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Overview of Experimental Setups in Spectroscopic Laboratory Measurements – the SpecTour Project

András Jung, Christian Götze & Cornelia Glässer, Halle (Saale)

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Summary: The spectral signatures differ in many ways; even for the same material the captured data is significantly influenced by data collection method, equipment and other parameters influencing the general experimental setup. Spectral measurements are primary information sources in hyperspectral remote sensing. Portable device-based spectroscopy has significantly accelerated high resolution data production and the risk of uncontrolled error propagation. The number of spectral library producers and users is increasing. The growing challenges of spectral libraries initiated the project SpecTour. SpecTour networks portable spectrometer users in order to provide an overview of their measurement routines, equipment, general attitudes and, most of all, the spectra. The project requires active attendance by its participants and is performed in a round-robin approach. The philosophy of the project is "Just measure like you always do!". The illumination parameters, workflow or other technical parameters are not predetermined, but the participants have to fill out a setup protocol. More than 36 spectrometers from Europe, Israel and USA have been involved in the experiment (last update: March 2012). All of the instruments are commercially available. The primary results show that the differences between the normalized spectra for the same reference panels are over 20 % and the quality of the spectra vary considerably. Evidence from the present and realistic measurement situation can be used to quantitatively highlight the lack of standards. This paper gives a general overview of the measurements and data acquisition techniques. The results of the setup protocols are evaluated and discussed here. The project is still running (SpecTour 2012) and is open to anyone who is an active field spectrometer user and would like to share spectra and practice.

Zusammenfassung: *Bei spektrometrischen Messungen werden oftmals für gleiche Objekte unterschiedliche Ergebnisse der Spektralsignaturen ermittelt.* Dabei können die Probenahme, die Laborausstattung und andere Parameter den Aufbau sowie den Ablauf des Experimentes beeinflussen. In der hyperspektralen Fernerkundung sind spektrale Messungen wichtige primäre Informationsquellen. Aufgrund der steigenden Anzahl von Nutzern und der dabei entstehenden spektralen Bibliotheken wird auch das Risiko von nicht aufgespürten Fehlern erhöht. Vor diesem Hintergrund ist das Hauptziel des Projektes „SpecTour" das Networking von Gruppen mit Spektrometern, um einen Überblick über ihre Messroutinen, ihre Ausstattung, die Gewohnheiten und die entstandenen Spektren zu schaffen. Das Projekt, angelegt als Ringversuch, benötigt eine aktive Beteiligung aller Teilnehmer. Die Philosophie des Projekts ist dabei „just measure like you always do!", d.h. die Beleuchtungsparameter, der Messaufbau sowie -ablauf werden nicht festgelegt. Alle Parameter werden aber in einem Messprotokoll festgehalten. Mehr als 36 im Handel verfügbare Spektrometer aus Europa, Israel und den USA sind bisher in dem Experiment zum Einsatz gekommen (Stand: März 2012). Die ersten Ergebnisse zeigen, dass zwischen den zu messenden Referenzmaterialien eine Variabilität von über 20 % auftritt. Ebenso sind Qualitätsunterschiede festzustellen. Die aktuelle Messsituation innerhalb der Community zeigt das Fehlen von Normen und Standards deutlich. Dieser Artikel präsentiert einen Überblick über die Auswertung der Messprotokolle aller bisherigen Teilnehmer. Das Projekt ist erreichbar unter SpecTour (2012). Jedem aktiven Nutzer von Feldspektrometern bieten wir die Möglichkeit, an diesem Experiment teilzunehmen.

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1 Introduction

Hyperspectral laboratory and field measurements were mostly made by expert groups until recent years. Profound changes can be recognized to date in hyperspectral remote sensing, which are characterized by the increasing number of spectrometers on the market and a growing scientific community. This community shows variability in technical and scientific background regarding the users' experience, equipment and applications. Due to this development nowadays we have a mixed user community ranging from beginners to experienced groups. Additionally, there are new and less experienced companies on the market for hyperspectral remote sensing.

Spectral records are stored and managed in databases such as the spectral database of the USGS or by working groups in own databases called spectral libraries. The quality is influenced and affected by many parameters. Exemplary studies investigated individual parameters and their influence on the spectral signature. The variability of the field of view (FOV) of spectral signals was analyzed by Caras et al. (2011). For reflectance spectra reference panels are usually used. A comparison of different reflectance standards were investigated by Sanches et al. (2009). It is of high importance that standards have a stable reflectance throughout the optical region. In the study of Castro-Esau et al. (2006) significant differences were found between different spectrometers depending on measurement and illumination geometry. Field spectrometers with full-range detectors show sensitivity changes following temperature changes (Markham et al. 1995). Detectors are often characterized by 'steps' between ranges which most frequently appear at the 'overlapping' regions (Milton et al. 2009). These can be reduced by a longer warm-up time. The GER3700 spectroradiometer (Brown et al. 2001) shows the changes of 'steps' in a three hour warm-up experiment. An analysis of the realistic technical environment in remote sensing laboratories does not exist yet. A "five-spectrometer-experiment" carried out under the same conditions in geometry and illumination showed that post correction methods could improve the comparability of the reflectance spectra (Jung et al. 2010, 2011).

Library spectra should be used as a reference for identification with no doubt to their quality and reliability. A spectral library is as good as its spectra and data structure. The development of spectral databases like SPECCHIO (Bojinski et al. 2003) shows also the need of standardized spectral libraries.

Our approach is focusing on the spectrometer user and the individual experimental setup. The object of our investigation was to analyze and compare spectrometric data using the same reference materials by different spectrometer users, because less attention has recently been paid to monitor and evaluate the individuality of the spectral measurements.

The analysis focuses on easy-to-capture technical parameters such as lamps, experiment setup and age-of-device. For the sake of simplicity, the laboratory seemed to be the most stable and suitable setting for the experiment. Furthermore, the concept of the experiment and initial conclusions with practical experiences are presented as well.

At this point it is important to note that development of a metadata structure, or best practice on how to archive spectral data, was not our intention, and a technical comparison or inter-calibration of the spectrometers was also not the focus of this work. In the literature there are comprehensive research studies focusing on calibration issues or database development with proven techniques and successful implementations (Schaepman & Dangel 2000, Hueni et al. 2009, Milton 1987, Milton et al. 2009).

SpecTour is a project of the German Society of Photogrammetry, Remote Sensing and Geoinformation (DGPF) and the Martin-Luther-University Halle-Wittenberg that investigates and analyses the variability of the measurement environments in laboratories in order to learn more about the real situation of spectral measurements in daily work. The round-robin test is not a tool to completely compensate low quality spectra or inappropriate measurement conditions (Price 1994, 1998). The goal of this paper is to communicate the present situation, a better understanding of the experimental setups and influences on spectral signals. Finally, we would like to minimize the knowledge gaps of spectrometer users.

2 Materials and Methods

This experimental is a round-robin test that involves different scientific groups to measure the same objects (four reference panels and one rock sample) in their own laboratory und environment. The participants vary from sophisticated experts to recently formed groups. The philosophy is "Just measure like you always do!". It was of high importance during the round-robin test to reflect and document the reality of the spectrometric laboratory measurements without any preliminary technical instructions but with the same reference panels. The test started in 2009 and it is still ongoing.

Up to now, the project has attracted 25 participants from six countries. The number of members is increasing since the project is ongoing and the community is growing. For more information about the participants, please visit SpecTour (2012).

The spectrometers deployed here are from industry leading manufacturers such as Analytical Spectral Devices (USA), FOSS NIRSystems (USA), LI-COR Biosciences (USA), Ocean Optics (USA) und Tec5 (Germany). The instruments vary in resolution, age, spectral range, technology and performance (Tab. 1). All of them were commercially available and active spectral library producers.

Tab. 1: Short technical overview of the involved spectrometers.

Spectrometer	**Spectral range (nm)**		**Light source**	
	350–1000	1000–2500	external	internal or contact
ASD FieldSpec Pro JR	**X**	**X**	**X**	
ASD FieldSpec Pro FR	**X**	**X**	**X**	**X** (with contact probe)
ASD FieldSpec 3	**X**	**X**	**X**	**X** (with contact probe)
ASD Handheld	**X**		**X**	
Tec5 HandySpec	**X**		**X**	
Ocean Optics HR2000+	**X**			**X**
FOSS XDS Rapid Content Analyzer	**X**			**X**
Li-Cor Li1800	**X**		**X**	

Tab. 2: Basic technical documentation of the experiment.

Basic setup information	Distance between reference and measurements unit (a) Distance between reference and the source of illumination (b) Angle between *a* and *b* (α)
Properties of the spectrometer	Name (serial number, type, version) Year of purchase Start of use Last calibration (when and where)
Properties of the lamp	Name (serial number, producer, type) Power (W) and voltage (V) values Operation since Total hours of operation
Administrative information	Name of the operator Date and place Affiliation and head of unit

In Tab. 2 we see which parameters were asked for documentation. These data were of high importance in understanding the experimental setups. Only those data were additionally recorded in the protocol that could not directly be derived from the spectra. Simplicity was important because of limited time and readiness. Consideration and documentation of all technical aspects of the measurement would have been beyond the capacity (of both the project and the participants) and would have been out of the original scopes as well.

The calibrated reference panels provide the most valuable details on the individuality of the measurements. The white reference measurement was taken with a calibrated 90 % reflectance panel, and this became the master reference for all further targets and samples. Each spectral measurement was repeated four times for the same target and saved separately. Before reflectance values were generated, the raw data or digital counts were also saved. The normalized reflectance factors were calculated and used for analysis.

Milton et al. (2009) noted that reflectance data would remain a convenient method to represent the energy interactions occurring at the surface. This approach was followed in this work and used for data interpretation. It is important to note that the real quantity acquired by the used spectrometers was the reflectance factor. The reflectance factor is the ratio of reflected and incident flux, irradiated under the same conditions (Nicodemus et al. 1977).

Each involved spectrometer collected 20 reflectance spectra (4 white, 4 grey, 4 black, 4 uncalibrated reference material and 4 chlorite) plus 4 reflectance spectra for the individual background materials. When chlorite was

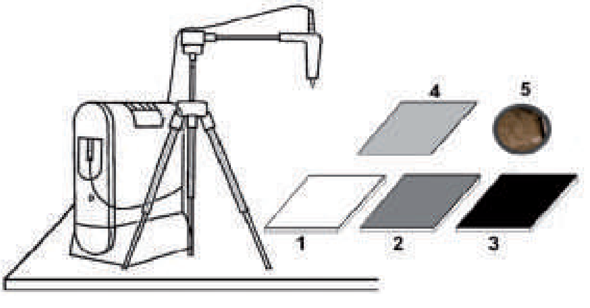

Fig. 1: Schematic illustration of the panels and targets with a field spectrometer in the laboratory, 1–3: calibrated panels, 4: uncalibrated reference panel, 5: chlorite.

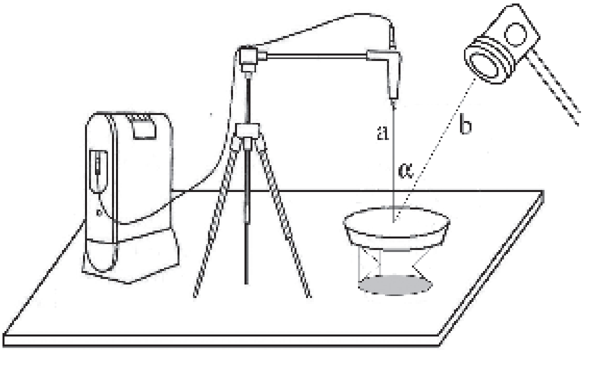

Fig. 2: Geometric parameters of the experiment protocol: a = distance between reference and measurements unit, b = distance between reference and the source of illumination, α = angle between a and b.

measured the size of the sample was often less than the FOV of the spectrometer and a spectrum-neutral background was needed, which was a challenge in many cases (Fig. 5).

The schematic illustration of the panels and targets with a spectrometer in a laboratory setup can be seen in Fig. 1. Fig. 2 shows the basic geometric parameters that were documented in the protocol (Tab. 2).

3 Reference Materials

Three calibrated reference targets (Fig. 1, 1–3) and two material samples (Fig. 1, 4–5) were measured by each participant. The two samples consisted of an uncalibrated reference target and a chlorite mineral (Chlorite schist, Great St. Bernard, Switzerland, $(Mg,Al,Fe,Mn)_3[(OH)_2Si_4O_{10}]*3Mg(OH)_2$). The calibrated targets had 5 %, 20 % and 90 % absolute reflectance.

The absolute reflectance values for the reference targets were defined in the following way: The hemispherical spectral reflectance was measured for the calibrated reference targets and the calibration was performed with a standard from U.S. National Institute of Standards and Technology (NIST), serial number 2044a-01-15. The absolute reflectance was determined by using a Perkin-Elmer Lambda 19 UV-VIS-NIR spectrometer (serial number: 1260) equipped with a 150 mm PTFE (Polytetrafluoroethylene) sphere, certified by the National Metrology Institute of Germany (PTB, Braunschweig, Calibration PTB 4.52-0208). The random error for the reference targets was 0.006 for 250–400 nm, 0.005 for 400–1100 nm, 0.006 for 1100–2200 nm and 0.010 for 2200–2500 nm. The size of the calibrated reference panels was 200 x 200 mm². The uncalibrated reference target shows typical reflectance properties in the visible spectral range and very characteristic features both in the NIR and SWIR (near and short wave infrared). Its size was also 200 x 200 mm². The chlorite sample (Fig. 4) with an average size of 50 x 50 mm² was an ideal mineral for a spectrometric round-robin test because it is robust and has easy-to-find absorption peaks and stand-alone features. The second reason to work with this sample was its small size. This pre-condition (50 x 50 mm²) was a challenge to the participants (because of FOV) and forced them to use individual background solutions, which strongly affected the final outcome and enriched the experiment with valuable information (Fig. 5).

The reference curves are presented (Fig. 3) to have basic spectral information on the reference panels and targets. It provides an illustration of the characteristics of the six curves (white, grey, black, uncalibrated, chlorite and background). The participants had to deliver these kinds of spectra after having finished the individual experiment with their own spectrometer. In Fig. 6 can be seen what kind of variety of the reflectance spectra were captured by individual measurements. As an example, three curves were shown in Fig. 6 to present obvious anomalies.

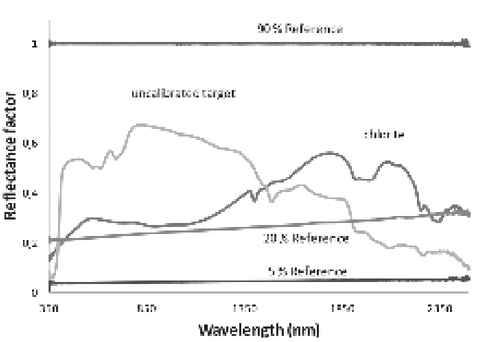

Fig. 3: The reference spectra and chlorite.

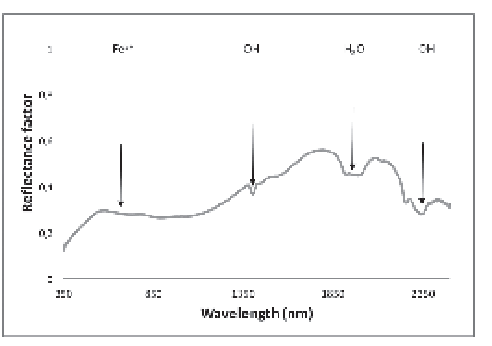

Fig. 4: Chlorite spectrum with absorption peaks.

4 Results

In this paper more attention is paid to general aspects and easy-to-recognize anomalies in the spectra and attitudes in the community. The results will be discussed through examples taken from the SpecTour database. The first one summarises the content of the protocols and highlights the tendencies of the user community. The second example will point out how important it is to be aware of the background materials when the FOV of the spectrometers exceeds the size of the sample. The third example shows typical errors for white reference measurements (Figs. 7 and 8). The SpecTour coordinators checked the spectra and gave feedback in case of anomalies. It helped localize and communicate typical problems and showed the advantages of a networking community.

4.1 *Evaluation of the Protocols*

The protocols of the experiment were of high significance for an understanding of the spectra and for the documentation of the non-spectral properties of a spectrometric measurement. These results came mostly from the measurements' protocol (Tab. 2 and Fig. 2) or from the header part of a measurement file. In Tab. 3 the geometrical properties of the individual measurement setup were summarised. Half of the participants worked with a target-measurement unit distance (P_a) of 21–30 cm, with a target-lamp distance (P_b) of 31–60 cm and with a lamp-to-measurement angle (P_α) of 36–45°. These dimensions document a typical laboratory environment and are achievable without extra investments. Another reason is the analogy to the field measurements which demand the source of illumination being significantly further away compared to the height of the measurement to guarantee diffuse irradiance conditions. In the laboratory real conditions are narrowed to compromises and feasible solutions.

Tab. 3: Geometric properties of the measurements.

Distance between target and measurement optic (cm)	% n=24
Contact (<1)	16
1–5	8
11–15	13
16–20	13
21–30	**50**

Distance between target and light source (cm)	% n=24
Contact (<1)	17
1–30	13
31–60	**50**
61–90	8
91–140	12

Angle between P_a and P_b in degree (°)	% n=25
Contact (<1)	16
15–25	12
26–36	8
36–45	**56**
46–55	8

n: number of elements (instrument or other parameters)
Contact: stands for measurement with distance up to 1 cm

Tab. 4: Auxiliary parameters of the spectra.

Integration time (ms)	% n=29
8	3
17	7
34	7
68	15
136	**62**
272	3
1000	3

Count of samplings before saving a measurement	% n=28
10	4
25	**50**
30	4
40	7
50	25
100	10

Considering the integration time it can be stated that more than 60 % of the participants operate with 136 ms. In many spectrometers the integration time is chosen automatically and manual adjustment is not needed. This avoids saturation and improves comparability. Another observed issue is "the count of samplings before saving". It points out how many measurements (samplings) were made and averaged before one spectrum was saved and shows that the saved spectra have different statistical robustness and half of the participants made 25 samplings before saving one spectrum (Tab. 4). According to the measurement protocol, most of the spectrometers were purchased between 2007 and 2009. This reflects a growing market and scientific interest (Tab. 5).

The number of calibrations is not very meaningful because most of the instruments were bought in the last 5–10 years (Tab. 5). Usually, the manufacturers recommend recalibrating the instrument every 2–3 years. However, as many instruments are quite new, 62 % of them have only been recalibrated once or twice. The frequency of recalibration also depends highly on budget and necessity in public research facilities.

In laboratories, artificial sources of illumination are commonly used. These illumination sources should be stable and robust over a long period of time. In this experiment, queries were made in reference to three parameters about lamps. The parameter "number of lamps" shows that more than 80 % of the participants use only one lamp in the laboratory setup (Tab. 6). One reason for this is that also in nature the sun is the "standalone source" of illumination. In some cases, the number of lamps is increased to minimise directional light effects and multiple shadowing for layered targets like vegetation. More than 60 % of the lamps had a power of 50 W. This power seems to be an appropriate solution that can service the observed 31–60 cm distance (P_b) and does not negatively affect vital or wet organic materials. A logical outcome is the year of the lamp's purchase that correlates with the

Tab. 5: Auxiliary parameters for the spectrometers.

Year of instrument purchase and last calibration	% n=30	% n=27
1991 – 1995	10	---
1996 – 2000	17	---
2001 – 2003	17	7
2004 – 2006	13	15
2007 – 2009	**37**	**59**
2010 – 2011	7	18

Number of calibrations	% n=16
1	**31**
2	**31**
3	13
5	6
6	13
7	6

n: number of elements (instrument or other parameters)

Tab. 6: Properties of illumination sources.

Number of lamps	% n=31
1	**84**
2	7
4	2
6	7

Power of light source (W)	% n=28
6.5	18
50	**63**
150	4
235	4
1000	7
2000	4

Year of purchase for light sources	% n=23
1997 – 2003	22
2004 – 2006	26
2007 – 2009	**43**
2010 – 2011	9

n: number of elements (instrument, lamp or other countable parameters) year of the spectrometer's purchase since most systems were obtained simultaneously and as a unit.

4.2 *Variability of Background Signals*

Multiple effects substantially influenced the chlorite spectra (Fig. 6). At the single spectrum level the integration time and the warm-up time of the instrument often were likely not to be properly addressed, which caused typical jumps (around 1000 nm and 1750 nm) in many spectra (Fig. 6, middle curve). The background and its interactions with the chlorite spectrum must be carefully discussed. The background was an unknown material behind the sample in almost all cases. The spectrometer user was asked to find the appropriate substance on his own in order to properly measure the chlorite sample. The ideal background in spectroscopy is a low reflectance material (<5 %) covering the range of 400–2500 nm (Fig. 5). Deployment of materials not meeting this requirement should be avoided. The example shows that there are no standards for background material (standard deviation of chlorite is 23 %). Unfortunately, not all spectrometer users are aware of this effect and do not pay enough attention to this (Fig. 5). It is evident that an inappropriate background can fundamentally change the reflectance values of a sample. Generally spoken, the spectrometer users need more information about what to consider when the FOV of the spectrometer exceeds the size of the sample.

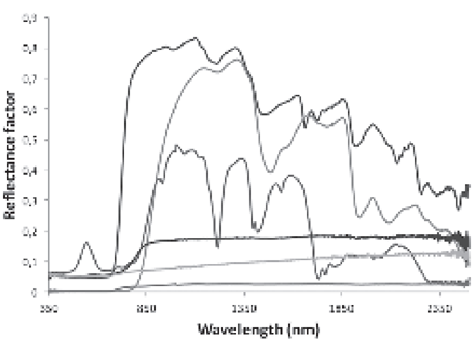

Fig. 5: Characteristics of 6 different background signals.

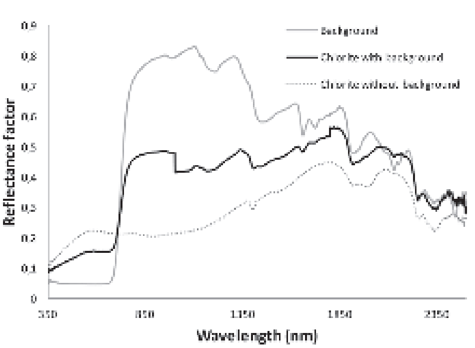

Fig. 6: Effect of background signals on chlorite.

4.3 *Variability of White Reference Signals*

Most of the white reference measurements seem to be appropriate at the present level of scaling (Fig. 7). Only one spectrum shows un-

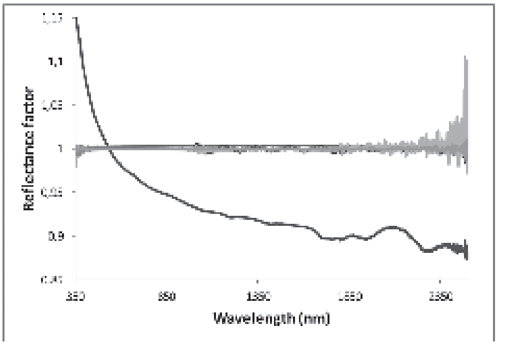

Fig. 7: White reference measurements.

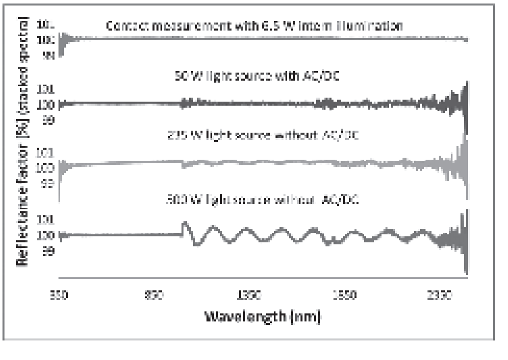

Fig. 8: Influence of light source effects (with or without AC/DC) on the reflectance factor of the white reference panel.

acceptable discrepancies and indicates a fundamental measurement failure.

In Fig. 8 four different reflectance curves are depicted (measurement on white panel) that are typically used by spectrometer users. The 6.5 W and 50 W sources were very common (70 % of the participants), but in the remaining 30 % of the measurements some uncommon phenomena could be observed. Five or six waves can be seen in the first SWIR detector of the spectrometer. The oscillations (sine wave) can be caused by an AC (alternating current) light source (ASD Manual 2007). It is a remarkable phenomenon to observe how electric adapters can influence the spectroscopic data. Laboratory lamps without AC/DC (direct current) adapters have a significant effect on the spectrum that was often overseen or neglected.

After taking the white reference measurement it is recommended to have a detailed look at the measured values to select and avoid malfunctioning signals.

The controlled illumination sources play a significant role in the in-door measurement practise, but they have a lower priority for spectrometer users who take the measurements mostly in the field and are less experienced in the laboratory.

5 Conclusions

This paper gives a brief overview on the diversity of laboratory environment and is more focused on the evaluation of the non-spectroscopic or auxiliary properties of the experiment. Some basic considerations could already be concluded from the present level of the analysis. It became evident that more technical communication is needed among spectroscopic laboratories. For newcomers training courses are necessary and standards or detailed reference books are still missing.

Taking part in the network increases the statistical robustness, helps the mapping procedure and avoids the typical anomalies of measurements.

Spectra must be evaluated regarding quality before entering the final spectral library. This quality is influenced and affected by many parameters, as we could see in this experiment as well. More attention has to be paid to background materials, interactions between white reference measurements and illumination sources. The high variance of background signals and their effects in mineral measurements provided surprising results. The AC/DC converter phenomenon was an interesting, although atypical, observation that can easily be eliminated through the use of a proper adapter. These results encourage us to network more intensively and effectively in the future.

6 Outlook

Our aim is to provide to the community recommendations regarding best practices, guidelines and participation in standardisation studies. Spectra are used as reference and reliability is the highest priority. The lack of measurement environment standards and the significant variability of the results encourage the detailed spectral analysis and interpretation of the parameters. Laboratory work does not cover the whole activity of a user. Field work is just as important as laboratory work and even more complicated. Open access to the results of the project will be available for teaching and training purposes. In the next level of this experiment the SpecTour project will be extended to field measurements.

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Addresses of the Authors:

Dr.-Ing. András Jung, Institut für Lasertechnologien in der Medizin und Messtechnik, Universität Ulm, D-89081 Ulm, Tel.: +49-731-1429997, e-mail: info@andrasjung.de

Dr. rer. nat. Christian Götze, Prof. Dr. Cornelia Glässer, Institut für Geowissenschaften und Geographie, Martin-Luther-Universität Halle-Wittenberg, Von-Seckendorff-Platz 4, D-06120 Halle (Saale), Tel.: +49-345-5526020/21, Fax: +49-345-5527168, e-mail: {christian.goetze}{cornelia.glaesser}@geo.uni-halle.de

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