

NAME

pyFAI-calib – pyFAI-calib

DESCRIPTIONusage: pyFAI-calib [options] **-w** 1 **-D** detector **-c** calibrant.D imagefile.edf

Calibrate the diffraction setup geometry based on Debye–Sherrer rings images without a priori knowledge of your setup. Most standard calibrants are directly installed together with pyFAI. If you prefer using your own, you can provide a "d-spacing" file containing the spacing of Miller plans in Angstrom (in decreasing order). Most crystal powders used for calibration are available in the American Mineralogist database: <http://rruff.geo.arizona.edu/AMS/amcsd.php>

positional arguments:

FILE List of files to calibrate

optional arguments:**-h, --help**

show this help message and exit

-V, --version**-o** FILE, **--out** FILE

Filename where processed image is saved

-v, --verbose

switch to debug/verbose mode

-c FILE, **--calibrant** FILE

Calibrant name or file containing d-spacing of the reference sample (MANDATORY)

-w WAVELENGTH, **--wavelength** WAVELENGTH

wavelength of the X-Ray beam in Angstrom

-e ENERGY, **--energy** ENERGYenergy of the X-Ray beam in keV ($hc=12.398419292\text{keV.A}$)**-P** POLARIZATION_FACTOR, **--polarization** POLARIZATION_FACTORpolarization factor, from **-1** (vertical) to **+1** (horizontal), default is None (no correction), synchrotrons are around 0.95**-b** BACKGROUND, **--background** BACKGROUND

Automatic background subtraction if no value are provided

-d DARK, **--dark** DARK

list of dark images to average and subtract

-f FLAT, **--flat** FLAT

list of flat images to average and divide

-s SPLINE, **--spline** SPLINE

spline file describing the detector distortion

-D DETECTOR_NAME, **--detector** DETECTOR_NAME

Detector name (instead of pixel size+spline)

-m MASK, **--mask** MASK

file containing the mask (for image reconstruction)

-n NPT, **--pt** NPT

file with datapoints saved. Default: basename.npt

--filter FILTER

select the filter, either mean(default), max or median

-l DISTANCE, **--distance** DISTANCE
sample-detector distance in millimeter

--poni1 PONI1
poni1 coordinate in meter

--poni2 PONI2
poni2 coordinate in meter

--rot1 ROT1
rot1 in radians

--rot2 ROT2
rot2 in radians

--rot3 ROT3
rot3 in radians

--fix-dist
fix the distance parameter

--free-dist
free the distance parameter

--fix-poni1
fix the poni1 parameter

--free-poni1
free the poni1 parameter

--fix-poni2
fix the poni2 parameter

--free-poni2
free the poni2 parameter

--fix-rot1
fix the rot1 parameter

--free-rot1
free the rot1 parameter

--fix-rot2
fix the rot2 parameter

--free-rot2
free the rot2 parameter

--fix-rot3
fix the rot3 parameter

--free-rot3
free the rot3 parameter

--fix-wavelength
fix the wavelength parameter

--free-wavelength
free the wavelength parameter

--saturation SATURATION
consider all pixel>max*(1-saturation) as saturated and reconstruct them

--weighted
weight fit by intensity, by default not.

--npt NPT_1D
Number of point in 1D integrated pattern, Default: 1024

--npt--azim NPT_2D_AZIM
Number of azimuthal sectors in 2D integrated images. Default: 360

--npt--rad NPT_2D_RAD
Number of radial bins in 2D integrated images. Default: 400

--unit UNIT
Valid units for radial range: 2th_deg, 2th_rad, q_nm⁻¹, q_A⁻¹, r_mm. Default: 2th_deg

--no-gui
force the program to run without a Graphical interface

--no-interactive
force the program to run and exit without prompting for refinements

-r, --reconstruct
Reconstruct image where data are masked or <0 (for Pilatus detectors or detectors with modules)

-g GAUSSIAN, **--gaussian** GAUSSIAN
Size of the gaussian kernel. Size of the gap (in pixels) between two consecutive rings, by default 100 Increase the value if the arc is not complete; decrease the value if arcs are mixed together.

--square
Use square kernel shape for neighbor search instead of diamond shape

-p PIXEL, **--pixel** PIXEL
size of the pixel in micron

The output of this program is a "PONI" file containing the detector description and the 6 refined parameters (distance, center, rotation) and wavelength. An 1D and 2D diffraction patterns are also produced. (.dat and .azim files)