

## **Response to reviewer's comments (D. Turner)**

We respond here to the comments that needed a more detailed answer other than addressing them in the publication itself.

### **1) Datapaper + Supplements – general comments:**

**1) While it is clear that there are linkages between the datasets, there is not linkage between all the topics. For example, the REE-related spectra match well with the Cu-related spectra, but not the Apliki site data. It is this reviewer's opinion that two ESSD papers could be written, perhaps best to match the REE and Cu mineral-focused spectra together in a single paper, and the Apliki site data by itself. That way, the target information is more consistent within the described datasets. In the present format, the four suites of data are all different in the physical nature of the samples and the (geo)chemical and mineral characterization.**

We are able to comprehend the reviewers argumentation and realize the difference between the here presented data sets. As we are planning to publish more spectral data of different origin and sample characteristics, the data paper is supposed to be a comprehensive overview of the spectral data acquisition in the GFZ laboratory. The datasets themselves do not have to have the same geochemical or mineral characterization, as their physical state and geochemistry is separately described in the data reports themselves. We therefore argue that the datapaper is presented as one conclusive umbrella publication that can be referred to when accessing the spectral data and geochemical data itself.

**2) The manuscript starts with some fairly sweeping comments in the introduction that could be toned down in the context of this contribution.**

You're completely right! We acknowledge the enthusiastic tone relating to our contribution to the accredited USGS libraries and toned it down. The rest of the introduction is a review of the associated methods and to the best of our knowledge in a neutral tone. When re-reading the manuscript we tried to re-structure section parts that detracted the reader.

**3) In order for the broader community to use any spectral library, documentation needs to be clear and there should be no ambiguity regarding data source or characterization methods.**

Your comments regarding the document were taken seriously and we cleared up the document based on your indications regarding the state of purity of the spectra, the mineral structure and the different geochemical analysis types. This should help the reader to clearly catch on the scope of this work. Again, the aim was to describe the

hyperspectral data acquisition in the laboratory that is consistent for all sample types. The geochemical analysis differences have been explained in detail (in the main paper and the data reports) and is dependent on the target material.

**4) In this sense, I also recommend splitting the paper into two discrete contributions so as to reduce the potential confusion over what methods were used on which samples.**

It is our aim to show the hyperspectral data acquisition and explain in detail how the hyperspectral laboratory work is conducted. The geochemical data for validation is not supposed to be of the same method of non-ambiguous.

**5) Furthermore, the samples that are rocks and not minerals need to be identified as such. For example, the monazite and synchysite spectra are not what I would have expected if these were mineral specimens. Since one of the principle uses of these spectra are as inputs to understand unknown spectra in other datasets, it is important to state their true nature.**

We cleared this in the data report as well as the ESSD paper. The REE-bearing minerals/minerals within a rock matrix. All of these samples are supplied with XRF data but not SEM. As these samples have been part of a number of diverse publications within the Ph.D. project of N.K. Bösche, and have been published and peer-reviewed, we did not re-analysis the samples. As the results based on these data (Bösche, 2015) and successful publications we wanted to share them with a broader community.

## **II) Datapaper Comments**

**Line 70. REE oxides are not minerals, though they are likely crystalline. Do you know the structure of these REE Oxides?**

You are correct, the REE-oxides are synthetic powders not in crystalline structure.

**Line 104. How did you validate the mineral species? (is related to the REE-bearing minerals)**

The minerals were not validated, the notation based on the supplier was assumed valid. The supplier (<http://www.seltene-mineralien.de>) offers analytical services with a modern REM-EDX technology and therefor we assume his specimen are analysed and the mineral species is validated before the sale.

**Line 108. How did you validate the mineral species? (is related to the Copper-bearing minerals)**

Mineral identification took place using microprobe analyses.

**Table 1. Why two suites for Copper bearing minerals? State why.**

Both supplemental entries are for one suite of samples. S4 is a table stating the sample origin, whereas S5 lists the sample Ids and photos.

**Line 345. 120 seconds isn't really short for a HHXRF**

The long duration of 120 seconds were chosen with the purpose to reduce the noise of the measurement.

**Line 121. "The sample preparation varied by sample type and depends on the material and the information of interest." This is a bit problematic. It is not that any one of the approaches isn't valid, but the presentation of the data as a collection should strive to have internally consistent methods.**

The hyperspectral data acquisition described in this document is the internally consistent method that is presented here. We are planning to publish more hyperspectral libraries in the future. All of these hyperspectral libraries will be compiled under the conditions as described here. The geochemically analysis is different not only based on the sample type but the level of detail required for the projects where our spectral libraries stem from. The geochemical analysis is presented only as a source of validation not as a data publication itself. Unfortunately our funding does not allow for the compilation of spectral libraries with consistent geochemical validation as the likes of the USGS Spectral Library Version 7 (Kokaly et al., 2017).

**Section 5.2 Why do you have two distinct descriptions for the JEOL unit at Potsdam?**

The University of Potsdam used two JEOL units, one for SEM and one for EMPA analyses. The EMPA analyses is described twice, one each for the sample type analyzed, as different measurement parameters were used.

**Line 272. Which standards? Same as above? If so, many of the Smithsonian materials are synthetic.**

SEM measurements are calibrated with pure copper and the EMPA measurements are calibrated with the standards mentioned in the text from the Smithsonian Institution and Astimex.

### **III) Apliki technical report:**

**To confirm above points, the “aquatic” sample above is not an aquatic sample. Instead, it was analyzed by aqua regia digestion, as described in the BVM analytical notes. Why was this one sample analyzed with a different method? The manuscripts need to have this item addressed.**

The internal BVMs sample preparation-/ analysis type groups by the required analysis method. These “analysis types” are namely “aquatic”, “rock” and “soil”. The measurement/ analysis type is chosen by the service provider “BVM Institute” on which we do not have any influence.

**It is unfortunate that your overlimit Cu samples were not re-analyzed for total Cu content, since this is a key focus for the Cu mine related samples.**

Yes, the BVM analysis limits were chosen in order to resolve sample copper content with lower limits. We honestly did not expect to have three samples with Cu content > 10.000 ppm. Unfortunately, the analysis could not be repeated.

**Figure 2. Maybe you could split this out into two plots, rocks and soils, so that the reader can maybe make a small assessment of the data without downloading and plotting the spectra?**

We’ve given the plot a larger space in document. Additionally the spectra are presented and shown in more detail in the Ph.D. thesis of Koerting (2020, in preparation).

#### **IV) Copper-bearing technical report:**

**Sample C3 has a typo in its name, where a “%” is used instead of “5”**

Unfortunately, we cannot find the typo, maybe it was fixed during our reworking of the document from review 01

**There are some samples that are not monomineralic, and this is important to state in the documentation. For example, “Malachite 1” has a whack of other minerals in the SEM image, so right away we know that the “Malachite” spectrum here is actually at least Malachite+pyroxene+quartz. Same for Azurite 2 and Chalcopyrite 3.**

You are absolutely right, the sample names were used from the names of the collection where the samples were retrieved from. We are adding this information to the technical report. All identified mineral phases of each sample are presented in the file “copper\_bearing\_minerals\_chemistry.pdf” in the published data. The samples in question are: A1, A3, L1, P3, B1, M2 & C3

#### **V) REE technical report:**

**You should include the anticipated crystal structure of these oxides. The work by White (1965?... off the top of my head) showed the importance of this variable for the resulting spectra. This is especially relevant in the context that Tb is listed as both 3+ and 4+.**

The synthetic REO powders were delivered by the supplier. The REE-bearing minerals and REO powders were published by (Bösche, 2015; Herrmann, 2019) and are described in detail in the reviewed works.

**Similar to the copper minerals, some of these samples are not monomineralic and instead are rocks, and therefore the spectra need to be identified as such. For example, the images you show in the EMPA data indicate that synchysite has a bunch of phases, as does ilmenite.**

You are absolutely right, the spectra of the REMin were supposed to be acquired only over the identifiable mineral surface in the hyperspectral imagery. The geochemical data indicate though, that some of the sampled area is not monomineralic. The geochemical data is supplied with the samples to show exactly that. We will note this in the geochemical part in the technical report.

**Do you have analyses of the monazite sample?**

Yes, we have the XRF analyses of the sample.