

**NAME**

pyFAI-calib – pyFAI-calib

**DESCRIPTION**

INFO:root:Enter, port=54321. usage: 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. You will need to provide a calibrant or a "d-spacing" file containing the spacing of Miller plans in Angstrom (in decreasing order). Calibrants available: quartz, Cr2O3, AgBh, CrOx, C14H30O, ZnO, Al, NaCl, cristobaltite, Si, Au, LaB6, CeO2, PBBA, alpha\_Al2O3 or search in the American Mineralogist database: <http://rruff.geo.arizona.edu/AMS/amcsd.php> The **---calibrant** option is mandatory !

**positional arguments:**

**FILE** List of files to calibrate

**optional arguments:**

**-h, --help**

show this help message and exit

**-V, --version**

show program's version number and exit

**-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, case sensitive !)

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

wavelength of the X-Ray beam in Angstrom. Mandatory

**-e ENERGY, --energy ENERGY**

energy of the X-Ray beam in keV ( $hc=12.398419292\text{keV.A}$ ).

**-P POLARIZATION\_FACTOR, --polarization POLARIZATION\_FACTOR**

polarization 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 comma separated dark images to average and subtract

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

list of comma separated 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. Default: 100mm

**--dist** DIST  
sample-detector distance in meter. Default: 0.1m

**--poni1** PONI1  
poni1 coordinate in meter. Default: center of detector

**--poni2** PONI2  
poni2 coordinate in meter. Default: center of detector

**--rot1** ROT1  
rot1 in radians. default: 0

**--rot2** ROT2  
rot2 in radians. default: 0

**--rot3** ROT3  
rot3 in radians. default: 0

**--fix-dist**  
fix the distance parameter

**--free-dist**  
free the distance parameter. Default: Activated

**--fix-poni1**  
fix the poni1 parameter

**--free-poni1**  
free the poni1 parameter. Default: Activated

**--fix-poni2**  
fix the poni2 parameter

**--free-poni2**  
free the poni2 parameter. Default: Activated

**--fix-rot1**  
fix the rot1 parameter

**--free-rot1**  
free the rot1 parameter. Default: Activated

**--fix-rot2**  
fix the rot2 parameter

**--free-rot2**  
free the rot2 parameter. Default: Activated

**--fix-rot3**  
fix the rot3 parameter

**--free-rot3**  
free the rot3 parameter. Default: Activated

**--fix-wavelength**  
fix the wavelength parameter. Default: Activated

**--free-wavelength**  
free the wavelength parameter. Default: Deactivated

**--tilt** Allow initially detector tilt to be refined (rot1, rot2, rot3). Default: Activated

**--no-tilt**  
Deactivated tilt refinement and set all rotation to 0

**--saturation SATURATION**  
 consider all pixel > max\*(1-saturation) as saturated and reconstruct them, default: 0 (deactivated)

**--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)