${CaNa_2}[Si_2](Si_3)O_{12}$
1915	_	100%	${CaNa_2}[Ti_2](Si_3)O_{12}$
1916	_	100%	${Na_3}[Al_2](P_3)O_{12}$
1917	_	No	${Ca_2Na}[Fe^{2+}_2](As^{5+}_3)O_{12}$
1918	Note: Synthes	ses: percentage giv	es the amount of the component

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

Table 8. Possible new species in the garnet supergroup.

1924	Relationship to known species	UM#	End-member formula	Criteria	(source)
1925	BITIKLEITE GROUP				
1926	Sn analogue of elbrusite		${Ca_3}[U_{0.5}^{6+}Sn_{0.5}^{4+}](Fe_{3}^{3+})O_{12}$	Sn/(Sn + Zr) = 0.93	(1)
1927	Nb analogue of usturite		${Ca_3}[NbZr](Fe^{3+}_3)O_{12}$	1.33 Zr, 0.05 Ti, 0.48 Nb pfu at <i>Y</i> site	(2)
1928	SCHORLOMITE GROUP				
1929	Al analogue of schorlomite		${Ca_3}[Ti_2](SiAl_2)O_{12}$	$A1/(A1+Fe^{3+}) = 0.65$	(3)
1930	(Ti analogue of kimzeyite)				
1931	GARNET GROUP			-	
1932	Mg analogue of morimotoite		${Ca_3}[TiMg](Si_3)O_{12}$	$Mg/(Mg + Fe^{2+}) = 0.63-0.64$	(4)
1933	Ga Ge analogue of grossular	UM1986-19	${Ca_3}[Ga_2](Ge_3)O_{12}$	2 Ge > 2 Si; 1 Ga > 1 Fe ³⁺ , 1 Al	(5)
1934	Ge analogue of grossular	UM1986-20	${Ca_3}[Al_2](Ge_3)O_{12}$	Criterion of ${}^{Z}Ge > {}^{Z}Si$ not met.	(5)

- Note: UM # refers to the list of valid unnamed minerals, update 2011-01 (Smith and Nickel 2007).
- 1936 Sources: (1) Galuskina et al. (2010a); (2) Zaitsev et al. (2010); (3) Koritnig et al. (1978); (4) Platt and
- 1937 Mitchell (1979); (5) Johan and Oudin (1986); Jambor et al. (1988b).

1938 Figure Captions

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Figure 1. Photographs of representative garnet supergroup minerals illustrating the diversity in appearance exhibited by the supergroup. A. Holtstamite, formula $\{Ca_3\}[Al,Mn^{3+}_2](Si_2)(\square)O_8(OH)_4$, as a yellow brown crystal between grains of Mn- and Cu-rich vesuvianite (purplish black) and calcite (white) in the holotype specimen from Wessels Mine, South Africa. Swedish Museum of Natural History specimen #19960380. Photo by U. Hålenius. B. Cryolithionite, end-member formula {Na₃}[Al₂](Li₃)F₁₂: a transparent, colorless single grain in yellowish-white fine-grained cryolite. Specimen size is 4.5 x 2 x 1.7 cm. From the type locality, Ivigtut Cryolite deposit, Ivittuut (Ivigtut), Kitaa, Greenland. Pavel M. Kartashov collection and photograph. C. Grossular, end-member formula {Ca₃}[Al₂](Si₃)O₁₂: 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 {Ca₃}[Cr³⁺₂](Si₃)O₁₂: 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 {Fe₃}[Al₂](Si₃)O₁₂: 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 {Ca₃}[Ti₂](SiFe³⁺₂)O₁₂: an incomplete crystal from the type locality, Magnet Cove, Hot Spring County, Arkansas. E.S. Grew collection and photograph. G. Manganberzeliite, end-member formula {Ca₂Na}[Mn²⁺₂](As⁵⁺₃)O₁₂, from the type locality, Långban, Sweden. The largest crystals are 3 mm across. Swedish Museum of Natural History specimen #19170722. M. Cooper photograph.

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

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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. Figure 4. Compositions of U-rich garnets (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 $\{Ca_3\}[U^{6+}_2](R^{2+}_3)O_{12}$ end-member. Yellow circle indicates the Sn-dominant analogue of elbrusite, which was included in the least-squares fit. Figure 5. Plot of the Y-site contents of 40 natural garnets with $TiO_2 > 12$ wt.% based on formulae normalized to 8 cations and 12 oxygen 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); 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 > Fe²⁺ (total for analysis) have been added only for compositions plotting in the morimotoite field. The square enclosing a triangle indicates the schorlomite in which ${}^{Z}Al > {}^{Z}Fe^{3+}$ and 0.55 Zr pfu reported by Koritnig et al. (1978); it is a possible new species, the Al-dominant analogue of schorlomite. Compositions are plotted under the assumption that Al preferentially is incorporated at the Z site (except from Fuka, see text).

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Figure 6. Y-site occupancy in species of the bitikleite group, including the possible unnamed Sndominant analogue of elbrusite. Placement of the divisions is indicated. 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. 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 $\{Y_3\}[R^{3+}_2](R^{3+}_3)O_{12}$ onto the plane defined by the components $\{Ca_3\}[Ti^{4+}R^{2+}](Si^{4+}_3)O_{12}, \{Ca_3\}[R^{3+}_2](Si^{4+}_3)O_{12}, \text{ and } \{Ca_3\}[R^{3+}_2](Si^{4+}_3)O_{12$ $\{(REE)_2Ca\}[R^{2+}_2](Si^{4+}_3)O_{12}$ (cf. Figure 7a, Grew et al. 2010). R^{2+} = Fe in morimotoite, Mg in menzerite-(Y); R^{3+} = Fe in and adite. Numbers refer to grains used for the crystal-structure refinement (SREF), optical measurements, and menzerite-(Y) sensu stricto (Mzr), including grain #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). 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.

2014 2015	Appendix 1. List of garnet species, end-member formulae, modifications, etymology, type localities; crystal structure refinements
2016	
2017	The following garnet species either have been previously accepted by the IMA-CNMNC or
2018	have been modified by the current garnet subcommittee. Modifications to the original garnet species
2019	descriptions are noted except for grandfathered species. One or two references are given for the
2020	crystal structure, either of natural material (when available) or of synthetic material, or both.
2021	Almandine
2022	End-member formula: $\{Fe^{2+}_3\}[Al_2](Si_3)O_{12}$
2023	Group: Garnet
2024	IMA number: Grandfathered.
2025	Modifications: None.
2026	Etymology: The "Alabandic carbuncles" of Pliny were so named as they were cut and polished in
2027	Alabanda (Dana 1837, 1892), an ancient city in what is presently Aydin Province, Turkey.
2028	Type locality: Not known.
2029	Crystal system, space group and structure refinement: Isometric, Ia-3d. Novak and Gibbs (1971);
2030	synthetic material: Armbruster et al. (1992).
2031	Original or oldest description: Known in ancient times. Name first used by D.L.G. Karsten in 1800
2032	(Dana 1892).
2033	Andradite
2034	End-member formula: $\{Ca_3\}[Fe^{3+}_2](Si_3)O_{12}$
2035	Group: Garnet
2036	IMA number: Grandfathered.
2037	Modifications: None.
2038	Etymology: For José Bonifácio de Andrada e Silva (1763 1838), the Brazilian mineralogist who
2039	described a variety under the name "allochroite" in 1800 (Dana 1892; Clark 1993).
2040	Type locality: Not known.
2041	Crystal system, space group and structure refinement: Isometric, Ia-3d. Armbruster and Geiger
2042	(1993).
2043	Original or oldest description: "allochroite" of de Andrada in 1800 and "melanite" of Werner in
2044	1800 (Dana 1892).
2045	Berzeliite
2046	End-member formula: $\{Ca_2Na\}[Mg_2](As^{5+}_3)O_{12}$
2047	Group: Berzeliite
2048	IMA number: Grandfathered.

- (DOI will not work until issue is live.) DOI: http://dx.doi.org/10.2138/am.2013.4201 Modifications: None. 2049 2050 Etymology: For Jacob Berzelius (1799 1848), a Swedish chemist. Type locality: Långban, Filipstad district, Värmland, Sweden. 2051 Crystal system and structure refinement: Isometric, *Ia-3d*. Hawthorne (1976); Nagashima and 2052 2053 Armbruster (2012). Original or oldest description: Kühn (1840). 2054 Bitikleite 2055 End-member formula: $\{Ca_3\}[Sb^{5+}Sn^{4+}](Al_3)O_{12}$ 2056 2057 Group: Bitikleite 2058 IMA number: 2009-052. 2059 Modifications: Originally described as bitikleite-(SnAl) with the same formula. Etymology: From Bitikle, the name of an old fortification near the type locality. 2060 2061 Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia. Crystal system, space group and structure refinement: Isometric, *Ia-3d*. Galuskina et al. (2010b). 2062 Original or oldest description: Galuskina et al. (2010b). 2063 2064 Calderite End-member formula: $\{Mn^{2+}_3\}[Fe^{3+}_2](Si_3)O_{12}$ 2065 Group: Garnet 2066 IMA number: Grandfathered. 2067 Modifications: None. 2068 Etymology: For James Calder, a member of the Asiatic Society of Bengal, originally applied to the 2069 rock containing the mineral (Piddington 1850). 2070 2071 Type locality: Either in Burdwan (Bardhaman) district, West Bengal State, or near Hazaribagh, 2072 Jharkhand State, India. Crystal system, space group and structure report: Isometric, *Ia-3d*. No structure refinement; 2073 structure optimization by distance least-squares refinement (Ottonello et al. 1996). 2074 Original or oldest description: Fermor (1909, 1926). 2075 2076 Cryolithionite End-member formula: $\{Na_3\}[Al_2](Li_3)F_{12}$ 2077 Group: ungrouped 2078 IMA number: Grandfathered. 2079
- 2081 Etymology: From the presence of Li and its relation to cryolite.

Modifications: None.

- Type locality: The Ivigtut cryolite deposit, Ivittuut (Ivigtut), Arsuk, Kitaa Province, Greenland. 2082
- 2083 Crystal system, space group and structure refinement: Isometric, *Ia-3d*. Geller (1971).

2084	Original or oldest description: Ussing (1904).
2085	Dzhuluite
2086	End-member formula: $\{Ca_3\}[Sb^{5+}Sn^{4+}](Fe^{3+}_3)O_{12}$
2087	Group: Bitikleite
2088	IMA number: 2010-64.
2089	Modifications: Originally described as bitikleite-(SnFe) with the same formula.
2090	Etymology: After Dzhulu Mountain near the type locality.
2091	Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia.
2092	Crystal system and space group: Isometric, <i>Ia-3d</i> . Structure not yet refined.
2093	Original or oldest description: Galuskina et al. (2011a).
2094	Elbrusite
2095	End-member formula: $\{Ca_3\}[U^{6+}_{0.5}Zr_{1.5}](Fe^{3+}_3)O_{12}$
2096	Group: Bitikleite
2097	IMA number: 2009-051.
2098	Modifications: Originally described as elbrusite-(Zr) with a formula $\{Ca_3\}[U^{6+}Zr](Fe^{3+}_2Fe^{2+})O_{12}$.
2099	Etymology: From the highest peak in Europe – Mount Elbrus (5642 m)
2100	Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia.
2101	Crystal system, space group and structure refinement: Isometric, <i>Ia-3d</i> . The structure of elbrusite
2102	has not yet been refined, but that of U-rich kerimasite has been refined (under the name "Fe-
2103	dominant analogue of kimzeyite", Galuskina et al. 2010a).
2104	Original or oldest description: Galuskina et al. (2010a).
2105	Eringaite
2106	End-member formula: $\{Ca_3\}[Sc_2](Si_3)O_{12}$
2107	Group: Garnet
2108	IMA number: 2009-054.
2109	Modifications: None.
2110	Etymology: From the Eringa River, a tributary of the Wiluy River.
2111	Type locality: Wiluy River, Sakha-Yakutia Republic, Russia. (63.0°N, 112.3°E).
2112	Crystal system, space group and structure refinement: Isometric, <i>Ia-3d</i> . Synthetic material: Mill' et
2113	al. (1977), Quartieri et al. (2006).
2114	Original or oldest description: Galuskina et al. (2010d).
2115	Goldmanite
2116	End-member formula: $\{Ca_3\}[V^{3+}_2](Si_3)O_{12}$
2117	Group: Garnet
2118	IMA number: 1963-003.

Modifications: None. 2119 2120 Etymology: For Marcus I. Goldman (1881-1965), a sedimentary petrologist with the U.S. Geological Survey. 2121 Type locality: Sandy (or South Laguna) mine area, Laguna, New Mexico, U.S.A. 2122 Crystal system, space group and structure refinement: Isometric, *Ia-3d*. Novak and Gibbs (1971); 2123 Righter et al. (2011). 2124 Original or oldest description: Moench and Meyrowitz (1964). 2125 2126 Grossular End-member formula: {Ca₃}[Al₂](Si₃)O₁₂ 2127 Group: Garnet 2128 2129 IMA number: Grandfathered. Modifications: None. 2130 2131 Etymology: From the color resembling gooseberry, *Ribes grossularia* (Dana 1892; Clark 1993). Type locality: Wiluy River, Sakha-Yakutia Republic, Russia. 2132 Crystal system, space group and structure refinement: Isometric, *Ia-3d*. Novak and Gibbs (1971). 2133 Synthetic material: Geiger and Armbruster (1997). 2134 Original or oldest description: A.G. Werner in 1808-1809. However, grossular was described earlier 2135 under other names, viz. as "Cinnamon Stone" (Kanelstein) from Sri Lanka by Werner in 1803-2136 1804 and as "Granat" by Pallas in 1793 (Dana (1892). 2137 2138 Henritermierite End-member formula: $\{Ca_3\}[Mn^{3+}_2](Si_2)(\square)O_8(OH)_4$ 2139 Group: Henritermierite 2140 2141 IMA number: 1968-029 Modifications: None. 2142 Etymology: For Henri-François-Émile Termier (1897-1989), a French geologist. 2143 Type locality: Tachgagalt mine, Morocco. 2144 Crystal system, space group and structure refinement: Tetragonal, $I4_1/acd$. Armbruster et al. (2001). 2145 2146 Original or oldest description: Gaudefroy et al. (1969). **Holtstamite** 2147 Formula: $\{Ca_3\}[Al_1Mn^{3+}_2](Si_2)(\square)O_8(OH)_4$ 2148 Group: Henritermierite 2149 IMA number: 2003-047. 2150 2151 Modifications: None. Etymology: For Dan Holtstam (b. 1963), a Swedish mineralogist. 2152 Type locality: Wessels Mine, Kalahari manganese field, South Africa. 2153

2154	Crystal system, space group and structure refinement: Tetragonal, I4 ₁ /acd. Hålenius et al. (2005)
2155	Original or oldest description: Hålenius (2004), Hålenius et al. (2005).
2156	Irinarassite
2157	End-member formula: $\{Ca_3\}[Sn^{4+}_{2}](SiAl_2)O_{12}$
2158	Group: Schorlomite
2159	IMA number: 2010-73.
2160	Modifications: None.
2161	Etymology: For Irina Rass (b. 1940), a Russian mineralogist.
2162	Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia.
2163	Crystal system and space group: Isometric, <i>Ia-3d</i> . Structure not yet refined.
2164	Original or oldest description: Galuskina et al. (2011b).
2165	Katoite
2166	End-member formula: $\{Ca_3\}[Al_2](\square_3)(OH)_{12}$
2167	Group: ungrouped
2168	IMA number: 1982-080.
2169	Modifications: None.
2170	Etymology: For Akira Kato (b. 1931), a Japanese mineralogist.
2171	Type locality: Campomorto quarry, Pietra Massa, Viterbo, Lazio, Italy.
2172	Crystal system, space group and structure refinement: Isometric, Ia-3d. Sacerdoti and Passaglia
2173	(1985); synthetic material (Lager et al. 1987).
2174	Original or oldest description: Passaglia and Rinaldi (1984).
2175	Kerimasite
2176	End-member formula: $\{Ca_3\}[Zr_2](SiFe^{3+}_2)O_{12}$
2177	Group: Schorlomite
2178	IMA number: 2009-29.
2179	Modifications: None.
2180	Etymology: For the Kerimasi volcano.
2181	Type locality: Kerimasi volcano, Gregory Rift, northern Tanzania.
2182	Crystal system, space group and structure refinement: Isometric, Ia-3d. Zaitsev et al. (2010), and
2183	under the name kimzeyite, Schingaro et al. (2001); synthetic material under the name kimzeyite
2184	(Whittle et al. 2007).
2185	Original or oldest description: Zaitsev et al. (2010). Under the name kimzeyite: Schingaro et al.
2186	(2001) and Galuskina et al. (2005); under the name "Fe-dominant analog of kimzeyite"
2187	(Galuskina et al. 2010a, b, c).
2188	Kimzeyite
	$\mathcal{C}\Lambda$

End-member formula: $\{Ca_3\}[Zr_2](SiAl_2)O_{12}$ 2189 2190 Group: Schorlomite IMA number: Not recorded. 2191 2192 Modifications: None. Etymology: For members of the Kimzey family, who were instrumental in obtaining and preserving 2193 mineral specimens from Magnet Cove. 2194 2195 Type locality: Kimzey quarry, Magnet Cove, Arkansas, U.S.A. 2196 Crystal system, space group and structure refinement: Isometric, Ia-3d. Munno et al. (1980) Original or oldest description: Milton and Blade (1958), Milton et al. (1961). 2197 2198 **Knorringite** End-member formula: $\{Mg_3\}[Cr^{3+}_2](Si_3)O_{12}$ 2199 2200 Group: Garnet 2201 IMA number: 1968-010. Modifications: None. 2202 Etymology: For Oleg von Knorring (1915-1994), a Russian mineralogist who worked in Finland 2203 2204 and the United Kingdom. Type locality: Kao kimberlite pipe, Butha-Buthe, Lesotho 2205 Crystal system, space group and structure refinement: Isometric, Ia-3d. Synthetic material: Juhin et 2206 2207 al. (2010). Original or oldest description: Nixon and Hornung (1968). 2208 2209 Majorite End-member formula: {Mg₃}[SiMg](Si₃)O₁₂ 2210 2211 Group: Garnet 2212 IMA number: 1969-018. Modifications: Formula originally given as {(Mg,Na)₃}[(Fe,Si,Al,Cr)₂](Si₃)O₁₂. 2213 Etymology: For Alan Major, who assisted A.E. Ringwood in experiments. 2214 Type locality: Coorara L6 chondrite (recovered in Western Australia). 2215 2216 Crystal system, space group and structure refinement: Isometric, *Ia-3d*. Synthetic material: Hazen et al. (1994). 2217 Original or oldest description: Smith and Mason (1970). 2218 2219 Manganberzeliite End-member formula: $\{Ca_2Na\}[Mn^{2+}_2](As^{5+}_3)O_{12}$ 2220 2221 Group: Berzeliite 2222 IMA number: Grandfathered. 2223 Modifications: See text.

(DOI will not work until issue is live.) DOI: http://dx.doi.org/10.2138/am.2013.4201 Etymology: The manganese analogue of berzeliite. 2224 2225 Type locality: Långban, Filipstad district, Värmland, Sweden. Crystal system, space group and structure refinement: Isometric, Ia-3d. Qualitative description of 2226 the structure: Bubeck and Machatschki (1935); Nagashima and Armbruster (2012). 2227 Original or oldest description: Igelström (1886, 1894). 2228 2229 *Menzerite-(Y)* End-member formula: $\{Y_2Ca\}[Mg_2](Si_3)O_{12}$ 2230 2231 Group: Garnet IMA number: 2009-050. 2232 2233 Modifications: None. 2234 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 2235 2236 is dominant among the sum of Y and the rare-earth elements. Type locality: Bonnet Island in Georgian Bay, near Parry Sound, Ontario, Canada 2237 Crystal system, space group and structure refinement: Isometric, *Ia-3d*. Grew et al. (2010). 2238 Original or oldest description: Grew et al. (2010). 2239 2240 Momoiite End-member formula: $\{Mn^{2+}_{3}\}[V^{3+}_{2}](Si_{3})O_{12}$ 2241 2242 Group: Garnet IMA number: 2009-026. 2243 2244 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). 2245 Etymology: For Hitoshi Momoi (1930-2002), the Japanese mineralogist who was the first to 2246 recognize $\{Mn^{2+}_3\}[V^{3+}_2](Si_3)O_{12}$ as a component in garnet 2247 Type locality: Kurase mine, Ehime Prefecture, Japan. 2248 Crystal system and space group: Isometric, Ia-3d. Structure not yet refined, but the atomic 2249 coordinates were predicted by Novak and Gibbs (1971). 2250 2251 Original or oldest description: Tanaka et al. (2010). 2252 *Morimotoite* End-member formula: {Ca₃}[TiFe²⁺](Si₃)O₁₂ 2253 2254 Group: Garnet IMA number: 1992-017. 2255 2256 Modifications: None.

Etymology: For Nobuo Morimoto (b. 1925), a Japanese mineralogist.

Type locality: Fuku, Bitchu-Cho, Okayama Prefecture, Japan.

Crystal system and space group: Isometric, *Ia-3d*. Structure not yet refined. 2259 2260 Original or oldest description: Henmi et al. (1995). 2261 End-member formula: $\{Ca_2Na\}[Mn^{2+}_2](V^{5+}_3)O_{12}$ 2262 Group: Berzeliite 2263 IMA number: 1986-011. 2264 Modifications: None. 2265 Etymology: For Andrea Palenzona (b. 1935), an Italian chemist. 2266 2267 Type locality: Molinello mine, Ne, Val Graveglia, Liguria, Italy. Crystal system, space group and structure refinement: Isometric, *Ia-3d*. Basso (1987); Nagashima 2268 2269 and Armbruster (2012). 2270 Original or oldest description: Basso (1987). 2271 Pyrope 2272 End-member formula: {Mg₃}[Al₂](Si₃)O₁₂ 2273 Group: Garnet 2274 IMA number: Grandfathered. Modifications: None. 2275 Etymology: From the Greek πνρωπός (pyropos) – firelike for its deep-red color. 2276 2277 Type locality: Bohemia (Czech Republic). Crystal system, space group and structure refinement: Isometric, *Ia-3d*. Novak and Gibbs (1971); 2278 2279 synthetic material: Armbruster et al. (1992). 2280 Original or oldest description: Recognized by Georgius Agricola (1546), but the name pyrope was 2281 introduced by A.G. Werner in 1800 (Dana 1892; Clark 1993). 2282 Schäferite End-member formula: $\{Ca_2Na\}[Mg_2](V^{5+}_3)O_{12}$ 2283 Group: Berzeliite 2284 IMA number: 1997-048. 2285 2286 Modifications: None. Etymology: For Helmut Schäfer (b. 1931), an amateur German mineralogist who discovered the 2287 mineral. 2288 Type locality: Bellberg volcano near Mayen, Eifel, Germany. 2289 Crystal system, space group and structure refinement: Isometric, *Ia-3d*. Krause et al. (1999). 2290 2291 Original or oldest description: Krause et al. (1999). 2292 Schorlomite End-member formula: {Ca₃}[Ti₂](SiFe³⁺₂)O₁₂ 2293

2294	Group: Schorlomite
2295	IMA number: Grandfathered.
2296	Modifications: Extensive; see main text.
2297	Etymology: For its resemblance to schorl.
2298	Type locality: Magnet Cove, Hot Springs County, Arkansas, U.S.A.
2299	Crystal system, space group and structure refinement: Isometric, Ia-3d. Chakhmouradian and
2300	McCammon (2005).
2301	Original or oldest description: Shepard (1846), Whitney (1849) and Rammelsberg (1850a,b).
2302	Spessartine
2303	End-member formula: $\{Mn^{2+}_3\}[Al_2](Si_3)O_{12}$
2304	Group: Garnet
2305	IMA number: Grandfathered.
2306	Modifications: None.
2307	Etymology: From the Spessart Mountains, Germany.
2308	Type locality: Sommer quarry, Wendelberg Mt., Spessart Mountains, Bavaria, Germany.
2309	Crystal system, space group and structure refinement: Isometric, <i>Ia-3d</i> . Novak and Gibbs (1971);
2310	for F-bearing, Smyth et al. (1990). Synthetic material: Geiger and Armbruster (1997).
2311	Original or oldest description: Recognized by M.H. Klaproth (1797), but the name spessartine was
2312	introduced by F.S. Beudant (1832) according to Dana (1892) and Clark (1993).
2313	Toturite
2313 2314	Toturite End-member formula: $\{Ca_3\}[Sn^{4+}_2](SiFe^{3+}_2)O_{12}$
2314	End-member formula: $\{Ca_3\}[Sn^{4+}_2](SiFe^{3+}_2)O_{12}$
2314 2315	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)O ₁₂ Group: Schorlomite
2314 2315 2316	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)O ₁₂ Group: Schorlomite IMA number: 2009-033.
2314 2315 2316 2317	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)O ₁₂ Group: Schorlomite IMA number: 2009-033. Modifications: None.
2314 2315 2316 2317 2318	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)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
2314 2315 2316 2317 2318 2319	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)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.
2314 2315 2316 2317 2318 2319 2320	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)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.
2314 2315 2316 2317 2318 2319 2320 2321	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)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, <i>Ia-3d</i> . Structure not yet refined. Original or oldest description: Galuskina et al. (2010c). <i>Usturite</i>
2314 2315 2316 2317 2318 2319 2320 2321 2322	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)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, <i>Ia-3d</i> . Structure not yet refined. Original or oldest description: Galuskina et al. (2010c). <i>Usturite</i> End-member formula: {Ca ₃ }[Sb ⁵⁺ Zr](Fe ³⁺ ₃)O ₁₂
2314 2315 2316 2317 2318 2319 2320 2321 2322 2323	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)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, <i>Ia-3d</i> . Structure not yet refined. Original or oldest description: Galuskina et al. (2010c). <i>Usturite</i> End-member formula: {Ca ₃ }[Sb ⁵⁺ Zr](Fe ³⁺ ₃)O ₁₂ Group: Bitikleite
2314 2315 2316 2317 2318 2319 2320 2321 2322 2323 2324	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)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, <i>Ia-3d</i> . Structure not yet refined. Original or oldest description: Galuskina et al. (2010c). **Usturite** End-member formula: {Ca ₃ }[Sb ⁵⁺ Zr](Fe ³⁺ ₃)O ₁₂ Group: Bitikleite IMA number: 2009-053.
2314 2315 2316 2317 2318 2319 2320 2321 2322 2323 2324 2325	End-member formula: {Ca ₃ }[Sn ⁴⁺ ₂](SiFe ³⁺ ₂)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, <i>Ia-3d</i> . Structure not yet refined. Original or oldest description: Galuskina et al. (2010c). <i>Usturite</i> End-member formula: {Ca ₃ }[Sb ⁵⁺ Zr](Fe ³⁺ ₃)O ₁₂ Group: Bitikleite

2329	Type locality: Upper Chegem caldera, Kabardino-Balkaria, North Caucasus, Russia.
2330	Crystal system and space group: Isometric, <i>Ia-3d</i> . Structure not yet refined.
2331	Original or oldest description: Galuskina et al. (2010b).
2332	Uvarovite
2333	End-member formula: $\{Ca_3\}[Cr^{3+}_2](Si_3)O_{12}$
2334	Group: Garnet
2335	IMA number: Grandfathered.
2336	Modifications: None.
2337	Etymology: For Count Sergei Semenovich Uvarov (1786-1855), a Russian historian.
2338	Type locality: Saranovskiy mine Biserskoye chromite deposit, Perm district, Urals, Russia (Pekov
2339	1998).
2340	Crystal system, space group and structure refinement: Isometric, <i>Ia-3d</i> . Novak and Gibbs (1971).
2341	For birefringent uvarovite: Wildner and Andrut (2001).
2342	Original or oldest description: Hess (1832).
2343	Yafsoanite
2344	End-member formula: $\{Ca_3\}[Te^{6+}_2](Zn_3)O_{12}$
2345	Group: ungrouped
2346	IMA number: 1981-022.
2347	Modifications: Introduced with the idealized formula $(Zn_{1.38}Ca_{1.36}Pb_{0.26})_{\Sigma=3.00}TeO_6$; current formula
2348	from Jarosch and Zemann (1989) and Mills et al. (2010).
2349	Etymology: From the acronym <u>Ya</u> kytskii <u>F</u> ilial <u>S</u> ibirskogo <u>O</u> tdeleniya <u>A</u> kademii <u>N</u> auk (Yakyt Filial
2350	of the Siberian Branch of the Academy of Sciences).
2351	Type locality: Kuranakh gold deposit, near Aldan, Yakutia, Russia (Pekov 1998).
2352	Crystal system, space group and structure refinement: Isometric, Ia-3d. Mills et al. (2010)
2353	Original or oldest description: Kim et al. (1982).
2354	

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

2357 OUTLINE OF RECOMMENDED PROCEDURE

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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 valency-imposed 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)

Appendix Table 1. Electron microprobe analysis with calculated Fe²⁺/Fe³⁺ ratio

	J			
2388		wt.%		ı per 12 O
2389	UO ₃	11.15	U^{6+}	0.282
2390	Nb_2O_5	0.87	Nb^{5+}	0.047
2391	Sb_2O_5	14.79	Sb^{5+}	0.661
2392	SiO_2	0.15	Si	0.018
2393	TiO_2	1.32	Ti	0.120
2394	ZrO_2	3.48	Zr	0.204
2395	SnO_2	16.20	Sn	0.777
2396	Al_2O_3	4.26	Al	0.604
2397	Sc_2O_3	0.13	Sc	0.014
2398	Fe_2O_3	20.96	Fe^{3+}	1.897
2399	MgO	0.03	Mg	0.005
2400	CaO	22.79	Ca	2.936
2401	FeO	4.35	Fe^{2+}	0.437
2402	Sum	100.48		8.000

Appendix Table 2. Site Allocation

 \boldsymbol{Z}

2406	Fe ²⁺	0.437	0.379
2407	Al^{3+}	0.604	0.604
2408	Fe ³⁺	1.897	1.897
2409	Si ⁴⁺	0.018	0.018
2410	Ti ⁴⁺	0.044	0.103
2411	Sum	3.000	3.000
2412	charge	8.625	8.793
2413			
2414		Y	
2415	Sc ³⁺ Ti ⁴⁺	0.014	0.014
2416		0.075	0.016
2417	Sn ⁴⁺	0.777	0.777
2418	Zr^{4+}	0.204	0.204
2419	Nb_{-}^{5+}	0.047	0.047
2420	Sb ⁵⁺	0.661	0.661
2421	U^{6+}	0.282	0.282
2422	Sum	2.060	2.000
2423			
2424		X	
2425	Ca	2.936	2.936
2426	Mg	0.005	0.005
2427	Fe ²⁺	0.000	0.059
2428	Sum	2.941	3.000

- 1. Si, Al, Fe³⁺, Fe²⁺ and sufficient Ti to fill Z2430
- 2. Sc, remaining Ti, Sn, Nb, Sb and U to Y. 2431
- 3. Ca and Mg to *X* 2432

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- Column 1 gives allocation from Appendix 4. Because of the assignment of Fe^{2+} to the Z site in 2433
- 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 Fe²⁺ to achieve stoichiometry. 2434
- 2435

Appendix Table 3. Dominant valences, constituents and percent of 2437 homovalent cations (from column 1 of Table 1) 2438

					,
2439	Site	Valence	Constituent	%	Identification
2440	\overline{Z}	+3	Fe	76	Bitikleite group
2441	Y	+5	Sb	93	Dzhuluite
2442	Y	+4	Sn	74	Dzhuluite
2443	\boldsymbol{X}	+2	Ca	99.8	Dzhuluite

Note: Y is constrained to have two occupants because of valency-

imposed double site-occupancy. 2445

Empirical formula from Table 2, column 1 (dominant cation for dominant valence in bold): 2447

 $\{Ca_{2.936}Mg_{0.005}\}[(Sn_{0.777}Zr_{0.204}Ti_{0.075})(Sb_{0.661}Nb_{0.047})U_{0.282}Sc_{0.014}]((Fe^{3+}_{1.897}Al_{0.604})Fe^{2+}_{0.437}(Ti_{0.044}Si_{0.047})U_{0.282}Sc_{0.014}]((Fe^{3+}_{1.897}Al_{0.604})Fe^{2+}_{0.437}(Ti_{0.044}Si_{0.014}Si_{0.014})Fe^{2+}_{0.$ 2448 $_{018}))O_{12}$ 2449

Empirical formula from Table 2, column 2 (dominant cation for dominant valence in bold): 2451

 $\{Ca_{2.936}Fe^{2^{+}}_{0.059}Mg_{0.005}\}[(Sn_{0.777}Zr_{0.204}Ti_{0.016})(Sb_{0.661}Nb_{0.047})U_{0.282}Sc_{0.014}]((Fe^{3^{+}}_{1.897}Al_{0.604})Fe^{2^{+}}_{0.379}(Fe^{2^{+}}_{0.016})$ 2452

 $Ti_{0.103}Si_{0.018})O_{12}$ 2453

Appendix Table 4. Proportions of generalized components 2456

Component	Maximum Proportion*	Proportion as independent variable [#]	Group or formula type
$\{R^{2+}_{3}\}[R^{6+}_{2}](R^{2+}_{3})O_{12}$	14.08%	12.62%	yafsoanite-type
${R^{2+}_{3}}[R^{4+}_{1.5}R^{6+}_{0.5}](R^{3+}_{3})O_{12}$	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. *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, $\{R^{2+}_3\}[R^{5+}R^{4+}](R^{3+}_3)O_{12}$.

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

Appendix Table 5. Electron microprobe analysis with calculated Fe²⁺/Fe³⁺ ratio

2478	analysis	with calcul	lated Fe ²	2+/Fe ³⁺ ratio
2479		Wt%		apfu per 12 O
2480	SiO ₂	26.16	Si	2.250
2481	TiO_2	16.52	Ti	1.069
2482	ZrO_2	1.31	Zr	0.055
2483	Al_2O_3	1.60	Al	0.162
2484	Fe_2O_3	17.07	Fe^{3+}	1.105
2485	FeO	3.44	Fe^{2+}	0.247
2486	MnO	0.48	Mn	0.035
2487	MgO	1.21	Mg	0.155
2488	CaO	31.54	Ca	2.907
2489	Na_2O	0.09	Na	0.015
2490	Sum	99.42	Sum	8.000

Appendix Table 6. Site Allocation

2493		Z
2494	Si	2.250
2495	Al	0.162
2496	Fe ³⁺	0.588
2497	Sum	3.000
2498	Charge	11.250
2499		Y
2500	Ti	1.069
2501	Zr	0.055
2502	Fe ³⁺	0.517
2503	Mg	0.155
2504	Fe^{2+}	0.204
2505	Sum	2.000
2506		X
2507	Fe^{2+}	0.043

2508	Ca	2.907
2509	Mn	0.035
2510	Na	0.015
2511	Sum	3.000

2513 1. Si to Z

2514 2. Al to Z

2515 3. Fe³⁺ to Z to bring total to 3 apfu, then Y

2516 4. Ca and Na to *X*

2517 5. Ti^{4+} , remaining Fe^{3+} , and Zr to Y.

2518 6. Mg: First to *Y*

2519 7. Fe^{$\frac{1}{2}$ +} First to Y to bring total to 2 apfu, then to X

2520 8. Mn^{2+} to X, which brings total X to 3 apfu

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Appendix Table 7. Dominant valences, constituents and percent of

2523 homovalent cations

2524	Site	Valence	Constituent	%	Identification
2525	\overline{Z}	+4	Si	100	Garnet group*
2526	Y	+4	Ti	95	Schorlomite
2527	X	+2	Ca	97	Schorlomite

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

2528 2529 2530

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

(Ca_{2.907}Fe²⁺_{0.043}Mn_{0.035})Na_{0.015} [(Ti_{1.069}Zr_{0.055})Fe³⁺_{0.517}(Fe²⁺_{0.204}Mg_{0.155})](Si_{2.250}(Fe³⁺_{0.588}Al_{0.162}))O₁₂]

25322533

Appendix Table 8. Maximum proportions of generalized components

		F -F	F
2534	Component	Proportion	Group and type
2535	$\{R^{2+}_{3}\}[R^{4+}_{2}](R^{4+}R^{3+}_{2})O_{12}$	37.5%	Schorlomite
2536	$\{R^{2+}_{3}\}[R^{3+}_{2}](R^{4+}_{3})O_{12}$	25.9%	Garnet: andradite-type
2537	$\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)O_{12}$	35.9%	Garnet: morimotoite-type
2538	$\{R^{+}_{2}R^{2+}\}[R^{4+}_{2}](R^{4+}_{3})O_{12}$	0.8%	Garnet: $\{Na_2Ca\}[Ti_2](Si_3)O_{12}$ -type
2539	Total	100.00%	

2540 2541 Note: The four generalized components are independent variables.

254325442545

2542

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.

2546 2547

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

254925502551

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Appendix Table 9. Electron microprobe

2552 analysis with calculated Fe^{2+}/Fe^{3+} ratio

2553		Wt%		apfu per 12 O
2554	SiO ₂	30.64	Si	2.820
2555	TiO_2	1.10	Ti	0.076
2556	Al_2O_3	4.87	Al	0.528
2557	Sc_2O_3	0.17	Sc	0.014
2558	V_2O_3	0.17	V	0.013

```
Cr_2O_3
                         0.04
                                    Cr
                                                   0.003
2559
                                    Fe<sup>3+</sup>
                         8.36
                                                   0.579
2560
         Fe_2O_3
                        16.93
                                      Y
                                                   0.829
2561
         Y_2O_3
                         0.00
                                                   0.000
2562
         La_2O_3
                                    La
2563
         Ce_2O_3
                         0.01
                                    Ce
                                                   0.000
2564
         Pr_2O_3
                         0.00
                                     Pr
                                                   0.000
                                    Nd
2565
         Nd_2O_3
                         0.12
                                                   0.004
2566
         Sm_2O_3
                         0.15
                                    Sm
                                                   0.005
         Eu<sub>2</sub>O<sub>3</sub>
                         0.01
                                    Eu
                                                   0.000
2567
2568
         Gd_2O_3
                         0.36
                                    Gd
                                                   0.011
                                    Tb
                         0.11
                                                   0.003
2569
         Tb_2O_3
                         1.52
2570
         Dy<sub>2</sub>O<sub>3</sub>
                                    Dy
                                                   0.045
         Ho<sub>2</sub>O<sub>3</sub>
                         0.63
                                    Но
                                                   0.018
2571
                         2.40
2572
         Er_2O_3
                                     Er
                                                   0.069
2573
         Tm_2O_3
                         0.38
                                    Tm
                                                   0.011
2574
         Yb_2O_3
                         2.03
                                    Yb
                                                   0.057
         Lu<sub>2</sub>O<sub>3</sub>
                         0.68
                                                   0.019
2575
                                    Lu
2576
         MgO
                         3.98
                                    Mg
                                                   0.546
2577
         CaO
                        13.92
                                    Ca
                                                    1.372
         MnO
                         0.85
                                                   0.066
2578
                                    Mn
                                    Fe^{2+}
2579
         FeO
                        11.84
                                                   0.911
2580
         Sum
                       101.26
                                  Sum
                                                   8.000
```

```
2582 Appendix Table 10. Site Allocation
```

```
Z
2583
2584
        Si
                       2.820
        Al
                       0.180
2585
2586
        Sum
                       3.000
2587
        Charge
                      11.820
                   Y
2588
2589
        Τi
                       0.076
        Al
2590
                       0.348
2591
        Sc
                       0.014
        V
2592
                       0.013
2593
        Cr
                       0.003
        Fe^{3+}
2594
                       0.580
        Mg
Fe<sup>2+</sup>
                       0.546
2595
                       0.422
2596
2597
        Sum
                       2.000
                  X
2598
        Y + REE
2599
                       1.072
2600
        Ca
                       1.372
2601
        Mn
                       0.066
        Fe<sup>2+</sup>
                       0.489
2602
2603
        Sum
                       3.000
```

- 2605 1. Si: First to *Z*
- 2606 2. Al to Z to bring total to 3 apfu, then Y
- 2607 3. Fe^{3+} to Y

2604

- 2608 4. Ca, Y, REE to X
- 2609 5. Al (after deducting Al at Z), Sc^{3+} , Ti^{4+} , V^{3+} , Cr^{3+} , Fe^{3+} to Y.
- 2610 6. Mg: First to *Y*

- 2611 7. Fe²⁺ First to Y to bring total to 2 apfu, then to X
- 2612 8. Mn^{2+} to X, which brings total X to 3 apfu

Appendix Table 11. Dominant valences, constituents and percent

of homovalent cations

2613

2614

2623

2625 2626

2627

2638

26392640

2641

26422643

2644

2645

2660 2661

2616	Site	Valence	Constituent	%	Identification
2617	\overline{Z}	+4	Si	100	Garnet group
2618	Y	+2	Mg	56	Menzerite-(Y)
2619	\boldsymbol{X}	+3	Y	77	Menzerite-(Y)
2620	\boldsymbol{X}	+2	Ca	71	Menzerite-(Y)

Note: *X* is constrained to have two occupants because of valency-

imposed double site-occupancy.

2624 Empirical formula (dominant cation for dominant valence in bold):

 $\{ (Ca_{1.372}Fe^{2^{+}}_{0.489}Mn_{0.066})(Y_{0.829}REE_{0.243}) \} [(Mg_{0.546}Fe^{2^{+}}_{0.422})(Fe^{3^{+}}_{0.579}Al_{0.348}Sc_{0.014}V_{0.013}Cr_{0.003})Ti_{0.076}] \\ [(Si_{2.820}Al_{0.180})O_{12}]$

Appendix Table 12. Proportions of generalized components

Component	Maximum Proportion*	Proportion as independent variable [#]	Group and type
${R_{2}^{3+}}{R_{2}^{3+}}[R_{2}^{3+}](R_{3}^{3+})O_{12}$	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. *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 Fe²⁺/Fe³⁺ ratio

2646		Wt%	apfu p	er 12 O
2647	SiO ₂	32.55	Si	2.681
2648	TiO_2	0.06	Ti	0.004
2649	Al_2O_3	20.13	Al	1.954
2650	Fe_2O_3	0.33	Fe ³⁺	0.020
2651	FeO	4.50	Fe^{2+}	0.310
2652	MnO	37.98	Mn^{2+}	2.650
2653	CaO	0.60	Ca	0.053
2654			Sum	7.672
2655	H_2O+	0.64	OH	0.352
2656	F	3.68	F	0.959
2657	O=F	-1.55	O	10.690
2658	Total	98.92	Sum	12.000

2659 Note: H₂O content by IR spectroscopy.

Appendix Table 14. Site Allocation

2662		Z
2663	Si	2.672
2664	vacancies	0.328
2665	Sum	3.000
2666	Charge	10.690
2667		Y
2668	Al	1.954
2669	Fe ³⁺	0.020
2670	Fe^{2+}	0.013
2671	Si	0.009
2672	Ti	0.004
2673	Sum	2.000
2674	_	X
2675	Mn^{2+}	2.650
2676	Fe^{2+}	0.297
2677	Ca	0.053
2678	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 *Y*

- 5. Fe²⁺ to *Y* to bring total to 2 apfu 6. Mn, Ca and remaining Fe²⁺ to *X*

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

Site	Valence	Constituent	%	Identification
\overline{Z}	+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):

 ${\bf Mn}_{2.650}{\bf Fe}_{0.297}{\bf Ca}_{0.053}{\bf Fe}_{0.020}{\bf Fe}_{0.020}^{3+}{\bf Fe}_{0.013}^{3+}({\bf Si}_{0.009}{\bf Ti}_{0.004}){\bf Si}_{2.672}\square_{0.328}{\bf O}_{10.690}{\bf F}_{0.959}{\bf OH}_{0.352}$

Appendix Table 16 Proportions of generalized components

Generalized Component	Maximum proportion*	Proportion as independent variable#	Group or formula type
$\{R_{-3}^{2+}\}[R_{-2}^{3+}](\square)_3(OH)_{12}$	2.93%	2.93%	katoite-type
$\{R^{2+}_{3}\}[R^{3+}_{2}](\square)_{3}F_{12}$	7.99%	7.99%	$\{Mn_3\}[Al_2](\square)_3F_{12}$ -type
$\{R_{2+3}^{2+3}\}[R_{4+2}^{3+2}](R_{4+2}^{4+2}\square)(OH)_4$	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.

> Example 5. Garnet JF22. "Majoritic" garnet included in diamond, Jagersfontein KIMBERLITE, SOUTH AFRICA (TAPPERT ET AL. 2005)

Appendix Table 17. Electron micro	probe
analysis with calculated Fe ²⁺ /Fe ³⁺ r	ratio

2715		Wt%	apfu p	er 12 O
2716	P_2O_5	0.09	P	0.006
2717	SiO_2	48.70	Si	3.525
2718	TiO_2	0.50	Ti	0.027
2719	Al_2O_3	9.65	Al	0.823
2720	Cr_2O_3	0.22	Cr	0.013
2721	Fe_2O_3	2.49	Fe^{3+}	0.135
2722	MgO	21.70	Mg	2.341
2723	CaO	5.73	Ca	0.444
2724	MnO	0.36	Mn	0.022
2725	FeO	9.46	Fe^{2+}	0.573
2726	Na_2O	0.65	Na	0.091
2727	Sum	99.55	Sum	8.000

2729 Appendix Table

2713 2714

2728

2749

2750

2751

2752 2753

2760

Mn

Fe

Mg Sum

		L		
2730	18.	Site	A1	location

2730	18. Site A	Illocation
2731		Z
2732	P	0.006
2733	Si	2.994
2734	Sum	3.000
2735	Charge	12.006
2736		
2737		Y
2738	Si	0.530
2739	Ti	0.027
2740	Al	0.823
2741	Cr	0.013
2742	Fe^{3+}	0.135
2743	Mg	0.472
2744	Sum	2.000
2745		
2746	-	X
2747	Na	0.091
2748	Ca	0.444

- Si and P to Z to a maximum of 3 apfu, overflow of Si to Y 2754 1.
- 2755 2.
- Ca and Na to XTi⁴⁺, Cr³⁺, Fe³⁺ to Y3. 2756
- Mg: First to Y to bring total to 2 apfu, then to X Fe²⁺ to X4. 2757
- 2758 5.
- Mn^{2+} to X, which brings total to 3 apfu 6. 2759
- 2761 Appendix Table 19. Dominant valences,

0.022

0.573

1.870

3.000

- constituents and percent of homovalent cations 2762
- 2763 Site Valence Constituent % Identification

2764	Z	+4	Si	100	Garnet group
2765	\boldsymbol{Y}	+3	Al	85	Pyrope
2766	\boldsymbol{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 $2R^{3+}$

2769 (Table 8).

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

 $\{(\mathbf{Mg_{1.870}} F e^{2^{+}}_{0.573} C a_{0.444} M n_{0.022}) N a_{0.091}\} [(\mathbf{Al_{0.823}} F e^{3^{+}}_{0.135} C r_{0.013}) (S i_{0.530} T i_{0.027}) M g_{0.472}] (\mathbf{Si_{2.994}} P_{0.006})$

Appendix Table 20. Proportions of generalized components

Component	Maximum Proportion*	Proportion as independent variable [#]	Group and type
${R^{1+}_{3}}[R^{3+}_{2}](R^{5+}_{3})O_{12}$	0.18%	0.18%	Berzeliite: $\{Na_3\}[Al_2](P_3)O_{12}$ -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: $\{Na_2Ca\}[Ti_2](Si_3)O_{12}$ -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 Fe²⁺/Fe³⁺ ratio

2794		Wt%		12 O
2795	SiO ₂	26.93	Si	2.319
2796	TiO_2	18.51	Ti	1.199
2797	ZrO_2	1.48	Zr	0.062
2798	Al_2O_3	0.97	Al	0.098
2799	Fe_2O_3	11.44	Fe^{3+}	0.741
2800	FeO	7.77	Fe^{2+}	0.559
2801	MnO	0.23	Mn	0.017
2802	MgO	0.87	Mg	0.112
2803	CaO	31.35	Ca	2.893
2804	Sum	99.54	Sum	8.000

Appendix Table 22. Site Allocation

2807		Z
2808	Si	2.319
2809	Al	0.098
2810	Fe ³⁺	0.583
2811	Sum	3.000
2812	Charge	11.319
2813		Y
2814	Ti	1 199

2815	Zr		0.062
2816	$\mathrm{Fe^{3+}}$		0.158
2817	Mg		0.112
2818	Fe ²⁺		0.469
2819	Sum		2.000
2820		\boldsymbol{X}	
2821	Fe^{2+}		0.091
2822	Ca		2.893
2823	Mn		0.017
2824	Sum		3.000
	-		

2834

2844

2847

2854 2855 2856

2860 2861

2862

- 2826 1. Si to Z
- 2827 2. Al to *Z*
- 2828 3. Fe³⁺ to Z to bring total to 3 apfu, then Y
- 2829 4. Ca to *X*
- 2830 5. Ti^{4+} , remaining Fe^{3+} , and Zr to Y.
- 2831 6. Mg: to *Y*
- 2832 7. Fe²⁺ First to Y to bring total to 2 apfu, then to X
- 2833 8. Mn^{2+} to X, which brings total X to 3 apfu

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

2837	Site	Valence	Constituent	%	Identification
2838	\overline{Z}	+4	Si	100	Garnet group
2839	Y	+4	Ti	95	Morimotoite
2840	Y	+2	Fe	81	Morimotoite
2841	X	+2	Ca	96	Morimotoite

Note: *Y* is constrained to have two occupants because of valency-

2843 imposed double site-occupancy.

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

2846 $\{Ca_{2.892}Fe^{2+}_{0.091}Mn_{0.017}\}[(Ti_{1.199}Zr_{0.062})(Fe^{2+}_{0.468}Mg_{0.112})Fe^{3+}_{0.159}](Si_{2.319}(Fe^{3+}_{0.583}Al_{0.098}))O_{12}$

2848 Appendix Table 24. Maximum proportions of generalized components

2849	Component	Proportion	Group
2850	${R^{2+}_{3}}[R^{4+}_{2}](R^{4+}R^{3+}_{2})O_{12}$	34.05%	Schorlomite
2851	${R^{2+}_{3}}[R^{3+}_{2}](R^{4+}_{3})O_{12}$	7.93%	Garnet: andradite-type
2852	$\{R^{2+}_3\}R^{4+}_3O_{12}$	58.01%	Garnet: morimotoite type
2853	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

2863 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: SiO₂, TiO₂, ZrO₂, SnO₂, UO₃, TeO₃, Sb₂O₅, As₂O₅, V₂O₅, Nb₂O₅, P₂O₅, Y₂O₃ (include REE₂O₃ as the equivalent proportion of Y₂O₃ along with the measured Y₂O₃ content), Al₂O₃, Sc₂O₃, Cr₂O₃, V₂O₃, FeO, Fe₂O₃ (but see below), ZnO, MnO, MgO, CaO, Na₂O, Li₂O, H₂O⁺ (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 V₂O₃ or V₂O₅.

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 Fe²⁺ and Fe³⁺ and Mn²⁺ and Mn³⁺ (this latter constituent only in the absence of Fe²⁺) on the basis of 12 anions, where the anions are the sum of O²⁻, (OH)⁻, and F⁻. If the user inputs some or all of the iron content as Fe₂O₃ (wt.%), then this calculation of Fe²⁺ and Fe³⁺, and Mn²⁺ and Mn³⁺, is not performed. In any case, the user should not input Mn₂O₃, 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, Th 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:

```
2900 Z > Y > X;

2901 Z = (As, V^{5+}, P, Li, Zn) > Si > Al > Fe^{3+} > Fe^{2+}, Ti;

2902 Y = (Zr, Sn, U, Te, Sb, Nb, Sc, Cr, V^{3+}) > (Si, Ti, Al, Mn^{3+}, Fe^{3+}) > Mg > Fe^{2+} > Mn;

2903 X = (Y, Ca, Na, Mn, Fe^{2+}) > 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 maximum content 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%.

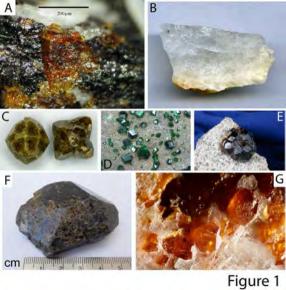
Having found the most abundant charge-balanced formula, the group to which it belongs is assigned (manuscript Table 1). From the assignment of the group, and from the site allocations of the cations, the principal cations that occupy the charge-balanced formula of that group are

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.



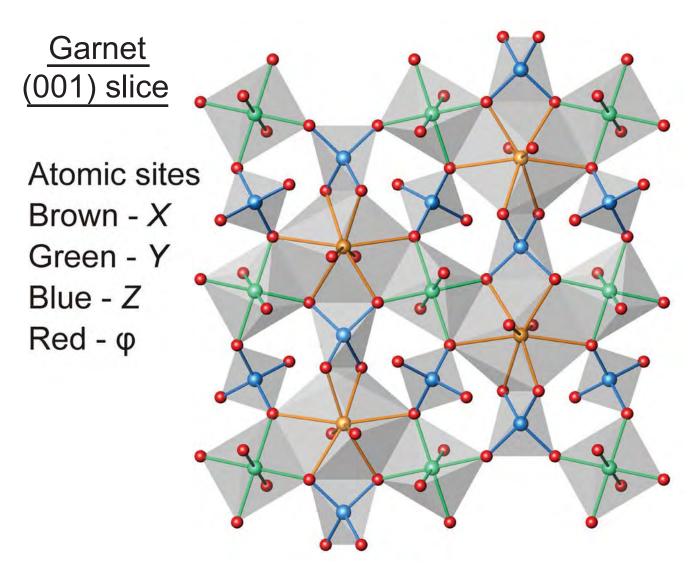
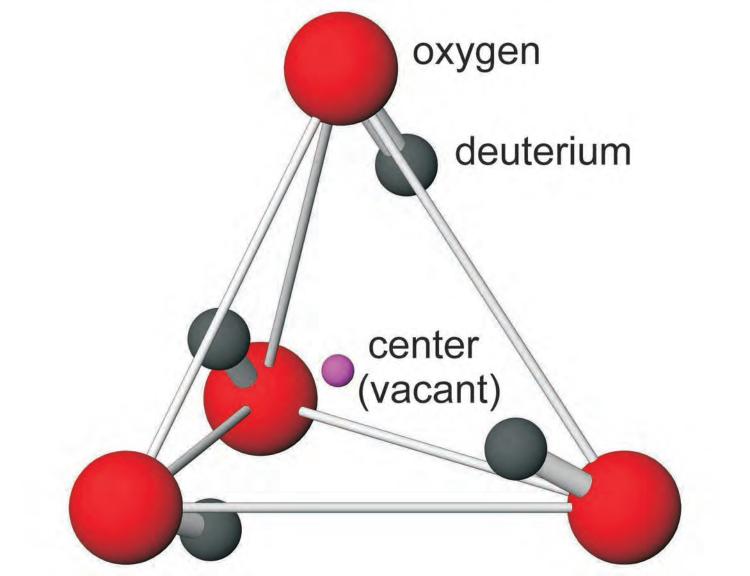
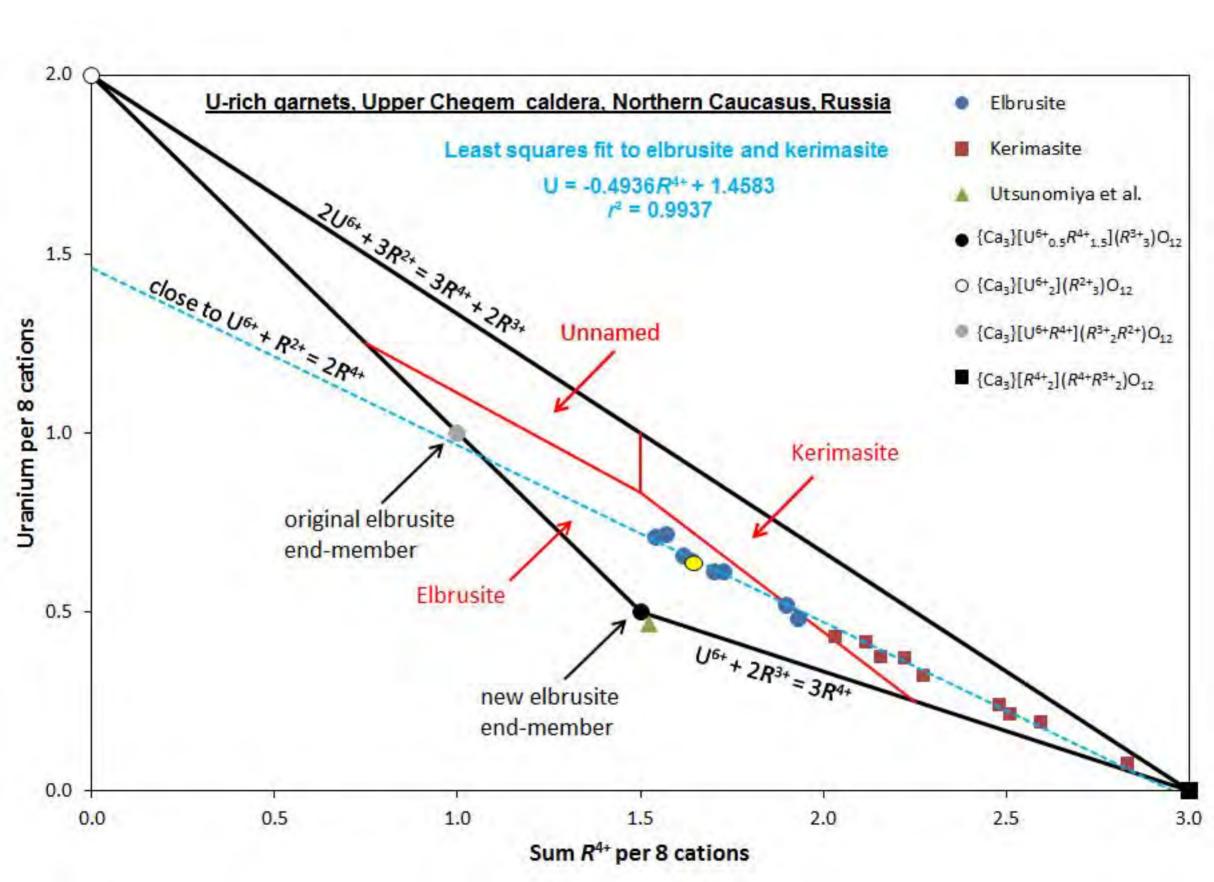
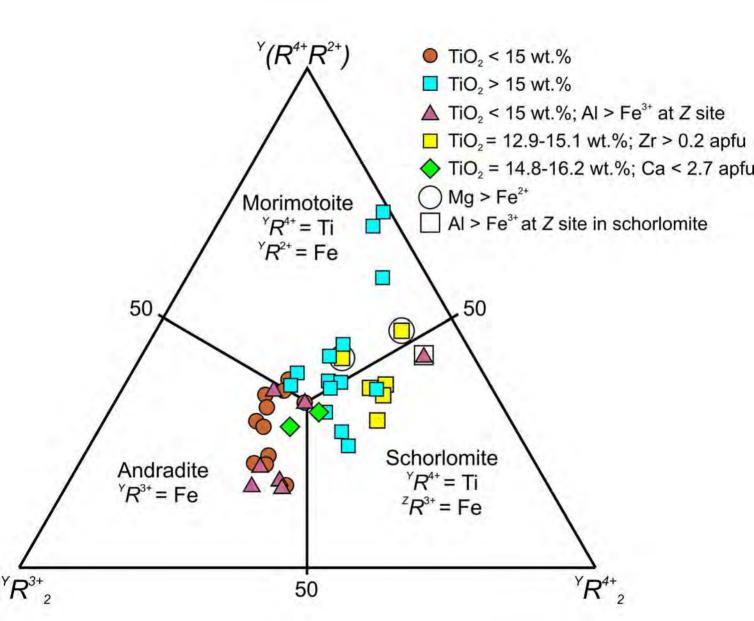


Figure 2







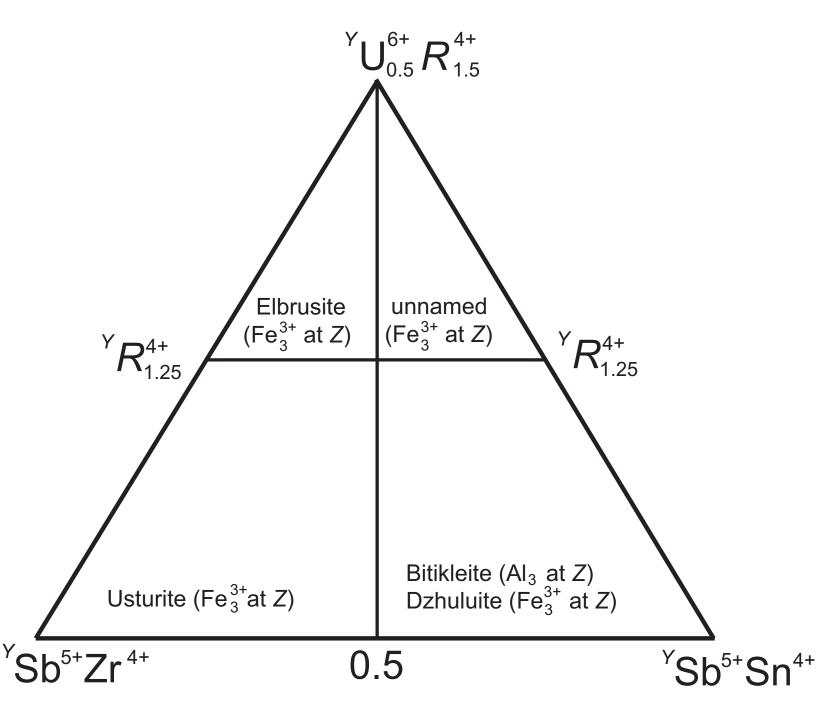


Figure 6

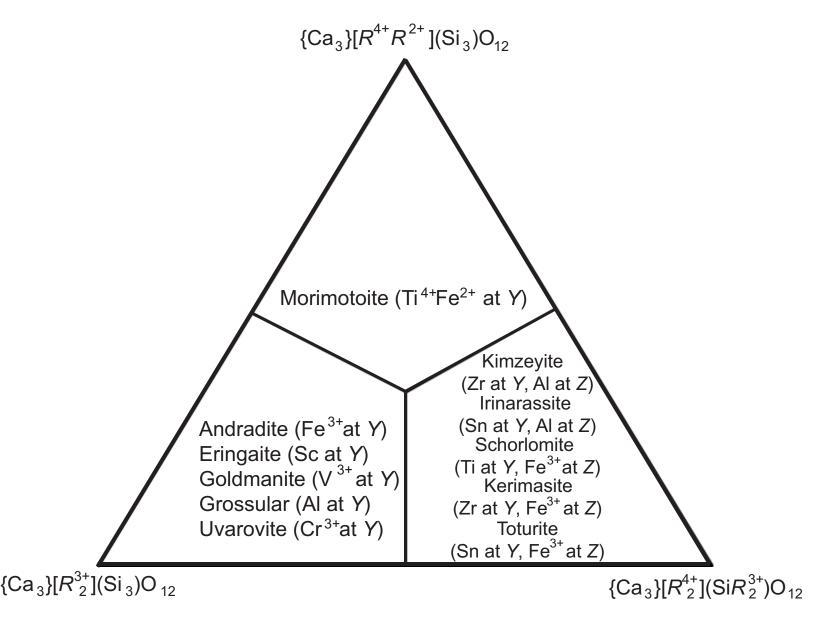


Figure 7

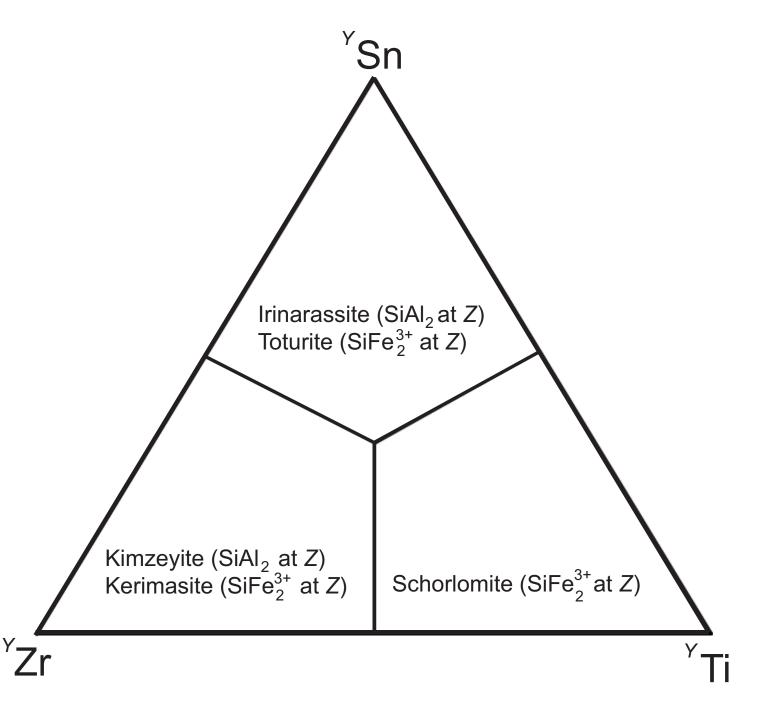


Figure 8

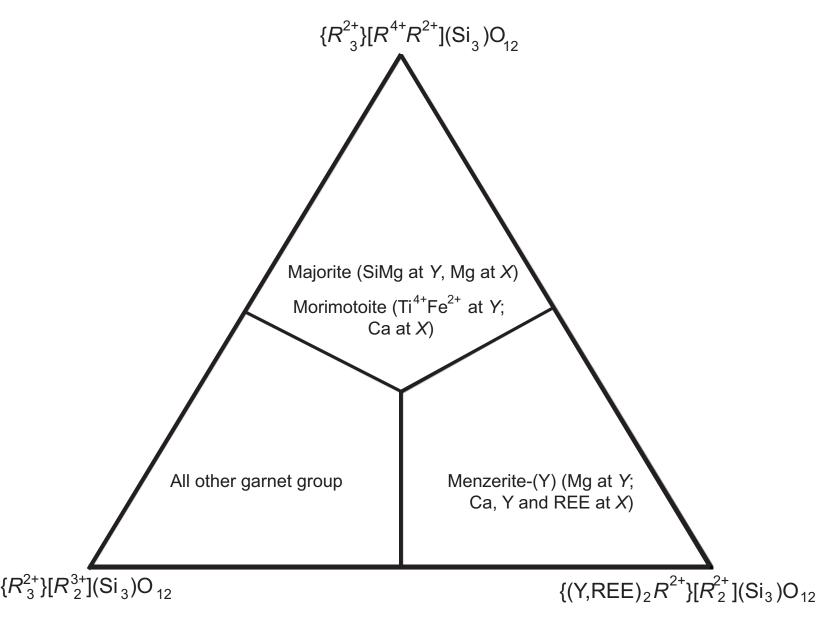


Figure 9

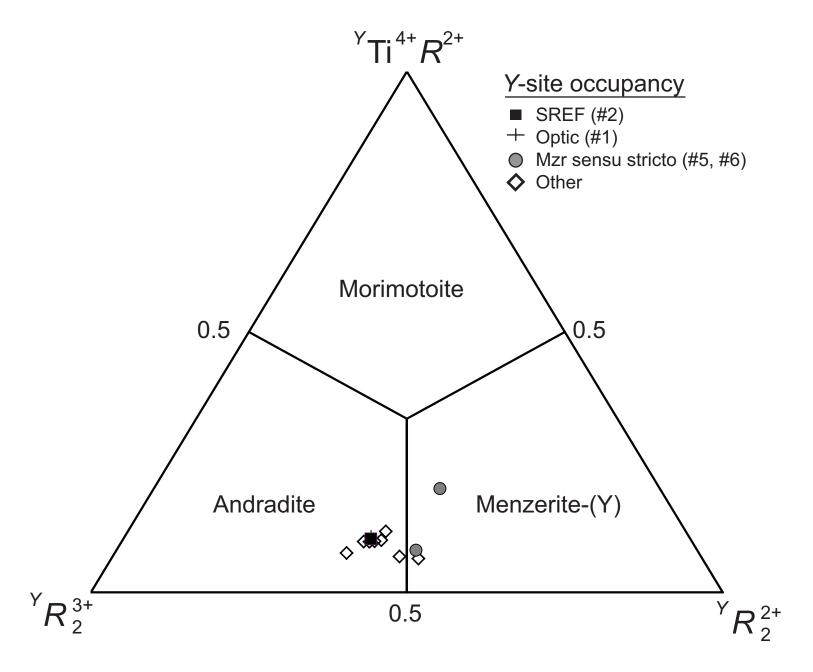


Figure 10

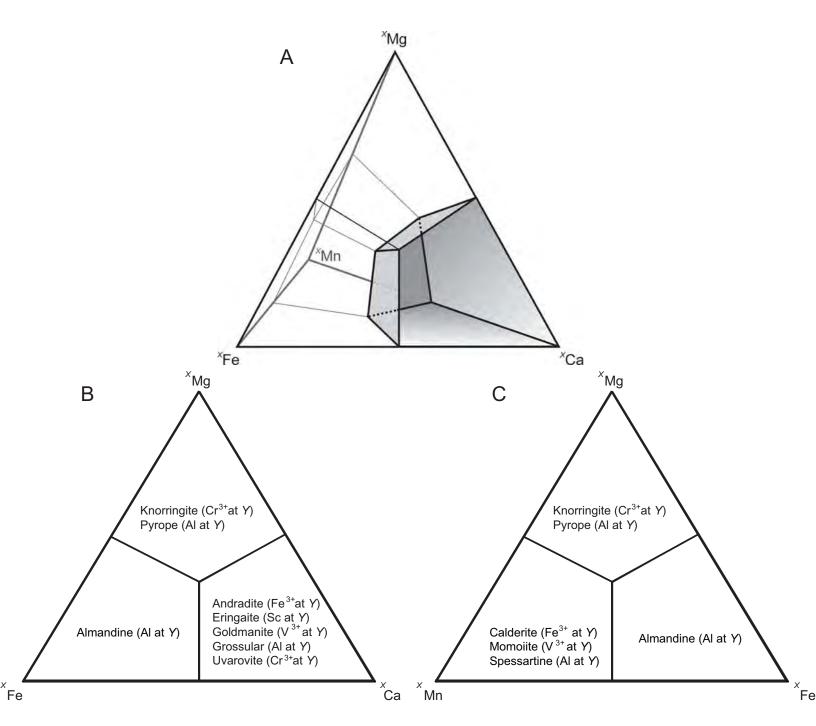


Figure 11