Technical Report: Mineral reflectance spectra and LIBS data of 18 lithium-bearing mineral samples (lepidolite, petalite and spodumene specimen)

(https://doi.org/10.5880/GFZ.1.4.2021.003)

Nicole Koellner[1*], Agnieszka Kuras[1], Constantin Hildebrand[1], Friederike Koerting[2], Friederike Kaestner[1]

1. *GFZ German Research Centre for Geosciences, Potsdam, Germany*
2. *Norsk Elektro Optikk AS – HySpex division, Oslo, Norway*

* *Corresponding author: nicole.koellner@gfz-potsdam.de*

Table of contents

1. License

2. Citation

When using the data please cite:

Koellner, N., Kuras, A., Hildebrand, C., Kaestner, F. and Koerting, F., (2021): Mineral reflectance spectra and LIBS data of 18 lithium-bearing mineral samples (lepidolite, petalite and spodumene specimen). GFZ Data Services. https://doi.org/10.5880/GFZ.1.4.2021.003

The spectral library presented here is part of a larger collection of spectral libraries including rare-earth minerals, rare-earth-oxides and copper-bearing mineral samples from mineral collections of the University of Potsdam (UP) and the Federal Institute for Geosciences and Natural Resources (BGR):

Koellner, N., Koerting, F., Horning, M., Mielke, C. and Altenberger, U. (2019). Mineral reflectance spectra and chemistry of 20 copper-bearing minerals, http://doi.org/10.5880/GFZ.1.4.2019.003

Koerting, F.; Herrmann, S.; Boesche, N. K.; Rogass, C.; Mielke, C.; Koellner, N.; Altenberger, U. (2019a). Mineral reflectance spectra and chemistry of 29 rare earth-bearing minerals and rare earth oxide powders including niobium- and tantalum-oxide powder, http://doi.org/10.5880/GFZ.1.4.2019.004

3. Abstract

The data set contains LIBS (Laser-Induced Breakdown Spectroscopy) emission spectra of 18 lithium-bearing minerals and their corresponding hyperspectral reflectance spectra. The data were collected within the research project LIGHTS (Lightweight Integrated Ground and Airborne Hyperspectral Topological Solutions, http://lights.univ-lorraine.fr/) which aims at developing a new exploration process for Li targets combining drone-borne hyperspectral data and field observations. Hyperspectral data were acquired with the HySpex system in a wavelength range of 414 - 2498 nm and are presented in a spectral library. Detailed information about the samples and area of spectral retrieval is presented in the data sheet below. The spectral library presented here expands the collection of spectral libraries including samples from rare-earth minerals, rare-earth-oxides (Koerting et al., 2019a) and copper-bearing minerals (Koellner et al., 2019) which are fully described in Koerting et al. (2021). These libraries aim to give a spectral overview of important resources and deposit mineralizations.

4. Samples

18 samples taken partly from the collections of the University of Potsdam (UP) and the Federal Institute for Geosciences and Natural Resources (BGR) and partly in the field during previous measurement campaigns were hyperspectrally measured and geochemically analysed by using a LIBS handheld analyzer. A description of the HySpex system in lab use can be found in Koerting et al. (2021).

The lithium-bearing mineral samples were measured without prior sample preparation as the surface of the minerals and the influence of the mineral structure were of interest (Figure 1). Figure 1 shows one HySpex scan of four lepidolite samples (Lep1, Lep2, Lep3, Lep4) displayed as a true color RGB image in order to show the untreated samples and the white reflectance (WR) panel needed for the hyperspectral measurements (WR 90%). Table 1 lists the lithium-bearing minerals, their original collection, their original sample name, the sample locations, a short sample description, a general formula of the analysed mineral, sample photos with the area of spectral sampling highlighted in red circles and plots of the corresponding reflectance spectra and the averaged spectra of the LIBS analyses. For each sample 64 LIB spectra were taken over a 8x8 pulse grid in the red circled area which was also used to obtain the reflectance spectrum, averaging (AVG) over a 5 by 5-pixel window. The resulting HySpex reflectance data were scaled from 0 - 1. A mean LIB spectrum per sample was calculated from the individual measurements.

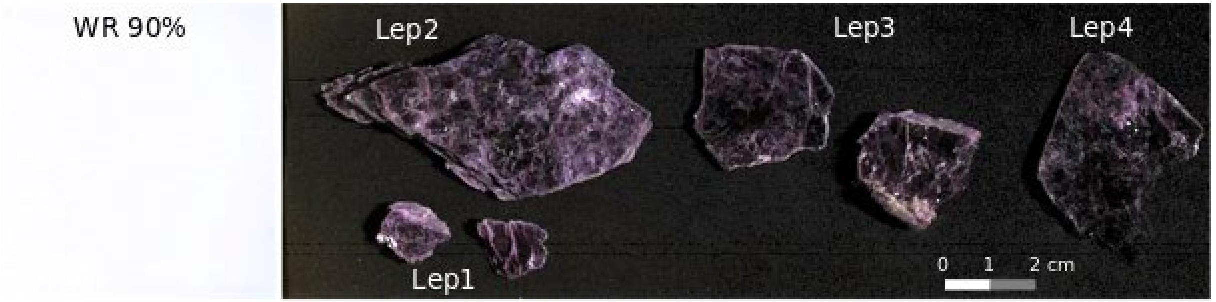


Figure 1: The HySpex scan, displayed as a true color RGB image, shows the lack of sample preparation. The scan includes 4 lepidolite samples and a white reflectance panel of 90% reflectance. Sample names and a scale bar were added.

Table 1: ***Overview of lithium-bearing minerals included in this publication****.*

(1) Sample ID*: Lep = Lepidolite, Ptl = Petalite, Spd = Spodumene,* ***(2) Collection****: "-" = field sample, UP = University of Potsdam, BGR = Federal Institute for Geosciences and Natural Resources (Spandau);* ***(3)*** *the area of spectral sampling for both reflectance and emission retrieval is highlighted in red.*

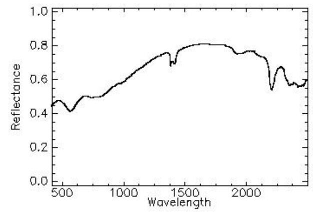
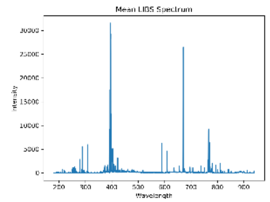
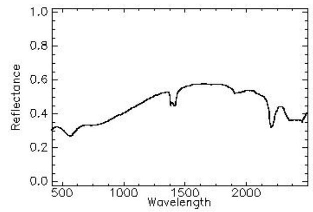
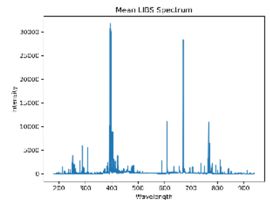
Sample ID (1)	Collec-tion (2)	Original sample ID/name	Sample locality	Sample description	Mineral formula	Photo of sample (3)	HySpex reflectance spectrum	SciApps Z-300 emission spectrum
Lep1	-	-	Høydalen Seter, Tørdal, Drangedal, Telemark, South Norway N 59°10'59.304'' E 8°45'34.788''	massive purple lepidolite flakes	$K(Li,Al)_3[(Si,Al)_4]O_{10}(OH,F)_2$			
Lep2	-	-	Høydalen Seter, Tørdal, Drangedal, Telemark, South Norway N 59°10'59.304'' E 8°45'34.788''	massive purple lepidolite flake	$K(Li,Al)_3[(Si,Al)_4]O_{10}(OH,F)_2$			

Table 1 (continued)

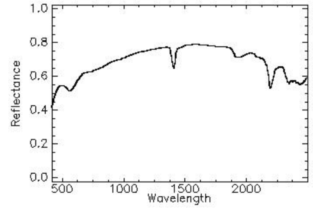
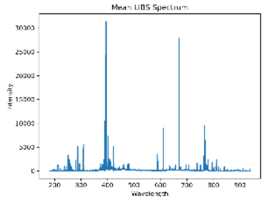
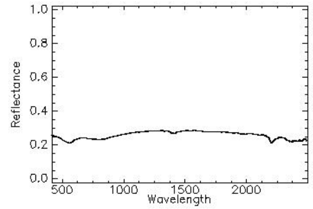
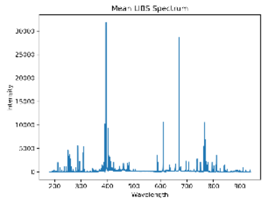
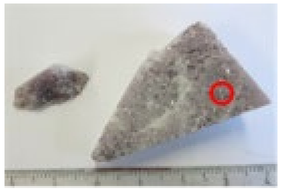
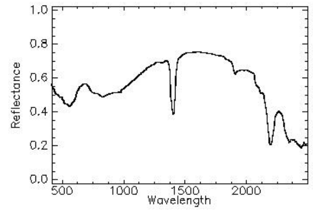
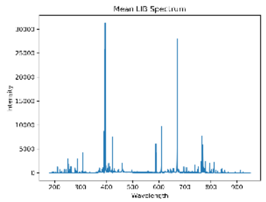
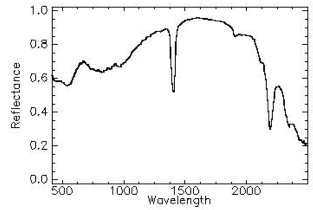
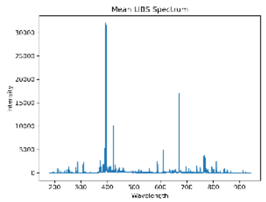
Sample ID [(1)]	Collection [(2)]	Original sample ID/name	Sample locality	Sample description	Mineral formula	Photo of sample [(3)]	HySpex reflectance spectrum	SciApps Z-300 emission spectrum
Lep3	-	-	Høydalen Seter, Tørdal, Drangedal, Telemark, South Norway N 59°10'59.304'' E 8°45'34.788''	massive purple lepidolite flakes	$K(Li,Al)_3[(Si,Al)_4]$ $O_{10}(OH,F)_2$			
Lep4	-	-	Høydalen Seter, Tørdal, Drangedal, Telemark, South Norway N 59°10'59.304'' E 8°45'34.788''	massive purple lepidolite flake	$K(Li,Al)_3[(Si,Al)_4]$ $O_{10}(OH,F)_2$			
Lep5	-	-	Tantalite Valley, Karas, Namibia S 28°142'51.5'' E 18°43'51.4''	massive, fine-grained, purple lepidolite in matrix	$K(Li,Al)_3[(Si,Al)_4]$ $O_{10}(OH,F)_2$			
Lep6	-	-	Tantalite Valley, Karas, Namibia S 28°142'51.5'' E 18°43'51.4''	massive, fine-grained, purple lepidolite in matrix	$K(Li,Al)_3[(Si,Al)_4]$ $O_{10}(OH,F)_2$			

Table 1 (continued)

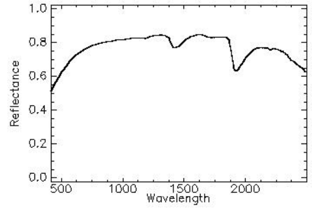
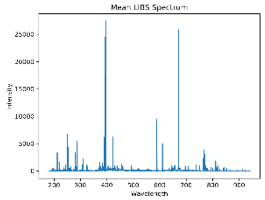
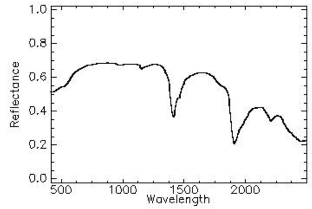
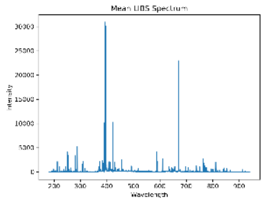
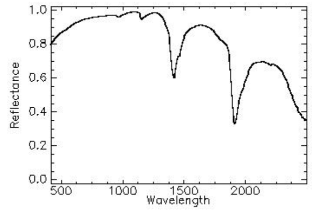
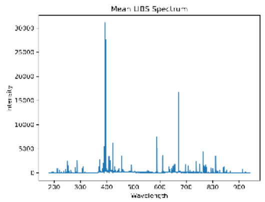
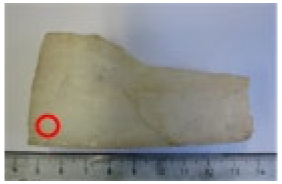
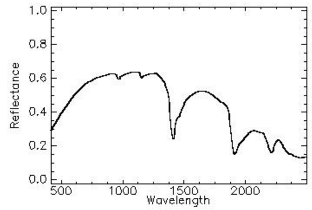
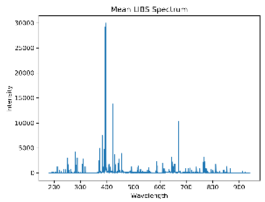
Sample ID [1]	Collec-tion [2]	Original sample ID/name	Sample locality	Sample description	Mineral formula	Photo of sample [3]	HySpex reflectance spectrum	SciApps Z-300 emission spectrum
Ptl1	UP	Petalite	Masvingo (Fort Victoria, Southern Rhodesia), Zimbabwe	massive aggregate of petalite, dirty white	$LiAlSi_4O_{10}$			
Ptl2	BGR	72275 Petalite	Karibib, Erongo, Namibia	colour transitions due to weathering, black tourmaline	$LiAlSi_4O_{10}$			
Ptl3	BGR	72287 Petalite	Karibib, Erongo, Namibia	massive aggregate of petalite, slightly translucent	$LiAlSi_4O_{10}$			
Ptl4	BGR	72281 white Petalite	Karibib, Erongo, Namibia	massive aggregate of white petalite, slightly weathered	$LiAlSi_4O_{10}$			

Table 1 (continued)

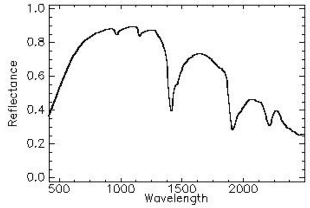
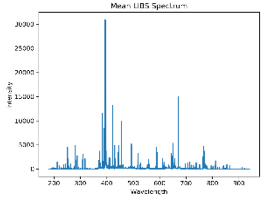
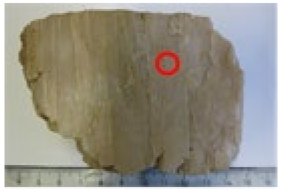
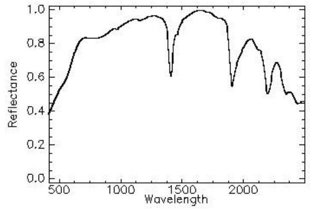
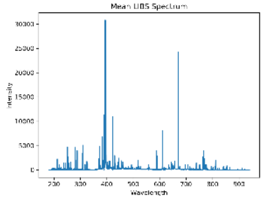
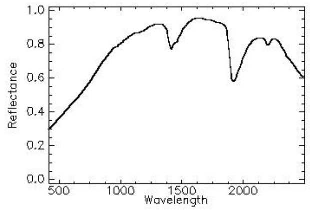
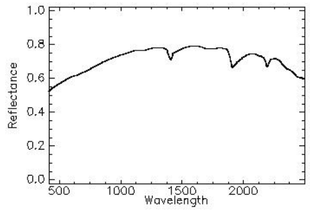
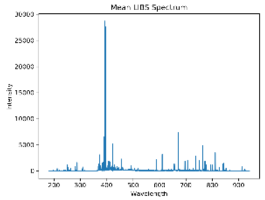
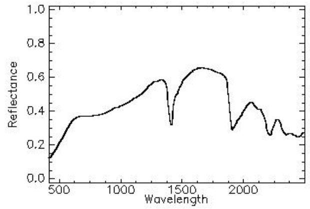
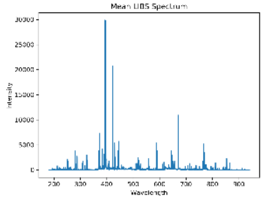
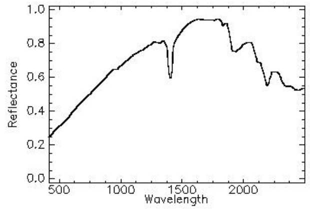
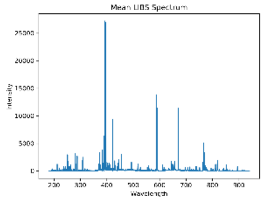
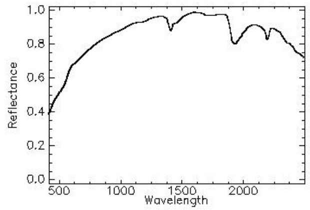
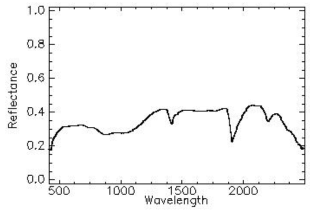
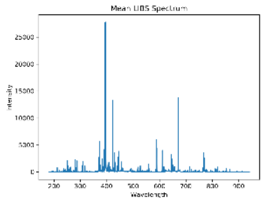
Sample ID [(1)]	Collec-tion [(2)]	Original sample ID/name	Sample locality	Sample description	Mineral formula	Photo of sample [(3)]	HySpex reflectance spectrum	SciApps Z-300 emission spectrum
Ptl5	BGR	72280 white Petalite	Karibib, Erongo, Namibia	massive aggregate of white petalite, slightly weathered	$LiAlSi_4O_{10}$			
Spd1	BGR	75247 red Spodumene	Labrador, Canada	massive aggregate of spodumene, light pink-brown	$LiAlSi_2O_6$			
Spd2	BGR	73299 Spodumene-pegmatite	Spodumene kopje, Namaqualand, Namibia	coarse-grained pegmatite containing spodumene, Li-mica and quartz	$LiAlSi_2O_6$			No LIBS spectrum available due to the rough surface of the sample.
Spd3	BGR	73303 massive Spodumene	Namaqualand, Namibia	massive aggregate of spodumene, light grey, dark grey veins	$LiAlSi_2O_6$			

Table 1 (continued)

Sample ID (1)	Collec-tion (2)	Original sample ID/name	Sample locality	Sample description	Mineral formula	Photo of sample (3)	HySpex reflectance spectrum	SciApps Z-300 emission spectrum
Spd4	BGR	75248 secondary Copper silicate	Labrador, Canada	coarse-grained aggregate of spodumene and copper silicate	$LiAlSi_2O_6$			
Spd5	BGR	75390 Spodumene	Australia	aggregate of large spodumene crystals	$LiAlSi_2O_6$			
Spd6	BGR	74785 Spodumene with columbite	Key Stone, Black Hills, South Dakota, USA, Elta Mine	coarse-grained aggregate of spodumene and mica	$LiAlSi_2O_6$			No LIBS spectrum available due to the rough surface of the sample.
Spd7	BGR	75262 green Spodumene with quartz	Labrador, Canada	massive aggregate of spodumene, light green	$LiAlSi_2O_6$			

5. Hyperspectral measurements

The HySpex VNIR-1600 and SWIR-320m-e (available at: (https://www.hyspex.com/hyspex-products, 2019)) are two line-scanning cameras that are mounted in parallel. They cover the range of the visible to near infrared (VNIR, 414 - 1000 nm) region and the short-wave infrared (SWIR, 1000 - 2498 nm) region and record an array-line of 1600 pixels (VNIR) and 320 pixels (SWIR) (push-broom scanning). Every pixel contains a spectrum with a spectral sampling number of 408 bands in total.

In laboratory mode, the HySpex 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 (45° illumination angle) are fixed, while the sleigh and the samples are moving through the focal plane (Rogass et al., 2017). Table 2 lists the main specifications of the HySpex system. For the measurements, the samples were placed on black cellular rubber without prior sample preparation. After data acquisition, the VNIR and SWIR data cubes were stacked and the reflectance was calculated on the basis of the white reference panel. Detailed descriptions of the laboratory setup, hyperspectral measurements, used parameters and data processing can be found in Rogass et al. (2017) and Koerting et al. (2021). For each sample a plane surface area was chosen to obtain the reflectance spectrum, averaging over a 5 pixel x 5 pixel window and scaling from 0 -1. The same area was used to perform LIBS analyses.

Table 2: ***Main specifications of the HySpex sensors VNIR-1600 and SWIR-320m-e.***

Sensor parameters	HySpex VNIR 1600	HySpex SWIR-320m-e
Wavelength range [nm]	414 - 993	967 - 2498
Number of Spectral Bands	160	256
Spectral resolution [nm]	3.5 - 6.0	5.6 - 7.0
Number of Pixels/Line	1600	320

6. Geochemical measurements

Laser-Induced Breakdown Spectroscopy (LIBS) is an analytical technique used for the determination of the elemental composition of materials. A focused, pulsed laser beam is directed at a sample surface, where laser energy absorption and material ablation produces high-temperature microplasma. Small amounts of the measured material are dissociated and ionized at the point of laser focus. During cooling atomic/ionic emissions in the plasma are generated. The integrated detector is used to spectrally/temporally resolve the signals from the plasma and records the emission lines of all elements present in the material. The resulting LIB spectrum represents the complete chemical composition of the analysed material (Miziolek et al., 2006). In this study LIBS data were collected using the SciAps Z-300 handheld analyzer with a wavelength range of 190 - 950 nm. The 50 Hz laser shots with 5-6mJ due every pulse and measures every element in the periodic table (available at: (https://sciaps.com/libs-handheld-laser-analyzers/z-300, 2021). The LIBS measurements were taken over an 8x8 pulse grid by using the Geochem Pro (Mining) App, resulting in 64 individual measurements per sample. The acquisition settings are listed in Table 3. For these 64 single shots, outliers and negative values were removed and the data were averaged to a mean spectrum for each sample. The samples Spd2 and Spd6 could not be measured due to the high roughness of their surfaces.

*Table 3: **Acquisition settings of the SciAps Z-300 handheld analyzer in Geochem Pro mode.***

Acquisition settings	
Test Rate	10 Hz
Test Locations	1 Locations
Cleaning Pulses Per Location	2 Shots
Data Pulses per Location	4 Shots
Argon Preflush Time	300 ms
Shots to Average	1

7. File description

The data are organised in two folders "hyperspectral-library" and "LIBS-data".

7.1. Folder "hyperspectral-library"

The reflectance spectra of the lithium-bearing minerals are presented in an ENVI® Spectral Library file format "GFZ_HySpex_lithium_minerals", associated header file "GFZ_HySpex_lithium_minerals.hdr" and a text file format "GFZ_HySpex_lithium_minerals.txt". The spectral library can be visualized in ENVI® as seen in Figure 2a, 2b and 2c. Figure 3 shows a section of the text file presenting the wavelength in column 1 and the reflectance values of the samples from column 2 onwards.

The additional file "lithium_bearing_minerals_hyperspectral_parameters.xlsx" provides a full over-view of the samples, their descriptions and the measurement parameters of the HySpex measurements. The Excel™ file header is described in Table 4.

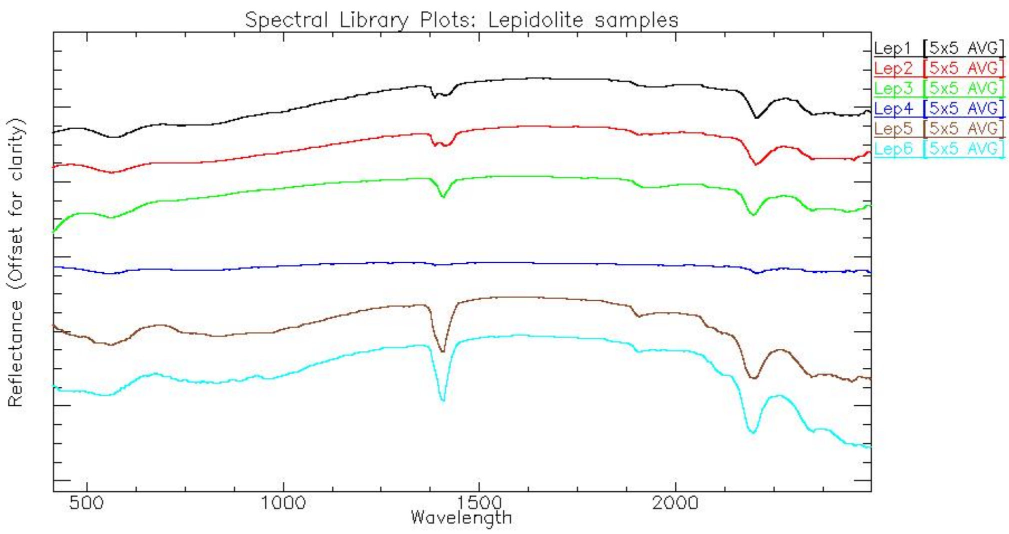


Figure 2a: Spectral library plot of the analysed lepidolite samples.

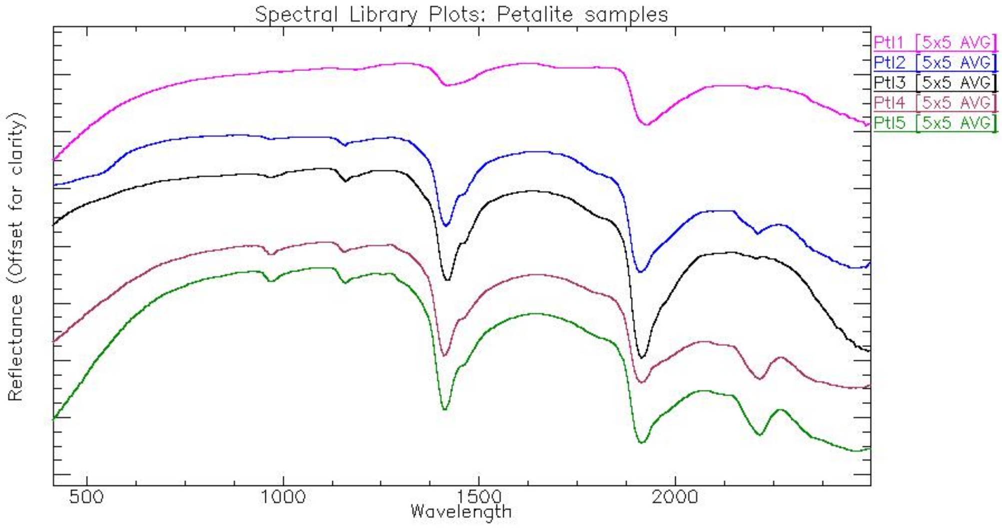


Figure 2b: Spectral library plot of the analysed petalite samples.

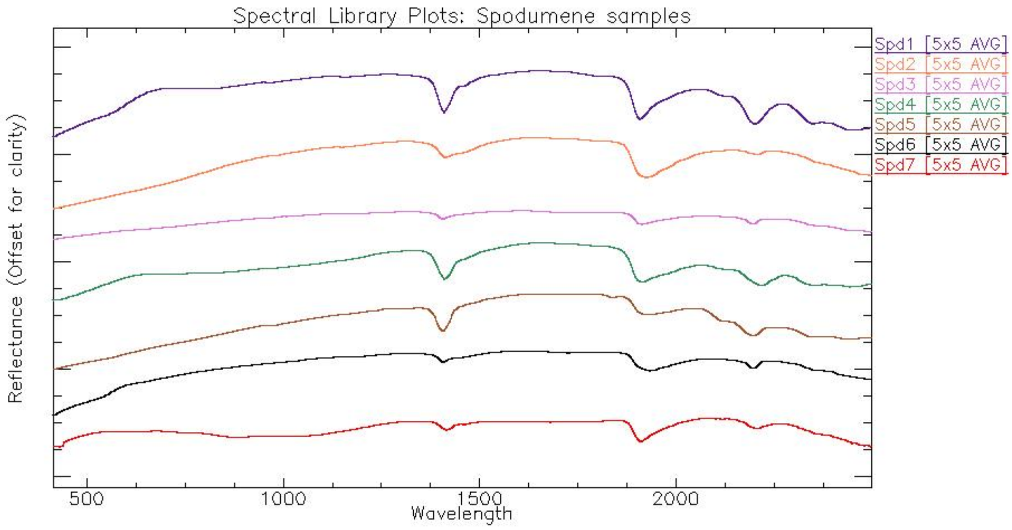


Figure 2c: Spectral library plot of the analysed spodumene samples.

```
ENVI ASCII Plot File [Wed May 26 15:45:20 2021]
Column 1: Wavelength
Column 2: Lep1 [5x5 AVG]~~1
Column 3: Lep2 [5x5 AVG]~~2
Column 4: Lep3 [5x5 AVG]~~3
Column 5: Lep4 [5x5 AVG]~~4
Column 6: Lep5 [5x5 AVG]~~5
Column 7: Lep6 [5x5 AVG]~~6
Column 8: Ptl1 [5x5 AVG]~~7
Column 9: Ptl2 [5x5 AVG]~~8
Column 10: Ptl3 [5x5 AVG]~~1
Column 11: Ptl4 [5x5 AVG]~~9
Column 12: Ptl5 [5x5 AVG]~~10
Column 13: Spd1 [5x5 AVG]~~11
Column 14: Spd2 [5x5 AVG]~~12
Column 15: Spd3 [5x5 AVG]~~13
Column 16: Spd4 [5x5 AVG]~~14
Column 17: Spd5 [5x5 AVG]~~15
Column 18: Spd6 [5x5 AVG]~~16
Column 19: Spd7 [5x5 AVG]~~17
   414.803009  0.443065  0.303317  0.415031  0.260625  0.570720  0.625163  0.512355  0.516809  0.795641
   418.440002  0.450820  0.307881  0.425747  0.259720  0.561363  0.620693  0.514448  0.516446  0.803780
   422.075989  0.456722  0.314918  0.438027  0.264158  0.551807  0.615521  0.519185  0.518401  0.806483
   425.713013  0.460574  0.318017  0.448881  0.259947  0.546158  0.610365  0.525002  0.519208  0.811322
   429.350006  0.462909  0.322299  0.457688  0.261505  0.542963  0.601149  0.529205  0.518784  0.815854
```

Figure 3: Detail of the ASCII file from the ENVI® spectral library.

Table 4: ***Explanation of the header of "lithium_bearing_minerals_hyperspectral_parameters.xlsx".***

Header of Excel™ file	Explanation
Sample ID	Sample name
Collection	Name of host institution of the sample Collection analysed in this study
Original sample ID/name	Original sample name from the collection
Sample locality	Origin of the sample
Sample description	description of visible alteration and style of mineralization
Mineral	Name of the analysed mineral
Formula	General mineral formula of the analysed mineral
Photo with highlighted area of spectra retrieval	Showing the location on the sample for LIBS and HySpex spectrum retrieval
HySpex spectrum name	Name of the spectrum, averaged over a window of 5 x 5-pixel
VNIR integration time (us)	Light exposure on VNIR sensor
VNIR frame period (us)	Time per line that the sensor allows data acquisition
VNIR frames	Number of frames measured
VNIR lens	VNIR lens used
SWIR integration time (us)	Light exposure on SWIR sensor
SWIR frame period (us)	Time per line that the sensor allows data acquisition
SWIR frames	Number of frames measured
SWIR lens	SWIR lens used
WR (%)	White reference standard used
SNR frame averaging	Number of frames that are averaged per measured frame
Temperature (°C)	Room temperature
Pressure (hPa)	Room pressure
Humidity (%)	Room humidity

7.2. Folder "LIBS-data"

The results of the LIBS analyses are given as an averaged mean spectrum per sample, accept samples Spd2 and Spd6. The averaged LIB spectra are provided as individual CSV files following the syntax "Sample ID_mean_spectrum.csv". Figure 4 shows a section of a CSV file presenting wavelength and intensity separated by comma.

```
wavelength,intensity
180.0,0.0
180.1,0.0
180.2,0.0
180.3,0.0
180.4,0.0
180.5,0.0
180.6,0.0
180.7,0.0
180.79999999999995,0.0
180.89999999999995,0.0
180.99999999999997,0.0
181.09999999999997,0.0
181.19999999999996,0.0
181.29999999999995,0.0
181.39999999999992,0.0
181.49999999999991,0.0
181.59999999999994,0.0
181.69999999999993,0.0
```

Figure 3: Detail of a CSV file from LIBS analyses.

8. Acknowledgements

We would like to thank the Helmholtz Centre Potsdam GFZ German Research Centre for Geosciences for providing the infrastructure and personnel support to conduct our research. The lab measurements were conducted within the LIGHTS (Lightweight Integrated Ground and Airborne Hyperspectral Topological Solutions) project which is funded by national research agencies under the EU H2020 ERAMIN-2 network. Our gratitude also goes to the University of Potsdam and the Spandau branch of the Federal Institute for Geosciences and Natural Resources (BGR) for supplying the mineral samples.

9. References

HySpex: Norsk Elektro Optikk AS HySpex VNIR1600 and SWIR320 m-e:, [online] Available from: https://www.hyspex.com/hyspex-products/ (Accessed 28 May 2021).

Koellner, N., Koerting, F., Horning, M., Mielke, C., & Altenberger, U. (2019). *Mineral reflectance spectra and chemistry of 20 copper-bearing minerals*. https://doi.org/http://doi.org/10.5880/GFZ.1.4.2019.003

Koerting, F., Herrmann, S., Boesche, N. K., Mielke, C., Koellner, N., & Altenberger, U. (2019a). *Mineral reflectance spectra and chemistry of 32 rare-earth minerals and rare-earth oxide powders including niobium- and tantalum-oxid powder.* https://doi.org/http://doi.org/10.5880/GFZ.1.4.2019.004

Koerting, F., Koellner, N., Kuras, A., Boesche, N. K., Rogass, C., Mielke, C., Elger, K., & Altenberger, U. (2021). A solar optical hyperspectral library of rare-earth-bearing minerals, rare-earth oxide powders, copper-bearing minerals and Apliki mine surface samples. *Earth System Science Data*, *13*(3), 923–942. https://doi.org/10.5194/essd-13-923-2021

Miziolek, A.W., Pallaschi, V., Schechter, I. (Eds.), 2006. Laser-Induced Breakdown Spectroscopy. Cambridge University Press. https://doi.org/10.1017/CBO9780511541261

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

SciAps: SciAps Inc. SciAps Z-300: [online] Available from: https://sciaps.com/libs-handheld-laser-analyzers/ (Accessed 28 May 2021).