A solar optical hyperspectral library of rare earth-bearing minerals, rare earth oxides, copper-bearing minerals and Apliki mine surface samples.

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Manuscript Comments

General

This contribution by Koerting et al includes a main paper, a supplement, and three datasets. The three datasets include description documents and multiple supporting data files. The three datasets also have their own publication citations as GFZ Data Services products, and the reviewer was required to source the information for the ESSD paper from the GFZ publications.

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.

Nevertheless, it is great that the raw data is being shared with the broader scientific community and that there is supporting data on the nature of the samples studied. These types of data can be important for academics, government and industry to carry out their tasks, whether that be in-field mine wall scanning or space-borne monitoring of mining activity in remote regions.

The manuscript starts with some fairly sweeping comments in the introduction that could be toned down in the context of this contribution. Formatting is not consistent, and there are simple typos and spelling mistakes that suggest the manuscript could have been reviewed again before submission (e.g., a single space before a period, abandoned commas). Sections are referred to as chapters, and appendices referred are not really appendices, but rather supplemental files that the reader must go find.

It is the reviewer's opinion that due to these observations, the manuscript should be given a re-read and edit by the authors to make it consistent with the journal structure and to address simpler non-technical issues that detract from the reading and scientific value of the data within. 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. 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. 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.

I am happy to see this data made available to the broader community, and another pass at cleaning it up will greatly improve its usefulness!

DT.

Specific

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

Line 101. Text indicates 99.9% of the specified REE, however, these samples are rare earth element oxides, and thus contain oxygen. Presumably the purity relates to not having other lanthanides, however, these are important distinctions to catch for data repositories. (clarification is given later, but as stated it still needs correction here)

Line 104. How did you validate the mineral species?

Line 108. How did you validate the mineral species?

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

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.

Line ~130. You need to have example images of REMin and REO samples like you do for the Cu and mine samples

Line ~130. I'm confused. Do the REMin spectra originate from one single pixel in the middle, or an average spectrum from more pixels?

Line 134. Be sure to reference these as copper-bearing, as copper itself is a mineral… in that sense, these are not all copper mineral samples, as they are other copper-bearing minerals too (e.g., azurite).

Line 136. Text speaks about geochemical sampling, but up to this point it didn't seem like the Cu minerals were analyzed geochemically at all?

Tables 2-4. What light source did you use? Halogen?

Line 205. You should state here whether you resize the VNIR or resize the SWIR images, since the spectra are supposed to be 5 x 5 averages… this could mean quite different numbers of ‘pixels’ depending on whether you are upsampling or downsampling.

Table 5. I see now that you’ve used the SEM and EMPA for Cu minerals

Line 261. The BSE images show differences in brightness from mean atomic number of the pixel, not light and heavy elements.

Line 263. This paragraph should be combined with the previous SEM paragraph.

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

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

Line 274. Why do you speak of limitations here of an EMPA, but not of the limitations for the Niton XL3t?

Line 290. There is an aquatic sample? But the documentation states that the aquatic sample is 1a… and your index shows a rock? And Figure 3 in the main manuscript shows the sample as a powder… Does “Aquatic” mean something else? Perhaps aqua regia digestion? This needs clarity and correction.

Line 335. You need to distinguish mineral specimens/samples from mineral species

Line 338. Is Misra et al the most appropriate reference for this statement? Maybe something more classical in the geological remote sensing literature?

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

Data Paper Comments

Generally speaking, the content of the PDFs can be cleaned up and typos addressed. In this review, I have not listed them.

Apliki

- 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.
- 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.
- 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?

Copper Minerals

- I see now how you've selected the small areas in the broader sample. This approach should be described in the main paper.
- Sample C3 has a typo in its name, where a "%" is used instead of "5"
    - This sample is also not just chalcopyrite, it is also bornite
- 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.
- Similarly with Azurite 2

REE oxides, minerals and Nb-Ta minerals

- 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+.
- In your spectral library, ilmenite is spelled incorrectly
- In your text, synchysite is spelled incorrectly
- 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.
- While it is not possible to do this validation with your other non-SEM samples, one can assume that this is true for at least the monazite sample, and likely your others that have multiple minerals in Table 1.
    - Your XRF data could be used to support this effort. For example, the high Sr in parisite suggests this is not only parisite and/or is another Sr-bearing REE-bearing carbonate phase.
    - Equally true about Zr in some samples
    - You need to critically evaluate the Niton data a bit more… for example the Ni values are suspect. In this sense, you need to clearly state how you're using that data to achieve your goals.
    - Similarly, it is not the voltage that preclude the analysis of other REE, but rather the fluorescence overlaps from other elements and the weakness of the L-lines that I suspect that unit is using to quantify the REEs.
    - https://www.bruker.com/fileadmin/user_upload/8-PDF-Docs/X-rayDiffraction_ElementalAnalysis/HH-XRF/Misc/Periodic_Table_and_X-ray_Energies.pdf
- "Xenotime a" is mislabeled in the XLS file
- Do you have analyses of the monazite sample?