Seismic properties and mineralogy of core samples from the COSC-1 borehole, Sweden

(https://doi.org/10.5880/GFZ.4.2.2020.009)

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2. Citation

When using the data please cite:

Kästner, F.; Wenning, Q.; Zappone, A.; Madonna, C.; Morales, L.F.G.; Pierdominici, S.; Berndt, C.; Schleicher, A.M.; Wilke, F.D.H. (2021): Seismic properties and mineralogy of core samples from the COSC-1 borehole, Sweden. GFZ Data Services. https://doi.org/10.5880/GFZ.4.2.2020.009

The data are supplementary material to:

Kästner, F., Pierdominici, S., Zappone, A., Morales, L. F. G., Schleicher, A. M., Wilke, F. D. H., & Berndt, C. (2021). Cross-scale seismic anisotropy analysis in metamorphic rocks from the COSC-1 borehole in the Scandinavian Caledonides. Journal of Geophysical Research: Solid Earth. https://doi.org/10.1029/2020jb021154

Kästner, F., Pierdominici, S., Elger, J., Zappone, A., Kück, J., & Berndt, C. (2020). Correlation of core and downhole seismic velocities in high-pressure metamorphic rocks: a case study for the COSC-1 borehole, Sweden. Solid Earth, 11(2), 607–626. https://doi.org/10.5194/se-11-607-2020

Wenning, Q. C., Almqvist, B. S. G., Hedin, P., & Zappone, A. (2016). Seismic anisotropy in mid to lower orogenic crust: Insights from laboratory measurements of Vp and Vs in drill core from central Scandinavian Caledonides. Tectonophysics, 692, 14–28. https://doi.org/10.1016/j.tecto.2016.07.002

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3. Data Description

Core samples have been taken for complementary laboratory seismic measurements and mineralogical analyses on whole rock core from the COSC-1 borehole, Sweden (UTM 63.3124, 13.5259). These samples were used to provide and characterize the seismic properties (i.e., seismic velocities and anisotropy) of the drilled rocks from the highly metamorphosed and deformed Seve Nappe Complex, an orogenic thrust zone in the Scandinavian Caledonides, in central Sweden. The laboratory seismic and mineralogical analysis in general comprises three distinct measurements (i.e., data sets), which will be described in detail in the following subsections:

1) P- and S-wave laboratory seismic measurements on three perpendicular core plugs, under different confining (hydrostatic) pressure conditions (10 + 6 samples)
2) Bulk mineralogy of core plugs using X-ray powder diffraction (XRD) and mineral chemical composition measurements using an electron probe micro-analyzer (EPMA, here microprobe), on 10 thin sections
3) Microstructural investigations based on electron-backscatter diffraction analyses on 5 thin sections

The laboratory seismic measurements were initially conducted on 6 samples by Wenning et al. (2016) and extended by another 10 samples by Kästner et al. (2020). Despite these authors were using the same sensor setup, the provided data files may differ due to individual acquisition parameters. Where different acquisition, processing, or calibration parameters are used this is indicated in the text using the abbreviations FK and QW referring to each examiner and their related sample measurements. International Geo Sample Numbers (IGSN) are provided for each core sample in the complete sample data table (Section 4.3.1).

3.1. Sampling method

3.1.1. Laboratory seismic analysis:

For the laboratory seismic analysis, 16 core samples of 15-20 cm length were cut from the almost 2.5 km long COSC-1 drill core at the BGR core repository, Berlin-Spandau (Germany). The subsequent sample preparation and laboratory seismic measurements were performed at the Rock Physics and Mechanics Laboratories of the ETH Zurich (Switzerland). From each sample, three mutually perpendicular core plugs were drilled using a diamond-coated drill bit corer with an inner diameter of 2.54 mm. The core plugs were drilled according to the structural axis of the core sample by visual inspection, i.e., with respect to the foliation and lineation, following the common practice notation: *x-axis* – parallel to lineation; *y-axis* – perpendicular to lineation and within the foliation plane; *z-axis* – perpendicular to the foliation plane spanned by *x* and *y*.

3.1.2. XRD measurements:

Sample powder of 10 core samples were prepared from remnants of the core plug's preparation procedure. This sample material was initially ground with a jaw crusher, and sieved to a grain size of < 62 µm. Subsequently, the powder was micronized to a homogeneous powder (< 10 µm) using a McCrone micronization mill. It was then loaded from the back side of the sample holder in order to provide a random distribution of the powdered material. The sample preparation and analysis were performed at the Geochemistry Laboratories of the GFZ Potsdam (Germany).

3.1.3. Thin sections:

Thin sections of 10 samples were prepared from the caps of the core's x-plugs, thus representing a slice in the sample's y-z plane, which is perpendicular to the foliation and lineation. These thin sections were polished with diamond solutions down to 0.25 µm grain size and subsequently carbon coated. Thin section preparation was performed at the Geochemistry Laboratories of the GFZ Potsdam (Germany). Five out of these 10 thin sections were selected for additional microstructural investigations using EBSD analysis at the Scientific Center for Optical and Electron Microscopy, ETH Zurich. To this end, the five selected thin sections were again polished down to colloidal silica levels of about 25 nm and coated with 3 nm of carbon.

3.2. Analytical procedures

The experimental procedure used to determine seismic velocities on core samples compares with that described in Kästner et al. (2020) and Wenning et al. (2016). In general, it is based on the investigation of seismic properties on pressurized samples using the pulse-transmission technique (e.g., Birch, 1960; Kern, 1990). In the following, we refer to the experimental setup as applied in Kästner et al. (2020)

Seismic velocities under different confining pressure were measured using a hydrostatic pressure vessel and corresponding acquisition system at the Rock Physics and Mechanics Laboratories, ETH Zurich. Previously prepared cylindrical core plugs were placed between metal-heads containing piezoelectric transducers (lead-zirconate ceramics) with a resonant frequency of 1 MHz, and buffer rods mounted such as to optimize the transmission of mechanical energy towards the specimen. The cores were jacketed in a polyolefin heat shrink tube and then submerged in oil, inside the pressurization chamber of the pressure vessel. The oil was pressurized using an air-driven fluid pump in conjunction with a compressor air system providing a precision of ±2 MPa. A wave generator connected to one of the two transducers produced a double-pulse input signal with 1 ms delay and 0.5 kHz pulse rate. It had a square shape of 0.2 µs width and an amplitude of 30 V (negative polarity).

Simultaneously, the wave generator sent a trigger impulse with the same pulse rate (0.5 kHz) to a PC card, which also acted as a wave analyzer. The analyzer used an impedance of 1 MΩ over a range of ±500 mV. The waveforms were recorded and saved with a sampling rate of 100 MHz (50 MHz for samples examined by QW). For the measurements, the pressure inside the vessel was incrementally increased up to 250 MPa (260 MPa for QW) in steps of 50 MPa and subsequently decreased in steps of 30 MPa from 240 MPa to 30 MPa (250 MPa to 40 MPa for QW). Acoustic waveforms, both during pressurization and depressurization cycles, were transferred to the computer for further processing without loss of resolution. Cables, transducers, and interfaces in the electronic system generally introduce a delay in the observed travel time, where $t_{observed} = t_{rock} + t_0$. As a result, a calibration had to be performed by measuring the travel times of the ultrasonic impulses (for P- and S-wave transducers, respectively) through steel cylinders of 24 mm, 29 mm, 39 mm, and 44 mm in length. The measured travel times are plotted against the cylinder lengths, extrapolated linearly, and the intercept time corresponding to 0 mm length are determined. These calibration measurements were conducted at 50 MPa, 100 MPa, and 200 MPa confining pressures. The system travel time (t_0) was determined by averaging the results obtained for the three different pressures. The calibration is performed by subtracting the system travel time t_0 from the measured travel time $t_{observed}$. System times determined and applied for present measurements are shown in Table 1. The polarization directions of the S-wave transducer setup are the following: y for the x plugs; z for the y plugs; and x for the z plugs (only for samples by FK). In addition, only for the six samples by QW, S waves were measured in two mutual perpendicular polarization directions for each core plug, that is: y, z for x plugs; y, z for x plugs; and x, y for z plugs.

Plug dimensions (i.e., cylinder length and diameter) were measured using a digital vernier caliper. The plug weight was determined using a laboratory precision balance. In addition, a He-gas pycnometer was used to measure the dry volume of each cylinder plug. Finally, the matrix density was calculated using the measured volume and weight of each core plug.

Table 1. P- and S-wave calibration of seismic laboratory measurements used for samples examined by FK and QW.

	FK – (10 samples)	**QW – (6 samples)**
P wave calibration (t_0)	1.57 µs	1.49 µs
S wave calibration (t_0)	10.62 µs	10.74 µs

X-ray powder diffractometry was performed with a Panalytical Empyrean XRD using a Bragg-Brentano geometry at 40 mA and 40 kV with CuKα radiation, and a PIXel3D detector at a step size of 0.013˚ 2θ from 4.6 to 85˚ 2θ and 60 s per step.

The quantitative chemical analyses were performed by a microprobe (JEOL Superprobe JXA-8230 with a LaB_6-cathode with an acceleration voltage of 15 kV, at 20 nA) equipped with five wavelength-dispersive spectrometers. Calibration of Si, Al, K, Na, Ca, Mg, Ti, Fe, Mn, Ba, Cr, Cl, and F was done using natural silicate and oxide minerals. Feldspar, phyllosilicates, and amphiboles were measured with a defocused probe size to prevent element migration and mineral destruction. Data correction taking into account the interactions of incident electrons with the target, matrix absorption and fluorescence was done with the a $\phi(\rho Z)$ correction scheme (CITZAF; Armstrong, 1995).

The five additional EBSD measurements were performed on colloidal-silica polished thin-sections, using a Thermofischer/FEI Quanta 200 FEG scanning electron microscope (SEM). The SEM is operating

a Hikari EDAX/TSL EBSD camera and TEAM software at the Scientific Centre for Optical and Electron Microscopy of ETH Zurich. Full-thin section orientation mapping was performed using a step size of 20 µm, acceleration voltage of 20 kV, and beam current of 8 nA at a working distance between 17 to 20 mm.

3.3. Data processing

Each recorded raw waveform was corrected by subtraction of the system travel time T_0 as determined from the calibration procedure. The applied calibration times are provided in Table 1. Due to the subtraction of the system travel time T_0, the waveforms may start at negative times, while the true waveform onset is at t = 0 µs. The calibrated waveforms for a complete pressure cycle (i.e., upgoing and downgoing pressure) are saved for P and S waves separately (see data file description, Section 4.1). No additional filters were applied.

X-ray diffractograms are provided for raw (uncorrected) data as well as for the modelled and refined diffractograms as used in Kästner et al. (2021). For the latter, Rietveld refinement for quantitative mineralogy was performed using the program *BGMN* (Bergmann et al., 1998) embedded in the open-source software *Profex* (Version 3.13.0; Doebelin and Kleeberg, 2015), which was calibrated for the used diffractometer.

Post-acquisition processing of the EBSD data involved the standardization of the confidence index (CI) using a minimum grain tolerance angle of 10° with a minimum of 10 indexed pixels per grain. Afterwards, a CI correlation between neighboring points was applied where pixels with a low CI (<0.1) were reassigned to the orientation and CI of the adjacent data point and to that with the highest CI in the individual grain.

4. File description

4.1. File inventory

Data sets are provided for the laboratory seismic and mineralogical analysis of samples taken from the COSC-1 drill core of the COSC drilling project. The following files are provided in this data publication:

- **2020-009_Kaestner-et-al_COSC-1_Sample_List.txt:** ASCII table including sample information and associated measurements. The table can be opened with arbitrary text editors or loaded into more comprehensive word processors such as *Microsoft Excel* or *LibreOffice Calculator*.
- **2020-009_Kaestner-et-al_COSC-1_Plug-Dimensions.txt:** ASCII table specifying the dimension of each core plug. This file contains the length, diameter, weight, volume, and calculated density of each core plug necessary to calculate the seismic velocity from the laboratory seismic experiment.
- **2020-009_Kaestner-et-al_COSC-1_Laboratory_Seismic_Measurements.zip:** Zip archive containing the P and S waveforms of all 16 core samples measured by Kästner et al. (2020) and Wenning et al. (2016), sorted into subfolders FK and QW, respectively. The including folders correspond to the sample name and contain the tab delimited ASCII text files for each of the three core plugs and measured wave phase, respectively (i.e., 3 files for the P waves and 3 to 6 files for the S waves). Each file name is composed as follows:

  COSC-1_SamplePlug_<Sample><Orientation>_<Phase>.dat

Here, **<*Sample*>** corresponds to the sample name as found in the sample list (cf. Section 4.3.1), **<*Orientation*>** the orientation of the core plug with respect to the sample's structural coordinate system, and **<*Phase*>** the considered wave type (either "*vP*" for P wave or "*vS*" for S wave). As an example, the file *"COSC-1_SamplePlug_106-1x_vP.dat"* contains the P waveform data for the x-oriented core plug of sample 106-1.

Each data file contains the measured waveform amplitudes for each pressure increment and decrement as a function of the travel time *t* in microseconds. The pressure is given in MPa.

- **2020-009_Kaestner-et-al_COSC-1_EPMA.txt:** This is a tab-delimited ASCII file with a table structure comprising the results of the chemical element analyses of each thin section sample from the microprobe. The first column contains the analyzed sample name labelled with an increasing point number. The elements are given as weight-percentage (wt%) of the associated oxides of the total composition (last column).
- **2020-009_Kaestner-et-al_COSC-1_XRD.zip:** This zip archive includes the XRD project files for 10 samples. The project files are provided as ASCII files (.dia), which were exported by the open-source software package *Profex* and contains the calibrated (measured) diffractograms as a function of 2θ, as well as the model diffractograms after applied Rietveld refinement. Each .dat file can be opened with an arbitrary text editor. For (quantitative) modal composition analysis these files can be loaded into the *Profex* Software (http://profex.doebelin.org/). The first row of each file contains information about the sample analysis and mineral phases after refinement. The actual data starts in the second row as tab-delimited, table-like data. The first four columns contain the diffraction angle, the measured diffractogram, the modelled diffractogram, and the calculated background intensity. All subsequent columns represent the individual mineral phases used for Rietveld refinement, which are listed in the first, explanatory line of the file (see Section 4.3.5 for details).
- **2020-009_Kaestner-et-al_COSC-1_EBSD.zip:** This zip archive contains the pre-processed EBSD data from five samples. Stored as EDAX ASCII files (.ang). These can be loaded, for example, with the *Matlab* toolbox MTEX (Mainprice et al., 2011). Each file contains a descriptive file header (indicated by an # symbol) providing information about the calibration of the EBSD system, phases used in the EBSD mapping containing the crystallographic constants and reflectors used in the identification of the diffraction patterns, and the data acquisition parameters such as grid specifications and sample name. The file description follows the measured data formatted as a space-delimited table (see data table in Section 4.3.6). For a correct importation in *Matlab* MTEX the EBSD files have to be loaded with the *ANG* interface flag *'convertEulertoSpatialReferenceFrame'*.

4.2. File naming convention

All file names clearly indicate the measurement procedure (e.g., "XRD" for X-ray diffractometry) and the sample or plug name (e.g., "149-4x") associated with that measurement.

The waveform data of the laboratory seismic measurements follow a special naming convention as described in the file inventory (Section 4.1). These special file names were chosen in order to facilitate the processing of the relatively large number of files, thus, making it more convenient for loading them into different programming languages such as *Python* or *Matlab*.

4.3. Description of data tables

4.3.1. 2020-009_Kaestner-et-al_COSC-1_Sample_List.txt

Column header	Unit	Description
Sample	-	Sample name or ID, corresponds to the core number and section
Box	-	Box number of the core section
Slot	-	Slot number within the core box
Section TOP	m	Meter-corrected depth of the top of the core section
Sample Depth	m	Meter-corrected depth of the center of the sample
Start in Section	cm	Start of the sample interval in the core section
End in Section	cm	End of the sample interval in the core section
Examiner	-	Principal examiner of the sample: QW: Wenning et al. (2016) FK: Kästner et al. (2020)
IGSN	-	International Geo Sample Number
Core lithology	-	Core lithology, modified after Lorenz et al. (2015)
Seismic Lab	-	Laboratory seismic P- and S-wave measurements
XRD/EPMA	-	Measurements using X-ray powder diffractometry and microprobe; N/A – not available
EBSD	-	Structural analysis using electron backscatter diffraction; N/A – not available

m = meter; cm = centimeter

4.3.2. 2020-009_Kaestner-et-al_COSC-1_Plug-Dimensions.txt

Column header	Unit	Description
Plug	-	Plug name, composed of the sample name and plug direction
Orientation	-	Orientation of the core plug with respect to the sample's reference coordinate system: x – parallel to foliation and parallel to lineation, y – parallel to foliation and perpendicular to lineation, z – perpendicular to foliation. A, B indicate that for this sample the lineation was not clearly detectable and may not concur with the actual structural axes.
Depth	m	Meter-corrected depth of the mean sample depth
Diameter	mm	Average cylinder plug diameter
Length	mm	Average cylinder plug length
Weight	g	Plug weight of dry cylinder plug
Volume	cm^3	Dry cylinder plug volume
Volume-SD	cm^3	Mean standard deviation of the volume measurement
Density	$g \cdot cm^{-3}$	Calculated (dry) matrix density derived from volume and weight measurements
Examiner	-	Principal examiner of the sample: QW: Wenning et al. (2016) FK: Kästner et al. (2020)

m = meter; cm = centimeter; mm = millimeter; g = gram

4.3.3. COSC-1_SamplePlug_<Sample><Orientation>_<Phase>.dat

Structure of waveform data file from laboratory seismic measurements (FK):

Column header	Unit	Description
t	µs	Travel time through the specimen
50-U	mV	Waveform amplitudes at 50 MPa pressure (upgoing pressure cycle)
100-U	mV	Waveform amplitudes at 100 MPa pressure (upgoing pressure cycle)
150-U	mV	Waveform amplitudes at 150 MPa pressure (upgoing pressure cycle)
200-U	mV	Waveform amplitudes at 200 MPa pressure (upgoing pressure cycle)
250-U	mV	Waveform amplitudes at 250 MPa pressure (upgoing pressure cycle)
240-D	mV	Waveform amplitudes at 240 MPa pressure (downgoing pressure cycle)
210-D	mV	Waveform amplitudes at 210 MPa pressure (downgoing pressure cycle)
180-D	mV	Waveform amplitudes at 180 MPa pressure (downgoing pressure cycle)
150-D	mV	Waveform amplitudes at 150 MPa pressure (downgoing pressure cycle)
120-D	mV	Waveform amplitudes at 120 MPa pressure (downgoing pressure cycle)
90-D	mV	Waveform amplitudes at 90 MPa pressure (downgoing pressure cycle)
60-D	mV	Waveform amplitudes at 60 MPa pressure (downgoing pressure cycle)
30-D	mV	Waveform amplitudes at 30 MPa pressure (downgoing pressure cycle)

µs = microseconds, mV = millivolt

Structure of waveform data file from laboratory seismic measurements (QW):

Column header	Unit	Description
t	µs	Travel time through the specimen
30-U	mV	Waveform amplitudes at 30 MPa pressure (upgoing pressure cycle)
80-U	mV	Waveform amplitudes at 80 MPa pressure (upgoing pressure cycle)
130-U	mV	Waveform amplitudes at 130 MPa pressure (upgoing pressure cycle)
180-U	mV	Waveform amplitudes at 180 MPa pressure (upgoing pressure cycle)
230-U	mV	Waveform amplitudes at 230 MPa pressure (upgoing pressure cycle)
260-U	mV	Waveform amplitudes at 260 MPa pressure (upgoing pressure cycle)
250-D	mV	Waveform amplitudes at 250 MPa pressure (downgoing pressure cycle)
220-D	mV	Waveform amplitudes at 220 MPa pressure (downgoing pressure cycle)
190-D	mV	Waveform amplitudes at 190 MPa pressure (downgoing pressure cycle)
160-D	mV	Waveform amplitudes at 160 MPa pressure (downgoing pressure cycle)
130-D	mV	Waveform amplitudes at 130 MPa pressure (downgoing pressure cycle)
100-D	mV	Waveform amplitudes at 100 MPa pressure (downgoing pressure cycle)
70-D	mV	Waveform amplitudes at 70 MPa pressure (downgoing pressure cycle)
40-D	mV	Waveform amplitudes at 40 MPa pressure (downgoing pressure cycle)

µs = microseconds, mV = millivolt

4.3.4. 2020-009_Kaestner-et-al_COSC-1_EPMA.txt

Column header	Unit	Description
Sample	-	Name of the analyzed sample
Point	-	Number of measurement on the same sample
SiO2	wt%	Abundance of silica
Al2O3	wt%	Abundance of aluminum
K2O	wt%	Abundance of potassium
Na2O	wt%	Abundance of sodium
CaO	wt%	Abundance of calcium
MgO	wt%	Abundance of magnesium
TiO2	wt%	Abundance of titanium
FeO	wt%	Abundance of iron
MnO	wt%	Abundance of manganese
BaO	wt%	Abundance of barium
Cr2O3	wt%	Abundance of chromium
Cl	wt%	Abundance of chlorine
F	wt%	Abundance of fluorine
Total	wt%	Cumulative abundance of detected elements
Min1	-	Associated, preliminary mineral group interpretation Am – amphibole; Ep – epidote; Mca – mica; Px – pyroxene; Fsp – feldspar; Cb – carbonate; Ttn – titanite; Op – opaque; Grt – garnet; Chl – chlorite; Qtz – quartz; Ilm – ilmenite; n.d. – not determined
wt% = weight percentage, all elements are given in their oxide state		

4.3.5. COSC-1_XRD_Sample_<SampleID>.dia

Column	Name	Unit	Description
1	Angle	Degrees of 2θ (°)	Diffraction angle measured with 0.013˚ step size
2	Data	Intensity (cps)	Measured diffractogram
3	Model	Intensity (cps)	Modelled diffractogram
4	Background	Intensity (cps)	Calculated background noise based on vendor-specific calibration file
5 and more	Phase names as listed in the file header (line 1)	Intensity (cps)	Contain the individual, phase-specific diffractograms used during Rietveld refinement
Data start in line 2; the first line in file includes sample information and refinement parameters			

4.3.6. COSC-1_EBSD_Sample_<SampleID>.ang

Column	Name	Unit	Description
1-3	Euler Angles	Radian (rad)	Three Euler angles (φ_1,θ, φ_2) that describe the orientation of each pixel
4	X	µm	X coordinate in sample
5	Y	µm	Y coordinate in sample
6-10	Image Quality	-	Contains a set of image quality parameters
11	CI	-	Confidence index
12-14	Data Quality	-	Parameters related to data quality
Data start right below the descriptive file header (i.e., first line without # symbol)			

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