

# Notes on converting 13-BMC single crystal data to CrysalisPro

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Input format

☒ Known CrysAlisPro format DECTRIS/PILATUS cbf

☐ Generic uncompressed image

Skip header bytes:  x=  y=  Pixel type: UNSIGNED SHORT (2 BYTES)

Frames info

Run digits: 0 Separator: None Frame: 3 nameFFF.ext

E:\CrysAlisPro\BMC\_En\_test2\oen\_1\_013\_00001.cbf Browse

E:\CrysAlisPro\BMC\_En\_test2\oen\_1\_013\_00340.cbf Browse

Show header 1st Show header last Import data from headers Run TC

Esperanto output

Images base name: oen\_1\_013\_00 Run #: 1

Rotation [deg]: ☐ 0 ☒ 90 ☐ 180 ☐ 270 ☐ Mirror

Detector info, Auto-gap detection

Pixel size [mm]: 0.1720 x0= 527.9 y0= 548.5 ☐ > 99999.0 overflow

☐ Use Auto-gap detection with value -1 Edit

Instrument info

Wavelength: User 0.43, 0.43, 0.43 Edit a1, a2, b ☒ Synchrotron: 0.4340 Edit lambda

Monochromator: MIRROR/SYNCHROTRON Polfact: 0.980 Edit polfact

Alpha, Beta [deg]: 50.0, 0.0 Edit

Omega0, Theta0, Kappa0 [deg]: 0.0, 0.0, 0.0 Edit

Detector dist. [mm]: 191.2 Edit Beam b2: 0.000 Edit

Gain: 1.0 Edit ☒ Thickn.: 1.0000mm Edit thk

Scan info ☒

Scan type: ☒ Phi Omega= 0.0 ☐ Omega Phi= 170.0

Scan: start, step, exp: -170.0, 1.0, 0.5 Edit Theta= 0.0 Kappa= 0

☒ Use frames in inverse order 1=last, 2=last-1... ☐ Scan scale err 1.000 Edit

Load Save

Help Cancel OK

Del = 0, Nu = 0

X0 = Dioplas X0+32 pixel (for CrysAlisPro square image padding)

Y0 = Dioplas Y0

Use frames in inverse order

Start = -(end phi angle)

If peak harvest still screw up, use "um i" command to update the detector info

## Input format

☒ Known CrysAlisPro format DECTRIS/PILATUS cbf☐ Generic uncompressed imageSkip header bytes:  x=  y=  Pixel type: UNSIG SHORT (2 BYTES)

## Frames info

Run digits: 0 Separator: None Frame: 3 nameFFF.ext

E:\CrysAlisPro\BMC\_En\_test3\oen\_1\_014\_00001.cbf

Browse

E:\CrysAlisPro\BMC\_En\_test3\oen\_1\_014\_00340.cbf

Browse

Show header 1st

Show header last

Import data from headers

Run TC

## Esperanto output

Images base name: oen\_1\_014\_00Run # 1Rotation [deg]: ☐ 0 ☒ 90 ☐ 180 ☐ 270 ☐ Mirror

## Detector info, Auto-gap detection

Pixel size [mm]: 0.1720 x0= 527.9 y0= 548.5 ☐ > 99999.0 overflow☐ Use Auto-gap detection with value -1

Edit

## Instrument info

Wavelength: User 0.43, 0.43, 0.43 Edit a1, a2, b ☒ Synchrotron: 0.4340

Edit lambda

Monochromator: MIRROR/SYNCHROTRON Polfact: 0.980

Edit polfact

Alpha, Beta [deg]: 50.0, 0.0 EditOmega0, Theta0, Kappa0 [deg]: 0.0, 0.0, 0.0 EditDetector dist. [mm]: 191.2 Edit Beam b2: 0.000 EditGain: 1.0 Edit ☒ Thickn.: 1.0000mm

Edit thk

Scan info ☒Scan type: ☒ Phi Omega= 0 ☐ Omega Phi= 170.0Scan: start, step, exp: 170.0, 1.0, 0.5 EditTheta= -20.0 Kappa= 0.0☒ Use frames in inverse order 1=last, 2=last-1...☐ Scan scale err 1.000 Edit

Load

Save

Help

Cancel

OK

For data collected at non-zero del angle, **Theta = - del**, Other parameters should be the same as zero-del.



## Peak hunting



Run list, image type and image directory

Run list: E:\CrysalisPro\BMC\_En\_test3\ESPERANTO\oen\_1\_014\_00

\*.esperanto

Image dir: E:\CrysalisPro\BMC\_En\_test3\ESPERANTO

#	type	start	end	width	exposure	omega	detector	kappa	phi	start	end
1	p	-170.00	170.00	1.00	0.50	0.00	-20.00	0.00	-	1,	340

Run list modification

By default the whole experiment will be evaluated.  
To modify this behaviour edit the run list -->

Edit start num of selected run

Edit end num of selected run

☐ Automatic threshold and background detection (preferred)

☐ Traditional peak hunting

☒ Smart peak hunting

☐ 3D peak extraction

Peak finding control

Threshold: 1000

7x7 average: 20

Overwrite existing peak hunting table

☒ Yes

☐ No

☐ Use background subtraction

Background evaluation control -> 25

Edit Re

25

Edit Fr

Binning for background evaluation:

☒ 1

☐ 2

☐ 4

☒ Reduce background accumulation to SHORT type (saves memory)

Resolution limits

☐ Skip peaks outside resolution limits

d-value (Ang): inf- 0.51  
2theta (deg): 0.00- 50.04

Edit res limits

☐ Apply float correction n/a

☐ Remove spikes

☒ weak

☐ strong

Help

Cancel

OK

Peak hunting: use smart