

Data collection with a mini kappa goniometer

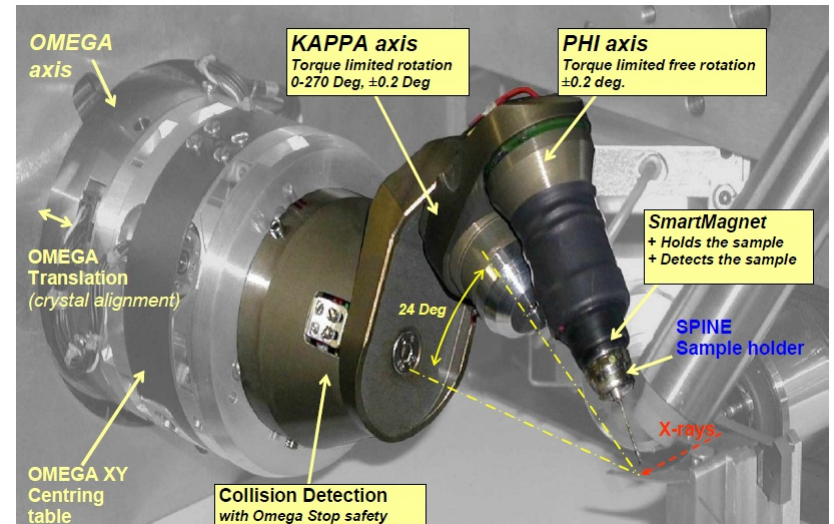
CCP4 Diamond course December 2014

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Mini kappa specifications

- Omega: main rotation axis
- Kappa, Phi: crystal alignment
 - stepper motors, ± 0.2 deg typical kappa/phi precision
 - backlash correction applied
- potential of collision
- Beamlines I04, I04-1



- typical SOC around $4 \mu\text{m}$
 - higher kappa angles more challenging
- SmartMagnet sample holder detection and control
- STAC, XOalign software for orientation calculations

Why use a mini kappa?

- crystal alignment/orientation
- help in point group determination
- get equivalent images from different crystals by reorienting them
- comparing crystals in the same orientation
- smart data collection strategies, better completeness of data
- reduced radiation damage by using smaller overall oscillation range
- optimised MAD data collection; Bijvoet pairs on the same frame
- improved high multiplicity SAD data collection protocols
- reducing/avoiding spot overlap, better spot separation
(long unit cell problem)
- multiple crystal data collection: collect only what has not been collected before

GDA crystal alignment

Software interface for GDA crystal alignment. The main window displays a live camera feed of a crystal sample, overlaid with a red crosshair indicating the alignment point. The interface includes several control panels:

- Camera Control:** Includes a Snapshot button, Zoom (5.0), and a Backlight button.
- Rotation:** Controls for Omega (-70.0 deg), Kappa (40.0 deg), and Phi (70.0 deg). Includes buttons for Move to zero, -90, +90, -180, +180, and Size (10.0 deg).
- Translation:** Readbacks for X (-472.3 micron), Y (88.5 micron), and Z (145.9 micron). Includes a Nudge panel with directional arrows and In/Out buttons, and a Size (10.0 mic) control.
- Lighting:** Sliders for Backlight Brightness (%) (33) and Frontlight Brightness (%) (0).

On the right side, there is an **Align** panel with buttons for Three Click Centring (Start, Cancel), 3-click centring complete, and Auto-centring (Xrec, Keyence Camera).

Dimensions of the crystal sample are indicated: 122.0 μm and 119.0 μm .

GDA data collection setup

Beamline I04 - Tel. +44 1235 778679 - GDA - 8.30.0

File Edit Run Window Help

Baton: Health: **Panic Stop**

Hutch Control:

Current Sample: Barcode:

Sample Robot: Robot Status:

Energy: Machine: Ring Current: Refill:

Wavelength: ID Gap:

Detector Distance:

Monitoring: Beamline: Script: Sample Control:

User feedback:

Samples Alignment Grid Scan Grid Scan Results Fluorescence Data Collection Line Scan Tools User Options Reset Layout

OAV View Data Collection Table Input

Visit Folder: Default Folder: Default Prefix:

Row Sel.	Sample ID	Code	Folder	Prefix	Holder	Position	Omega Start (°)	Omega Oscillation (°)	Omega Delta (°)	Kappa (°)	Phi (°)	Number of Images	Time per Image (s)	Maximum Resolution (Å)	Dis (m)
	smapl_8				2	8	0.00	0.500	45.00	20.000	55.000	3	0.040	2.0670	400.0

Centre the sample

New sample loaded. Manually centre using the 'Centre the sample' view, and press 'Centring complete' to resume data collection.

Data Collection Settings

Scan Control

Sample

Barcode:

Holder:

Position:

Files

Visit directory:

Folder:

Prefix:

☒ Automatic run number

Run number:

Comment:

Axes

Start:

Oscillation:

Total oscillation:

Delta:

Kappa:

Phi:

Image

Number of images:

Exposure time: s

Total exposure time: s

First image number:

Beam and Detector

Maximum resolution: Å

Detector distance: mm

Wavelength: Å

Energy: eV

☐ Use current energy

Transmission: %

Aperture and Beamstop

Aperture:

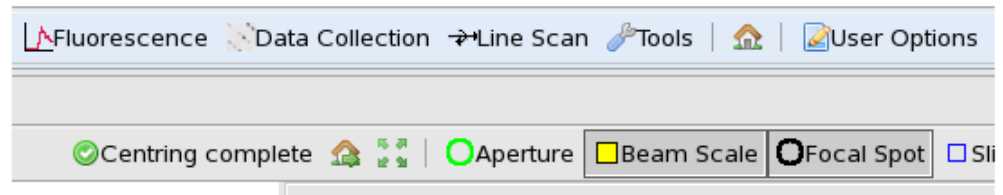
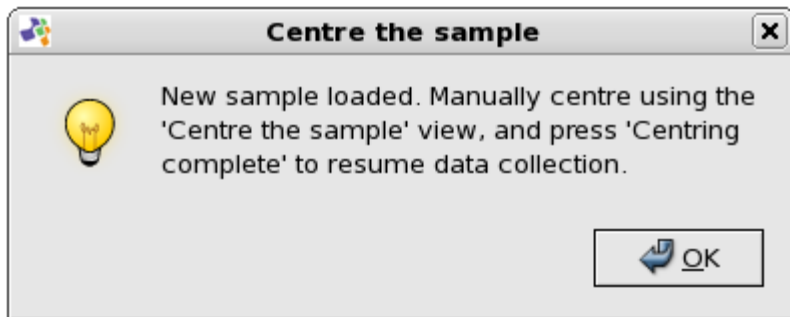
Beamstop:

Omega Start (°)	Omega Oscillation (°)	Omega Delta (°)	Kappa (°)	Phi (°)	Number of Images	Time per Image (s)
0.00	0.500	45.00	20.000	55.000	3	0.040

Paused Script Queue - paused

How to use the mini kappa ?

When a new sample is loaded the Keyence and OAV autocentring are run, then kappa is moved to 0 deg. If kappa/phi values which are different from 0 deg are requested in the data collection table, then a centring request pop-up window will appear and the user has to centre the sample in the Sample Control tab. This step is required because of the mechanical properties of the mini kappa which causes the sample to move away from the crosshair if kappa and/or phi are moved.



XOalign, crystal alignment calculations

Quick Mosflm Strategy Results

Spacegroup	Refined unit cell parameters (Å/degrees)						Est Mosaicity
	a	b	c	α	β	γ	
P4	57.992	57.992	150.453	90.000	90.000	90.000	0.20

Description	Phi Start	Phi Oscillation	No Of Images	Phi End	Completeness	Resolution
Native	21.0°	1.5°	60	111.0°	1.00	1.56Å
Anomalous	21.0°	1.5°	60	111.0°	0.98	1.56Å

XOalign Crystal Alignment Results

Independent Solutions for DLS I04 MiniKappa goniometer:

a*	b*	c*	
66.857	85.934	23.539	Angles between crystal axes and Phi axis
47.654	45.070	77.414	" " " " and BEAM at Datum
66.899	84.730	23.763	" " " " and Omega axis

Solutions for Datum positions: c*, a*

First axis (c*) along rotation axis, second axis (a*) along beam

Omega	Kappa	Phi
29.133	63.085	48.097

Solutions for Datum positions: c*, b*

First axis (c*) along rotation axis, second axis (b*) along beam

Omega	Kappa	Phi
119.133	63.085	48.097

For more details see [log](#).



Data collection information management

Data Collection Parameters			
Wavelength:	1.3051Å	Resolution:	1.6Å
Omega Start:	0°	Omega Oscillation:	0.1°
Time Per Image:	0.1s	Transmission:	4.9019%
Number Of Images:	3600	Overlap:	0°
Beam Size X:	90µm	Beam Size Y:	45µm
Kappa:	161.47°	Phi:	170.382°
Comments:	(-100,-1144,-746) Aperture: Large		

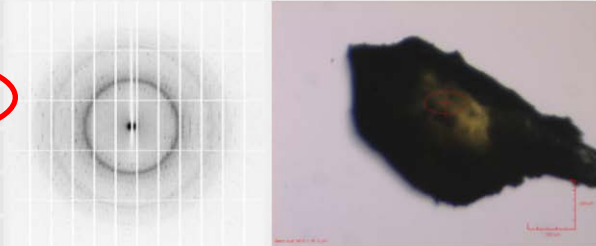
```

###CBF: VERSION 1.5, CBFlib v0.7.8 - PILATUS
data_fer1_a_b_1_0001
_array_data.header_convention "PILATUS_1.2"
_array_data.header_contents
;
# Detector: PILATUS 2M, S/N 24-0107 Diamond
# 2012-05-31T11:35:16.399
# Pixel_size 172e-6 m x 172e-6 m
# Silicon sensor, thickness 0.000320 m
# Exposure_time 0.1964000 s
# Exposure_period 0.1964000 s
# Tau = 199.1e-09 s
# Count_cutoff 493212 counts
# Threshold_setting: 7000 eV
# Gain_setting: mid gain (vrf = -0.200)
# N_excluded_pixels = 255
# Excluded_pixels: badpix_mask.tif
# Flat_field: (nil)
# Trim_file: p2m0107_E14000_T7000_vrf_m0p20.b
# Image_path: .../data/2012/cm5700-2/20120531
# Comment: Mini kappa in use
# Wavelength 0.92088 Å
# Detector_distance 0.25194 m
# Beam_xy (733.24, 839.50) pixels
# Flux 0
# Filter_transmission 0.4350
# Start_angle 68.3000 deg.
# Angle_increment 0.2000 deg.
# Polarization 0.998
# Kappa 123.4480 deg.
# Phi 158.6200 deg.
;
    
```

Close

05-12-2014 12:23:12 - 20141205/Thau_12/data1/Thau_12_1_####.cbf

Sample: <u>Thau_12</u>	Ω Start: 75.0°
Ω Osc: 0.15°	Ω Overlap: 0°
No. Images: 300	κ: 63.085° φ: 48.097°
Resolution: 1.60Å	Wavelength: 0.9795Å
Exposure: 0.050s	Transmission: 15.01%
Beamsize: 90x45µm	Type: Data Collection
Comment: (-671,477,748) Aperture: Large	

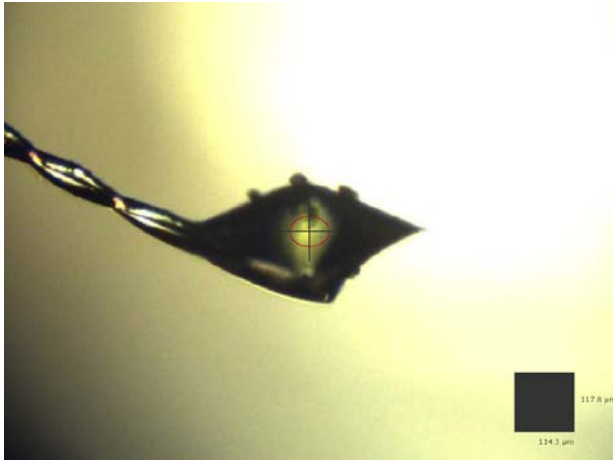


Thu Oct 31, 2013 - 20:51:44

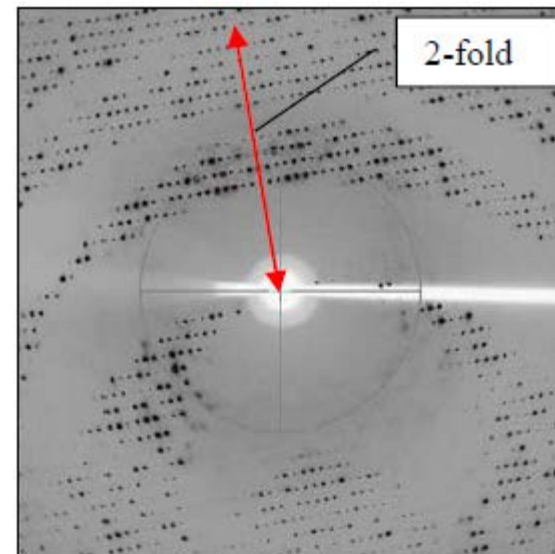
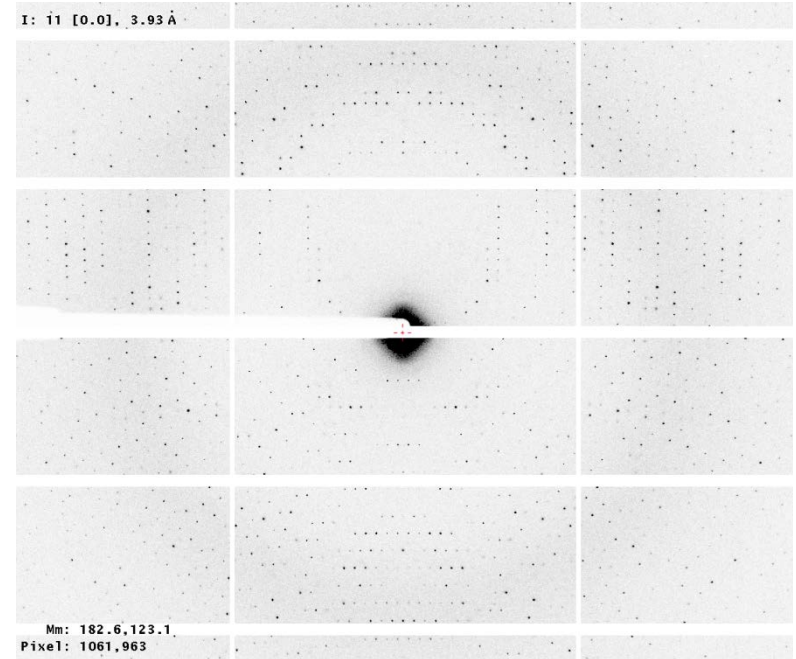
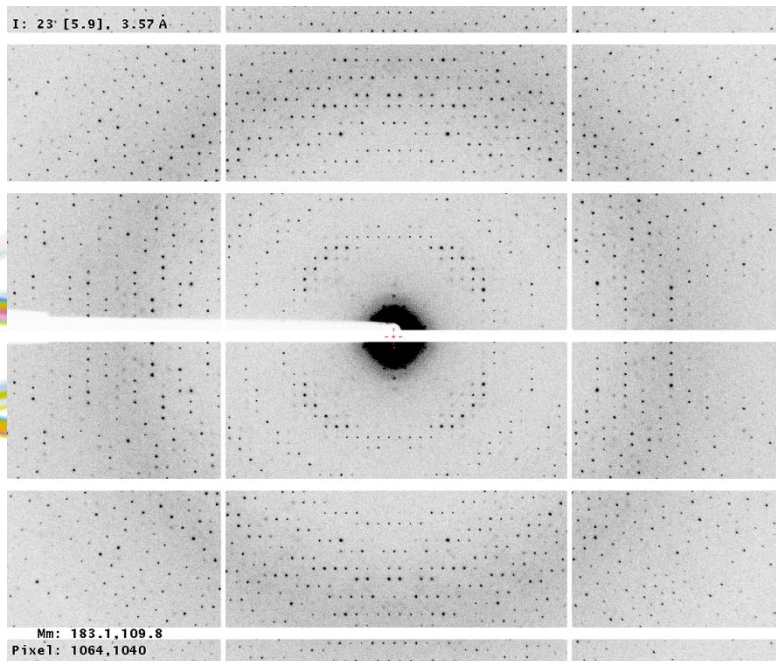
[20131031/mini kappa/glu2/data2/glu2_K161_P170_1_####.cbf](#)

No. Images:	3600	Resolution:	1.60Å
Exp. Time:	0.1s	Trans:	4.90%
Omega Osc:	0.1°	Wavelength:	1.3051Å
Kappa:	161.47°	Phi:	170.382°
Comments:	(-100,-1144,-746) Aperture: Large		
Fast_dp Status:	✓	Xia2 Status:	✓✓✓
Running:	Fast_ep 😊	MrBUMP 😊	DIMPLE ✓

Crystal alignment, diffraction pattern

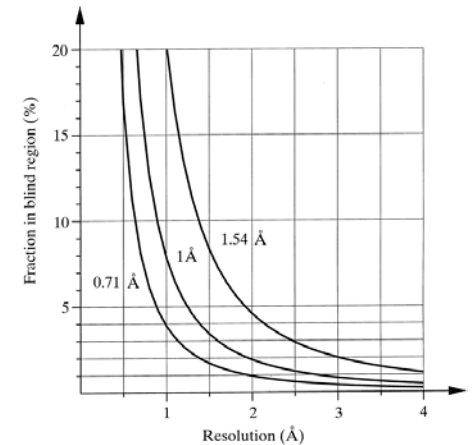
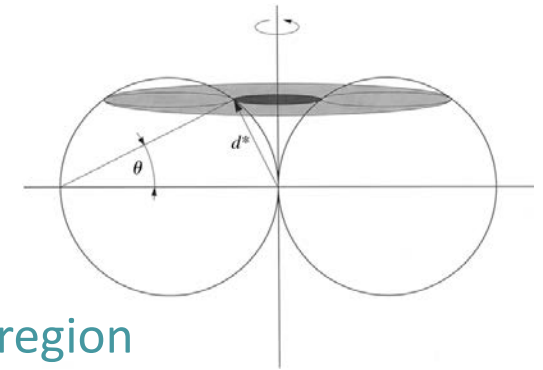
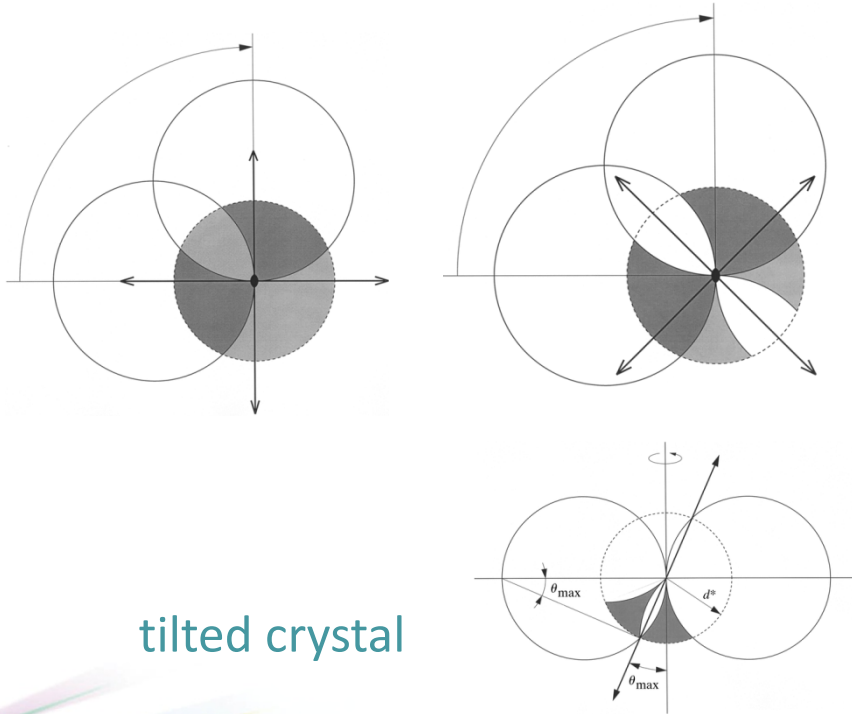


symmetry axes



Data collection strategy, data range, completeness

- Z. Dauter, Acta Cryst. (1999) D55, 1703-1717



Point group	Native data	Anomalous data
1	180 (any)	$180 + 2\theta_{\max}$ (any)
2	180 (b); 90 (ac)	180 (b); $180 + 2\theta_{\max}$ (ac)
222	90 (ab or ac or bc)	90 (ab or ac or bc)
4	90 (c or ab)	90 (c); $90 + \theta_{\max}$ (ab)
422	45 (c); 90 (ab)	45 (c); 90 (ab)
3	60 (c); 90 (ab)	$60 + 2\theta_{\max}$ (c); $90 + \theta_{\max}$ (ab)
32	30 (c); 90 (ab)	$30 + \theta_{\max}$ (c); 90 (ab)
6	60 (c); 90 (ab)	60 (c); $90 + \theta_{\max}$ (ab)
622	30 (c); 90 (ab)	30 (c); 90 (ab)
23	~ 60	~ 70
432	~ 35	~ 45

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New-ISPyB

Old-ISPyB

Shipping Samples

Sample Holders

Sample Changer

Remote Access

Short Visits

Data Collection Software

Mini Kappa

Using the Mini Kappa

Crystal Orientation

Calculations

Data Analysis

Data Backup

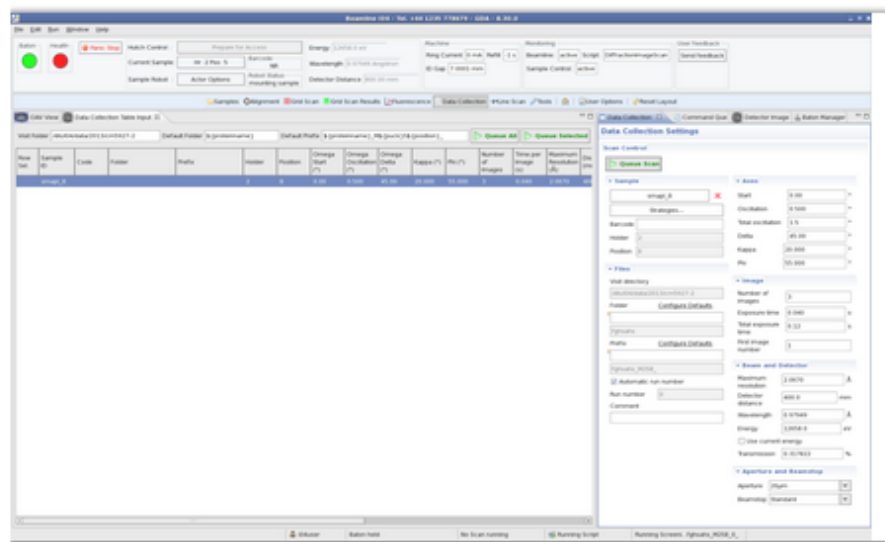
Webcams

Beamline Schematic

Resources

Using the Mini Kappa

In the RCP client kappa and phi values can be entered either in the data collection table or in the data collection form. If a value is changed in the table the form will be updated automatically and vice versa. Values can be entered within the allowed range, kappa: 0-250 deg, phi: 0-360 deg.



When a new sample is loaded the Keyence and OAV autocentring are run, then kappa is moved to 0 deg. If kappa/phi values which are different from 0 deg are requested in the data collection table, then a centring request pop-up window will appear and the user has to centre the sample in the Sample Control tab. This step is required because of the mechanical properties of the mini kappa which causes the sample to move away from the crosshair if kappa and/or phi are moved.

Omega Start (°)	Omega Oscillation (°)	Omega Delta (°)	Kappa (°)	Phi (°)	Number of Images	Time per Image (s)
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