

# 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: UNSIG SHORT (2 BYTES)

Frames info

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

E:\CrysAlisPro\BMC\_En\_test3\oen\_1\_013\_00001.cbf Browse

E:\CrysAlisPro\BMC\_En\_test3\oen\_1\_013\_00340.cbf Browse

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

Press after find files

Esperanto output

Images base name:  Run #

Rotation [deg]:  0  90  180  270  Mirror

Detector info, Auto-gap detection

Pixel size [mm]:  x0=  y0=   >  overflow

Use Auto-gap detection with value -1 Edit

Instrument info

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

Monochromator: MIRROR/SYNCHROTRON Polfact: 0.980 Edit polfact

Alpha, Beta [deg]:  Edit

Omega0, Theta0, Kappa0 [deg]:  Edit

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

Gain:  Edit  Thickn.: 1.0000mm Edit thk

Scan info

Scan type:  Phi  Omega

Scan: start, step, exp:  Edit

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

Load

Save

Help

Cancel

OK

Del = 0, Nu = 0

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

Y0 = 1044 - Dioptas 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  cbf Generic uncompressed imageSkip header bytes:  x=  y=  Pixel type: 

## Frames info

Run digits:  Separator:  Frame:  nameFFF.extE:\CrysAlisPro\BMC\_En\_test3\oen\_1\_014\_00001.cbf E:\CrysAlisPro\BMC\_En\_test3\oen\_1\_014\_00340.cbf 

## Esperanto output

Images base name:  Run #: Rotation [deg]:  0  90  180  270  Mirror

## Detector info, Auto-gap detection

Pixel size [mm]:  x0=  y0=   >  overflow Use Auto-gap detection with value -1 

## Instrument info

Wavelength:  0.43, 0.43, 0.43   Synchrotron: 0.4340 Monochromator:  Polfact: 0.980 Alpha, Beta [deg]: 50.0, 0.0 Omega0, Theta0, Kappa0 [deg]: 0.0, 0.0, 0.0 Detector dist. [mm]: 191.2  Beam b2: 0.000 Gain: 1.0   Thickn.: 1.0000mm Scan info Scan type:  Phi Omega=   Omega Phi= Scan: start, step, exp: -170.0, 1.0, 0.5  Theta=  Kappa=  Use frames in inverse order 1=last, 2=last-1...  Scan scale err 1.000 

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 -&gt; 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 limitsd-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