

1. Response to editor's comments

1) Reply to comments in Feb. 2021

Comment 1: Please modify or discard Figure 13 Figure 13 shows examples of reflectance spectra, however, it remains unclear to the reader what is displayed: the naming of the spectra are numbers that do not appear as codes in the table, the Y-axis does not show the scaling of the unit of reflectance (that would be here 0-1 * scaling factor), you could either add in figure 13 the labels that you also present in the tables or discard figure 13.

Answer: Figure 13 has been modified; the full sample names have been added in the legend (e.g. "Apl1_A_13b [5x5AVG]" instead of "13b")

The data scaling has been added in the caption (between 0-10000).

Comment 2: Please add information on the scaling factor that you use for your reflectance data as - a sentence in the manuscript, e.g. would fit well in 3.3 Hyperspectral Data Processing - a sentence in your data publication abstracts at GFZ data services reflectance is expressed either as 0-100 % or 0 -1 unitless (as the theoretical ratio of outgoing energy / radiance versus incoming energy / radiance) in the case of your published data sets, reflectance is expressed unitless with a scaling factor that needs to be described in the manuscript text and in the data publication abstracts.

Answer: The scaling from 0 – 10.000 is based on the HySpex sensor calibration and the Reflectance Retrieval Routine described in Rogass et al., 2017. We added the information regarding this unitless scaling in Chapter 3.3 of the manuscript as well as in the caption of Figure 13, where the scaling of the spectra appears. As the other figures showing the spectral libraries are stacked, here the scaling is not shown.

The information regarding the scaling were added to the data reports hosted on the GFZ Data Service website and are already online. This information is added in the Abstract as well as the "Hyperspectral Measurement" section.

2) Reply to comments in Nov. 2020

General comment by the authors: As the repetition of information in the supplements and the technical report seems to cause confusion, we have decided to delete the supplements and only refer to the technical reports that present all of the needed detailed information regarding the samples.

Question: Requirements are to enhance the usability of the published data collections and the manuscript following the referees' and editorial recommendations.

Question: Please upload the revised version with i) new answers to the referees as in the current version of answers to the reviewers it becomes not clear if and how all referee points have been addressed, e.g. please list what edits and changes you could made in the published data collection

Answer: the revised answers will be uploaded as "_comments_v2"

Question: and with ii) the new manuscript version with track changes included.

Answer: We will do that and upload them separately

i) In general

Q: The ESSD manuscript describes a spectral library collection without in this moment visualising the data in form of spectral library plots and without a user-friendly overview on the content per collection.

i) provide more detailed tables on the content of the spectral library collections in the main text, e.g. provide the name of the minerals per collection in overview tables in the ESSD manuscript

ii) provide plots (e.g. stacked or group associated) of the spectral library collections in the main text. You can also add more specific details in the appendix

A: Added these info in the manuscript from line 510 to line 548.

We added a chapter 4 “results”, presenting the spectral libraries, the spectral entries and a plot for each spectral library. All of this information can be found in more detail in the technical reports provided on the data platform and we’re again citing these technical reports.

II) Data publication

Q: in the data collection enhance the ascii files. Now the ascii spectral library files are directly exported from the ENVI spectral libraries.

Enhancement of ascii files: you have the possibility to add more codes and explanations: please add – in addition to the ENVI spectral library code name of the reflectance spectra – at least another code that is also clearly the same code in a linked chemical measurement, please add also a column for the general name of the mineral / element.

A: The ascii files are directly being exported from the spectral libraries in ENVI. The ASCII files and samples are now better described in the technical reports of the data. In addition, the header in the ASCII files define the columns in the data file. The tables in the technical reports list all these information for each sample and are provided on the DOI landing page of the data publication.

Q: Specifically for the copper bearing minerals you need a clearly identifying code system so that the geochemistry and reflectance spectra can be linked.

A: This has been done in the new technical reports and spectral libraries that will be uploaded as version 2 of the data and technical reports. Here, each technical report lists the samples of the spectral library in a table. We have added a column with the spectrum name for each sample for the copper and REO and REMin samples, now all samples (including the Apliki samples) are clearly named and the spectra names clearly identify the samples. In addition, we have included sample overview tables of all data publications in the manuscript section 4.

Q: If you intend to keep the Apliki mine spectral library collection in this ESSD manuscript you need to provide a linkage to the other data collections, e.g. you could do this in the form of mineral interpretation

A: Lines 583 – 587, we’ve added that the sample collections themselves are independent from each other in line 219 – 262 (the line numeration is off, somehow this happens in the template?). Our manuscript aims to explain the method of spectral data collection by the HySpex system and present different datasets for a wider community based on the HySpex sensor characteristics. However, to make the description of the Apliki samples more comparable with the copper and REE samples, we have added a general description of the sulphide deposits of the Apliki Mine to the Technical Report and an additional column describing the mineralogy based on qualitative XRD analysis in Table 1 of the Technical Report.

Q: Please consider the Referees comment: The authors should also explain exactly what they mean by geochemical validation-to show the composition of the samples, or to show a relationship between composition and absorption minima?

and make more clear in the text how you apply the term ‘validation

A: we’ve added this in line 214-218: “The samples are presented as reflectance spectral libraries and their geochemical composition. Sample nominations are based on the geological collection of origin or sample abbreviations from the field sampling. The sample nomination is not an interpretation of the presented geochemical data. The datasets are independent of each other, the reflectance spectra can be seen as a spectral expression of the existing geochemical data. Neither the geochemistry nor the reflectance spectra are interpreted or correlated to each other.

III) specific requirements:

Q: Abstract: please name how many samples are in the specific collections each

A: added in lines 23 - 29, “The spectral libraries and corresponding geochemistry are published via GFZ Data Services with the following DOIs: <http://doi.org/10.5880/GFZ.1.4.2019.004> (13 REE-bearing minerals and 16 oxide powders, Koerting et al. (2019a)), <http://doi.org/10.5880/GFZ.1.4.2019.003> (20 Copper-bearing minerals,

Koellner et al. (2019)), and <http://doi.org/10.5880/GFZ.1.4.2019.005> (37 Copper-bearing surface material samples from the Apliki copper-gold-pyrite mine in Cyprus, Koerting et al. (2019b)). All spectral libraries are united and comparable by the internally consistent method of hyperspectral data acquisition in the laboratory.”

Q: Introduction: Please change the focus of your introduction: in your manuscript, the introduction leads into the direction of hyperspectral imaging, specifically on future hyperspectral satellite missions such as EnMAP and future imaging spectroscopy applications that could make use of the spectral libraries. While this can be a part of the introduction substantial information is not provided yet.

A: We have changed the order of the different sections within the introduction. It should now be clear why hyperspectral satellite missions are needed for the geology applications that we refer to. Here, specifically from line 145 - 154.

Q: Please introduce in the introduction the REE- and copper bearing target minerals / rock assemblages that are your published data collection in which ore deposits they occur and for what these elements are used for. Explicitly show which spectral libraries on REE and / or copper bearing target minerals are available, e.g. USGS, NASA-Jet Propulsion Laboratory Library, Canada Geological Survey published dataset (with citations)

A: In our opinion a full intro into the different spectral libraries goes too much into detail, similar to a review of the existing libraries. We've added why our spectra and samples can contribute to commonly known libraries and how we aim to make them available for other hypspx users. This can be found in line 156 - 162.

Q: The description of the future ENMAP satellite acquisition principle is not relevant for this ESSD publication, please delete:

'The image scenes are acquired by a moving line scanner mounted on the satellite, which records the spatial dimension (x- and y-dimension) line by line, as well as the wavelength dimension (z-dimension). Each pixel therefore represents the full spectral range of the sensor. The sensor's movement along a rotation or a movement axis provides spatially continuous imaging spectroscopy data.'

A: this has been deleted, as suggested.

Q: Better to show that spectral reflectance measurements and characteristics are clearly based on physics by citing some literature on mineral spectroscopy and also the reason of absorption in the VIS (electronic transitions) and the SWIR (molecular vibrations) instead of to descriptive sentences e.g. 'Variations along the spectral domain of the data are visible as concave indentions, often referred to as "absorption bands". – They are absorption bands

A: We've added the information and citations about mineral spectroscopy from line 43 - 89.

Q: L36 in this study -> change into this data collection

A: This has been changed

Q: Methods: please combine chapters 3, 4 and 5 to one chapter method with subchapters – may be add more tables

A: Has been changed and adjusted

Q: add a chapter 'results'. Here you can provide plots (e.g. stacked or group associated) of the spectral library collections

A: We added a chapter 4 "results", listing the samples, relevant information, spectra names and a plot for each spectral library. All of this information can be found in more detail in the technical reports provided on the data platform and we're again citing these technical reports.

Q: Discussion –

You provide discussion chapters on accuracies

Here is also the opportunity on a short chapter for an overview what your data collection provides to the user of the data collections, where you can better bring the Apliki spectral library into the context of this manuscript.

A: Added briefly in line 636 - 640

Q: Please note: there is nowhere a requirement about spectral analyses on spectral characteristics.
A: *It's not clear to us what you mean here. Do you mean that we do not discuss the spectral characteristics or correlate spectral features to the minerals from the collections or their geochemistry? We do not aim to discuss the spectra, we simply aim to provide the spectra of each material and the geochemistry of the same material without interpreting if e.g. the mineral denomination from a certain collection is correct or if the spectrum of the sample corresponds correctly to the geochemical data.*

Q: Throughout the text: reflectance spectra (instead of spectra)
A: *Has been cleared up/ "reflectance" was added*

2. Authors responses to Jeanne Percival - Reviewer Comments:

(Comments in bold, answers in regular script.)

1) Datapaper + Supplements

1) The authors should also explain exactly what they mean by geochemical validation-to show the composition of the samples, or to show a relationship between composition and absorption minima?

In order to avoid confusion with the term validation, we now refer to the geochemical analyses as a possibility for the user to check/interpret the spectra. The hyperspectral spectra and corresponding geochemistry are independent of each other, the reflectance spectra can simply be seen as a spectral expression of the existing geochemical data. Neither the geochemistry nor the reflectance spectra are interpreted or correlated to each other.

2) These data sets should be available as the spectral library was made available, or somewhere there should be a note as to how to access the files as a guest.

The data is openly available on the GFZ data service website and licenced with a CC BY 4.0 Licence. There might have been an issue with the firewall of the user's computer or with server maintenance? We had a system update in spring 2020 at GFZ Data Services.

3) "elemental" from a hyperspectral viewpoint, I would see Fe as the main element observed (i.e., in gossans), as REE-bearing minerals tend to be in trace amounts, very small, hence seeing the NIR signature may be masked by other minerals such as clays or carbonates etc.

This is just meant as a basic introduction for hyperspectral data uses and not tailored to outcrops or weathered surfaces. The mapping meant here is not only for rock outcrop scan or satellite imagery but also in laboratory scans and in these scans, we do have REE mineral specimen that need to be mapped. Here, the spectrum depends on the element content and is not covered by clay etc. as if found in the field. You are right, in field imagery, the major element mapped is Fe but in laboratory scans, other elements like Nd embedded in monazite can be mapped.

4) Line 46: should references be in chronological order from oldest to youngest? + Turner et al 2014a is out of order in the ref list.

We've changed this in the references

5) Fig. 1: This is very good and provides a good image of what your paper is about. Suggest that the spectral pattern for chalcopyrite be a darker colour, cannot see the yellow; also the malachite should be a continuous line like the other three.

We changed the malachite to a continuous line. The color-coding itself is based on the mapping colors in fig. A+B. We changed the line thickness so that the spectrum is well visible in yellow but corresponds to the colors from A and B.

6) Line 84-88: Delete, as this is repeating what noted earlier. Add the last sentence to the end of the previous paragraph. "The spectral libraries...." after the url address.

We hoped that this part helps to lead the reader through the chapters of the manuscript and aims to explain the structure. The previous paragraph has been rewritten, so there is not repetition anymore (see lines 220 - 226)

7) Table 1 is not really necessary-you can summarize that info in the text.

We decided to delete the supplements, as the information is repetitive to the technical reports of the dataset and seem to have been confusing. Therefore, Table 1 was also deleted and any reference to the supplements.

8) Table 2-4 Suggest combining Tables 2, 3 and 4 into 1 as many parameters are common. So you can have more columns relative to each of the different mineral groups.

We changed that. Now we show the common parameters in Table 1 and the different dataset parameters in Table 2-3 (page 10, starting at line 390).

9) Table 5: The header "Concentration level determination" does not relate to what you have placed in the rows. What are they? All you do is re-reference the data sets. Likely this Table is not critical to the paper.

We changed this to "geochemical analysis". This table should give an easy to read overview of the different geochemical analyses used for the different sample types

10) Line 227-233: This is repeated in the data set paper, why include this detail here. If this is the preferred place, then shorten that in the data set paper. Principles of XRF analysis are not really needed, can refer to a paper on this subject

As we explained all instruments used, e.g HySpex, we aimed to explain every analysis method shortly in order to save the reader from cross referencing too many papers. We think that the data should be understandable by just accessing the Gfz Data Service website, where the technical reports are provided, without knowledge of the data paper.

11) Table 6: What about adding in the probable interferences for analysing the LREE with a hand- held XRF instrument. This provides very little information to the reader.

The XRF analysis is based on Bösche (2015) dissertation with more information on the XRF measurements. We've now added the citation.

12) List background count times on EPMA, especially for the trace elements.

The REE EPMA method is based on Lorenz et al. (2019) and was developed by her at the university as part of her PhD Thesis. Therefore, we are not able to forward the method before her Ph.D. is finished.

13) Line 254: Measuring F in fluorapatite is problematic using EPMA. At a minimum, the Area-Peak Factors method should be used otherwise result is usually spuriously-high values.

Lorenz et al., 2019 say "Fluorine, as one of the least-stable components in apatite, was measured first during the analytical scheme. To reduce halogen migration, counting times for F were reduced to 6 s on peaks and 3 s on backgrounds. The EPMA data were reduced with the PRZ-XXP correction routine".

14) Line 268-274: delete, and any additional information incorporate with the EPMA section.

We added both EPMA explanations together now, it is done for the two different sample groups with different parameters and correction routines (copper and REE) (lines 466 - 529, section 3.4.2)

15) Line 290: why was one sample analysed using “aquatic” What is so different about it-this is worth explaining. The code info is better placed in the data sheets information.

We deleted the tables from the data paper and instead added them in the data description of the technical report. The info for the aquatic analysis is also added in there. “Sample 1a belongs to a group of samples where only the weathered crust was extracted for analysis. Only sample 1a is provided here. The aquatic analysis has a very low detection limit and was chosen due to the expected depleted element content.”

16) Table 8 and 9: Is this really important? You have not noted any samples numbers in the text so there is information for the reader in table 8. This should be in an Appendix if deemed critical. Describe the analyses and how they are done –that is more important.

The tables were deleted from the paper.

17) References: Turner et al, 2014a is out of order, Turner 2015 should be first (single author). Leave a space between Tong et al and the turner reference.

We’ve redone the references and changed the order.

18) Line 310-314: Only certificate info provided as validation for the REO powders For REE minerals, there is no table comparing the results from the XRF vs. EPMA and indicating if the results are actually comparable. For the geochem analyses by BVM there is no information on how good the data is, no comparison of duplicates, no CRM’s, unless this is also held in the University site.

REO powders are only characterized by the certificates which can be found in the corresponding technical report As we do not interpret or correlate the different datasets, XRF and EPMA are not compared. The standards measured by BVM are provided in the Excel TM files, apparently the standard measurements reached the expected results. Therefore, no information on the quality of the analysis was given by BVM.

Sample	decimal lat	decimal long	Method	WGHT	LF300	LF300	LF300	LF300	LF300	LF300	LF300	LF300	LF300
			Analyte	Wgt	SiO2	Al2O3	Fe2O3	MgO	CaO	Na2O	K2O	TiO2	P2O5
			Unit	KG	%	%	%	%	%	%	%	%	%
			MDL	0.01	0.01	0.01	0.04	0.01	0.01	0.01	0.01	0.01	0.01
			Type										
AP/1-A - 1f	35,077	32,84275	Soil	0.07	45.44	15.86	12.79	5.11	7.65	2.37	1.01	1.00	0.07
AP/1-A - 2a	35,076867	32,84275	Soil	0.11	40.72	8.00	31.22	2.67	0.75	0.31	0.67	0.38	0.20
AP/1-A - 3a	35,076983	32,843083	Soil	0.11	44.66	14.20	15.25	4.87	3.74	1.15	0.86	0.74	0.05
AP/1-A - 3b	35,077	32,84305	Soil	0.08	49.15	11.83	13.91	5.40	3.59	0.85	0.51	0.58	0.05
AP/1-A - 4a	35,076967	32,843067	Soil	0.03	33.97	10.29	10.62	9.96	8.00	0.22	0.02	0.24	0.01
AP/1-A - 4b	35,077	32,843033	Soil	0.06	42.68	16.01	13.35	8.08	2.80	0.83	0.42	0.50	0.02
AP/1-A - 6a	35,076967	32,8431	Soil	0.09	44.32	12.76	19.85	4.44	0.99	0.65	1.77	0.42	0.03
AP/1-A - 6b	35,07695	32,8432	Soil	0.13	45.93	14.81	14.24	5.49	5.43	1.63	0.85	0.79	0.07
AP/1-A - 6c	not available	not available	Soil	0.11	43.27	8.94	25.45	4.54	0.79	0.31	0.48	0.27	0.02
AP/1-A - 6d	not available	not available	Soil	0.11	39.93	12.47	24.96	4.30	1.19	0.53	1.24	0.41	0.06
AP/1-A - 13b	35,076117	32,8434	Soil	0.12	57.20	13.23	14.08	3.77	0.71	0.35	0.08	0.82	0.03
Pulp Duplicates													
AP/1-A - 6d	not available	not available	Soil	0.11	39.93	12.47	24.96	4.30	1.19	0.53	1.24	0.41	0.06
AP/1-A - 6d	not available	not available	REP										
AP/1-A - 4a	35,076967	32,843067	Soil	0.03	33.97	10.29	10.62	9.96	8.00	0.22	0.02	0.24	0.01
AP/1-A - 4a	35,076967	32,843067	REP		34.28	10.20	10.53	9.92	7.93	0.22	0.02	0.24	<0.01
Preparation Duplicates													
AP/1-A - 4b	35,076967	32,843067	Soil	0.06	42.68	16.01	13.35	8.08	2.80	0.83	0.42	0.50	0.02
AP/1-A - 4b	35,076967	32,843067	DUP		42.54	16.09	13.35	8.12	2.81	0.83	0.43	0.50	0.02
Reference Materials													
STD GS311-1			STD										
STD GS910-4			STD										
STD SO-19			STD		60.47	13.98	7.38	2.94	5.95	4.07	1.31	0.70	0.31
STD SO-19			STD		60.60	13.91	7.47	2.90	5.92	4.02	1.30	0.70	0.32
STD SO-19			STD		60.23	14.03	7.60	2.95	5.99	3.98	1.29	0.70	0.31
STD SO-19			STD		60.51	13.95	7.47	2.92	5.96	4.02	1.29	0.70	0.30
BLK			BLK										
BLK			BLK		0.03	<0.01	<0.04	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
BLK			BLK		0.01	<0.01	<0.04	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Prep Wash													
QUARTZ_KRA			Prep Blank		98.24	0.52	0.76	0.03	<0.01	<0.01	0.12	0.09	<0.01

19) Line 337: provide information on how to obtain easy access to this geochemical data.

The data links are provided in the paper, it might have been possible that a server maintenance did not allow you access the data. All data is provided via the DOI link to GFZ Data Services and not another source (e.g. university website or similar).

II) Technical Report REE:

1) What is really needed, is to identify which REE corresponds to which reflection-as in Turner’s 2015 thesis (and published papers 2014). This is the test for validation.

As we do not interpret or correlate the datasets with/to other data we do not provide information to identify distinct peaks of different rare earth elements. We only want to provide full spectra for the VNIR and SWIR range in form of a spectral library. The spectrum of each mineral is unique.

2) I do not see REO analyses in any table, certainly not in Table 5.

The sample analyses are the purity certificates in table 5, technical report starting page 9

“Table 5: Chemical composition of the REO powders provided by certificates of purity (Bösche, 2015; Herrmann, 2019).”

3) I could not access geochemical data by XRF nor EPMA.

All data was and is freely available via the DOI links. GFZ Data Services, however, had a system update probably corresponding with your unsuccessful attempts to access the data. We apologise for this. For the revised version, we have thoroughly restructured the three technical reports and published a new version of the DOI.

III) Copper-bearing mineral report:

1) I believe this is the place where that should be held, and maybe the Supplement does not need to be so extensive with images.

We have now decided to delete the supplements altogether. Everything is provided in the separate technical reports of the datasets which are closely cross-referenced with the article.

2) For this set of data, I was able to open the EPMA results as well as the SEM images and EDS analyses. I assumed that the EPMA of the 25 analyses match the samples depicted in the SEM file, however that was not the case. It would be very useful in the EPMA files to indicate the sample name using the abbreviations provided (A1, A2, A3, etc.) for cross-reference. Also, as you have several samples of one mineral, averaging their mineral chemistry and calculating an actual mineral formula would be most useful. This can be also calculated for the individual samples.

The sample names have all been changed to include the abbreviations (A1_Azurite, A2_Azurite, ..) provided. We did not average the three measurements of the EPMA in the data text-file themselves, as the data publication is supposed to provide raw, unchanged data. A mean however is provided in the table listing all samples (both, in the data paper and the technical report)

3) What is the XRD trace of this mineral?

XRD trace is not provided for any of the samples in the article. The copper-bearing samples originate from the university of Potsdam and the BGR and could only be analysed by non-destructive methods. It is not a new mineral but based on our measurements we do not feel confident to notate it. Instead we provide the geochemistry and spectrum.

4) No issues with the spectral data; can open the data files. What validation has been done between the spectral signature of a sample and its geochemistry?

None, we only provide the data. The spectrum for each sample is provided, each sample is geochemically described by its geochemical information and in the copper-bearing minerals and the REE samples by the sample denomination provided by the collection holder or the sample re-seller. The reflectance spectra can be seen as a spectral expression of the existing geochemical data. We repeatedly point out now, that the geochemical data should be looked at when denominating the spectra, the sample "names" are only suggestions from the seller or the the originator of the collection (e.g. lines 214 - 218)

5) Why not summarize the chemistry in a table and indicate calculated formula for each mineral? What are the ore minerals?

EPMA and SEM were now combined in the technical report stating the general formula of the mineral that was measured. Pulp duplicates are mentioned in the geochemistry Excel™ file for each BVM analysis method.

IV) Apliki samples:

1) Table 2: we added the missing information

2) Table 3 and Table 4 were also in the main paper-they are not really important here; provide a web address. I think a description of the method is more valuable to the reader. Also, need to provide accuracy and precision information, there is no mention of duplicate or CRMs being analysed. Geochem data could not be accessed.

We seperated the tables from the main paper and provided them here. As each analysis group has different steps of analysis but some of them are similar it makes sense to us to provide the analysis methods in a table format. The data is accessible via GFZ Data Services.

3) What validation has been done between the spectral signature of a sample and its geochemistry? None, in this paper we only describe the data that is accessible, no interpretation whatsoever is provided either here or in the article.

3. Authors responses to David Turners - Reviewer Comments:

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 data sets presented here. As we are planning to publish more spectral data of different origin and sample characteristics, this article is mainly focussing on 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. The introduction has now been restructured to introduce the datasets more clearly and explain the aim of presenting different data collections.

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 restructure 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.

We have taken your comments regarding the document seriously and 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. 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 are 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. All datasets are united and comparable by the method of hyperspectral data acquisition in the laboratory. We have added substantial new information to the Apliki Technical Report that makes the information on samples and spectral libraries of Apliki more comparable to the other two spectral libraries. As mentioned above, the main aim of this manuscript is to describe the method that was used to create all three spectral libraries.

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 in the ESSD paper. The REE-bearing minerals/ minerals within a rock matrix. All of these samples are supplied with XRF data but not all were measured with SEM. As these samples have been part of a number of diverse publications within the Ph.D. project of N.K. Bösche, 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. We have now excluded the Monazite sample and all corresponding information from the data, resulting in 13 REMin samples instead of 14.

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. The technical report now states this clearly.

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

For the REE-bearing Minerals the notation from the supplier was assumed valid. The supplier (<http://www.seltene-mineralien.de>) offers analytical services with a modern REM-EDX technology and therefore, we assume the specimen he analysed and the mineral species were validated before the sale.

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

Mineral denomination is based on microprobe analyses.

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

The supplements were deleted, the copper bearing minerals are described in a revised table in the technical report.

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 geochemical 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 for the users to check or interpret the hyperspectral data and not as a data publication itself. Unfortunately our funding does not allow for the compilation of spectral libraries with consistent geochemical validation as is possible for 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 are 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 did 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 the document and added a subset of the spectral library to showcase some of the spectra. Additionally the spectra are presented and shown in more detail in the Ph.D. thesis of Koerting (2021, awaiting defence).

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 added 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_Azurite, A3_Azurite, L1_Linarite, P3_Plancheite, B1_Brochantite, M2_Malachite & C3_Chalcopyrite

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) and 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 provided the XRF analyses of the sample in Version 1 of the technical report + data. After a revision, we, however, decided to exclude the Monazite from the data in the new version of the data and the technical report.