## NAME

pyFAI-calib − pyFAI-calib

## DESCRIPTION

INFO:root:Enter, port=54321. INFO:root:Enter. 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: Ni, CrOx, NaCl, Si_SRM640e, Si_SRM640d, Si_SRM640a, Si_SRM640b, Cr2O3, AgBh, Si_SRM640, CuO, PBBA, alpha_Al2O3, SI_SRM640c, quartz, C14H30O, cristobaltite, Si, LaB6, CeO2, LaB6_SRM660a, LaB6_SRM660b, LaB6_SRM660c, TiO2, ZnO, Al, Au 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=12.398419292keV.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

**−i** FILE, **−−poni** FILE
file containing the diffraction parameter (poni−file). MANDATORY for pyFAI−recalib!

**−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_nmˆ−1, q_Aˆ−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)