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

5 Friederike Koerting[1], Nicole Koellner[1], Agnieszka Kuras[1], Nina K. Boesche[1], Christian Rogass[1], Christian Mielke[1], Kirsten Elger[1], Uwe Altenberger[2]

[1] GFZ German Research Centre for Geosciences, Potsdam, 14473, Germany
[2] University of Potsdam, Institute of Geosciences, Potsdam, 14476, Germany

Correspondence to: Friederike Koerting (koerting@gfz-potsdam.de)

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)).

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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 prospection. 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; Bösche, 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.
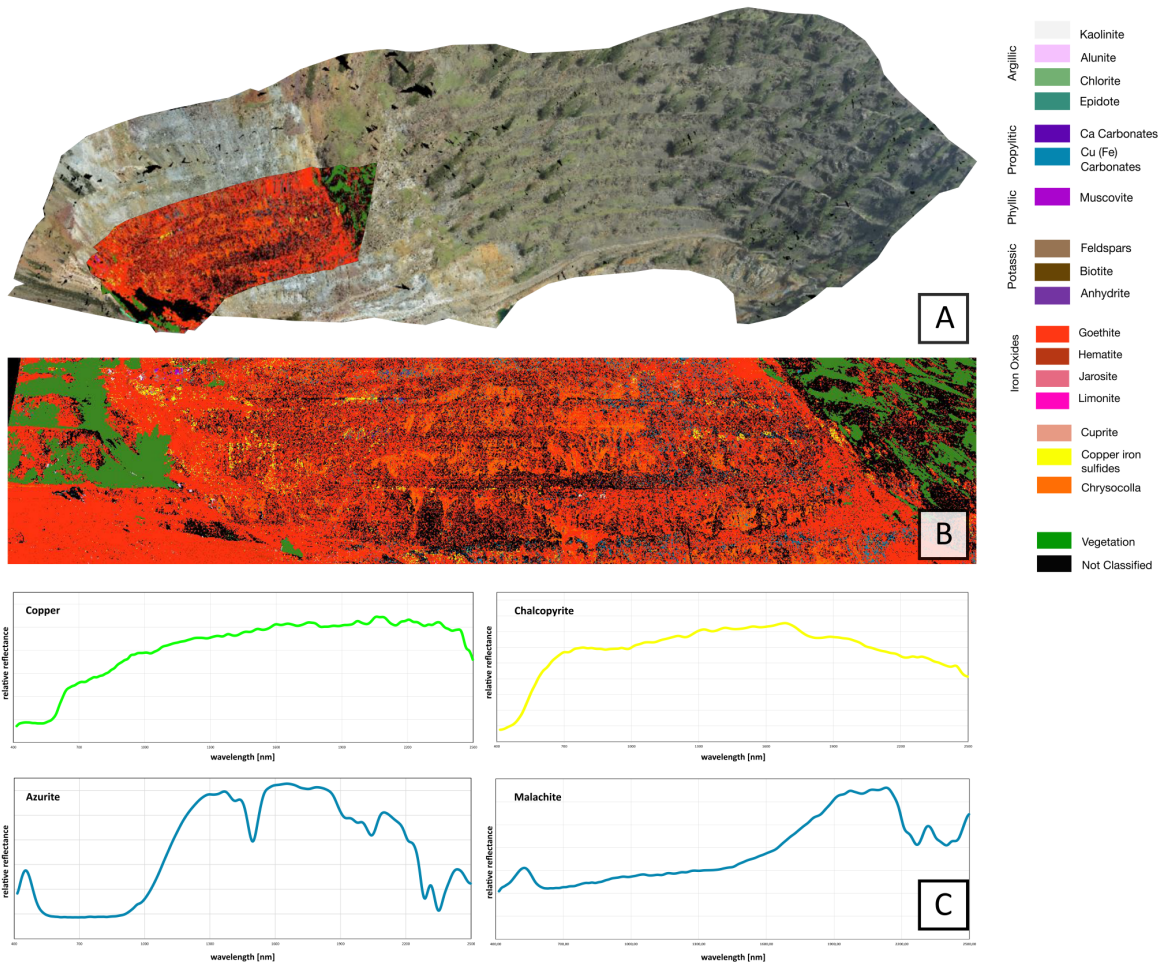
Figure 1: Example for the application of a spectral library. A) 3D modelling based on 79 RGB images and one RGB HySpex scene from the Apliki mine in the Republic of Cyprus. The mineral analysis from B) is stacked on the 3D model for visualization purposes. B) Analysis based on HySpex scene analyzed by 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).

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 grainsize 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 specimen 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.

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 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

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 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..

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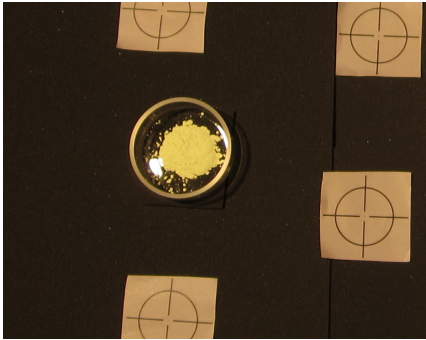
Figure 2: Holmium-oxide powder in the laboratory HySpex setting in a quartz glass petri dish underlain by black cellular rubber. Geometric markers for the pre-processing were placed alongside the sample.

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

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 ≥85% of the sample was < 75μm. 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.
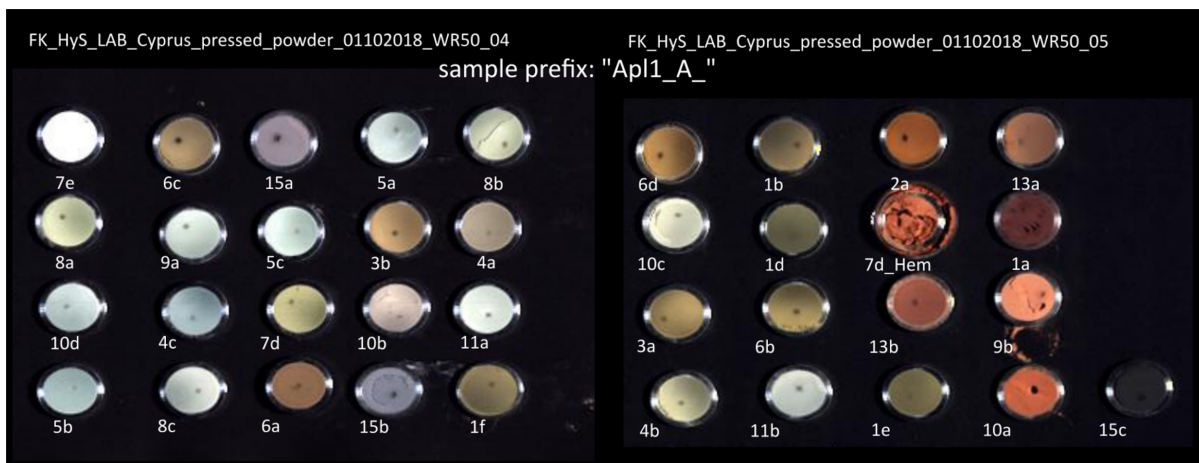
Figure 5: Showing the Apliki mine samples prepared as powder tablets.

4. HySpex Data Recording

The HySpex VNIR-1600 and SWIR-320m-e (technical description available at: (hyspex.no/products/disc.php, 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±0.5°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).
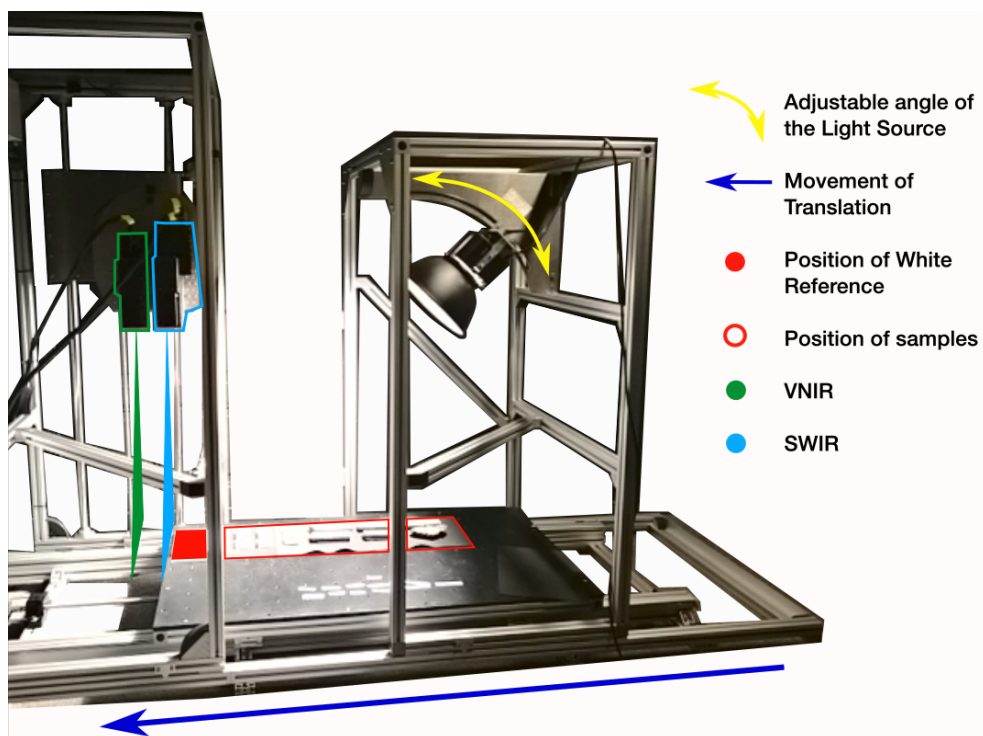
Figure 6: The HySpex translation stage setup (Körting, 2019).

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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 [μs]	30 000	5 000
Frame period [μs]	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 [µs]	120000 - 140000	15000 – 20000
Frame period [µs]	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 [µs]	60000	10000
Frame period [µs]	60060	239282

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.

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.

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

large area drift detector (GOLDD). The maximum excitation voltage of the XL3t device is 50 kV, which means out of the 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 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)

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

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 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 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.

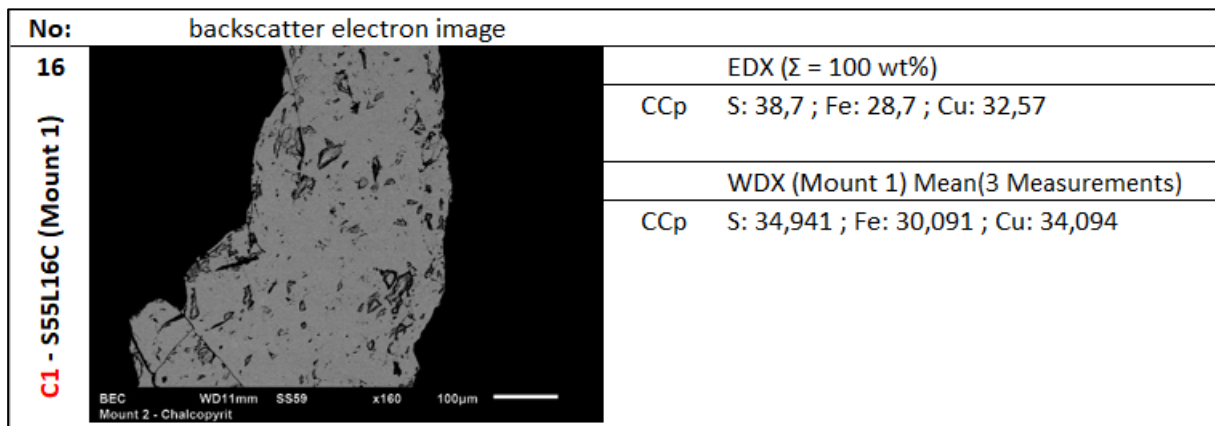
260 An example analysis for copper-bearing mineral sample C1 can be seen in Figure 7 and Table 7, the full SEM and EPMA data files are documented in (Koellner et al., 2019).

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 Kα, P Kα, Ca Kα), albite (Na Kα), fayalite (Fe Kα, Mn Kα), wollastonite (Si Kα), omphacite (Al Kα), LaPO$_4$ (La Lα), PrPO$_4$ (Pr Lβ), CePO$_4$ (Ce Lα), NdPO$_4$ (Nd Lβ), YPO$_4$ (Y Lα), EuPO$_4$ (Eu Lα), SmPO$_4$ (Sm Lβ), LuPO$_4$ (Lu Lα), GdPO$_4$ (Gd Lα), ErPO$_4$ (Er Lβ), DyPO$_4$ (Dy Lβ), YbPO$_4$ (Yb Lα), HoPO$_4$ (Ho Lβ), monazite (Th Mα, U Mβ, Tb Lα), uranothorite (U Mβ), crocoite (Pb Mβ). The EPMA data were reduced using the software-implemented PRZ-XXP data-correction routine, which is based

280 on the φ(ρz) 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

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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 (2σ) 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
310   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

315   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
320   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

325   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
330   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
335   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);
340   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 (www.enmap.org)[1]
	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 push broom 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
	Smithonian Institution	Smithsonian Institution Department of Mineral Sciences, reference material from the Smithonian Microbeam Standards
	Astimex Standards Ltd.	Astimex produces standards suitable for electron probe and scanning electron miscroscop X-ray analysis.
	BVM	Bureau Veritas Minerals is an industry leader in the analysis of minerals for the Exploration and Mining industries. BVM is a service-provider company that provides mineral preparation and laboratory testing services.
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™

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.

11. Competing interests

The authors declare no conflict of interest

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380 publication of the Apliki mine surface data is associated to this MoU.

13. References

385   Boesche, N., Rogass, C., Lubitz, C., Brell, M., Herrmann, S., Mielke, C., Tonn, S., Appelt, O., Altenberger, U. and Kaufmann, H.: Hyperspectral REE (Rare Earth Element) Mapping of Outcrops—Applications for Neodymium Detection, Remote Sens., 7(5), 5160–5186, doi:10.3390/rs70505160, 2015.

Boesche, N. K.: Hyperspectral Rare Earth Element Mapping of Three Outcrops at the Fen Complex, Norway: Calcitic, Dolomitic, and Ankeritic Carbonatites, in Rare Earths Industry - Technological, Economic, and Environmental Implications, edited by I. B. De Lima and
390   W. L. Filho, p. 434, Elsevier Inc. [online] Available from: https://www.elsevier.com/books/rare-earths-industry/borges-de-lima/978-0-12-802328-0, 2015.

Bösche, N. K.: Detection of Rare Earth Elements and Rare Earth Oxides with Hyperspectral Spectroscopy, University of Potsdam. [online] Available from: http://nbn-resolving.de/urn:nbn:de:kobv:517-opus4-85363, 2015.

Bureau Veritas: Bureau Veritas Metals, Minerals & Environmental Schedule of Services & Fees 2020. [online] Available from:
395   http://acmelab.com/wp-content/uploads/2020/02/BV_Fees-Schedule-2020_USD_v3_07Feb2020.pdf, 2020.

Clark, R. N.: Spectroscopy of rocks and minerals, and principles of spectroscopy, Remote Sens. earth Sci. Man. Remote Sens., 3, 3–58, doi:10.1111/j.1945-5100.2004.tb00079.x, 1999.

Clark, R. N.: Imaging spectroscopy: Earth and planetary remote sensing with the USGS Tetracorder and expert systems, J. Geophys. Res., 108(E12), 5131, doi:10.1029/2002JE001847, 2003.

400   Guanter, L., Kaufmann, H., Segl, K., Foerster, S., Rogass, C., Chabrillat, S., Kuester, T., Hollstein, A., Rossner, G., Chlebek, C., Straif, C., Fischer, S., Schrader, S., Storch, T., Heiden, U., Mueller, A., Bachmann, M., Mühle, H., Müller, R., Habermeyer, M., Ohndorf, A., Hill, J., Buddenbaum, H., Hostert, P., Van Der Linden, S., Leitão, P. J., Rabe, A., Doerffer, R., Krasemann, H., Xi, H., Mauser, W., Hank, T., Locherer, M., Rast, M., Staenz, K. and Sang, B.: The EnMAP spaceborne imaging spectroscopy mission for earth observation, Remote Sens., doi:10.3390/rs70708830, 2015.

405   Heinrich, K. F. J. and Newbury, D. E.: Electron probe quantitation edited by K.F.J. HEINRICH and D.E. NEWBURY (Plenum Press New York, 1991), Microsc. Microanal. Microstruct., doi:10.1051/mmm:0199200302-3029500, 1991.

Herrmann, S.: Capacity of Imaging Spectroscopy for the characterisation of REO , REE bearing minerals & primary REE-deposits., 2019.

Hunt, G. R.: Spectral signatures of particulate minerals in the visible and near infrared, Geophysics, doi:10.1190/1.1440721, 1977.

Hunt, G. R.: Spectroscopic Properties of Rocks and Minerals, in Practical Handbook of Physical Properties of Rocks and Minerals, edited
410   by R. S. Carmichael, pp. 599–669, CRC Press., 1982.

Hunt, G. R. and Ashley, R. P.: Spectra of altered rocks in the visible and near infrared, Econ. Geol., doi:10.2113/gsecongeo.74.7.1613, 1979.

hyspex.no/products/disc.php: Norsk Elektro Optikk AS HySpex VNIR1600 and SWIR320 m-e:, [online] Available from: https://www.hyspex.no/products/disc/vnir-1600.php (Accessed 18 June 2019), 2019.

415   Iwasaki, A., Ohgi, N., Tanii, J., Kawashima, T. and Inada, H.: Hyperspectral Imager Suite (HISUI)-Japanese hyper-multi spectral radiometer, in International Geoscience and Remote Sensing Symposium (IGARSS)., 2011.

Koellner, N., Koerting, F., Horning, M., Mielke, C. and Altenberger, U.: Mineral spectra and chemistry of 20 copper-bearing minerals., 2019.

Koerting, F., Herrmann, S., Boesche, N. K., Mielke, C., Koellner, N. and Altenberger, U.: Mineral spectra and chemistry of 32 rare-earth
420   minerals and rare-earth oxide powders including niobium- and tantalum-oxid powder., 2019a.

Koerting, F., Rogass, C., Koellner, N., Horning, M. and Altenberger, U.: Mineral spectra and chemistry of 37 copper-bearing surface samples from Apliki copper-gold-pyrite mine in the Republic of Cyprus., 2019b.

Kokaly, R. F., Clark, R. N., Swayze, G. A., Livo, K. E., Hoefen, T. M., Pearson, N. C., Wise, R. A., Benzel, W. M., Lowers, H. A., Driscoll, R. L. and Klein, A. J.: USGS Spectral Library Version 7. [online] Available from: https://pubs.er.usgs.gov/publication/ds1035, 425   2017.

Körting, F.: Development of a 360 ° hyperspectral drill core scanner Test of technical conditions and validation of high-resolution near-field analysis of crystalline basement rocks using COSC-1 core samples., 2019.

Lorenz, M., Altenberger, U., Trumbull, R. B., Lira, R., Luchi, M. L. De, Günter, C. and Eidner, S.: Chemical and textural relations of britholite- And apatite-group minerals from hydrothermal REE mineralization at the Rodeo de los Molles deposit, Central Argentina, Am. 430   Mineral., doi:10.2138/am-2019-6969, 2019.

van der Meer, F. D., van der Werff, H. M. A., van Ruitenbeek, F. J. A., Hecker, C. A., Bakker, W. H., Noomen, M. F., van der Meijde, M., Carranza, E. J. M., de Smeth, J. B. and Woldai, T.: Multi- and hyperspectral geologic remote sensing: A review, Int. J. Appl. Earth Obs. Geoinf., doi:10.1016/j.jag.2011.08.002, 2012.

Mielke, C., Rogass, C., Boesche, N., Segl, K. and Altenberger, U.: EnGeoMAP 2.0—Automated Hyperspectral Mineral Identification for 435   the German EnMAP Space Mission, Remote Sens., 8(2), 127, doi:10.3390/rs8020127, 2016.

Rogass, C., Koerting, F. M., Mielke, C., Brell, M., Boesche, N. K., Bade, M. and Hohmann, C.: Translational imaging spectroscopy for proximal sensing, Sensors (Switzerland), 17(8), doi:10.3390/s17081857, 2017.

Swayze, G. A., Clark, R. N., Goetz, A. F. H., Livo, K. E., Breit, G. N., Kruse, F. A., Sutley, S. J., Snee, L. W., Lowers, H. A., Post, J. L., Stoffregen, R. E. and Ashley, R. P.: Mapping advanced argillic alteration at Cuprite, Nevada, using imaging spectroscopy, Econ. Geol., 440   109(5), 1179–1221, doi:10.2113/econgeo.109.5.1179, 2014.

Tong, Q., Xue, Y. and Zhang, L.: Progress in hyperspectral remote sensing science and technology in China over the past three decades, IEEE J. Sel. Top. Appl. Earth Obs. Remote Sens., doi:10.1109/JSTARS.2013.2267204, 2014.

Turner, D., Rivard, B. and Groat, L.: Rare earth element ore grade estimation of mineralized drill core from hyperspectral imaging spectroscopy, in 2014 IEEE Geoscience and Remote Sensing Symposium, pp. 4612–4615, IEEE., 2014a.

445   Turner, D. J.: Reflectance spectroscopy and imaging spectroscopy of rare earth element-bearing mineral and rock samples., 2015.

Turner, D. J., Rivard, B. and Groat, L. A.: Visible and short-wave infrared reflectance spectroscopy of REE fluorocarbonates, Am. Mineral., doi:10.2138/am.2014.4674, 2014b.