

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, cristobalite, 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 ($hc=12.398419292keV.A$).

-P POLARIZATION_FACTOR, --polarization POLARIZATION_FACTOR

polarization factor, from **-1** (vertical) to **+1** (horizontal), default is None (no correction), synchrotrons are around 0.95

-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 $> \max * (1 - \text{saturation})$ 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)