Example

December 18, 2020

1 Experimental setup

SIRIUS Beamline : Experiment 1234

Example

- Type: Proposal
- Safety: Yellow
- Date: 12/12/2020

- Main proposer: Hemmerle
- Local contact: Myself
- Users (on site): Home office
- Recording directory: recording/

- Machine:
  - Current: 450 mA
  - Mode: Top-up

- Optics:
  - DCM: Si111
  - MGM: Not used
  - M1: M1-A Pt Track
  - M2: M2 Pt Track
  - M3: No M3
  - M4: M4 Pt Track

- Beam:
  - Fixed/Variable energy: Fixed
  - Energy (keV): 8
  - Wavelength (nm): 0.155
  - Harmonic: 12
  - Polarisation: LH
  - Phase (deg): 0
  - Horizontal focalisation: False
  - Vertical focalisation: True
  - Horizontal beamsize (mm): 2
  - Vertical beamsize (mm): 0.5

- Monitors and XBPM:
  - mon1:

  - mon2:
  - mon3:
  - mon4: thick diamond
  - Detectors: Pilatus on delta0

- Remarks: This is an example.

2 Beamline alignment

Here we show functions used during beamline aligment.

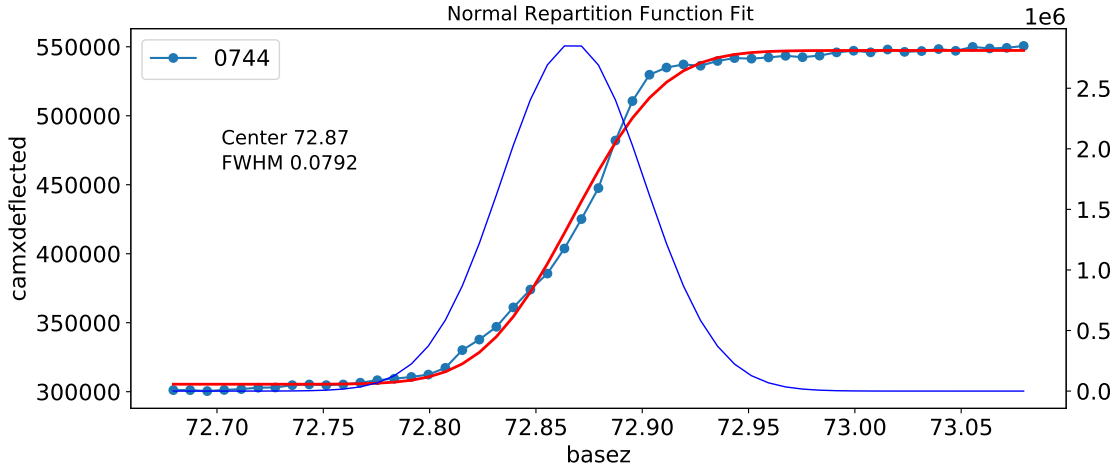
LaTeX formula can be used:

$$\frac{786 - 558}{2 \times 2069} \times 0.0355 = 1.9mrad$$

2.1 Subsection

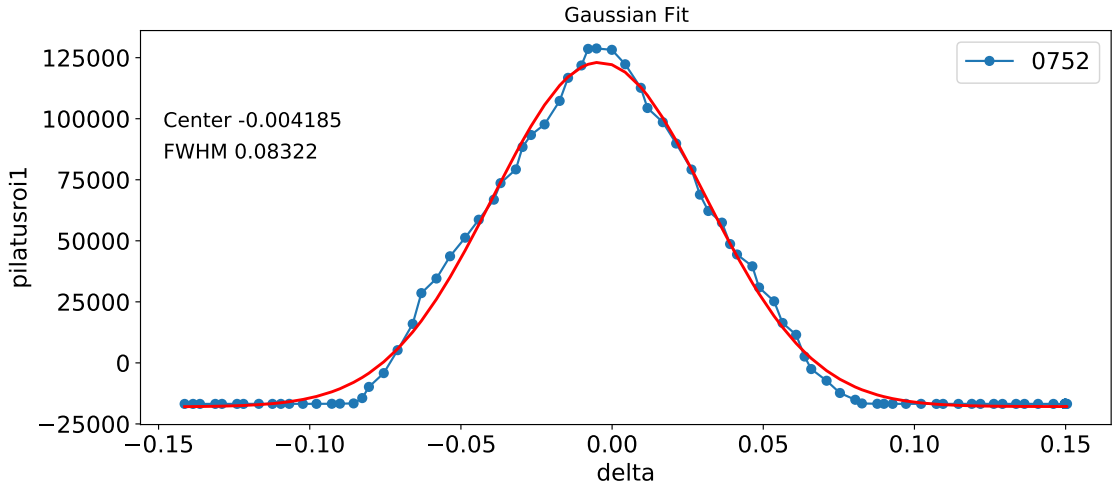
2.1.1 SIRIUS_2020_03_11_0744: dscan basez -.2 .2 50 .1

Fit with erf function.

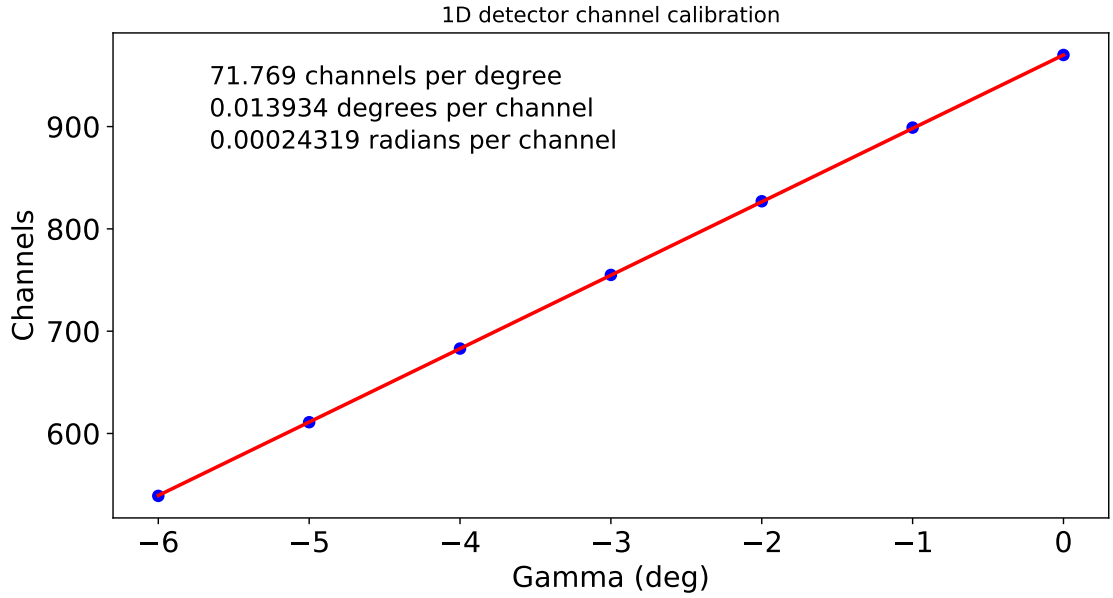


2.1.2 SIRIUS_2020_03_11_0752: One can edit the scan info here as well

Fit with a gaussian.



2.2 Calibration thetaz



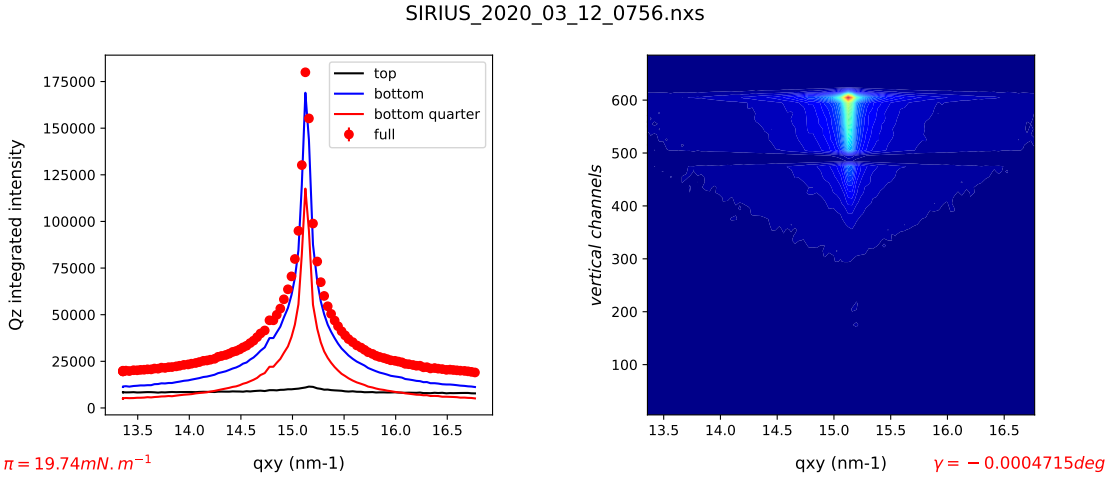
3 GIXD

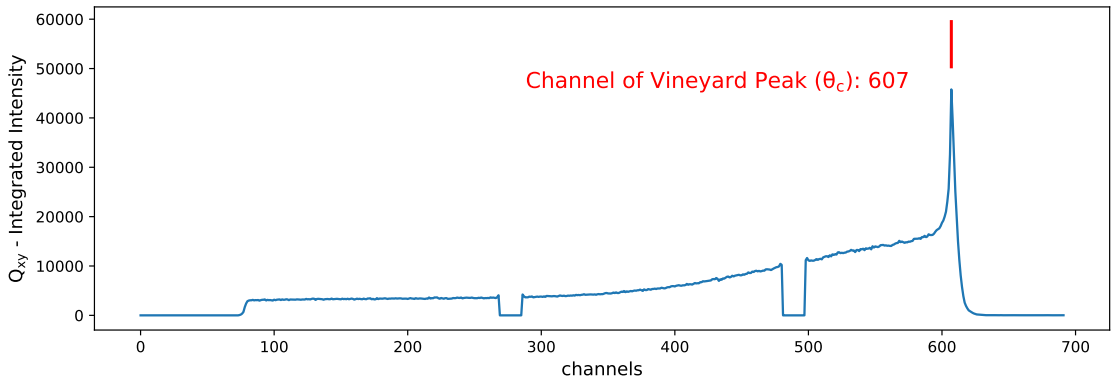
3.0.1 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

Extraction of the Vineyard.

- Open Nexus Data File :

```
recording/SIRIUS_2020_03_12_0756.nxs
. Number of data points:  101
. Available Counters:
        0  -------->  delta
        1  -------->  zs
        2  -------->  gamma
        3  -------->  hu36energy
        4  -------->  xs
        5  -------->  energydcm
        6  -------->  current
        7  -------->  mon2
        8  -------->  surfacepressure
        9  -------->  areapermolecule
        10  -------->  qxy
        11  -------->  pilatus
        12  -------->  pilatusroi1
        13  -------->  integration_time
        14  -------->  sensorsRelTimestamps
        15  -------->  sensorsTimestamps
. Pilatus data found, (column 11, alias pilatus)
. qxy data found, (column 10, alias qxy)
. Valid data between points 0 and 100
. Surface pressure data found, mean value 19.74 ± 0.006163 mN/m
. Area per molecule data found, mean value 0.3557 ± 3.866e-05 nm2 per
molecule
. Gamma motor data found, mean value -0.0004715 deg
```






```
Data not saved. To save data, run a GIXD on the scan.
Channel0: 607
```

3.0.2 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

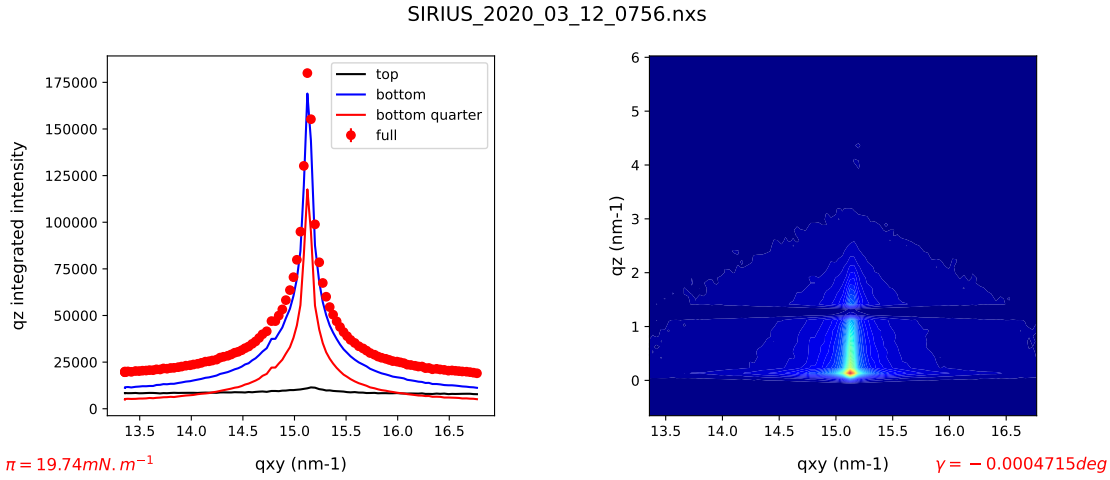
Classic GIXD with:

$$q_{xy} = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right)$$

Generates:
- SIRIUS_2020_03_12_0756_1D_qz.dat for each binning
- SIRIUS_2020_03_12_0756_1D.dat
- SIRIUS_2020_03_12_0756_1D.mat for each binning
- SIRIUS_2020_03_12_0756_1D.moy for each binning

3.0.3 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

```
        . Absorbers:
29 - Vide
```



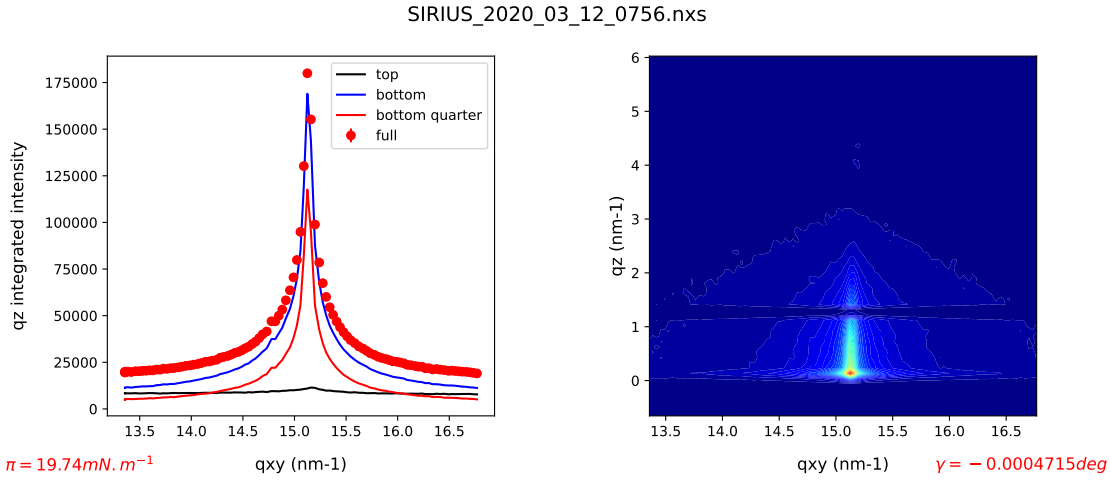
3.0.4 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

It is possible to print all info on the scan and the counters.

3.0.5 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

```
- Open Nexus Data File :
        recording/SIRIUS_2020_03_12_0756.nxs
        . Number of data points:  101
        . Available Counters:
                0  -------->  delta
                1  -------->  zs
                2  -------->  gamma
                3  -------->  hu36energy
                4  -------->  xs
                5  -------->  energydcm
                6  -------->  current
                7  -------->  mon2
                8  -------->  surfacepressure
                9  -------->  areapermolecule
                10  -------->  qxy
                11  -------->  pilatus
                12  -------->  pilatusroi1
                13  -------->  integration_time
                14  -------->  sensorsRelTimestamps
                15  -------->  sensorsTimestamps
        . Pilatus data found, (column 11, alias pilatus)
        . qxy data found, (column 10, alias qxy)
        . Valid data between points 0 and 100
```

```
        . Surface pressure data found, mean value 19.74 ± 0.006163 mN/m
        . Area per molecule data found, mean value 0.3557 ± 3.866e-05 nm2 per
molecule
        . Gamma motor data found, mean value -0.0004715 deg
```



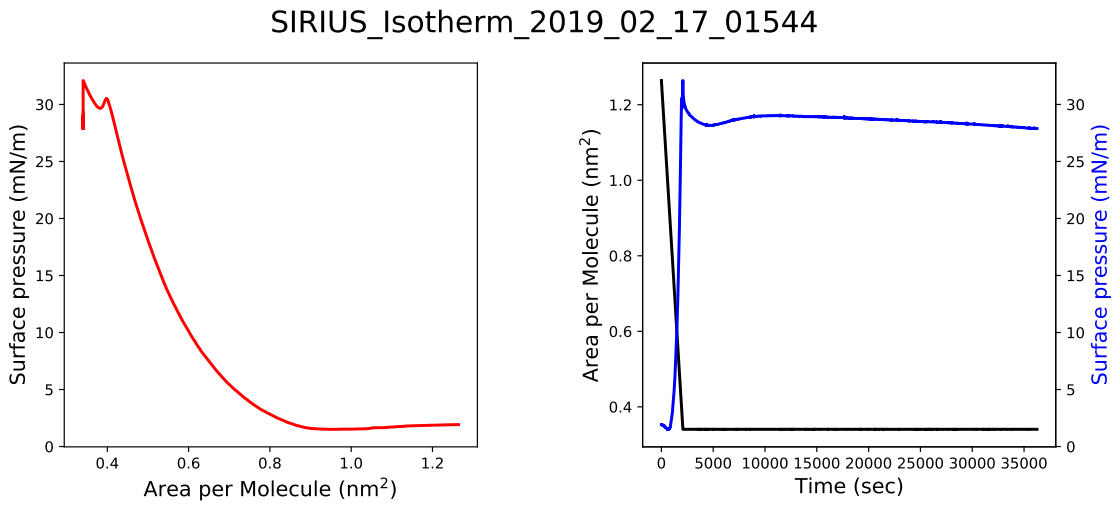

```
        . Original, non binned, matrix saved in:
         working/SIRIUS_2020_03_12_0756_1D.mat
        . Scalar data saved in:
         working/SIRIUS_2020_03_12_0756_1D.dat
        . qz values saved in:
        working/SIRIUS_2020_03_12_0756_1D_qz.dat10
        . Binned matrix saved in:
         working/SIRIUS_2020_03_12_0756_1D.mat10
        . XYZ data saved in:
         working/SIRIUS_2020_03_12_0756_1D.moy10
        . qz values saved in:
        working/SIRIUS_2020_03_12_0756_1D_qz.dat20
        . Binned matrix saved in:
         working/SIRIUS_2020_03_12_0756_1D.mat20
        . XYZ data saved in:
         working/SIRIUS_2020_03_12_0756_1D.moy20
        . qz values saved in:
        working/SIRIUS_2020_03_12_0756_1D_qz.dat40
        . Binned matrix saved in:
         working/SIRIUS_2020_03_12_0756_1D.mat40
        . XYZ data saved in:
         working/SIRIUS_2020_03_12_0756_1D.moy40
```

4 Isotherm

4.0.1 SIRIUS_Isotherm_2019_02_17_01544: isotherm 1.97 46 35000 1

Plot the isotherm. Generates SIRIUS_Isotherm_2019_02_17_01544.dat

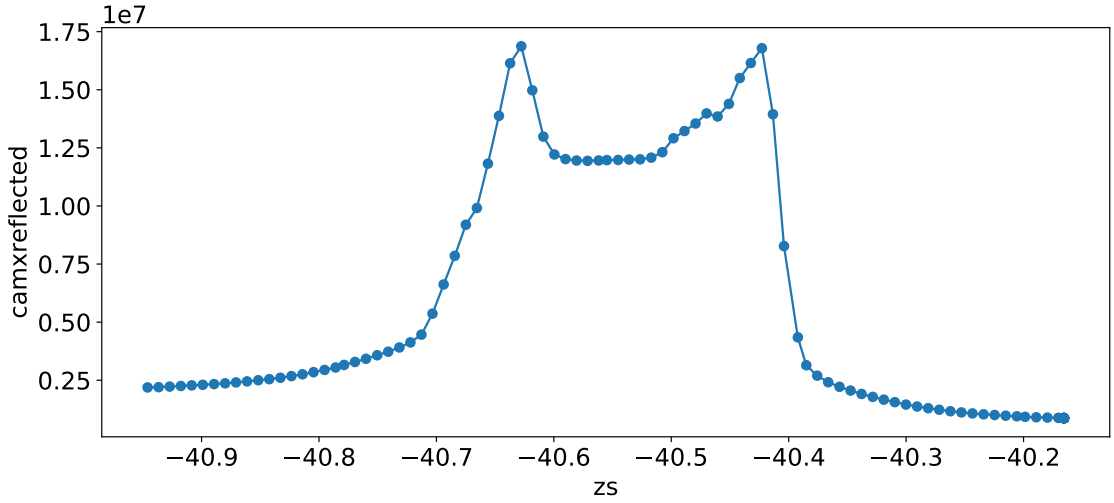
4.0.2 SIRIUS_Isotherm_2019_02_17_01544: isotherm 1.97 46 35000 1



5 1D plot

5.0.1 SIRIUS_2020_03_12_0760: run cont_regh.ipy

Add a 1D plot by clicking on ”’Add plot to report”’.
Generates SIRIUS_2020_03_12_0760.dat

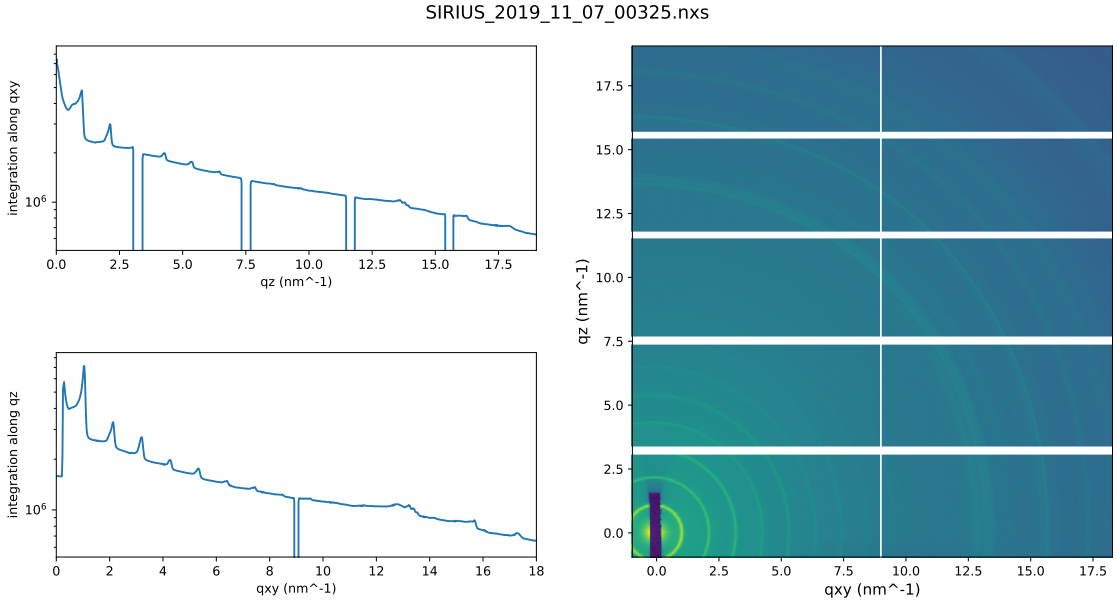


6 GIXS

6.0.1 SIRIUS_2019_11_07_00325: tscan 10 10

GIXS: q_z vs q_{xy}.
Image and profiles with the approximation $q_{xy} = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right)$.
Generates:
- SIRIUS_2019_11_07_00325_pilatus_sum.tiff
- SIRIUS_2019_11_07_00325_pilatus_sum.mat
- SIRIUS_2019_11_07_00325_integrated_qz.dat
- SIRIUS_2019_11_07_00325_integrated_qxy.dat

```
. Absorbers: 29 - Vide
. Gamma is forced to the value : gamma = 0
. Delta is forced to the value : delta = 11.578
```

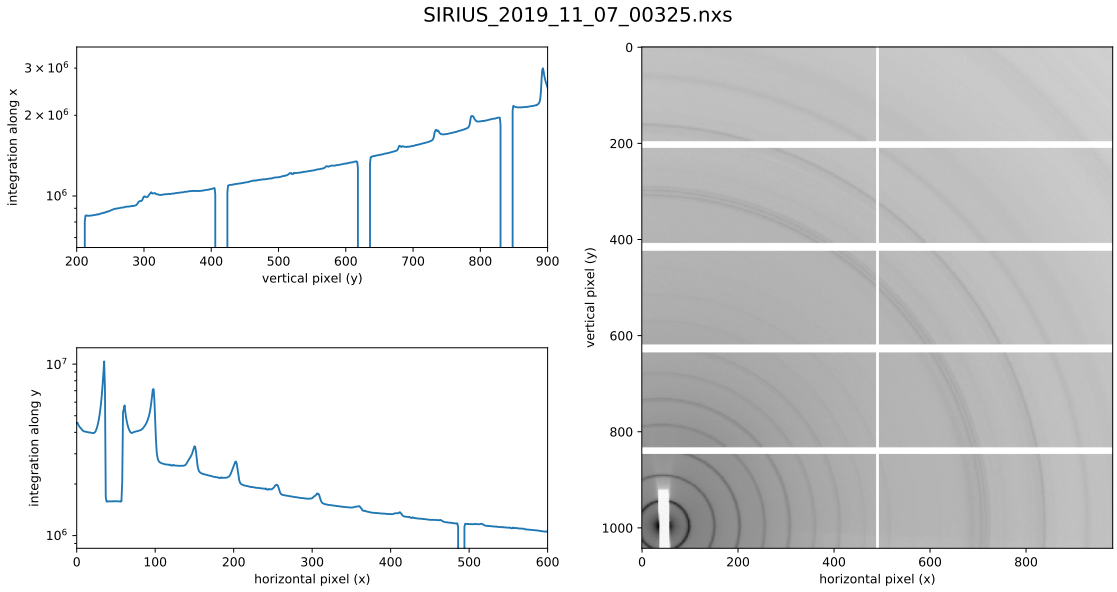


7 Plot pilatus

7.0.1 SIRIUS_2019_11_07_00325: tscan 10 10

Plot the sum of the images from the Pilatus (time integration).
Generates:
- SIRIUS_2019_11_07_00325_pilatus_sum.tiff
- SIRIUS_2019_11_07_00325_pilatus_sum.mat
- SIRIUS_2019_11_07_00325_integrated_x.dat
- SIRIUS_2019_11_07_00325_integrated_y.dat

```
. Absorbers: 29 - Vide
```



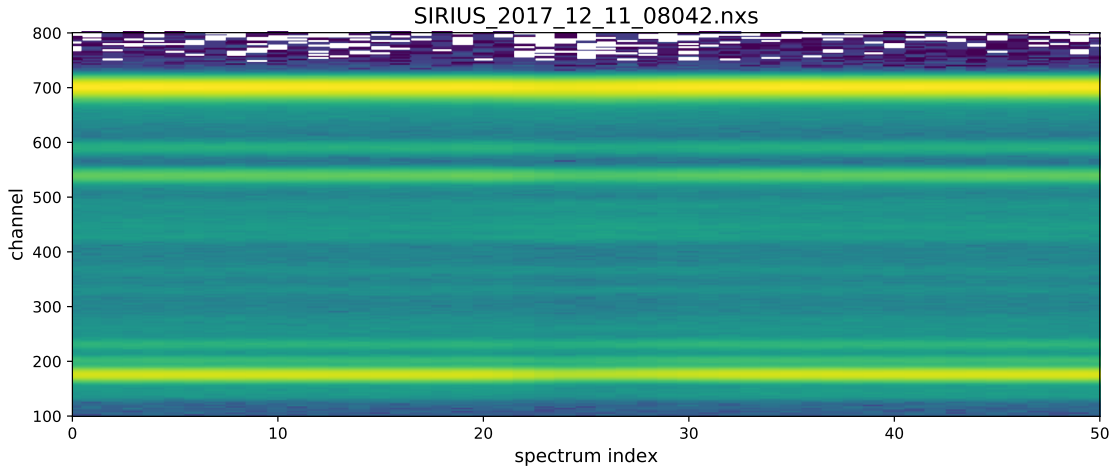
8 XRF

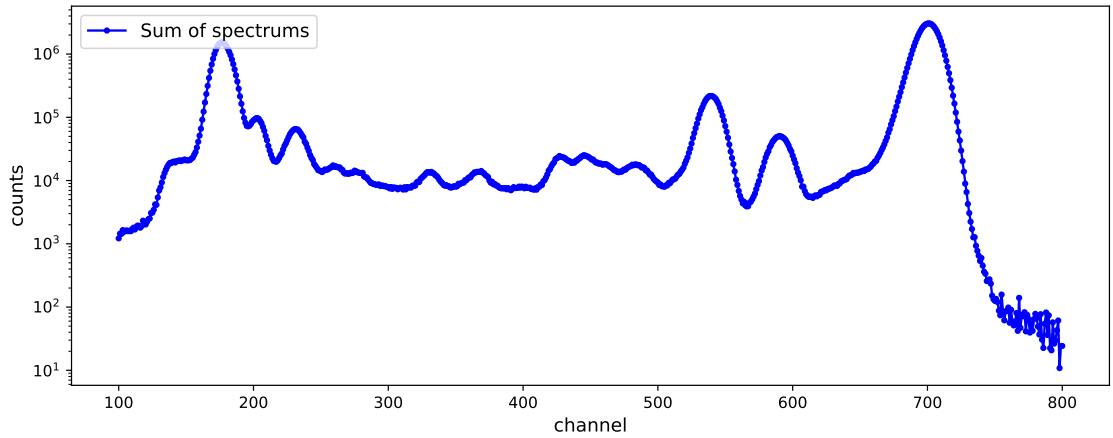
8.0.1 SIRIUS_2017_12_11_08042: run xsw7.ipy

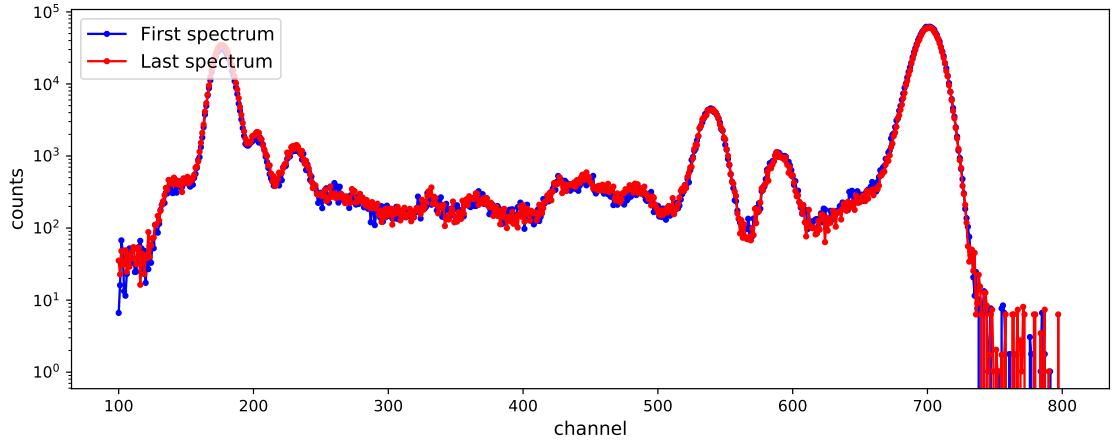
Plot XRF from the 4-elements detector, in channels and without peak identification.
Generates:
- SIRIUS_2017_12_11_08042_fluospectrum.mat for each element
- SIRIUS_2017_12_11_08042.dat

8.0.2 SIRIUS_2017_12_11_08042: run xsw7.ipy

```
. Absorbers: Al 200micron
```


SIRIUS_2017_12_11_08042.nxs
channel
spectrum index

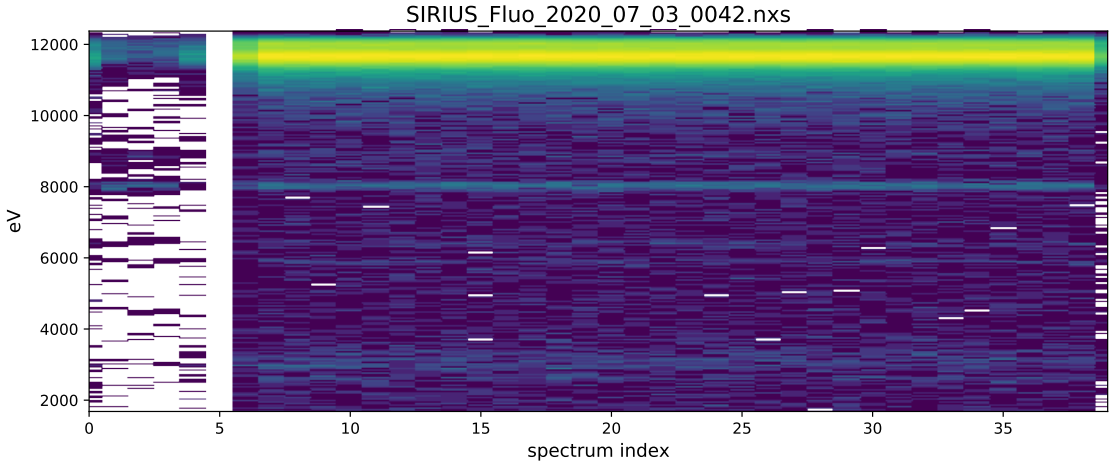

Sum of spectrums
counts
channel

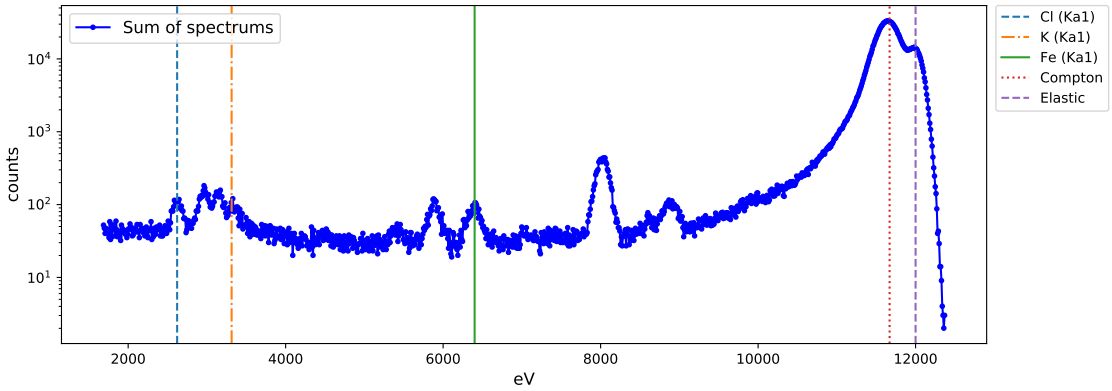

First spectrum
Last spectrum
counts
channel

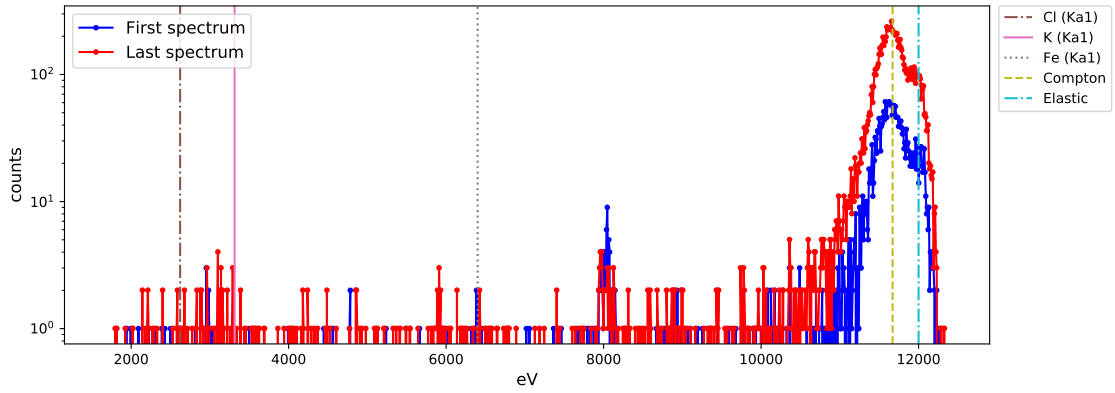
8.0.3 SIRIUS_Fluo_2020_07_03_0042: tscan 500 30

Plot XRF from the 1-element detector, in eVs and with peak identification.
Generates:
- SIRIUS_Fluo_2020_07_03_0042_fluospectrum04.mat
- SIRIUS_Fluo_2020_07_03_0042.dat

```
. Absorbers: Al 800micron
```







9 Insert script

Script inserted (with automatic scan numbering) using ”‘Insert script”’.

9.0.1 script_with_loop.ipy

```
%shopen
%amove delta -40
%run reset_motors.ipy
%amove delta -35
%continuous_ascan delta -35 -25 250 5 #123
%run reset_motors.ipy
for i in range(4):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #124 #126 #128 #130
    %run reset_motors.ipy
    %run cont_regh_abs.ipy #125 #127 #129 #131
for i in range(3):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #132 #135 #138
    %run reset_motors.ipy
    %run cont_regh_abs.ipy #133 #136 #139
    %run cont_regh_abs.ipy #134 #137 #140
for i in range(2):
    %amove delta -20
    %tscan 10 100 #141 #142

%continuous_ascan delta -35 -25 250 5 #143
%amove delta -40
%shclose
```

10 Insert positions

Positions extracted from the logs, using ’‘Insert positions”’.

10.0.1 wm zs

zs
-40.9178

10.0.2 wm diffracto

deltacodeur	euchi	euth	euphi	kappa_h	kappa_k
	1.00196	-89.57961	90.42039	-0.00580	-0.08252
Degrees	deg	deg	deg		

kappa_l	qxy	qxy0	qz	basexPoint	basexTrait
-0.18486	2.0556	23.82	-0.92	-15.7275	-15.7274
	nm-1	nm-1	nm-1		

basezPlan	basezPoint	basezTrait	basepitch	baseroll	basex
71.1257	71.1257	71.1257	-0.0000	0.000	-15.727
			mrad	mrad	mm

baseyaw	basez	alphax	alphay	delta	delta0
-0.000	71.126	0.2998	0.2000	-2.9110	-34.2322
mrad	mm				

deltaa	etaa	gamma	kappav	mu	kphi
0.0000	0.0000	1.2997	1.3080	-179.9997	0.0000

thetaa	thetah	komega	xs	ky	ys
0.0000	0.0185	0.0000	0.0000	-0.1000	0.0000

kz	zs	kx
0.0000	-41.9999	-0.1000

11 Insert commands

Commands extracted from the logs, using ”‘Insert commands”’.

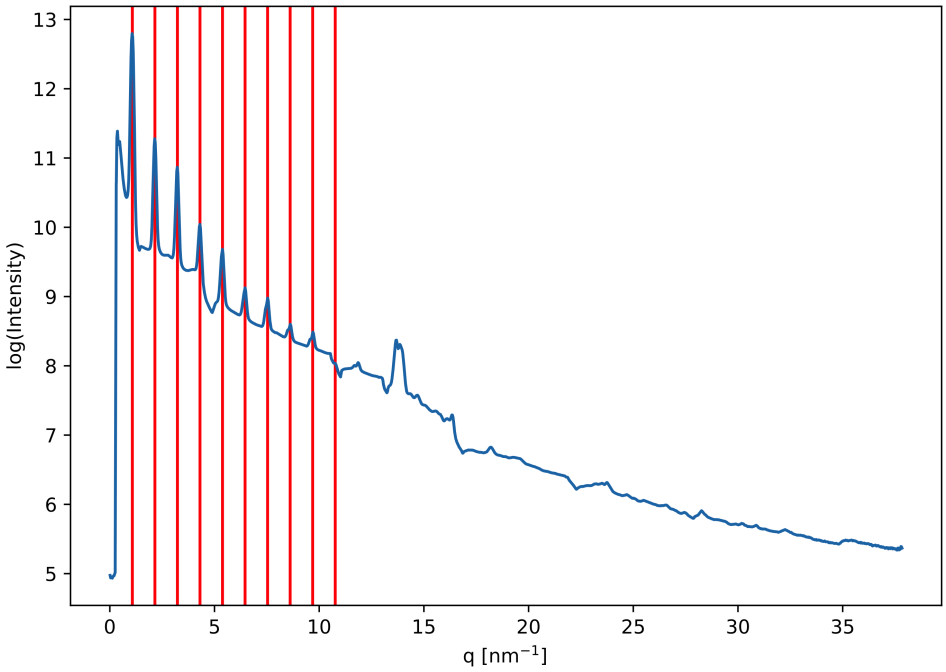
```
Wed, 11 Mar 2020 16:46:47 ct 1
Wed, 11 Mar 2020 16:46:56 dmove basez 1
Wed, 11 Mar 2020 16:47:01 ct 1
Wed, 11 Mar 2020 16:47:05 dmove basez 1
Wed, 11 Mar 2020 16:47:09 ct 1
Wed, 11 Mar 2020 16:47:13 dmove basez -5
Wed, 11 Mar 2020 16:47:26 ct 1
Wed, 11 Mar 2020 16:47:30 dmove basez 1
Wed, 11 Mar 2020 16:47:35 ct 1
Wed, 11 Mar 2020 16:47:53 dscan basez -1 0 50 .1 #741
```

12 Convert logs

Human-readable logs generated in the folder /working/readable_logs/ by clicking on ”‘Convert logs”’.

13 Insert an image

Using the command “Insert image”.



14 Export to pdf

PDF generated by clicking on ”‘Export to pdf”’.