



LoKI STAP Update

Instrument progress
23rd October 2024

PRESENTED BY THE LOKI TEAM

2024-10-11



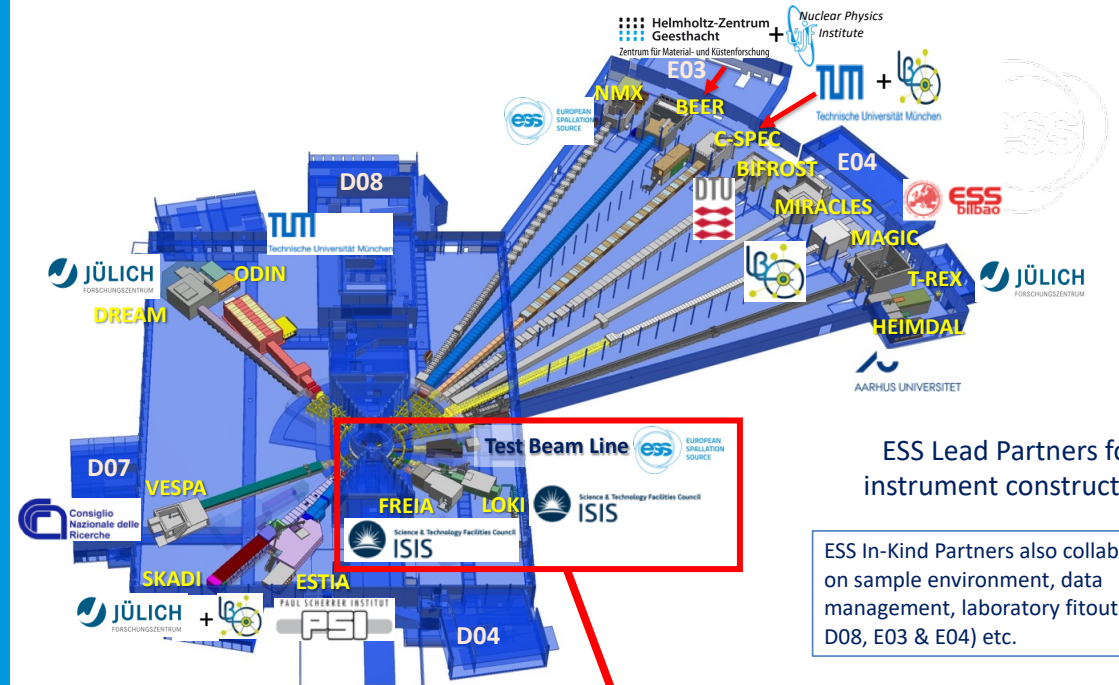
LoKI team

Lead engineer :	Jim Nightingale
Installation package leader :	Clara Lopez
Instrument scientist :	Judith Houston
Instrument data scientist :	Oliver Hammond *
Instrument operations engineer :	Hannah Burrall *
Commissioning scientist (in-kind) :	<i>Position cancelled, after a late decision by the candidate to not come</i>
Second instrument scientist :	<i>Recruitment at ESS to begin soon</i>

** New since the last in person STAP*

1

Installation activities



ESS Lead Partners for instrument construction

ESS In-Kind Partners also collaborate on sample environment, data management, laboratory fitout (D04, D08, E03 & E04) etc.



LoKI Status Overview

Items which are concerns to the timeline



Detectors

Vessel, **mechanical frames and most modules** installed
All detector components, including beamstop installed, *awaiting cable connections and testing*

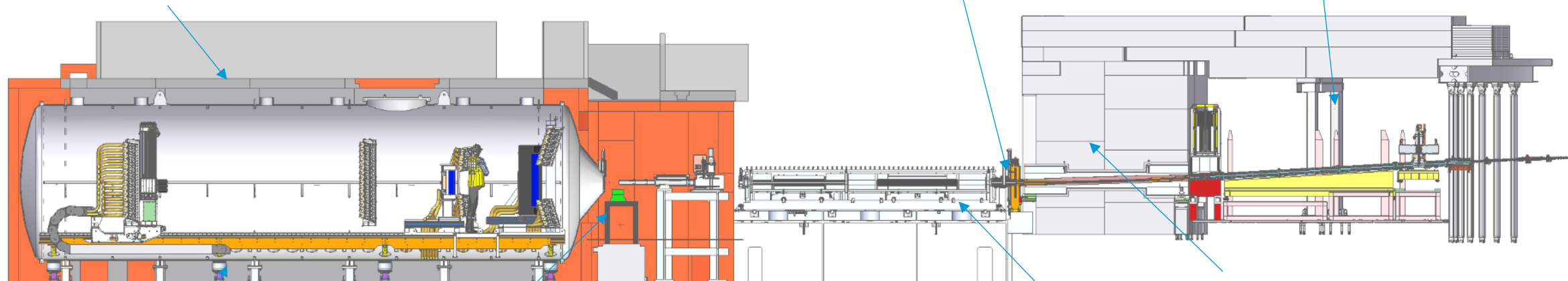
Utilities

Electrical services, utilities, PSS and network being installed and almost complete in all cases
Energisation is imminent – *although causing delays to commissioning*

Chopper 2
Installed

In-bunker

All components installed, awaiting final alignment checks



BWI
Insert installed

Cave Shielding

- Steel is installed
- Concrete roof is installed

Sample Area

- Stack awaiting installation
- Snout system about to begin installation
- Door and roof installed

Beam monitors

- First 2 monitors awaiting installation
- *Other 3 monitors awaiting final assembly (risk to timeline)*

Bunker-to-cave

- Collimation tank installed and vacuum tested
- Collimation selectors and slits installed and undergoing final testing before commissioning

Installations in the last year

Pumps and racks installed

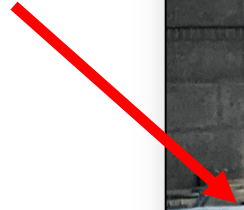
Door and roof mechanism installed

All detector mechanical structures including beamstop installed



Installations in the last year

In bunker equipment



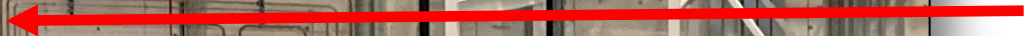
Collimation including selectors with guides and slit sets



Racks for motion, choppers, PSS, ICS, vacuum installed



Utilities and electrical



Installations in the last year



- Selector, guides and slit sets installed and have been motion tested locally
- Chopper 2 and Collimation vessel vacuum section tested
- Proceeding shortly with final installation of the shielding

Installations in the last year

Sample area

- Almost all utilities are now installed.
- Floor installed.
- Ready for sample stack and snout (including laser, monitor, extendable snout) to be installed in the coming months



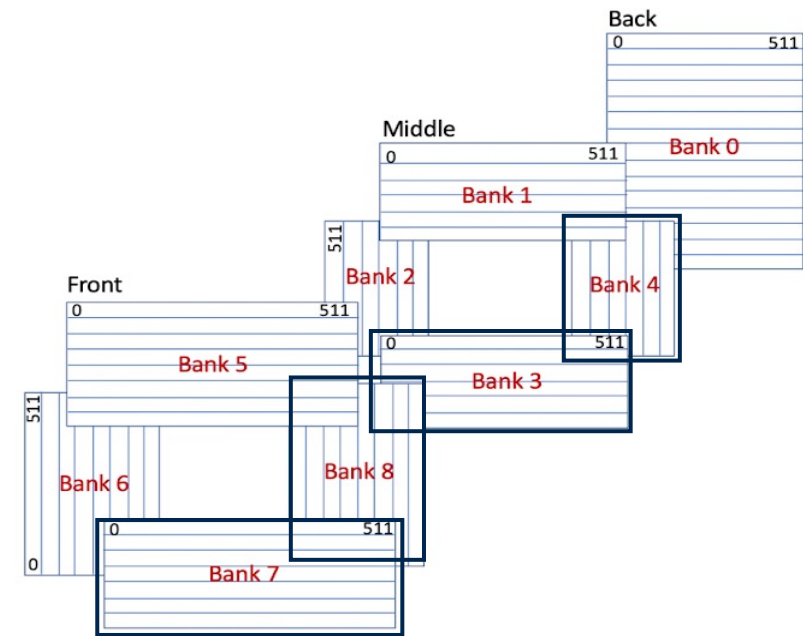
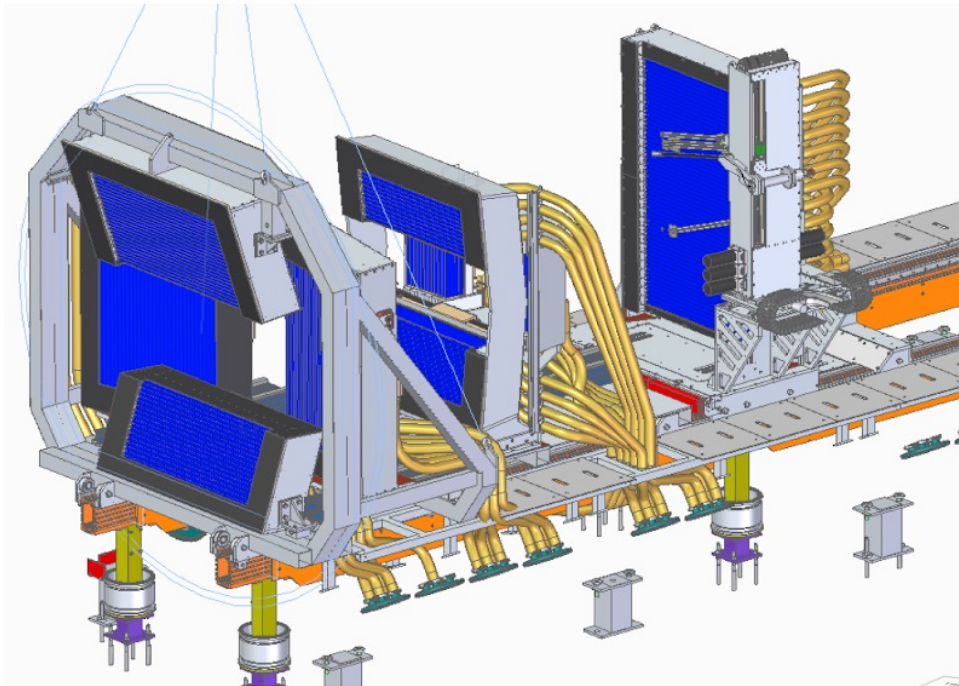
Detector update



- Almost all mechanical infrastructure installed including: all the frames, most of the modules, beamstop mechanism, air hoses, racks on hutch roof
- Detector group are now completing cable connections to patch panels, models and racks.
- Detector carriage and beam stop mechanism undergoing motion testing

Detector upgrade update

- All cables and mechanical structures are at ISIS, and tubes are arriving from PTI (USA).
- 65% of modules are complete at ISIS.
- Electronics already at ESS. External cables from detector vessel to racks are already in place
- On target to made March 2025 delivery.



Installations planned for the next 6 months



- Remaining detector modules and cabling
- Sample area components including sample stack and snout components
- Beam monitors
- Racks for the in-bunker components



LOKI sample snout

Cold commissioning

Pre-requisites before cold commissioning can begin:

- Energisation of electrical rack (*should be imminent...*)
- Energisation of ICS rack (*should be imminent...*)
- Energisation of individual technical racks
- Components, e.g. motion, choppers, detectors, have passed local testing
- Instrument control computer is set-up in the hutch

Assuming the above, we expect to begin CC in the following order:

- Chopper 2 (out of bunker)
- Collimation section including selectors and slit sets
- Chopper 1 (in bunker) and heavy shutter
- Sample area motion
- Detector motion including detector carriage and beamstop mechanism
- Detectors



Other progress

- TG3 (design) milestone passed
- All TG4 (final manufacture) documentation submitted by ISIS
- Major issues remaining:
 - Still awaiting energization. This then delays energization of racks, local testing by the technical groups, and finally the start of cold commissioning with instrument control software.
 - Detector quality gate
 - Monitor delivery from ISIS
- Outstanding deliveries: 3/5 monitors
- Current installation complete date (TG5) is **Spring 2025**

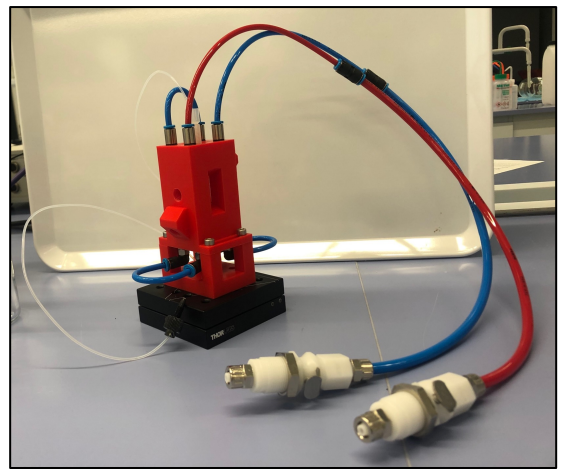
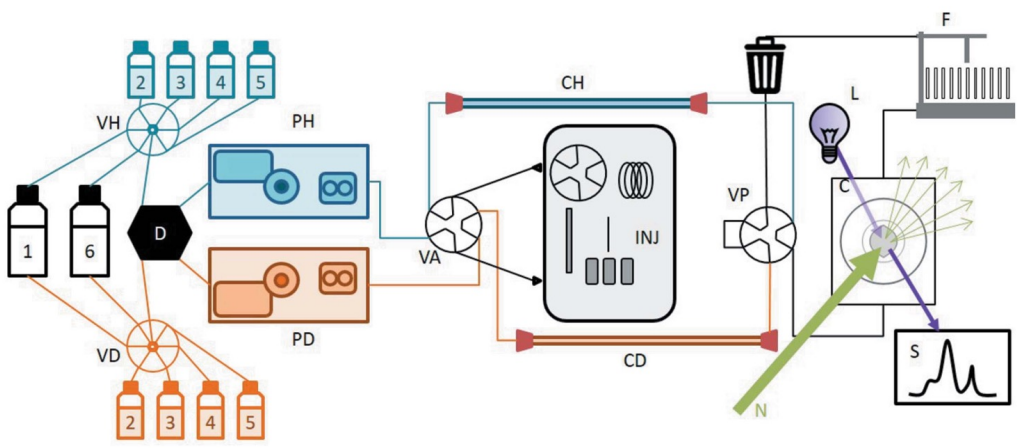
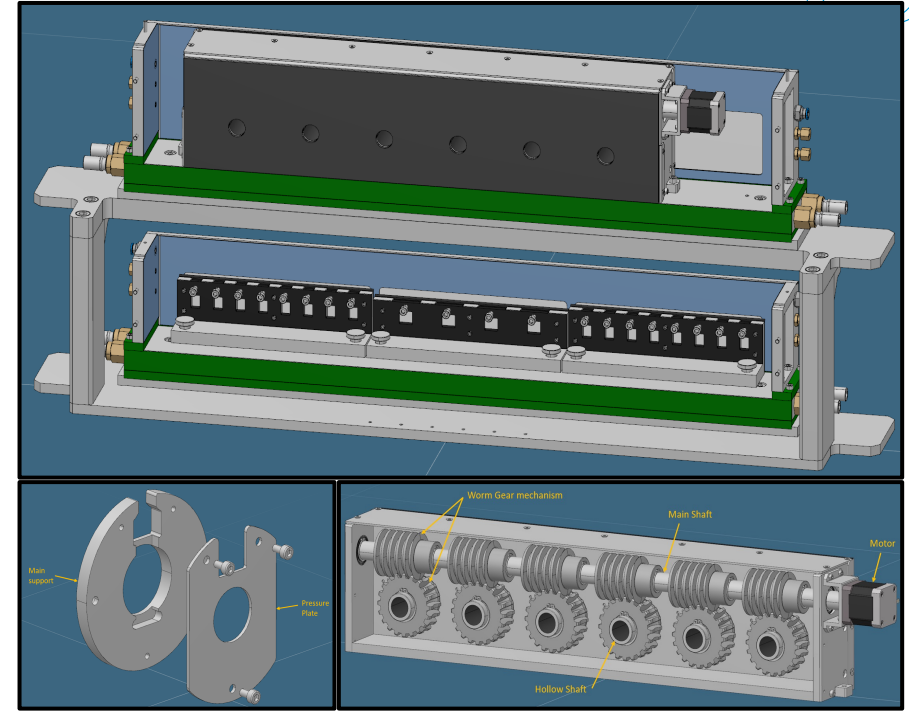


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Sample environment

General sample environment updates

- **Thermostated cell holder** and **rotating cell holder** components manufactured and about to begin assembly.
- **Rheometer** integration is underway and making progress (ESS pool equipment). Sub-pulse project with Uppsala on-going with ISIS
- **Size-exclusion chromatography** set-up delayed due to loss of post-doc.
- **NURF (in situ spectrometers and continuous flow cell)** cell prototyped and devices integrated.



(a) Ann Martel's SEC set-up (J. Appl. Cryst. (2023). 56)

Sample environments

Changes from last update



Priority	Sample Environment System (SES)	Phase	Date Needed	Status
1	Thermostated sample changer for quartz cuvettes	HC	Q1 2025	Components arriving to site for assembly
1	Cell tumblers/rotating sample holders	HC	Q1 2025	B4C painting of inner components complete, awaiting assembly
1	Flow cell (including HPLC pumps)	HC	Q3 2025	Jasco HPLC integrated
2	In situ techniques, as spectrometer attachments to the flow-through cell	ES	Q4 2025	Integration finished
2	Size Exclusion Chromatography	ES	Q4 2025	Post-doc no longer available to do project looking at other oportunities
2	Rheometer	ES	Q1 2025	Anton Paar - still undergoing integration at ESS
3	Stopped-flow cell	ES	Q3 2025	In-kind device from Estonia (Biologic) undergoing testing at ESS
4	Individually thermostated cuvette rack	ES	Q2 2025	Prototype exists and integrated at ESS
4	Goniometer(s)	ES	Q1 2026	ESS to purchase
4	Dismountable 'sandwich'-style cells (ESS)	ES	Q4 2025	Designs exist. Just to be sent for manufacture
4	Warm Bore Cryomagnet 2.5T	SOUP	Q1 2028	Delivered to site
4	Stress/stretching rig (ESS)	SOUP	Q1 2028	ESS colaboration(s) to develop different rigs
4	Cryostat – dilution fridge less than 1K	SOUP	Q1 2028	
4	Cryostat wet	SOUP	Q1 2028	



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LOKI Data Reduction Update

2024-10-11

LOKI Data Pipeline Updates



- Loss of SANS IDS Wojciech at the beginning of April. New IDS **Oliver Hammond** started mid-September and is getting up to speed
- Data reduction and direct beam script in Mantid have been transferred to SCIPP, and the workflow optimised

Published online here:

<https://scipp.github.io/esssans/user-guide/loki/loki-iofq.html>

Wavelength bands

```
[10]: workflow[WavelengthBands] = sc.linspace("wavelength", 1.0, 13.0, 11, unit="angstrom")
da_bands = workflow.compute(BackgroundSubtractedIofQ)
da_bands
```

```
[10]: scipp.DataArray (10.93 KB)
```

► Dimensions: (band: 10, Q: 100)

▼ Coordinates:

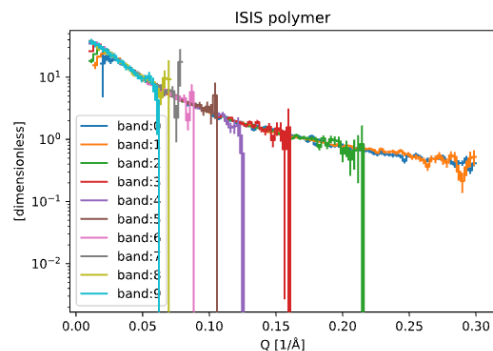
L1	()	float64	m	25.610000610351562	
Q	(Q [bin-edge])	float64	1/Å	0.01, 0.013, ..., 0.297, 0.3	
gravity	()	vector3	m/s ²	[0. -9.80665 0.]	
incident_beam	()	vector3	m	[0. 0. 25.61000061]	
wavelength	(wavelength [bin-edge], band)	float64	Å	1.0, 2.2, ..., 11.800, 13.0	

▼ Data:

(band, Q)	float32	1	nan, nan, ..., nan, nan	
			$\sigma = \text{nan, nan, ..., nan, nan}$	

```
[11]: pp.plot(sc.collapse(da_bands, keep="Q"), norm="log", title="ISIS polymer")
```

```
[11]:
```



Porous Silica

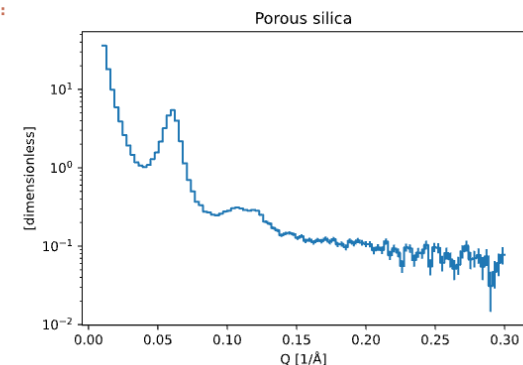
```
[15]: workflow[Filename[SampleRun]] = loki.data.loki_tutorial_porous_silica_sample_run()
workflow[Filename[TransmissionRun[SampleRun]]] = (
    loki.data.loki_tutorial_porous_silica_transmission_run()
)
```

```
# Beam center
workflow[BeamCenter] = sans.beam_center_from_center_of_mass(workflow)
```

```
# I(Q)
da = workflow.compute(BackgroundSubtractedIofQ)
da.plot(norm="log", title="Porous silica")
```

```
Downloading file '60385-2022-02-28_2215.nxs' from 'https://public.esss.dk/groups/scipp/ess/loki/2/603'
Downloading file '60384-2022-02-28_2215.nxs' from 'https://public.esss.dk/groups/scipp/ess/loki/2/603'
```

```
[15]:
```



GUI progress

Still in the prototype phase.

- DMSC have been working on the GUI for the data reduction interface for LOKI
- The GUI (made of widgets) are generated from the workflow (sciline) graph. This means that if we change something in the workflow, the GUI will automatically follow/be updated.
- This will be discussed in more detail at the DMSC STAP.

Published online here:

<https://scipp.github.io/essans/user-guide/loki/workflow-widget-loki.html>

```
[1]: # Import loki submodule to register workflow
from ess import loki # noqa: F401
from ess.reduce import ui

# Prepare a container for accessing the results computed by the GUI
results = {}

# Initialize the GUI widget
widget = ui.workflow_widget(result_registry=results)
widget
```

[1]: Workflow: LokiAtLarmorTutorialWorkflow

▼ Typical Outputs

- BackgroundSubtractedIofQ
- BackgroundSubtractedIofQxy
- IofQ[SampleRun]
- IofQxy[SampleRun]
- IofQ[BackgroundRun]
- IofQxy[BackgroundRun]
- MaskedData[BackgroundRun]
- MaskedData[SampleRun]
- WavelengthMonitor[SampleRun, Incident]
- WavelengthMonitor[SampleRun, Transmission]
- WavelengthMonitor[BackgroundRun, Incident]
- WavelengthMonitor[BackgroundRun, Transmission]

► Extended Outputs

Run Clear Output

scipp.DataArray (3.75 KB)

► Dimensions: (Q: 100)

▼ Coordinates:

L1	()	float64	m	2	☰
Q	(Q [bin-edg...	float64	1/Å	0	☰
gravity	()	vector3	m/s^2	[☰
incident_beam	()	vector3	m	[☰
wavelength	(wavelength...	float64	Å	2	☰

▼ Data:

	(Q)	float32	1	4	☰
					σ

Refresh Parameters

CorrectForGravity

NeXusDetectorName larmor_detector

NeXusMonitorName[Incident] monitor_1

NeXusMonitorName[Transmission] monitor_2

TransformationPath transform

PixelMaskFilename /home/runner/.cache/ess/loki/2/mask_new_

PixelShapePath pixel_shape

ReturnEvents

<enum 'UncertaintyBroadcastMode'> UncertaintyBroadcastM

Filename[SampleRun] /home/runner/.cache/ess/loki/2/60339-2

Filename[TransmissionRun[SampleRun]] /home/runner/.cache/

Filename[EmptyBeamRun] /home/runner/.cache/ess/loki/2/603

angstrom start: 2 stop: 12 nbins: 300

1/angstrom start: 0,01 stop: 0,3 nbins: 100

None DirectBeam

x = -0,02914868 y = -0,01816138 unit: m