

Garnet Manuscript Reviewer Comments

All responses to the reviewers from the authors are indicated in **bold text**.

Reviewer 1:

Citation: <https://doi.org/10.5194/essd-2023-45-RC1>

General Comments

The manuscript reports on a database of chemical analyses, ages, localities, paragenesis, P-T conditions etc. of garnets and some preliminary interpretations.

1) The dataset could be indeed be very interesting if obviously wrong entries would be eliminated, and a more convincing quality control would be used, e.g. by calculation of garnet species or end-members from the analyses.

Only a very small part of the data presented in the database is new and original. The quality of the new data is very good. However, the authors have also included analyses of inclusion minerals as “garnet” analyses in the database. I cannot see any use of including such obvious wrong analyses in the data set.

A similar problem is that the authors include data from older peer reviewed publications (the “dark data”) that are clearly in the original publication not identified as garnet, but as whole rock analyses of garnet-bearing rocks, such as quartzites. These include:

Project ID 43-52 are not spessartine mineral analyses but so-called “coticles”, i.e. garnet-bearing quartzites and one of the authors, KC, has even included bulk analyses of slates and volcanic rocks as “garnet” analyses (see Herbosch et al. 2016, Table 3). Project ID 146-171 are quartzite whole rock analyses, not garnets (Reinecke et al. 1986 not Reincke as stated in the database).

Thus, whole rock analyses were included in the data set as mineral analyses. These were avoidable errors of the authors. These inconsistent data must be eliminated.

We agree with the reviewer that these are erroneous samples and should not be included. We did a thorough check of the dataset and included all changes below:

Notes:

- Deleted samples from Herbosch et al 2016 (Project ID 43-52).
- Deleted sampled from Reinecke et al 1986 (Project Id 146 - 171).
- Added more specific paragenesis to Schönig et al. (2018) (Project ID 1081 - 1373).
- Added 4 Grossular samples from Naimo et al (2003).
- Andradite samples in Katerinopoulou (2009) were excluded in silica confidence interval.
- Andradite samples had a difficult time with the silica confidence interval (range of SiO₂: 29 - 32 wt%).
- Added temperature data to Plümper et al. (2014).

- Russell et al. (1999) has more data but cannot find repository: A database of titanian andradite compositions is available from JKR or GMD or via ftp [<http://perseus.geology.ubc.ca/>].
- Updated the Russell et al. (1999) Geological Context column (Project ID 1587-1590).
- Added 3 rim analyses from Marks et al. (2008) (Project ID's: 1620, 1623, 1625).
- Updated the following columns for both Marks et al. 2008 papers (Project ID 1606-1625): Notes, Mineral, Zone, Area, Geological Context, Analysis Method.
- Updated the Title and Journal columns for Marks et al. (2008) (Project ID 1606-1617).
- Silica confidence interval excluded kimzeyites from Beard and Drake (2007) (range of SiO₂: 23 - 35 wt%).
- Sieck et al. (2019) paragenesis of "rhyolitic flows, ignimbrite" -> "Rhyolite" and added P&T data.
- Pribavkin, Avdonina, and Zamyatin (2012) added samples (origin ID) 16, 17, & 18.
- Added 20 samples to Patranabis-Deb, Schieber, and Basu (2009).
- Deleted repeat of Beard & Drake (2007) (Project ID 1987 - 1995; 58-66 MG).
- Deleted repeat of Jamtveit et al. (1997) and Naimo et al. (2003).
- Von Knorring (1986) changed paragenesis from "Unknown" to "Skarn".
- Mueller and Delor (1991) changed paragenesis from "Skarn veins" to "Skarn".
- Ghosh and Morishita (2011) hydrothermal alteration of the peridotite led to garnet formation -> updated paragenesis.
- Added Age, Temp, Pressure to Kotkova and Harley (2010)
- Updated paragenesis in Inglis et al. (2017) and Zeh & Gerdes (2014)..
- Added age, temp, pressure and paragenesis to Wang et al. (1999).
- Added temp and pressure to Enami et al. (1993).
- Added garnet species names to literature from Locock (2008) but there is still no age, temp, pressure, or paragenesis.
- Marked Project ID 3314-3330 and 3461-3463 as repeats (they are part of Locock (2008)'s dataset).
- Updated varietal name for Project ID: 2085-2095.
- The Kimzeyites and Elbrusites in Galuskina et al (2010) are excluded from SiO₂ intervals (anomalously low SiO₂ ~3 wt. % for high UO₃ ~20 wt. %).
- Added age, temp, pressure to Kawakami et al. (2019).
- Added 17 foliated eclogite samples to Li et al. (2018).
- Added Age, Paragenesis, and Garnet name to Salnikova et al. (2019), SiO₂ excludes some of these andradites.
- Added temperature to Salnikova et al. (2019).
- Added 95 samples from Philpotts et al. (1972), Huang et al. (2020), Zhang et al. (2022).
- Deleted original EMPA inclusions: chromite, dark almandine, light almandine, dark uvarovite.
- Fixed total and our total wt. % columns.
- Removed the Silica Confidence Interval.
- Evaluated all the garnet sample analyses and reclassified them using the spreadsheets from Locock (2008) and Grew et al. (2013) to calculate the end-member species and provide a Quality Index from the geochemical data.

2) The authors use a “Silica Confidence Interval” (SCI) method to exclude samples of questionable composition from further analysis. This method seems to identify the above mentioned whole rock analyses of quartzites as unlikely of garnets and analyses of minerals that are not garnets but pyroxenes or spinel group minerals from the EarthChem database. However, it also seems to eliminate analyses, e.g. of henritermierites (Project ID 60-61), titanian andradites, schorlomites, kimzeyites, katoite-rich (hydro)grossulars of high quality! Thus, the SCI method is not very useful if the mineral species is not considered. Partial analysis of inclusions and garnet, a concern of the authors, will often not be identified correctly by this method.

A much better method to evaluate the quality of garnet analyses would be to calculate the end-member species from the chemical analysis using the approach of Locock (2008) and Grew et al. (2013) and calculate a “Quality Index” as suggested by Locock (2008). See Hawthorne (2021, *Can. Mineral.* 59, 169ff).

We agree with this comment from the reviewer and evaluated all of the garnets using a combination of the spreadsheets from Locock (2008) and Grew et al. (2013). In the list above, we flagged some examples of samples that were erroneously excluded using the silica confidence interval. We decided to instead, remove erroneous samples (such as Herbosch et al. (2016) and Reinecke et al. (1986)) with the full list of dataset changes listed above. We eliminated the silica confidence interval since we should not exclude the samples of low SiO₂ wt% from the dataset such as kimzeyites and elbrusites (Galuskina et al., 2010).

3) The discussion and interpretation of the data set is focused mainly on frequency plots of major (and some minor) elements and on the binary correlations of elements for various “material types” (igneous, metamorphic, detrital and unknown), in my view, the least reliable categorization of garnets (see below).

The dataset is heavily biased by garnets from the mantle (mostly brought to the surface by volcanic rocks) and by a study of garnets in a single amphibolite from the crust. The authors do not eliminate these overrepresented data in their data evaluation or weight them accordingly. Thus, any meaningful evaluation of the data must consider or correct for the bias.

The interpretation of the data, the main part of the manuscript, is therefore not very insightful. The interpretation of observed correlations between two elements as binary series of two garnet species on the other hand, is trivial if only binary correlations are studied. Why not use multivariate statistical methods or explore ternary compositions? The lengthy discussion of the binary element correlations and the frequency plots of strongly biased data stands in contrast to the few new insights gained from the analysis of the database. Some of the conclusions are probably wrong (see below).

We thank the reviewer for the thoughtful suggestion. To clarify, the purpose of this paper is solely to be a data description paper, rather than a multivariate analysis of the data present. The correlation coefficient plots were intended to solely show any users of the dataset what data and geochemical samples are currently present in this version of the dataset. Given that the purpose of these plots caused confusion for the reviewer, we have removed them and any discussion relating to them from the paper. We do not intend to analyze or draw any conclusions from the data. We intend only to provide this dataset to future researchers who may wish to use it for their own work or to upload their own garnet geochemical analyses to a larger mineralogical repository.

Further, we did initially create ternary diagrams of the data to show the distributions of garnet geochemistry present. However, our coauthor Frank Spear found significant biases by using ternary diagrams based on the idealized end-member species and

proposed a more thorough way to visualize the distributions is by creating correlation coefficient plots of the measured major oxides. Therefore, any researcher who needed to identify a range of geochemical properties would have a better way to interpret whether this dataset is useful to them. We have removed this discussion based on the reviewer's feedback.

4) The discrimination between an igneous and a metamorphic origin for mantle garnets is a question of semantics and ambiguous. I would rather suggest that the authors discuss garnets from distinct "paragenesis" instead of their "material types". See for example the approach of Krippner et al. (2014 Sed. Geol. 306, 36ff) - a relevant publication not cited by the authors. Igneous versus metamorphic origin of Earth's mantle materials: The authors (and the sources they use) classify all ultramafic/peridotitic materials as "igneous" and all eclogites as "metamorphic". This is an arbitrary decision. If a fertile mantle lherzolite is partially molten, a basaltic liquid extracted and then crystallizes within the upper mantle, it will have an eclogite-like mineral paragenesis consisting of pyrope- and grossular-rich almandine garnet and an omphacitic clinopyroxene. The authors will classify the rock and garnet as "metamorphic", although it is obviously an igneous rock and mineral. An ultramafic rock of bridgmanite-ferropericase composition from the lower mantle that is brought by diapirism into the upper mantle will be transformed in solid state thus by a metamorphic process into a rock of garnet-bearing peridotite paragenesis. Thus, the discrimination between (and discussion of) compositions of igneous and metamorphic rocks makes little sense in the realm of mantle rocks, the overwhelming lithology in the database. This problem can also be seen in the material type classification of majorite analyses from inclusions in diamonds (see below). Thus, similar to the authors' use of the class "detrital", I would suggest that the authors use the term "mantle" in the category "Material". But it is recommended that the authors discuss the garnet compositions of distinct paragenetic assemblages not the ambiguous "Materials".

We agree with the reviewer that this classification distinction is a little complicated, however, we adopted this column "Material" directly from the EarthChem repository. For the sake of data continuity, we would like to respect their decisions and data classification of their 61,294 samples and maintain this column and all designations. We agree with the reviewer that the classification of igneous vs metamorphic in the example they describe is highly subjective and complicates the interpretation of this data. We recommend that users of the dataset keep this limitation in mind, and we highlighted this limitation in the methods section of the text: "We recommend examining each of the petrogenetic attributes collectively as well as individually to best characterize the data with cluster analysis. It should also be noted that how each of the attributes are classified remains a subject of debate as they are highly subjective and vary over time and between authors. For example, the distinction between igneous and metamorphic rocks can be arbitrary when various mantle processes at various depths can be responsible for a specific rock's mineralogy and texture."

Similarly, they classified all of their samples as a general "garnet" for the mineral name, therefore we must maintain this classification and instead added an additional column, "Species," to reflect the mineral species classification based on the spreadsheets from Locock (2008) and Grew et al. (2013) and added a "Quality Index" column. Hopefully these addition addresses some of the reviewer's concerns.

Specific comments:

line 112: Goldmannite is defined as the $\text{Ca}_3\text{V}_3+2\text{Si}_3\text{O}_{12}$ endmember, not as $\text{Ca}_3[\text{V,Al,Fe,Ti}]_2\text{Si}_3\text{O}_{12}$. It might (and it always does) contain additionally tri- or tetravalent cations in the octahedral site such as Al, Fe^{3+} and Ti^{4+} or very rarely Ti^{3+} , but these elements are not essential (e.g. Grew et al. 2013) and should not be reported in the formula of a mineral species.

Accepted and incorporated: “There are also reported rare instances of goldmanite ($\text{Ca}_3\text{V}^{3+}_2\text{Si}_3\text{O}_{12}$), eringaite ($\text{Ca}_3\text{Sc}_2\text{Si}_3\text{O}_{12}$), and rubinite ($\text{Ca}_3\text{Ti}_2\text{Si}_3\text{O}_{12}$) occurring in chondrite meteorites (Hazen et al., 2008; Grew et al., 2013; Morrison and Hazen, 2020).”

line 119: First formation of almandine around 4.0 to 3.5 Ga: Some of the Hadean zircons (> 4.0 Ga) are probably derived from felsic continental crust (e.g. Zhong et al. 2023 Comm. Earth and Env. <https://doi.org/10.1038/s43247-023-00731-7> and references therein) that could also contain almandine. I can see no indication for this late suggested appearance of almandine (and spessartine).

Accepted and incorporated: “Almandine ($\text{Fe}_3\text{Al}_2\text{Si}_3\text{O}_{12}$) possibly first formed around 4.4 to 3.3 Ga as it is indicative of felsic igneous environments, occurs in medium- to low-grade metamorphic terrains and is typically found in pegmatites, granite, mica schist, or gneiss (Deer et al., 1982; Nesse, 2013; Zhong et al., 2023). A transition from stagnant lid to present day active lid plate tectonics occurred between 4.4-2.5 Ga (Cawood et al., 2022). The appearance of spessartine ($\text{Mn}_3\text{Al}_2\text{Si}_3\text{O}_{12}$), which occurs in uplifted regional metamorphic environments, most likely occurred around 3.6-2.5 Ga during which lateral tectonics initiated and the lithosphere went from variable to uniformly rigid (Hazen et al., 2008; Bauer et al., 2020; Hawkesworth et al., 2020; Cawood et al., 2022).”

line 124: Uvarovite does not occur or form in “igneous environments”. It is rather a typical metasomatic or better hydrothermal mineral (see e.g. Melcher et al. J. Petrol. 38, 1419ff and Farré-de-Pablo et al. 2021 Mineralium Deposita 57, 955ff and references therein).

Accepted and incorporated: “Uvarovite is rare and occurs in chromite-rich metasomatic or hydrothermal environments (Deer et al., 1982; Farré-de-Pablo et al., 2022; Melcher et al., 1997; Nesse, 2013).”

line 435: The authors use the category ‘almandine-pyrope’ for garnets near 50-50 compositions. An approach not supported by the IMA convention, but in my (and some other’s) view quite useful in practice. But what is the meaning of - and the reason to include - the category ‘pyrope-almandine’ then (see e.g. Fig.1)? I would suggest to merge these two categories and those of the other intermediate species with “flipped” composite names.

We decided to take the reviewers feedback and merge these categories in the dataset for simplicity. We would prefer to list the category that is slightly more prevalent first (i.e., ‘pyrope-almandine’), however, we recognize that this complicates the categories and combined them under one notation (‘almandine-pyrope’).

See new text: “There are 37 IMA-recognized structural garnet species and 14 silicate garnets, however, there are 32 categories of mineral names within the dataset which includes the combination of end-members such as ‘Almandine-Grossular’ and ‘Almandine-Pyrope’ for samples near 50-50 in composition as well as the simplified term ‘Garnet’ for unidentified samples. For samples that reported a near 50-50 composition, we standardized the naming convention to one category. For example, sample analyses that reported ‘Pyrope-Almandine’ are included in ‘Almandine-Pyrope’ for simplicity.”

Fig.1: The authors should eliminate the following “Mineral” categories, as they are meaningless:

“Andradite-Grandit” (single entry): “grandite” is not a garnet species but an acronym derived from grossular-andradite for garnets of the grossular-andradite join. Thus, andradite-grossular-andradite makes no sense.

“Piemontite-Spessartin” (15 entries): “piemontite is a Mn-rich species of the epidote family not a garnet. The reported analyses have 0.4 to 2.2 % K₂O and more than 70% SiO₂ and only very minor MnO and Mn₂O₃ concentrations (<3 wt%). This is a very clear misidentification by Chiama et al. The original publication (Reinecke et al. 1985 not Reincke et al. 1985) unambiguously says “piemontite-spessartine and spessartine quartzite”. Thus these analyses are bulk XRF analyses of various quartzites and not garnet mineral analyses! The garnet analyses are presented for this locality in Reinecke (1986) in the same journal, but they were not included in the database. Why and how the authors have selected this source?

- **These values were removed.**

line 679-683 and Fig 6a: The discussion of age distributions in terms of mineral evolution is in my view misleading. The overwhelming majority of garnet “ages” relate to mantle xenoliths transported by explosive volcanism to the surface and the reported ages are overwhelmingly the ages of the kimberlite eruptions. As the timing of kimberlite volcanism is in almost all cases unrelated to garnet growth in the mantle rocks, the discussion of age distribution is meaningless for age distribution of garnet growths. Thus, only age values of directly dated garnets should be evaluated here.

We agree that the garnet “ages” is misleading and few literature sources directly dated the garnet samples and instead provided only general ages of the formation or host rock in the literature. We removed this discussion and figures based on the reviewer’s comments that this is “meaningless.”

line 765: For metasomatic garnets, dominated by skarn assemblages, a significant correlation between Fe³⁺ and Al³⁺ is found that is later interpreted as representing the binary substitution between andradite and grossular. The other significant correlation between Fe³⁺ and Si is not discussed. Why? This correlation is simply a consequence of interpreting mass-percentages instead of molar units or endmembers. Andradite with a full occupancy of Si on the tetrahedral site has only 35 mass-% SiO₂, while grossular lacking any katoite (or hydrous) component has 40 mass-% SiO₂. Thus, the negative correlation of Fe³⁺ and Si is simply a consequence of the interpretation of mass percentages and is not related to any substitution of Si by Fe³⁺.

- **This discussion of the correlation coefficients plots was removed.**

line 927: the moderate to weak correlation for Mg-Si in the “metamorphic matrix” “may be caused by majorite analyses”. The correlation coefficient is only 0.126. The 156 majorite analyses in the database are classified as extraterrestrial (4 entries), igneous (28 entries), metamorphic (39 entries) and unknown (85 entries). All igneous and unknown majorites are inclusions in diamonds. 22 of the “metamorphic” majorites are also inclusions in diamonds and the remaining 17 analysis formed in an amphibolite with an impact setting. Here you can see the significant problem of categorizing of materials from the mantle. In the category “metamorphic” 24,601 garnet analyses are plotted and the 39 majorite analyses from a metamorphic setting should be responsible for the moderate to weak correlation between Mg and Si? I doubt that. The correlation is again related to effects of discussing mass-percentages instead of molar proportions. Thus, I strongly recommend to discuss molar proportions or endmembers.

- **This discussion of the correlation coefficients plots was removed.**

line 935-6. “Unknown” matrix: “The Mg - Si relationship represents majorite garnets”. Here the correlation coefficient Mg-Si is much higher (0.491). Again, only 85 majorite analysis should influence the correlation of 9476 garnets? It is more probable that garnets with high pyrope

content, the most common Mg-rich endmember garnet, also have higher Si values, as pyrope is the garnet with the highest Si content on a mass or weight basis.

- **This discussion of the correlation coefficients plots was removed.**

References: Where are the full references of all the publications cited in the database? I have checked some and found many typos, especially in the new additions from the authors.

- **A list of references for the dataset itself is added as a supplemental file and these references are also cited directly in the dataset. Corrections and typos were included in version 2 of the dataset and a documentation of the changes is included above.**

Reviewer 2:

All responses to the reviewer from the authors are indicated in bold text. We would like to kindly thank the reviewer for their thorough review of both the dataset as well as the manuscript. Their comments made both significantly stronger and we hope that our revisions are satisfactory.

Citation: <https://doi.org/10.5194/essd-2023-45-RC2>

This is to present a comprehensive dataset of geochemical characteristics of garnet. The authors have treated 95,588 (!) garnet samples from various sources and compiled their geochemical characters combined with other properties. It is useful without doubt for people who are interested in garnet if used carefully at their responsibility. There are, however, some questions and issues that should be more clearly stated in the dataset.

We appreciate this reviewer's recognition of the value of our compiled database.

1. The area of the data sources of garnet analyses. I would greatly appreciate the authors' effort to collect so many garnet analyses, but the area of their search is not so clear. Have they searched garnet analyses in the sources written in English? I have seen many garnet analyses in papers written in non-English languages. What was the authors' strategy for data collection?

We searched for English-written literature sources only and added a mention of this to the paper. Certainly, there are thousands of more garnet sample analyses that are published in non-English written literature and we certainly would appreciate if non-English speakers donate their data to this repository in the future!

2. The most serious point is that the attributes the authors used are various in character. Some of them, especially those related to petrogenesis or origin, are highly interpretative and totally depend on authors' interpretation of source literature. They can be, however, changed with time in future studies. In addition, the origins of garnet, igneous, metasomatic and metamorphic, are sometimes difficult to determine, especially in deep-seated rocks.
3. Similar issue. The grouping of "Petrogenesis attributes" (Table 3) are somewhat confusing. "Type" is composed of five attributes, but four of those (Xenolith, Amphibolite, Xenocryst and Volcanic) are not the same in kind to each other: xenoliths

and xenocrystals are fragments of rocks and minerals, respectively, in igneous (especially volcanic) rocks. So, xenocrysts (and possibly xenoliths) are in part “volcanic”. Amphibolite is a name of one of metamorphic facies, and is the name of the rocks of amphibolite facies. Of course, we can find “Xenolith” or “Amphibolite” in “Volcanic” rocks. It is unbelievable for me the largest number of garnet analyses have been from rocks of “Unknown” “Type”. This may mean that selection of attributes in terms of “Type” is not appropriate.

The ‘type’ of material consists of 56 unique categories, the ones listed by the reviewer are the 5 most prevalent in the dataset listed in table 3 (now table 2). We changed some of the wording and presentation of the dataset to make it clear that there are more options than the 5 listed.

Overall, we agree that this is an issue and that the interpretation of the Material, Type, Composition, and Paragenesis attributes are highly subjective and often can vary due to individual interpretation of the literature. We settled on using these categories due to the format of the EarthChem dataset and since all their samples already came with the mentioned classifications and distinctions applied, we did not attempt to reclassify any sample analyses that originate from data repositories for the sake of data continuity. Hopefully authors that use this data resource will carefully consider these limitations and can provide more insight in the future from their geochemical signatures.

4. The list of attributes as “Paragenesis” in Table 3 is especially embarrassing. “Schist” may represent metamorphic rocks with schistosity irrespective of composition. Others (Kimberlite, Peridotite, Lherzolite and Harzburgite) are classified based on composition or modal assemblage of minerals. There are “schistose peridotites”. Is “Peridotite” representative of coarse-grained olivine-rich rocks, which are not referred to mineral assemblage or modal compositions by original authors? It is incredible, possibly meaning some unreliable descriptions. “Lherzolite” and “Harzburgite” are of course included in “Peridotite”.

Again, these are classifications that originated from the EarthChem repository that we did not attempt to alter due to data continuity. We recommend that researchers that use this dataset in the future keep this in mind as it is an important limitation.

5. I propose to consider “Massif” or something like that instead of “Amphibole” and others to represent non-xenolithic metamorphic or igneous rocks. “Amphibolite” should be included in “Paragenesis” and included in “Schist”. “Lherzolite” and “Harzburgite” should be discarded and included in “Peridotite” to avoid confusion.

We recommend that these distinctions are adopted in future uses of the data, however, EarthChem requested that we maintain data continuity and therefore, we cannot change these classifications in the overarching dataset.

We added additional text in the results and discussion section to address the limitations mentioned by the reviewer:

“Nevertheless, there are some limitations regarding the classifications of the petrogenetic and paragenetic attributes that must be considered when evaluating this dataset. First, these distinctions are simplified and could be subjective to each authors

interpretation. For example, within the 'Type' category of 'Xenoliths', these rock fragments could consist of different formation processes (such as fragments of amphibolite/granulite/eclogite facies) that were captured in a volcanic sequence. Thus, their Type as a Xenolith would not represent the individual formation processes of the garnets within the host rock. Second, some classifications of paragenesis do not contain compositional information. For example, a 'Schist' does not consider the compositional origin of the parent rock and therefore could be a peridotite with a foliated texture. Finally, these classifications and distinctions were adopted from the EarthChem repository to maintain data continuity. Therefore, this dataset provides the original classifications applied to the data donated to the repository – presumably from the original authors themselves, although this cannot be guaranteed. For example, while Peridotite is listed as a category within paragenesis, so are Lherzolite and Harzburgite which are types of peridotites. We recommend that these categories be grouped together when analysing this dataset further. Ideally, a system of properly representing the rock-type origin and individual mineral formation processes should be developed to prevent misinterpretation of samples within large datasets such as this one.

There could be other limitations other than the specific examples mentioned here. We recommend that any researchers using this dataset for their own work carefully consider the petrogenetic and paragenetic categories as well as original sources of the data.”