

## **Response to reviewer's comments (J. Percival)**

### **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?**

The hyperspectral spectra are presented for different surface materials without any interpretation. The geochemical analyses are there to support the characterization of the samples and not to validate the spectra. We do not aim to present the relationship between composition and absorption minima we only aim at providing hyperspectral datasets of minerals and mixed surface materials that area also geochemically characterized. Geochemistry and spectra of e.g. Apliki can be used separately in order to characterize the area with the provided GPS data.

**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. There might be issues with the firewall of the user's computer.

**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.**

This is based on the template of the ESSD citation, which is in alphabetical order

**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.**

I changed the malachite to a continuous, the color coding is based on the mapping colors in fig. A+B, therefor I only changed the line thickness so that the spectrum is well visible in yellow.

**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.**

This does not seem a repetition for us, as it just least through the chapters of the manuscript and aims to explain the structure. The previous paragraph explains which is provided in the scope of this datapaper + data publications.

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

The table is supposed to give a quick overview of the included supplements and is easier to read.

**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.**

As these tables relate to measurements of three different sets of samples and three different data description reports, these tables should stay separated. The measurement parameters are also provided separately in Excel TM files in the data.

**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 tis geochemical analysis. Again, this table should only 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. The data set papers are only “technical reports” on the g fz data services website. The data should be understandable by just accessing this website without knowledge of the datapaper.

**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 informations 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 Ph.D. 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.**

see Lorenz et al., 2019 "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 EMPA data were reduced with the PRZ-XXP correction routine.

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

EMPA explanation is done for the two different sample groups with different parameters and correction routines (copper and REE).

**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.**

this is based on the ESSD template and resulting reference list from mendeley desktop

**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 supplements. XRF and EPMA will not be compared as the scope of this paper is only to provide data and not to interpret/compare them. The standards measured by BVM are provided in the Excel TM files, apparently the standard measurements reached the expected results therefor no information on the quality of the analysis was given by BVM/ is necessary.

Sample	decimal latiti	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.

This based on the firewall on your computer (?) and not the accessibility of the repository.

#### 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.**

The scope of the data publication is not 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 4.

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

Again, this should be in the open access gfz data-service repository

#### 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 believe the images should be in both reports. We have a complete data paper describing all samples, therefore it makes sense that these samples are at least shown in the supplements.

**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.**

We did not average the three measurements of the EPMA as the data publication is supposed to provide raw, unchanged data. We did however provide 3 EPMA measurements of each sample seen the SEM images if the user wants to average the analysis he can do so. In the SEM PDF, the averaged EPMA is provided in comparison with the SEM.

**3) What is the XRD trace of this mineral?**

XRD trace is not provided for any of the samples in the datapaper. 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 samples and its geochemistry?**

None, we only provide the data

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

Because the EPMA analysis was done in two programs for the oxides and sulphides + native copper separately. Therefore the analysis will be given separately. The ore minerals are the sulphides and native copper.

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 cut 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 has to be accessible.

**3) What validation has been done between the spectral signature of a samples 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 data datapaper.

## **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.

# A solar optical hyperspectral library of rare earth-bearing minerals, rare earth oxide powders, copper-bearing minerals and Apliki mine surface samples

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10

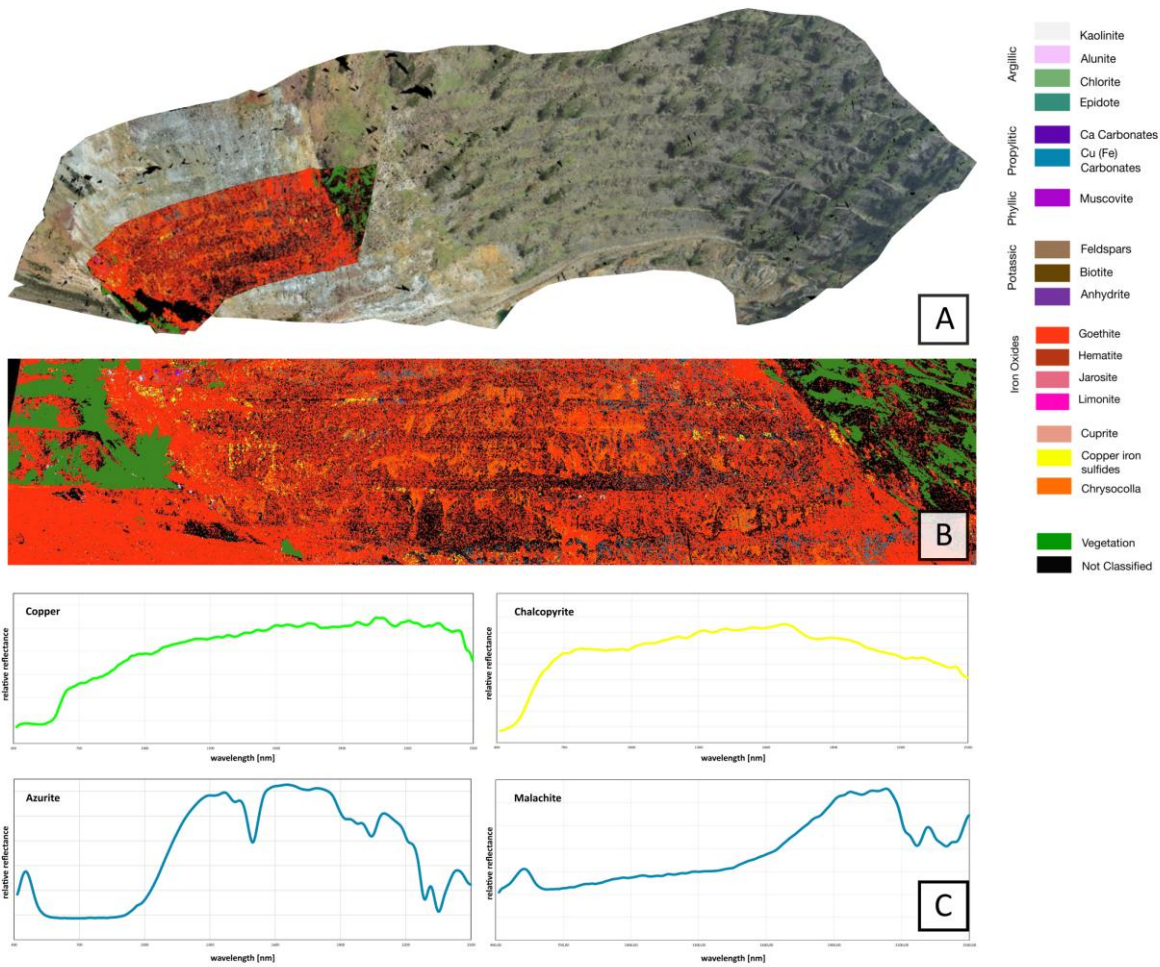
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**Abstract.** Mineral resource exploration and mining is an essential part of today's high-tech industry. Elements such as rare  
15 earth elements (REE) and copper are, therefore, in high demand. Modern exploration techniques from multiple platforms  
(e.g. space- and airborne), to detect and map the spectral characteristics of the materials of interest, require spectral libraries  
as an essential reference. They include field and laboratory spectral information in combination with geochemical analyses  
for validation. Here, we present a collection of REE- and copper-related hyperspectral spectra with associated geochemical  
information. The libraries contain spectra from rare earth element oxides, REE-bearing minerals, copper-bearing minerals  
20 and mine surface samples from the Apliki copper-gold-pyrite-mine in the Republic of Cyprus. The samples were measured  
with the HySpex imaging spectrometers in the visible near infrared (VNIR) and short wave infrared (SWIR) range (400 –  
2500 nm). The geochemical validation of each sample is provided with the spectra. The spectral library is openly available to  
assist future mineral mapping campaigns and laboratory spectroscopic analyses. 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>  
25 (REE-bearing minerals and oxide powders,(Koerting et al., 2019a)), <http://doi.org/10.5880/GFZ.1.4.2019.003> (Copper-  
bearing minerals,(Koellner et al., 2019)), and <http://doi.org/10.5880/GFZ.1.4.2019.005> (Copper-bearing surface material  
from the Apliki copper-gold-pyrite mine in Cyprus,(Koerting et al., 2019b)).

30

## 1. Introduction

Reflectance spectroscopy is based on measuring the reflected solar radiation from a material of interest. It uses photosensitive detectors to record and analyse light reflected or scattered from the surface. The reflected light is unique for each material and acts like a spectral “fingerprint”. Spectral libraries are comprehensive collections representing optical properties of materials in a specific wavelength range. In this study, the spectra were collected under standardized laboratory or field conditions and include geochemical validation of the materials. Spectral libraries are essential in the field of reflectance spectroscopy for example, for mapping purposes. The results are hyperspectral images that serve for the detection and mapping of element or mineral occurrences in natural and in man-made surfaces. Examples for applications are large-area satellite or aerial surface mapping for geological exploration in early-stage field prospecting. Future hyperspectral imaging satellites will provide the necessary data quality requirements to successfully map rare earth elements (REEs), copper deposits and other resources from space. These satellites will play an important role in the future of geological exploration, to help mapping large mineralized areas in remote regions (Mielke et al., 2016; Swayze et al., 2014). Several global mapping satellite missions will be launched in the next few years. Amongst them are the German EnMAP, the Chinese CCRSS-A and the Japanese HISUI missions (Guanter et al., 2015; Iwasaki et al., 2011; Tong et al., 2014). For those missions, the imaging spectroscopy community is currently developing methodologies for e.g. the detection of REEs in the image spectra (Boesche et al., 2015; Boesche, 2015; Börsche, 2015; Herrmann, 2019; van der Meer et al., 2012; Turner et al., 2014a, 2014b; Turner, 2015). Hyperspectral data can be acquired by ground- or UAV-based outcrop scans to study an ore body’s surface geometry and mineral distribution (Figure 1) and can be applied in the laboratory on thin sections, hand samples, as well as drill core to analyse and visualize zonation at a smaller scale.



55 **Figure 1: Example for the application of a spectral library. A) 3D modelling based on 79 RGB images and one RGB HySpex scene from the Apliki mine in the Republic of Cyprus. The mineral analysis from B) is stacked on the 3D model for visualization purposes. B) Analysis based on HySpex scene analyzed by EnGeoMap 2.0 using a custom-made spectral library from USGS spectra (Mielke et al., 2016). C) Example of hyperspectral spectra from copper-bearing minerals as presented in (Koellner et al., 2019).**

60 The methods developed for the upcoming hyperspectral satellite missions like EnMap (Guanter et al., 2015) use image spectra as a database for their analysis. 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. Variations along the spectral domain of the data are visible as concave indentions, often referred to as "absorption bands". They are characteristic for the measured surface material and

enable its identification and quantification (Clark, 2003). The recorded spectral information is a function of the chemical and physical properties of the target material and the sensor setup itself. Typical copper-bearing hyperspectral spectra are shown in Figure 1C.

We are presenting four spectral library files and their geochemical validation. The library files present the spectral information of three different mineral groups: (1) REE-bearing minerals and (2) synthetic REE-oxide powders (Koerting et al., 2019a), (3) copper-bearing minerals without any sample preparation (Koellner et al., 2019) and (4) powders of copper-bearing surface material from the Apliki copper-gold-pyrite mine in the Republic of Cyprus with the corresponding GPS position of the samples (Koerting et al., 2019b). Spectrally, the libraries cover the full wavelength range of the solar optical range (414 nm – 2498 nm). We aim to contribute to the already existing, accredited libraries, e.g. the USGS Spectral Library (Hunt, 1977; Kokaly et al., 2017). The geochemical validation for each sample type is explained in the methods. The two REE libraries (Koerting et al., 2019a) consist of the spectra of 16 rare earth oxide (REO) powders and 14 REE-bearing minerals (REMin). In addition, the spectra of niobium- and tantalum oxide powders are provided, which will further not be mentioned individually but be included in the term “REO”. The third spectral library includes 20 copper-bearing minerals (Koellner et al., 2019) and the fourth spectral library contains 37 surface samples from the Apliki copper-gold-pyrite mine site in the Republic of Cyprus (Koerting et al., 2019b). A list of all the samples can be found in the supplements.

The outline of this document follows the necessary line of knowledge to successfully make use of the here presented spectral libraries. Section 2 includes a description of the analyzed materials and Section 3 informs about the sample preparation and spectra collection. Section 4 describes the hyperspectral data acquisition, covering the processing of the data and spectral measurement parameters and Section 5 presents the geochemical analyses of the samples. Section 6 discusses the parameters influencing the data. The spectral libraries can be downloaded as an ASCII \*.txt file format and as binary spectral library files format \*.sli with its associated header files \*.hdr. A separate data description and the geochemical analysis results are included as data reports in the data publications (Koellner et al., 2019; Koerting et al., 2019a, 2019b).

## 2. Materials

The REE sample material includes 16 REO powders (REO) and 14 REE-bearing minerals (REMin). The REO powders belong to a series of rare earth metals and compounds (REacton®) and were purchased from Alfa Aesar. All REO powders contained at least 99.9% of the REE oxide, as per the seller-supplied concentration certificates. The concentration certificate information can be found in the data description of (Koerting et al., 2019a). The REO powders were obtained as high-purity materials with a grain size of <63 µm. The REMin samples (ore minerals) were purchased from Gunnar Färber Minerals, an online trader of mineral specimens. The mineral notation is based on the sample name provided by Gunnar Färber Minerals. The supplier offers analytical services with a modern REM-EDX technology and therefore we assume his specimens are analyzed and the mineral species is validated before the sale. The X-Ray Fluorescence (XRF) data presented in the data

description of (Koerting et al., 2019a) should be consulted to validate the given mineral nomination noted by Gunnar Färber Minerals. A sample list for the REMin can be found in S1 and S2, for the REO in S3 of the Supplement.

100 The copper-bearing minerals belong to collections of the University of Potsdam (UP) and the Federal Institute for Geosciences and Natural Resources (BGR), a samples list can be found in the appendix (S4-S5). The minerals were measured hyperspectrally with no sample preparation, the sample photos and geochemical analysis are provided in the data description for (Koellner et al., 2019). The Apliki mine surface samples were collected (Koerting et al., 2019b) in March 2018 during a field campaign of the Geological Survey Department of the Republic of Cyprus (GSD) and the GFZ German Research Centre for Geosciences (GFZ). Surface material in the mine was collected and prepared for geochemical analysis by Bureau Veritas Minerals (BVM). The powdered samples were measured hyperspectrally, a sample list including photos  
105 from the in-situ conditions of the samples can be found in S6 of the supplement and in (Koerting et al., 2019b). An overview on sample types and their corresponding sample description in the supplements are listed in Table 1.

**Table 1: Table of sample material and where to find the corresponding sample description tables.**

Sample Material	Sample description in Supplements
REMin	S1, S2
REO	S3
Copper-bearing minerals	S4, S5
Apliki mine powders	S6

### 110 3. Sample Preparation and spectra collection

The sample preparation varied by sample type and depends on the material and the information of interest. This is based on the research projects that the samples stem from and for which the spectral and geochemical data was acquired.

The spectra for each sample were manually extracted from the hyperspectral image scenes using an averaging number of pixels and were compiled in a spectral library. Thereby, each spectrum of a spectral library represents an average spectrum  
115 of the material, depending on the sample size and spectral homogeneity. The extraction of the spectra is explained in detail in each data description (Koellner et al., 2019; Koerting et al., 2019a, 2019b).

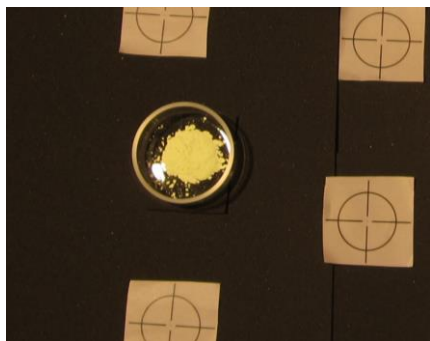
The REO powders were measured in 100% quartz glass petri dishes underlain by black cellular rubber, each powder was measured separately. Figure 2 shows the measurement setup of holmium-oxide powder as an example for the REO powders..

120 The REE-bearing minerals were measured separately. Figure 3 shows the xenotime sample (brownish single crystal embedded in quartz) as an example for the REMin samples. The REMin samples were measured without sample preparation



on black cellular rubber as shown for the copper-bearing minerals in Figure 4. For all measurements, the final spectral analyses were spatially reduced to the centre pixels averaging each identified REE-bearing mineral or a 5x5 pixel average spectrum centred on the REO powder sample. Shadow effects from the sidewalls of the boxes could therefore be minimized.

125 One representative spectrum of every sample was produced for the spectral library. In order to improve the signal-to-noise ratio and reduce the influence of outlier pixels, an average spectrum of sample-covering pixels was produced (Herrmann, 2019).



130 **Figure 2: Holmium-oxide powder in the laboratory HySpex setting in a quartz glass petri dish underlain by black cellular rubber. Geometric markers for the pre-processing were placed alongside the sample.**



**Figure 3: Xenotime embedded in quartz as an example for the REE-bearing mineral samples.**

135

The copper-bearing mineral samples were measured with no sample preparation as the variable surface of the minerals and the influence of the mineral structure was of interest. Figure 4 shows an example scan of a part of the copper-bearing minerals. Table S5 in the supplements shows the area for the geochemical sampling encircled in yellow. The same area was used to obtain the spectrum, averaging over a 5 by 5 pixel window.



Figure 4: Showing HySpex scan “MH\_FK\_LAB\_Cudetect\_008\_09012018\_WR20” as an example to highlight the lack of sample preparation.

The Apliki mine samples were crushed and powdered so that  $\geq 85\%$  of the sample was  $< 75\mu\text{m}$ . Homogenized powders were measured as pressed powder tablets (Figure 5). The area to obtain the sample’s spectra was chosen over a 5 by 5 pixel window, in the centre of the powder tablet to minimize influences from the tablet’s metal frame. The dark spots in each tablet were caused by previous measurements with a laser induced breakdown spectrometer (LIBS). The hyperspectral sample spots were chosen in order to exclude the measurement points of the LIBS in the spectral footprint. In case of broken powder tablets like “7d\_Hem”, the shadowed, rough surface areas were also excluded from the spectral sampling.

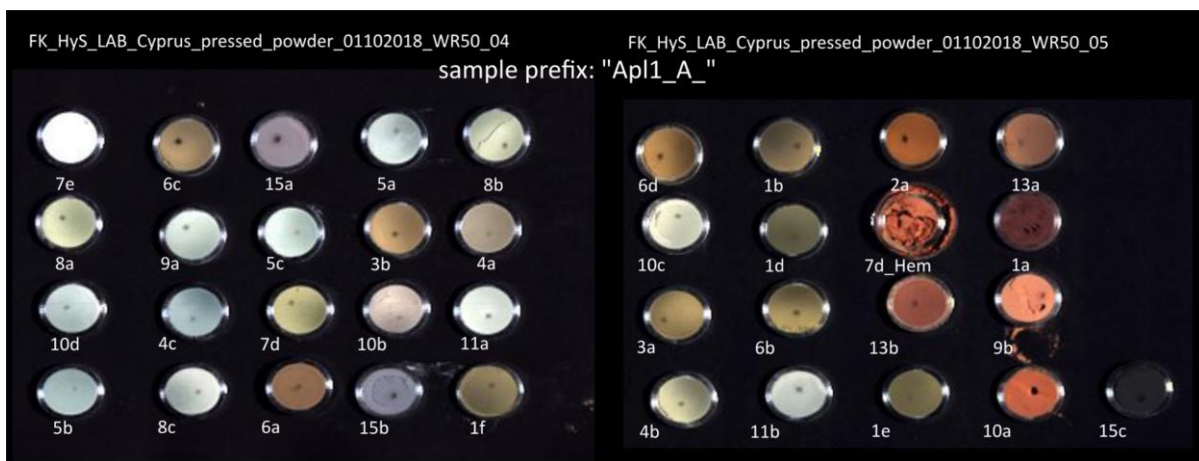


Figure 5: Showing the Apliki mine samples prepared as powder tablets.

#### 4. HySpex Data Recording

The HySpex VNIR-1600 and SWIR-320m-e (technical description available at: [hyspex.no/products/disc.php](http://hyspex.no/products/disc.php), 2019)) are two line-scanning cameras mounted in parallel. They cover the range of the visible to near infrared (VNIR, 414 – 1000 nm) and the short-wave infrared (SWIR, 1000 – 2498 nm). They record an array-line of 1600 pixel (VNIR) and 320 pixel (SWIR) (push-broom scanning). Every pixel contains a spectrum with a total spectral sampling number of 408 bands in total. The HySpex cameras are provided with two acquisition modes, one for airborne data collection and one for laboratory measurements. In laboratory mode, the cameras are combined with a trigger pulse-moving sleigh (translation stage) of definable frame period (depending on the integration time of every array-line acquisition). The configuration of the translation stage framework, the cameras and the light source (Halogen GX6.35, 2 x 1000 W, 45° illumination angle) are fixed, while the sleigh and the samples are moving through the focal plane (Rogass et al., 2017).

The reflectance level of a white reference panel, placed in line with the samples, is chosen according to the albedo of the samples. The higher the albedo of the sample, the higher is the diffuse reflectance factor of the white reference panel that is chosen. For the REE samples (REMin and REO), a white reference panel of 95% reflectance was used, because most of the samples were bright, white powders of a high albedo, this is based on test measurements of (Bösche, 2015; Herrmann, 2019).

The Apliki samples required a 50% reflectance white reference panel, whereas the copper-bearing minerals were measured using a 20% reflectance white reference panel. Both the geometrical setup and the heat up time of the lamp influence the configuration of the light source. The maximum illumination was obtained with a certain angle of 45° between incident light and the vertical plane. The distance between the lamp and the HySpex cameras was higher compared to the distance between samples and sensor to ensure diffuse illumination and to avoid thermal influence on the cameras and the samples. The integration time (= measurement time for each image line) was tested to be as high as possible to suppress the impact of signal uncorrelated gaussian white noise and at the same time as low as needed to avoid detector saturation. For all measurements the integration time was chosen with respect to the sample albedo. The used settings for the REMin and REOs are listed in Table 2, the settings for the copper-bearing minerals in Table 3 and for the Apliki mine samples in Table 4. The laboratory is equipped with black-painted walls and doors, as well as black curtains to avoid reflected light from surfaces other than the sample, an example setup can be seen in Figure 6. The laboratory conditions were kept stable, the air temperature was regulated to  $21 \pm 0.5^\circ\text{C}$  and the humidity was below 70% for all measurements. Black cellular rubber is used as a base material for all samples for hyperspectral data acquisition. It reflects less than 5% on average of the incoming radiation.

Detailed descriptions for the GFZ' standard measurements and the process chain can be found in (Rogass et al., 2017).

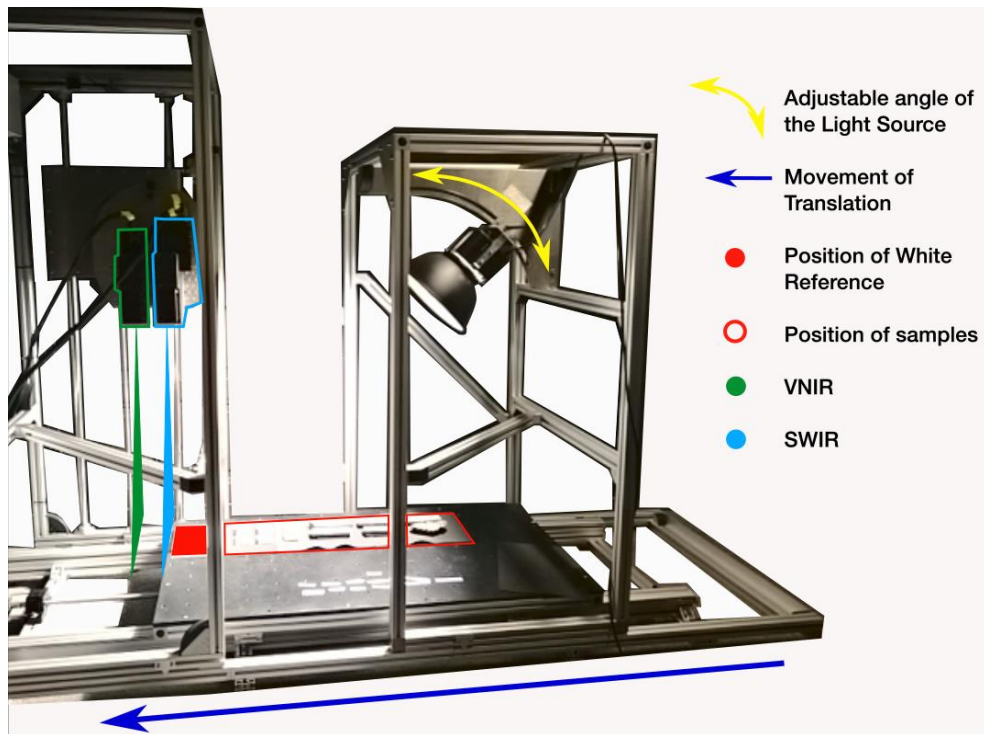


Figure 6: The HySpex translation stage setup (Körting, 2019).

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Table 2: HySpex settings for laboratory measurements of the REO and REMin (Koerting et al., 2019a, modified after (Bösche, 2015; Herrmann, 2019)).

HySpex settings		
Lamp arrangement	45°	
Distance, sample to sensor	1 m	
Sensor arrangement head to head	1m lenses, eq on VNIR	
Wavelength range	414 to 2498 nm	
	VNIR	SWIR
Sampling interval	3.7	6
Radiometric resolution	12 bit	14 bit
Light source	Halogen GX6.35, 2 x 1000 W	
	VNIR (1600 px)	SWIR (320 px)
Frames	variable	variable
Integration time [ $\mu$ s]	30 000	5 000
Frame period [ $\mu$ s]	31 000	123 506

**Table 3: HySpex settings for laboratory measurements of the copper-bearing minerals (Koellner et al., 2019).**

HySpex settings		
Lamp arrangement	45°	
Distance, sample to sensor	30cm	
Sensor arrangement head to head	30cm lenses, eq on VNIR	
Wavelength range	414 to 2498 nm	
	VNIR	SWIR
Sampling interval	3.7	6
Radiometric resolution	12 bit	14 bit
Light source	Halogen GX6.35, 2 x 1000 W	
	VNIR (1600 px)	SWIR (320 px)
Frames	variable	variable
Integration time [ $\mu$ s]	120000 - 140000	15000 - 20000
Frame period [ $\mu$ s]	120062 - 141004	478334 - 561768

**Table 4: HySpex settings for laboratory measurements of Apliki mine powdered samples (Koerting et al., 2019b).**

HySpex settings		
Lamp arrangement	45°	
Distance, sample to sensor	1 m	
Sensor arrangement head to head	1m lenses, eq on VNIR	
Wavelength range	414 to 2498 nm	
	VNIR	SWIR
Sampling interval	3.7	6
Radiometric resolution	12 bit	14 bit
Light source	Halogen GX6.35, 2 x 1000 W	
	VNIR (1600 px)	SWIR (320 px)
Frames	variable	variable
Integration time [ $\mu$ s]	60000	10000
Frame period [ $\mu$ s]	60060	239282

## 205 Hyperspectral Data Processing

Each measurement run produces one VNIR and one SWIR 3D-data cube. The three dimensions are the two spatial x,y- and the spectral z-dimension. The 3D image cubes are produced, by moving a homogeneous reflecting white reference panel and the samples through the focal plane of the two sensors. The VNIR image cube is resized to the spatial dimensions of the SWIR data cube, co-registered and stacked with the SWIR data cube resulting in a continuous image cube with the spectral range of 414 – 2498 nm. In order to produce a reflectance image, the image pixel that show the white standard were averaged to a one-line reference spectrum. The reflectance was calculated by dividing every image line spectrum by its reference spectrum from the reflecting white reference panel. A detailed description for the laboratory set-up and processing can be found in (Rogass et al., 2017). The software ‘HySpex ground’ is used to perform the measurements and the software ‘HySpex rad’ is used to perform the radiometric calibration on the image data.

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### 5. Geochemical Sample Analysis for Sample Characterization

Depending on the sample type, the geochemical analysis methods differ. The methods used for each sample type, can be found in Table 5.

220 Table 5: Sample type and corresponding geochemical characterization method.

Sample type	Geochemical Analysis
REO (Koerting et al., 2019a)	Laboratory certificates
REMin (Koerting et al., 2019a)	X-Ray Fluorescence (XRF), Electron probe microanalyzer (EPMA) analyses
Copper-bearing minerals (Koellner et al., 2019)	Scanning electron microscope (SEM), EPMA
Apliki mine samples (Koerting et al., 2019b)	Bureau Veritas Mineral Analysis

#### 5.1 Thermo Niton XL3t (XRF)

The geochemical validation measurements for the REMins were performed using an X-Ray Fluorescence (XRF) instrument - Thermo Niton XL3t (Fisher Scientific, 2002). The XL3t is a lightweight, hand-held XRF analyzer. The measurement principle follows the principle of X-Ray fluorescence, where the sample inbound X-Rays excite electrons to a higher energy level in the sample material. Energy in form of XRF radiation is released when these electrons return to their original state. The frequency of this radiation is characteristic for the measured chemical element and its intensity is correlated to the concentration level. The intensity of each element is detected as counts per second by the detector, a geometrically optimized

225

large area drift detector (GOLDD). The maximum excitation voltage of the XL3t device is 50 kV, which means out of the  
230 full REE suite only four light REEs can be detected (Lanthanum, Cerium, Praseodymium and Neodymium).

The XL3t spectrometer is attached to a lead shielded sample chamber, in which samples with a diameter smaller than 3.3 cm  
can be placed. Mineral samples can be directly placed in the chamber; powdered samples have to be placed in sample tubes  
(2.5 cm diameter). The sample tubes are made of plastic with a plastic foil on the bottom. The plastic cannot be detected by  
XRF and therefore not interfere with the measurements. A built-in camera of the XL3t enables the precise location of the  
235 measuring spot. The software used for the measurements is named “NDTr” and the measurement mode was “mining and  
exploration”. The concentration levels are provided along with a balance value. “Balance” represents counts per seconds that  
could not be attributed to one of the measured elements. Table 6 shows the measurement modes and filters used. In-depth  
description of the XL3t and the XL3t-results for each sample can be found in (Bösche, 2015; Herrmann, 2019)

240 **Table 6: Settings used for the Thermo Niton XL3t X-ray fluorescence device (Bösche, 2015).**

Thermo Niton XL3t Setting	
Measurement mode	Test all geo
Filter	Main, Low, High, Light
Filter measurement time	30 seconds each

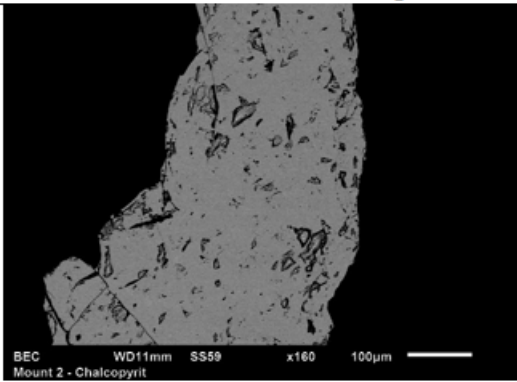
## 5.2 Scanning Electron Microscope (SEM) and Electron Probe Microanalyzer (EPMA)

### Copper-bearing minerals

245 In order to obtain information about the zonation and internal fabrics of the copper-bearing minerals a fully automated JEOL  
JSM-6510 scanning electron microscope (SEM) (20kV acceleration voltage) at the University of Potsdam was used. A back-  
scattered electron detector displays compositional variation in the imaging area based on the mean atomic number of the  
pixel. An energy dispersive X-ray spectrometer (EDX, Oxford Instruments INCAx-act) attached to the instrumentation  
provides quantitative elemental analysis of single spots. After calibrating with pure copper, a wide spectrum of elements can  
250 be identified. Based on previous results, divergences of up to 5 weight % can be expected, which for quantitative analysis is  
acceptable.

In order to approximate the values for copper a JEOL JXA-8200 electron probe microanalyzer (EPMA) at the University of  
Potsdam was used. The electron microprobe is equipped with five wavelength-dispersive X-ray spectrometers (WDX) and  
255 was operated with a 20 kV accelerating voltage, a 20 nA current, and a beam diameter of 2 µm. The analytical counting  
times were 20/10 s for the element peak and 10/5 s for background positions. Analyses were calibrated using  
silicates/sulphides obtained from the Smithsonian Institution and Astimex. Quantifying elements of a lower atomic mass  
than boron is not possible, carbon cannot be measured either.

260 An example analysis for copper-bearing mineral sample C1 can be seen in Figure 7 and Table 7, the full SEM and EPMA data files are documented in (Koellner et al., 2019).

No:		backscatter electron image	
16 C1 - S55L16C (Mount 1)		EDX ( $\Sigma = 100$ wt%)	
		CCp	S: 38,7 ; Fe: 28,7 ; Cu: 32,57
		WDX (Mount 1) Mean(3 Measurements)	
		CCp	S: 34,941 ; Fe: 30,091 ; Cu: 34,094

265 Figure 7: Sample C1 SEM and EPMA analysis example

Table 7: Sample C1 EPMA analysis example, up to 3 measurement spots for each sample (C1-S55L16c-1 – 3 in the “comment column”). Element concentrations reported as wt%.

Al	Hg	Fe	Cu	Si	S	Mn	Total	Comment
-	0.035	30.002	33.98	-	34.805	0.002	98.824	C1-S55L16c-1
-	0	30.193	34.108	0.003	34.931	0.004	99.239	C1-S55L16c-2
-	0.001	30.077	34.194	-	35.086	-	99.358	C1-S55L16c-3

## 270 REE-bearing Minerals

Some of the REMin (xenotime, bastnaesite, fluorapatite, synchysite and ilmenite) were additionally analyzed by using a JEOL JXA-8200 electron microprobe (EPMA) at the University of Potsdam based on a method developed by (Lorenz et al., 2019). The conditions used for the analysis were: 20kV acceleration voltage, 20nA beam current and a beam size of 2 µm. Counting times were between 10 s - 20 s on peak for major elements and 50 s for REE and other trace elements.



275 The following spectral lines and mineral standards from Smithsonian and Astimex were used: fluorapatite (F K $\alpha$ , P K $\alpha$ , Ca  
K $\alpha$ ), albite (Na K $\alpha$ ), fayalite (Fe K $\alpha$ , Mn K $\alpha$ ), wollastonite (Si K $\alpha$ ), omphacite (Al K $\alpha$ ), LaPO<sub>4</sub> (La L $\alpha$ ), PrPO<sub>4</sub> (Pr L $\beta$ ),  
CePO<sub>4</sub> (Ce L $\alpha$ ), NdPO<sub>4</sub> (Nd L $\beta$ ), YPO<sub>4</sub> (Y L $\alpha$ ), EuPO<sub>4</sub> (Eu L $\alpha$ ), SmPO<sub>4</sub> (Sm L $\beta$ ), LuPO<sub>4</sub> (Lu L $\alpha$ ), GdPO<sub>4</sub> (Gd L $\alpha$ ), ErPO<sub>4</sub>  
(Er L $\beta$ ), DyPO<sub>4</sub> (Dy L $\beta$ ), YbPO<sub>4</sub> (Yb L $\alpha$ ), HoPO<sub>4</sub> (Ho L $\beta$ ), monazite (Th M $\alpha$ , U M $\beta$ , Tb L $\alpha$ ), uranothorite (U M $\beta$ ), crocoite  
280 on the  $\phi(\rho z)$  method (Heinrich and Newbury, 1991).

### 5.3 Apliki mine surface sample analysis

The Apliki mine samples were analyzed by Bureau Veritas Minerals – Mineral Laboratories Canada (BVM) using their  
standard packages (Bureau Veritas, 2020). The samples were pulverized and analyzed for major, minor and trace elements  
285 using ICP-MS and ES. The internal BVMs sample preparation-/ analysis type groups by the required analysis method. These  
“analysis types” are namely “aquatic”, “rock” and “soil”. The sample numbers, associated analysis type and internal BVM  
analysis codes can be found in the technical report of the Apliki mine surface sample data (Koerting et al., 2019b).

## 6. Validation and Discussion

290 Technical validation of the results in terms of sample material properties, systematic errors and variation of measurements  
(experimental error) are given below.

### Sample Material Properties

295 The REO powders were certified to contain at least 99.9% of the corresponding REO. The certificates are listed in (Koerting  
et al., 2019a). The REE mineral samples were geochemically analyzed using the Thermo Niton XL3t (Fisher Scientific,  
2002) device. The resulting element concentrations and the measurement error ( $2\sigma$ ) are provided in Koerting et al. (2019a).  
The validation for the copper-bearing minerals can be found in Koellner et al. (2019) and the Apliki mine sample validation,  
analyzed by BVM, can be found in Koerting et al. (2019b).

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### Systematic Errors of hyperspectral data acquisition

Systematic errors are discussed based on instrument drift, calibration and optimization of measurements. Initializing a warm-  
up phase of optical components, detectors and lamps, reduced influences due to instrument drift. Additionally, laboratory  
conditions were monitored to ensure a stable temperature and humidity. The HySpex cameras and the reference standards are  
305 factory calibrated once per year. Measurements used for the final spectral library were collected within one calibration time  
span to ensure equal acquisition conditions. For HySpex, averaging multiple measurements minimizes variations in the data.  
An average (median) of 500 to 800 pixel spectra was taken for the HySpex REE and REO spectra. This number relates to the  
maximum number of non-disturbed pixels per sample region of interest (e.g., pixels that were not shadowed from the sample

holder side walls, etc.). For the copper-bearing minerals and the Apliki mine powders a 5x5 average pixel window was chosen over the area of interest. For these samples using a smaller pixel number for the average was necessary as the sampling of the copper-bearing minerals for geochemical validation occurred over a small area of the sample and the Apliki mine powder tablets were too small to ensure a larger homogenous area.

### Measurements variation

Variations of measurements were not only based on instrument calibrations or drift. They can also occur due to the detector geometry or geochemical properties of the minerals. These variations may appear as a shift of the peak positions of the absorption bands. This means, different hyperspectral sensors will show variations in the spectrum of the same material. By only using one set of hyperspectral sensors, the HySpex VNIR and SWIR, these shifts will not appear in our data sets. They might show when comparing our spectra of a material with spectra taken from a different instrument. For the copper-bearing minerals, the sample spectra also differ when comparing different samples of the same mineral species (e.g. “Malachite”) to each other. The spectral signal differs, for example, due to changes in geochemistry, physical appearance e.g. crystallization and degree of weathering (Clark, 1999; Hunt, 1982; Hunt and Ashley, 1979).

### XL3t systematic errors

The XL3t is internally calibrated and provides an internal warm-up phase to guarantee stable measurement conditions. Unlike the spectrometer measurements, experimental error was only provided for the XL3t. In order to reduce the experimental error, a long duration measurement time of 120 seconds was set. The XL3t collects the emitted radiation from the sample using four different filters. While the sample was irradiated, each filter measures counts per second within a time span of 30 seconds. Next, the average counts per second were internally transformed to ppm. The irradiation of, in total, 120 seconds per sample was empirically tested to enable short measurement duration in combination with the lowest achievable standard deviation of concentration level.

## 7. Data Availability

The spectral libraries are published under the Creative Commons Attribution International 4.0 Licence (CC BY 4.0) via GFZ Data Services. Due to the different types of samples, we present the following three data publications: (1) 32 rare-earth minerals and rare-earth oxide powders including niobium- and tantalum-oxide powder (Koerting et al., 2019a), <http://doi.org/10.5880/GFZ.1.4.2019.004>); (2) Mineral spectra and chemistry of 20 copper-bearing minerals (Koellner et al., 2019); <http://doi.org/10.5880/GFZ.1.4.2019.003>) and (3) Mineral spectra and chemistry of 37 copper-bearing surface samples from Apliki copper-gold-pyrite mine in the Republic of Cyprus (Koerting et al., 2019b); <http://doi.org/10.5880/GFZ.1.4.2019.005>).

## 8. Sample Availability

The samples provided by the BGR are available through the collection of the BGR Spandau by their sample name in table S5 in the supplements (<https://www.gewis.bgr.de>). The samples provided by the GFZ and UP belong to projects and have to be requested separately.

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## 9. Appendices

**Table A1: List of less commonly known terms and their abbreviations used throughout the paper**

Terms	Abbreviation	Description
Abbreviation	REE	Rare Earth Element
	REO	Rare Earth Oxide
	REMin	Rare Earth Element bearing Mineral
	VNIR	Visible light and near infrared
	SWIR	Short wave infrared
	XRF	X-Ray fluorescence
	EnMAP	Environmental Mapping and Analysis Program: future earth observation satellite mission ( <a href="http://www.enmap.org">www.enmap.org</a> ) <sup>1</sup>
	CCRSS-A	China Commercial Remote Sensing Satellite System: future earth observation satellite mission
	HISUI	Hyperspectral Imager Suite: future earth observation satellite mission
Instruments	HySpex VNIR-1600	HySpex pushbroom spectrometer, VNIR camera
	HySpex SWIR-320m-e	HySpex pushbroom spectrometer, SWIR camera
	HySpex ground	HySpex operational software for laboratory and near-field application
	HySpex rad	HySpex calibration software to transform raw DN into radiance data
	Thermo Scientific Niton XL3t	Thermo Scientific Inc. X-Ray fluorescence analyzer (NITON TM XL3t)

	NDTr	Thermo Scientific Inc. NITON TM operational software
	JEOL JXA-8200	Electron probe microanalyzer (EPMA)
	JEOL JSM-6510	Scanning electron microscope (SEM)
	Oxford Instruments INCAx-act	Energy dispersive X-ray spectrometer (EDS)
Registered brands, Copyrights and/ or other protected terms	REacton®	Series of rare earth metals and compounds
	Alfa Aesar	Manufacturer and supplier of chemicals for research and development (today: Thermo Scientific Inc.)
	Gunnar Färber Minerals	Supplier of mineral specimen
	REEMAP	Rare Earth Element MAPping: Research project for the development of a modular multi-sensor processing chain for modern imaging spectrometers to detect REEs
	Smithsonian Institution	Smithsonian Institution Department of Mineral Sciences, reference material from the Smithsonian Microbeam Standards
	Astimex Standards Ltd.	Astimex produces standards suitable for electron probe and scanning electron microscope X-ray analysis.
Research and federal institutes	BGR	Federal Institute for Geosciences and Natural Resources
	GSD	Geological Survey Department, Ministry of Agriculture, Rural Development and Environment, Republic of Cyprus
	UP	University of Potsdam
	GFZ	German Research Centre for Geosciences
Registered Trademarks	Excel™	Microsoft Excel™

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## 10. Author contributions

*Apliki mine and copper-bearing minerals:* Friederike Koerting designed the Apliki sample related study, performed and supervised the measurements for Marcel Hornings' data and the Apliki samples and wrote the manuscript. Nicole Koellner designed the copper sample study, supervised the measurements and performed the geochemical analysis at the University of Potsdam. Marcel Horning performed most of the measurements on the copper samples and prepared the spectral copper library. Pia Brinkman prepared the Apliki sample powder tablets. Christian Mielke, Agnieszka Kuras, Constantin Hildebrand and Friederike Klos prepared parts of the spectral libraries. *REE minerals and REOs:* Nina K. Boesche designed the REE study, performed some measurements, and supervised the REE measurements. Sabrina Herrmann prepared the samples and conducted most of the measurements. Christian Rogass developed and applied the HySpex post-processing chain. Christian Mielke and Kirsten Elger helped revising the manuscript. Uwe Altenberger supervised the studies and gave some valuable comments on the manuscript.

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## 11. Competing interests

The authors declare no conflict of interest

## 12. Acknowledgements

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# Supplements to: A Solar Optical Hyperspectral Library of Rare Earth-bearing minerals, RE-Oxide powders, copper-bearing minerals and Apliki mine surface samples. Sample Descriptions.

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## TABLE OF CONTENTS

	<b>Table S1: Rare Earth Mineral sample name, formula, size and provenance</b>	2
	<b>Table S2: REE-bearing mineral sample name and sample photo.</b>	3
15	<b>Table S3: Rare Earth Oxide Powders, Suppliers, Product Number and Lot Number.</b>	5
	<b>Table S4: Copper and copper-bearing minerals, abbreviation, alteration, collection, collection locality</b>	6
	<b>Table S5: Copper and copper-bearing minerals listed with their sample name, collection and the area of sampling for EDX/WDX analyses and spectra retrieval</b>	7
20	<b>Table S6: Apliki mine surface samples, including description, coordinates of sampling in March 2018 in the Republic of Cyprus and a field photo of the sample.</b>	12
	<b>References</b>	17











The spectral libraries and corresponding geochemistry of the samples listed here are published via GFZ Data Services with the following DOIs: <http://doi.org/10.5880/GFZ.1.4.2019.004> (REE-bearing minerals and REO powders, (Koerting et al., 2019a)), <http://doi.org/10.5880/GFZ.1.4.2019.003> (copper-bearing minerals, (Koellner et al., 2019)), and <http://doi.org/10.5880/GFZ.1.4.2019.005> (copper-bearing surface samples from the Apliki copper-gold-pyrite mine in Cyprus, (Koerting et al., 2019b)).







Table S1: Rare Earth **-bearing mineral sample name, formula, size and provenance, modified after (Bösche, 2015; Herrmann, 2019).**

Rare Earth Mineral	Formula	Mineral size	Collection Locality
Baropyrochlore. Fluorapatite	$(\text{Ba, Sr})(\text{Nb, Ti})_2(\text{O,OH})_7$	0.5 x 0.2 cm	Mina Boa Vista. Catalao. Goias/Brazil
Bastnaesite (Ce)	$\text{Ce}[\text{F} \text{CO}_3]$	3 x 1.3 cm	Zagi Mountain. Warzal Dam. Pechawar. North-West Frontier Prov./Pakistan
Gadolinit (Y). Synchysite (Y). Fluorite	$\text{Y}_2\text{Fe}_2+\text{Be}_2\text{O}_2(\text{SiO}_4)_2$	1.1 x 0.7 cm	White Cloud Pegmatite. South Platte. Jefferson Co. Colorade/USA
Monazite (Sm) incl. <b>Monazite (Nd)</b>	$\text{SmPO}_4. (\text{Nd,Ce, La})(\text{P, Si})\text{O}_4, \text{Ca}(\text{Ce, La})_2(\text{CO}_3)_3\text{F}_2$	0.2 x 0.2 cm	Svodovyi. Grubependity Lake. Maldynyrd Range. Prepolar Ural. Komi Republic. Russia
Parisite (Nd) incl. Parisite (Ce)	$\text{Ca}(\text{Nd, Ce, La})_2(\text{CO}_3)_3\text{F}_2$	2.6 x 1.6 cm	Mountain Pass Mine. Ivanpah Mts. San Bernardino Co. California/USA
Polycrase (Y)	$(\text{Y,Ca,Ce,U,Th})(\text{Ti,Nb, Ta})_2\text{O}_6$	0.5 x 0.1 cm	Puotevare Pegmatite. Tjalmejaure Lake. Jokkmokk Lappland/Northern Sweden
Synchysite (Y)	$\text{CaY}(\text{CO}_3)_2\text{F}$	1.5 x 2.5 cm	White Cloud Pegmatite. South Platte. Jefferson Co. Colorade/USA
Xenotime (Y) (a)	$\text{Y PO}_4$	0.7 x 0.3 cm	Novo Horizonte. Ibitiara. Bahia/Brazil
Xenotime (Y) (b)	$\text{Y PO}_4$	1.2 x 0.4 cm	Novo Horizonte. Ibitiara. Bahia/Brazil
Aegirine. "Acmite"	$\text{NaFe}^{3+}[\text{Si}_2\text{O}_6]$	4.5 x 2.5 cm	Rundemyr. Øvre Eiker. Buskerud. Norway/TYP
Fluorapatite. Albite	$\text{Ca}_5(\text{PO}_4)_3\text{F}, \text{NaAlSi}_3\text{O}_8$	1.2 x 0.5 cm	Golconda Mine. Governador Valadares. Doce Valley. Minas Gerais/Brazil

40 Table S2: REE-bearing minerals within mineral assemblage; Sample name and sample photo. REE-bearing samples are not mono-minerals, instead the REE-bearing minerals were singled out in the hyperspectral and geochemical measurements.

Rare earth –bearing mineral sample	Sample Photo	Rare earth –bearing mineral sample	Sample Photo
Baropyrochlore. Fluorapatite		Polycrase (Y)	
Bastnaesite (Ce)		Synchysite (Y), Microcline, Quartz	
Gadolinite (Y) Synchysite (Y), Fluorite		Xenotime (Y) (a)	
Monazite (Sm) incl. Monazite (Nd)		Xenotime (Y) (b)	
Parisite (Nd) incl. Parisite (Ce)		Aegirine, "Acmite"	

Rare earth –bearing mineral sample	Sample Photo	Rare earth –bearing mineral sample	Sample Photo
Fluorapatite, Albite		Illmenite	
Fluorite		Zircon	

**Table S3:** Rare Earth Oxide Powders, Suppliers, Product Number and Lot Number. Certificates of purity can be found in the data description (Koerting et al., 2019a).

Rare Earth Oxide Powder, Supplier	Product Number	Lot Number
Lanthanum (III) oxide, REacton	11272	B08X015
Cerium (IV) oxide, REacton	11372	L07S057
Neodymium (III) oxide, REacton	11250	C02W029
Samarium (III) oxide, REacton	11229	61200836
Europium (III) oxide, REacton	11299	A16Z001
Gadolinium (III) oxide, REacton	11290	A13W016
Terbium (III,IV) oxide, REacton	11208	J24Q019
Dysprosium (III) oxide, REacton	11319	61300733
Holmium (III) oxide, REacton	11280	J11X030
Erbium (III) oxide, REacton	11310	61000356
Thulium (III) oxide, REacton	11198	F25S060
Ytterbium (III) oxide, REacton	11191	61201069
Lutetium (III) oxide, REacton	11255	G14X082

Yttrium (III) oxide, Sigma-Aldrich	204927	MKBL2030V
Niobium (V) oxide, Alfa Aesar	11366	L18Y022
Tantalum (V) oxide, Alfa Aesar	14709	I14Y039




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**Table S4: Copper and copper-bearing minerals, abbreviation, alteration, collection, collection locality (Koellner et al., 2019).**


Sample	Visible alteration	Collection	Collection locality
K1	slightly altered	University of Potsdam	Furnace, Luebeck, Germany
A1	altered, nodular	University of Potsdam	Cheroy near Lyon, France
A2	altered	University of Potsdam	Tsumeb near Otavi, Namibia
A3	strongly altered	BGR Spandau	Cornberg near Fulda, Germany
M1	altered, nodular	BGR Spandau	L'Etoile du Congo Mine, Katanga, Kongo
M2	strongly altered	BGR Spandau	Henderson Mine, Clear Creek Country, USA
M3	altered	BGR Spandau	Tsumeb near Otavi, Namibia
M4	strongly altered	BGR Spandau	Ogonja Mine in Okahandja, Namibia
M5	lightly altered, spicular	BGR Spandau	Siegen, Germany
C1	strongly altered	BGR Spandau	Füsseberg Mine, Siegerland, Germany
C2	slightly altered	BGR Spandau	Erzgebirge, Slovakia
C3	tarnished	BGR Spandau	Henderson Mine, Clear Creek Country, USA
C4	slightly altered	University of Potsdam	Cornwall, England, GB
C5	altered	University of Potsdam	Clausthal, Harz, Germany
P1	slightly altered	University of Potsdam	Jordan
P2	slightly altered	University of Potsdam	Jordan
P3	slightly altered	University of Potsdam	Jordan
B1	slightly altered, powdered	BGR Spandau	Altenberg, Slovakia
F1	slightly altered	BGR Spandau	Kotterbach near Witkow, Poland



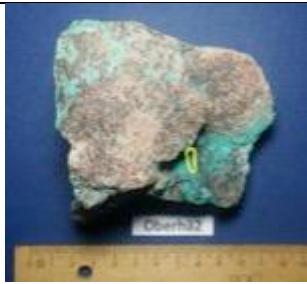

L1	slightly altered, spicular	Uni Potsdam	Unknown location
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50 **Table S5: Copper and copper-bearing minerals listed with their sample name and collection (University of Potsdam = UP, BGR Spandau = BGR) and the area of sampling for EDX/WDX analyses and spectra retrieval (Koellner et al., 2019).**


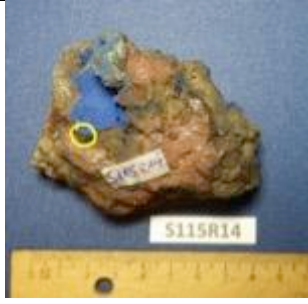

Sample	Sample name (collection)	Material	Formula	Spectra and sampling location
K1	600-1 (UP)	Copper	Cu	
A1	2458 (UP)	Azurite	$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$	
A2	2437 (UP)	Azurite	$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$	
A3	S101L7 (BGR)	Azurite	$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$	

Sample	Sample name (collection)	Material	Formula	Spectra and sampling location
M1	S134R8 (BGR)	Malachite	$\text{Cu}_2[(\text{OH})_2\text{CO}_3]$	
M2	S131L5 M (BGR)	Malachite	$\text{Cu}_2[(\text{OH})_2\text{CO}_3]$	
M3	S131R4 (BGR)	Malachite	$\text{Cu}_2[(\text{OH})_2\text{CO}_3]$	
M4	S132L2 (BGR)	Malachite	$\text{Cu}_2[(\text{OH})_2\text{CO}_3]$	
M5	S55L16 M (BGR)	Malachite	$\text{Cu}_2[(\text{OH})_2\text{CO}_3]$	

Sample	Sample name (collection)	Material	Formula	Spectra and sampling location
C1	S55L16 C (BGR)	Chalcopyrite	$\text{CuFeS}_2$	
C2	S115R12 (BGR)	Chalcopyrite	$\text{CuFeS}_2$	
C3	S131L5 C (BGR)	Chalcopyrite	$\text{CuFeS}_2$	
C4	7534 (UP)	Chalcopyrite	$\text{CuFeS}_2$	

Sample	Sample name (collection)	Material	Formula	Spectra and sampling location
C5	7526 (UP)	Chalcopyrite	$\text{CuFeS}_2$	
P1	Oberhä (UP)	Plancheite	$\text{Cu}_8\text{Si}_8\text{O}_{22}(\text{OH})_4 \cdot \text{H}_2\text{O}$	
P2	Oberhä2 (UP)	Plancheite	$\text{Cu}_8\text{Si}_8\text{O}_{22}(\text{OH})_4 \cdot \text{H}_2\text{O}$	
P3	Oberhä3 (UP)	Plancheite	$\text{Cu}_8\text{Si}_8\text{O}_{22}(\text{OH})_4 \cdot \text{H}_2\text{O}$	



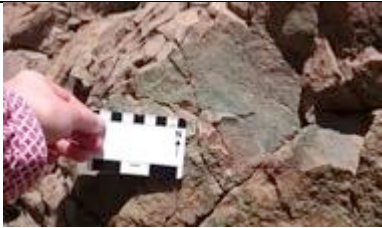









Sample	Sample name (collection)	Material	Formula	Spectra and sampling location
B1	S115R3 (BGR)	Brochantite	$\text{Cu}_4(\text{SO}_4)(\text{OH})_6$	
F1	S115R14 (BGR)	unknown	-	
L1	9542 (UP)	Linarite	$\text{PbCu}(\text{SO}_4)(\text{OH})_2$	






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**Table S6:** Apliki mine surface samples, including description, coordinates of sampling in March 2018 in the Republic of Cyprus and a field photo of the sample (Koerting et al., 2019b).






Sample	Description	Decimal latitude	Decimal longitude	Photo
<i>Apl1_A_1a</i>	Grey green "fresh" surface	35,077033	32,842833	
<i>Apl1_A_1b</i>	hematite coloured weathering crust	35,077017	32,842833	
<i>Apl1_A_1d</i>	"fresh" dark green weathering crust	35,077017	32,842833	
<i>Apl1_A_1e</i>	yellow-ish orange weathering crust	35,077033	32,8428	
<i>Apl1_A_1f</i>	"soil formation", gravel	35,07700	32,84275	

Sample	Description	Decimal latitude	Decimal longitude	Photo
<i>Apl1_A_2a</i>	<i>waste, soil</i>	35,076867	32,84275	
<i>Apl1_A_3a</i>	<i>yellow-ish weathered, soil</i>	35,076983	32,843083	
<i>Apl1_A_3b</i>	<i>brown-ish weathered, soil</i>	35,077	32,84305	
<i>Apl1_A_4a</i>	<i>white, small grained gravel,</i>	35,076967	32,843067	
<i>Apl1_A_4b</i>	<i>grey, small grained gravel</i>	35,077	32,843033	

Sample	Description	Decimal latitude	Decimal longitude	Photo
Apl1_A_4c	grey-green, weathering crust	35,077	32,842633	
Apl1_A_5a	grey-medium, weathering crust	35,076983	32,843167	
Apl1_A_5b	grey-dark, weathering crust	35,07705	32,843167	
Apl1_A_5c	grey-light, weathering crust	35,077083	32,843183	
Apl1_A_6a	Red-ish brown, soil, gravel	35,076967	32,8431	
Apl1_A_6b	Red-ish brown, soil	35,07695	32,8432	All samples from same spot, see 6a
Apl1_A_6c	Red-ish brown	not available	not available	All samples from same spot, see 6a
Apl1_A_6d	Red-ish brown, soil	not available	not available	All samples from same spot, see 6a

Sample	Description	Decimal latitude	Decimal longitude	Photo
Apl1_A_7d	<i>Grey, crust unstable</i>	35,076967	32,84325	
Apl1_A_7d _Hem	<i>Red, hematite</i>	35,076967	32,84325	
Apl1_A_7e	<i>blue crystal</i>	35,076833	32,843217	
Apl1_A_8a	<i>grey, small grained gravel</i>	35,076917	32,8433	
Apl1_A_8b	<i>grey, small grained gravel</i>	35,076933	32,84335	

Sample	Description	Decimal latitude	Decimal longitude	Photo
Apl1_A_8c	grey, soil-ish,	35,076917	32,8433	
Apl1_A_9a	light green weathering crust	35,076883	32,843333	
Apl1_A_9b	hematite vein	35,076833	32,843317	
Apl1_A_10a	white with pink, weathering crust	35,076733	32,843383	
Apl1_A_10b	white with purple, weathering crust	35,076833	32,843383	
Apl1_A_10c	green-ish veins	35,07685	32,843333	

Sample	Description	Decimal latitude	Decimal longitude	Photo
Apl1_A_10 d	White evaporate crust	35,076833	32,84335	See overview photo from 10c, no detail photo available
Apl1_A_11 a	Grey, weathering crust	35,076783	32,843533	
Apl1_A_11 b	Green, weathering crust	35,076767	32,843517	
Apl1_A_13 a	red, rock	35,076133	32,843333	
Apl1_A_13 b	red, gravel, weathered hillside rock	35,076117	32,8434	
Apl1_A_15 a	dark blue crystalline crust	35,076133	32,843217	
Apl1_A_15 b	light blue rock+ blue crust	35,076133	32,843217	See sample Apl1_A_15a

Sample	Description	Decimal latitude	Decimal longitude	Photo
Apl1_A_15 c	<i>black pyrite</i>	35,076133	32,843217	See sample Apl1_A_15a

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80

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