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DRILLING PROGRAM

ICDP Data Set Report 2

# Explanatory remarks on the data sets of the master thesis: "Analysis of element behavior in mylonites of the Seve Nappe of the Scandinavian Caledonides using different core scanning methods"

Johannes Hierold, Friederike Körting, Tina Kollaske,
Christian Rogass, Ulrich Harms

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# ICDP Data Set Report COSC-1

# Explanatory remarks on the data sets of the master thesis: “Analysis of element behavior in mylonites of the Seve Nappe of the Scandinavian Caledonides using different core scanning methods”

**J. Hierold**[1, 2]

[1] Scientific Drilling, GFZ German Research Centre for Geosciences, Potsdam, Germany

[2] University of Greifswald, Institute for Geography and Geology, Germany

**Abstract**

**The International Continental Scientific Drilling Program (ICDP) performed a dual-phase scientific drilling project to investigate mountain-building processes called Collisional Orogeny in the Scandinavian Caledonides (COSC). The borehole COSC-1 was drilled through the Lower Seve Nappe, as the first of two 2.5 km deep drill holes close to Åre, central Sweden. The recovered rocks comprise a 1650 m thick suite of high grade gneisses and amphibolites with clear Seve Nappe affinities, while the lower 850 m comprise rather homogenous mylonitic gneisses with interfingered K-rich phyllonite bands of cm to several m size and some intercalated amphibolites. The different lithologies all crosscut the core in a subhorizontal direction with foliation of gneisses and phyllonites in the same direction. Albite and garnet porphyroblasts with pressure shadows show syndeformational growth and the same sub-horizontal alignment.**

**The focus was to detect chemical and mineralogical differences in mylonitic and host rocks and to relate these differences to either metasomatism and deformation or inherited source rock variance. Another goal of this work is to compare chemical core scanning instruments. For this purpose, two different µ-Energy-Dispersive X-Ray Fluorescence (µ-EDXRF), Laser Induced Breakdown Spectroscopy (LIBS) and hyperspectral imaging techniques served to measure seven samples from the lower 850 m of the COSC-1 core.**

**This report will explain the data sets gained during this study. The metadata will be presented in an additional file including XRF data from the AVAATECH XRF core scanner in a text file as well as data sets of the other used devices in original file formats.**

**Related Work**

Lorenz, Henning; Rosberg, Jan-Erik; Juhlin, Christopher; Bjelm, Leif; Almqvist, Bjarne; Berthet, Théo; Conze, Ronald; Gee, David G.; Klonowska, Iwona; Pascal, Christophe; Pedersen, Karsten; Roberts, Nick; Tsang, Chinfu (2015): COSC-1 operational report - Operational data sets. GFZ Data Services. DOI: http://doi.org/10.1594/GFZ.SDDB.ICDP.5054.2015

Hierold, Johannes; Körting, Friederike; Kollaske, Tina; Rogass, Christian; Harms, Ulrich (2016) "Analysis of element behavior in mylonites of the Seve Nappe of the Scandinavian Caledonides using different core scanning methods" – Operational data sets. GFZ Data Services. DOI: http://doi.org/10.5880/ICDP.5054.001

Hierold, Johannes (2016): Analysis of element behavior in mylonites of the Seve Nappe of the Scandinavian Caledonides using different core scanning methods, Master Thesis, (Scientific Technical Report STR; 16/07), Potsdam: GFZ German Research Centre for Geosciences. DOI: http://doi.org/10.2312/GFZ.b103-16070

**Coordinates of the COSC-1 drill site:** 63.4063 N, 13.203057 E

# Table of Contents

# 1. Common Conventions for All Data

- Throughout all data sets the common naming convention used is ― Expedition, Site, Hole (the Expedition ID 5054 is used for COSC). See more details and example at the end of this report.
- Throughout all data sets the common date and time format used is ―Day Month Year Hours:Minutes:Seconds The time zone is CET (Central European Time), hours are in 24-hours notation.
- Persistent identifiers (IGSN, International Geo Sample Number) are used in data sets showing sample material from the drill core and borehole. The uppermost IGSN in the hierarchy are available via http://hdl.handle.net/10273/ICDP5054EHW1001 (COSC 1 hole A), http://hdl.handle.net/10273/ICDP5054EHX1001 (COSC 1 hole B) and http://hdl.handle.net/10273/ICDP5054EH02001 (COSC 1 hole C). For more general information about IGSN please visit http://www.igsn.org.
- Throughout all data sets with measured values the metric unit system is used as described in Lorenz et al. (2015c)
- The COSC project has the ICDP project (expedition) number 5054.
- The COSC-1 site has the site number 1.
- The deep drill hole has the hole designation A, the 100-m observation drill hole the designation B, and the 50-m observation drill hole the designation C.
- Sections in the core box are successively numbered from the top of the core run downwards, beginning at 1 for each core run. All analysed core sections have been split longitudinal.
- Depth is the driller depth in the bore hole measured from the surface in m.

The Sample-id is following these definitions and directly related to the relational database structure of the Drilling Information System DIS (Conze, 2015)

Example:
5054-1-A-550-3-1682.057
Project-Site-Hole-Core Run-Section-depth measured from surface in m

# 2. Cores, Sections, and Boxes

- CORE is the complete core run recovered from the core barrel.
- SECTION of a core run is defined by the actually used core box layout. Top and bottom of a core section is defined by top or bottom of the core run and/or the top or bottom of a box slot.

## 3. Core Samples

The following table shows the core samples investigated within the master thesis.

The IGSN can be resolved e.g. for sample 5054-1-A 550-3 using the URL-link: http://hdl.handle.net/10273/ICDP5054EX2Z501

| IGSN | Sample-ID | Short form of sample | Depth from top of section [m] | Length [cm] | Used devices for investigation |
|---|---|---|---|---|---|
| ICDP5054EX2Z501 | 5054-1-A 550-3 | 550 | 1682.057 | 15.5 | EDXRF; LIBS; AVAATECH XRF scanner; HySpex |
| BGRB5054RX25201 | 5054-1-A 578-6 | 578 | 1802.50 | 15 | AVAATECH XRF scanner |
| ICDP5054EX3Z501 | 5054-1-A 625-7 | 625 | 2077.20 | 19 | EDXRF; LIBS; AVAATECH XRF scanner; HySpex |
| BGRB5054RX15201 | 5054-1-A 641-3 | 641 | 2170.17 | 35 | AVAATECH XRF scanner |
| BGRB5054RX05201 | 5054-1-A 658-6 | 658 | 2273.46 | 17.5 | AVAATECH XRF scanner |
| ICDP5054EX4Z501 | 5054-1-A-689-2 | 689 | 2456.46 | 18 | EDXRF; LIBS; AVAATECH XRF scanner; HySpex |
| BGRB5054RXZ4201 | 5054-1-A 691-2 | 691 | 2469.26 | 16 | AVAATECH XRF scanner |

## 4. Sample Orientation

In almost all cases the samples are correctly orientated vertically. The only exception is the data set of the AVAATECH XRF measurements. Here the core samples have been analysed horizontally. In this case the top of the core is on the left-hand side, whereas the bottom of the core is on the right-hand side.

## 5. Energy Dispersive X-Ray Fluorescence (EDXRF) Data (BRUKER)

EDXRF geochemical data of the selected core sections with µ-EDXRF core scanner Tornado M4 by Bruker were measured in July 2015 at the BGR in Hannover. The measured values show the intensities of the detected elements including the major elements: Si, Ti, Al, Fe, Mn, Mg, Ca, Na, K, P and the trace elements: Ba, Cl, Co, Cr, Cu, Nb, Ni, Pb, Rb, S, Sr, V, Y, Zn and Zr. An electric voltage of 49 kV and a current of 597 µA were used to register with a very high resolution of 50 µm on the entire half core surface with a measuring time per point of 2 ms.

More information about the analyzing device Tornado M4 by Bruker is available via: https://www.bruker.com/fileadmin/user_upload/8-PDF-Docs/X-rayDiffraction_ElementalAnalysis/mXRF/Flyers/Fly_m4_tornado_2p_en_rev1_lores.pdf

## 6. Hyperspectral Data

The hyperspectral data were acquired using a hyperspectral camera by HySpex Norsk Elektro Optikk, Norway. Two sensors have been used to detect wavelength in a range from 400 – 2500 nm. After the reflectance retrieval, the HySpex data was analysed by the PRISM program, “**P**rocessing **R**outines in **I**DL for **S**pectroscopic **M**easurements”, a software package for hyperspectral mineral analyses created by the USGS (http://pubs.usgs.gov/of/2011/1155/) which is a freely available add-on of the remote sensing software "ENVI". Within PRISM, an incorporated algorithm called MICA (“**M**aterial **I**dentification and **C**haracterization **A**lgorithm”) was used to identify best fits with reference spectra of known minerals of a spectral library. The library spectra were retrieved from splib06a (Clark et al., 2007) which is provided by the USGS (http://speclab.cr.usgs.gov/spectral.lib06/ds231/). The available mineral spectra are of different degrees of "purity" which is explained in (Clark et al. 2007). A list of the available spectra can be found via http://speclab.cr.usgs.gov/spectral.lib06/ds231/datatable.html.

In addition, the data were processed using an algorithm to identify Fe and Fe-bearing minerals (Mielke, et al., 2014).

## 7. Laser Induced Breakdown Spectroscopy (LIBS) Data

LIBS measurements have been realized in July 2015 at the BGR in Hannover using a prototype LIBS core scanner by Lasertechnik Berlin. The measurements have been conducted with a resolution of 0.2 mm. Two laser beams per measuring point were shot onto the sample surface and the accumulated signal was detected by the spectrograph. The data values represent the intensity of the detected element, including the major elements: Si, Ti, Al, Fe, Mn, Mg, Ca, Na, K, P and the trace elements B, Ba, Ca, Co, Cr, Cu, Li, Nb, S, Y and Zr.

Additional information about the used device is available via: http://www.ltb-berlin.de/?id=1 (LTB Lasertechnik Berlin)

The LIBS mineral map derived by Hierold, (2016) relies on the assumption that the presence and intensities of certain elements could be used as proxies for certain minerals. **Muscovite** was mapped for the regions showing high K and Al intensities and no Fe or Mg intensities. Calcite is correlated to regions which show very high intensities of Ca but no other elements and **K-feldspar** was assumed as a combination of high K intensities, low Na and the absence of Fe. As Deer et al, (1992) states, a diversity of elements can substitute elements in the mineral due to changes in P-T-conditions or the surrounding rock. In reality, Calcite (CaCO3) can substitute Ca with other elements like (Mg, Fe, Sr, Ba, Mn, Co and Zn). Muscovite with the general formula $KAl_2Si_3O_{10}(OH)_2$ can substitute elements like (Na, Rb, Cs, Ca and Ba) for K and (Mg, Fe, Mn, Li, Cr, Ti and V) for Al. OH can also be substituted by F. K-feldspar with the general formula of KAlSi3O8 can substitute elements like Ti, Fe, Mg, Ba, Ca and Na (Deer et al., 1992).

The difference in the mineral mapping between the LIBS and the EnGeoMap mapping is not due to the EnGeoMap algorithm or the hyperspectral mapping approach but clearly based on the oversimplification of the LIBS mineral mapping. Hierold (2016) based his mineral modelling on the presence and absence of only 1-4 elements. Additionally, the intensities of these elements were taken as a proxy to determine the presence of a certain mineral. For example, by excluding every other element but Ca to map calcite, only the pure calcite minerals were mapped and all variations of calcite were neglected.

## 8. X-Ray Fluorescence (XRF) Data (AVAATECH)

XRF measurements with the AVAATECH core scanner have been performed as line scans on the selected core sections at the core repository in Berlin/Spandau. The measured values show the intensities of the elements Mg, Al, Si, S, Cl, K, Ca, Ti, Cr, Mn, Fe and Rh.

Additional information about the used device and the core repository in Berlin-Spandau, is available via: http://www.avaatech.com/ (Website AVAATECH)

http://www.bgr.bund.de/DE/Themen/Sammlungen-Grundlagen/Bohrkernlager/Bohrkernlager_kontinentale_Forschungsbohrungen/Bohrkernlager_kontinentale_Forschungsbohrungen_inhalt.html?nn=1871576
(Website Core Repository Berlin Spandau)

## 9. Evaluation Software ENVI

The evaluation of all data measured with the techniques introduced above was performed with the processing software package ENVI "Environment for Visualizing Images" of Harris Geospatial Solutions. The program can import different types of image formats combined with the additional raster information. Statistical information can be calculated and illustrated in tabular form or as graphs. Additionally, data sets can be exported for other programs such as Microsoft Excel.

The used data formats for ENVI where .bsq, and .tiff and the related meta information is stored in *.hdr files

More information about ENVI is given in the master thesis of J. Hierold (2016) or via http://www.exelisvis.com/docs/using_envi_Home.html.

## 10. References


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Lorenz, H., Rosberg, J.E., Juhlin, C., Bjelm, L., Almqvist, B.S.G., Berthet, T., Conze, R., Gee, D.G., Klonowska, I., Pascal, C., Pedersen, K., Roberts, N.M.W. and Tsang, C.F. (2015c): COSC-1 operational report: Explanatory Remarks on the Operational Data Sets. Potsdam, ICDP Data Set Report. GFZ German Research Centre for Geosciences, http://doi.org/10.2312/icdp.2015.001

Mielke, C. et al., 2014. Spaceborne Mine Waste Mineralogy Monitoring in South Africa, Applications for Modern Push-Broom Missions: Hyperion/OLI and EnMAP/Sentinel-2. Remote Sensing, 6, pp. 6790-6816. http://doi.org/10.3390/rs6086790

## 11. List of available data sets

The provided data (size: 2.37 GB) are structured into four folders:

- 01_EDXRF-Tornado-M4_Data
- 02_Hyperspectral_Data
- 03_LIBS_Data
- 04_XRF_Avaatech_Data

### 11.1. Energy Dispersive X-Ray Fluorescence (EDXRF) Data (BRUKER)

The folder **"01_EDXRF-Tornado-M4_Data"** (size: 2.29 GB) contains the following data:

- EDXRF_TIFF_FORMAT
- EDXRF_550.bcf
- EDXRF_625.bcf
- EDXRF_689.bcf

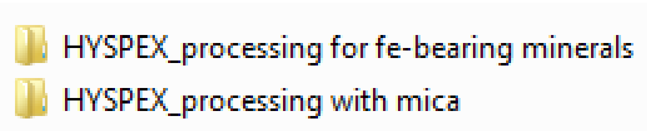
The original Energy Dispersive X-Ray Fluorescence (EDXRF) data set by the Tornado M4 core scanner by Bruker is provided in .bcf file format and can only be opened with the associated software from Bruker. You will find three .bcf files for the three main samples 550, 625 & 689.

However, the element distribution maps created with the Bruker software were saved in .tiff format to make analysis with the frequently used evaluation software ENVI possible. The figures show the distribution of the detected element as well as its intensity. In the folder EDXRF_TIFF_FORMAT you will find three subfolders for the three main samples 550, 625 & 689. Each subfolder contains 24 tiff-images that show the distribution and intensity of the detected Element, e.g. the tiff-file EDXRF_550_Al stands for the distribution of aluminum in Sample 550.

| Filename | Extension | Format | Size | Note |
|---|---|---|---|---|
| EDXRF_TIFF_FORMAT | file folder | file folder | 110 MB | contains the three subfolders 550, 625 & 689 |
| EDXRF_550 | .bcf | BCF-File only possible to open with associated software from Bruker | 573 MB | maps provide content of analysed elements |
| EDXRF_625 | .bcf | BCF-File only possible to open with associated software from Bruker | 825 MB | maps provide content of analysed elements |
| EDXRF_689 | .bcf | BCF-File only possible to open with associated software from Bruker | 836 MB | maps provide content of analysed elements |

## 11.2. Hyperspectral data

The folder **"02_Hyperspectral_Data"** (size: 258 KB) contains the following data:




The post-processed hyperspectral data set is provided in .bsq format and can be opened with the evaluation software ENVI. You will find two folders with hyperspectral data sets, one is to analyse Fe-bearing minerals, the other to analyse different types of phyllosilicates. Each folder contains six files, including two different formats per sample (main samples 550, 625 & 689). These are .bsq and .hdr format. The header file (-hdr) includes all of the spatial and spectral information which are used as a base for the algorithm to access the data in the .bsq format. To open the actual spectral dataset by ENVI it has to be ensured that all two files related to one image are kept altogether in one folder.

The folder **“HYSPEX_processing for fe-bearing minerals”** (size: 127 KB) contains the following files:

| **Filename** | **Extension** | **Format** | **Size** | **Content** |
|---|---|---|---|---|
| HYSPEX_550-fe-bearing | .bsq | bsq binary | 26 KB | file to be opened with e.g. ENVI |
| HYSPEX_550-fe-bearing | .hdr | HDR-file | 3 KB | Header file |
| HYSPEX_625-fe-bearing | .bsq | bsq binary | 35 KB | file to be opened with e.g. ENVI |
| HYSPEX_625-fe-bearing | .hdr | HDR-file | 3 KB | Header file |
| HYSPEX_689-fe-bearing | .bsq | bsq binary | 34 KB | file to be opened with e.g. ENVI |
| HYSPEX_689-fe-bearing | .hdr | HDR-file | 3 KB | Header file |

The folder **“HYSPEX_processing with mica”** (size: 131 KB) contains the following files:

| **Filename** | **Extension** | **Format** | **Size** | **Content** |
|---|---|---|---|---|
| HYSPEX_550-with-mica | .bsq | bsq binary | 29 KB | file to be opened with e.g. ENVI |
| HYSPEX_550-with-mica | .hdr | HDR-file | 3 KB | Header file |
| HYSPEX_625-with-mica | .bsq | bsq binary | 37 KB | file to be opened with e.g. ENVI |
| HYSPEX_625-with-mica | .hdr | HDR-file | 3 KB | Header file |
| HYSPEX_689-with-mica | .bsq | bsq binary | 31 KB | file to be opened with e.g. ENVI |
| HYSPEX_689-with-mica | .hdr | HDR-file | 3 KB | Header file |

## 11.3. Laser Induced Breakdown Spectroscopy (LIBS) data

The folder **“03_LIBS_Data”** (size: 82,3 MB) contains the following data:

| Filename | Extension | Format | Size | Content |
|---|---|---|---|---|
| LIBS_550-all-elements | .bsq | bsq binary | 18426 KB | file to be opened with e.g. ENVI |
| LIBS_550-all-elements | .hdr | HDR-file | 1 KB | Header file |
| LIBS_625-all-elements | .bsq | bsq binary | 23658 KB | file to be opened with e.g. ENVI |
| LIBS_625-all-elements | .hdr | HDR-file | 1 KB | Header file |
| LIBS_689-all-elements | .bsq | bsq binary | 21875 KB | file to be opened with e.g. ENVI |
| LIBS_689-all-elements | .hdr | HDR-file | 1 KB | Header file |

The LIBS data set is provided in .bsq and .hdr formats and can be opened with the evaluation software ENVI. The header file (-hdr) includes all of the spatial and spectral information which are used as a base for the algorithm to access the data in the .bsq format. To open the actual spectral dataset by ENVI it has to be ensured that all two files related to one image are kept altogether in one folder.

The bands represent the following elements:

| Band | Element_wavelength [nm] | Band | Element_wavelength [nm] |
|---|---|---|---|
| 1 | Al_309.2839 | 26 | Nb_416.8130 |
| 2 | Al_396.1520 | 27 | P__603.4040 |
| 3 | B__434.5000 | 28 | P__604.3120 |
| 4 | Ba_455.4033 | 29 | S__921.2865 |
| 5 | Ba_493.4077 | 30 | Si_288.1580 |
| 6 | C__909.4830 | 31 | Si_390.5520 |
| 7 | Ca_393.3660 | 32 | Si_634.7100 |
| 8 | Ca_396.8470 | 33 | Ti_337.2800 |
| 9 | Co_340.5120 | 34 | Ti_498.1730 |
| 10 | Cr_520.6040 | 35 | Y__395.0360 |
| 11 | Cu_324.7540 | 36 | Y__437.4940 |
| 12 | Cu_327.3960 | 37 | Zr_339.1980 |
| 13 | Fe_373.4864 | 38 | Zr_343.8230 |
| 14 | Fe_404.5813 | 39 | Ba_455.4033 |
| 15 | K__766.4900 | 40 | Ba_493.4077 |
| 16 | K__769.8960 | 41 | Co_340.5120 |
| 17 | Li_670.7910 | 42 | Cr_520.6040 |
| 18 | Mg_383.8292 | 43 | Cu_324.7540 |
| 19 | Mg_518.3604 | 44 | Cu_327.3960 |
| 20 | Mn_403.3070 | 45 | Mn_403.3070 |
| 21 | Mn_403.4490 | 46 | Mn_403.4490 |
| 22 | Na_588.9950 | 47 | P__603.4040 |
| 23 | Na_819.4824 | 48 | S__921.2865 |
| 24 | Nb_353.7480 | 49 | Zr_339.1980 |
| 25 | Nb_407.9730 | 50 | Zr_343.8230 |

The numbers behind the elements represent the characteristic wavelength in nm of the detected element.

## 11.4. AVAATECH XRF data

The folder **“04_XRF_Avaatech_Data”** (size: 225 KB) contains the following data:

| Filename | Extension | Format | Size | Content |
|---|---|---|---|---|
| XRF_AVAATECH_DATA | .txt | Text-file | 100 KB | Data information in raw text format |
| XRF_AVAATECH_DATA | .xlsx | Excel-file | 127 KB | Data information in excel sheet |

The AVAATECH XRF data sets are provided in ASCII (.txt) and Microsoft Excel (.xlsx) formats. Both files contain information of all analysed samples.

Table: Explanation of the metadata part

| Column Name | Data Type | Description | Validation Text | Unit |
|---|---|---|---|---|
| EXPEDITION | Numeric | expedition number | integer value | # |
| SITE | Numeric | site number | integer value | # |
| HOLE | Text | code for hole | text string of max. 1 character (A_Z) | # |
| CORE | Numeric | core identifier | integer value >=1 | # |
| SECTION | Numeric | section number | integer value >=1 | # |
| IGSN | Text | International Geo Sample Number | text string of max. 15 characters | # |
| MEASUREMENT-DATE | Triple | date of measurement | date in UTC | dd-mmm-yyyy |
| MEASUREMENT-TIME | Triple | time of measurement | time in UTC | hh:mm:ss |
| LIVETIME | Numeric | live time measured | integer value | sec. |
| REALTIME | Numeric | real time measured | integer value | sec. |
| X_POSITION | Numeric | distance in X-direction | integer value | cm |
| Y_POSITION | Numeric | distance in Y-direction | integer value | cm |
| SLIT_DC | Numeric | slit size in X-direction | integer value | mm |
| SLIT_CC | Numeric | slit size in Y-direction | integer value | mm |
| TOTALCPS | Numeric | total counts/ second | integer value | # |
| ELEMENT_AREA | Numeric | counts of element per detected area | integer value | # |