## Single-Crystal X-ray Diffraction

I) Data ReductionII) Structural Analysis

#### Open the .par file



#### Import your data



Knov	vn format selector (1.0.2	2)
	Known formats with vali	id headers
	🔿 Dtrek (Rigaku)	rigaku - CCD/Pilatus, no curved IP
	C MAR/Rayonix	marNNNN, pck, img - IP, CCD, Rayonix with Mar formats
	Saxi (Bruker)	sax, sfrm - smart (with unwarp format), Apex, Photon2/50/100
	C Dectris	$cbf$ - simple $\ldots$ setup with single spindle type PX
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NDTE: Using CrysAlisPro you can process only SAXI images from APEX1/2, Photon2/50/100 detectors!

Browse E:\frames\guest\DBA4AgBiBr8\Rigaku training\mo\_DBA4AgBiBr8\_01\_0001.sfm

Last do SAXI do file ----

1

2

3

Browse E:\frames\guest\DBA4AgBiBr8\Rigaku training\mo\_DBA4AgBiBr8\_07\_0096.sfm

NOTE: The CMOS detectors Photon2/50/100 are having gaps, which can be inspected in the \*\_am\_RR\_FFFE.stm files. CAP is adding these gaps. Furthermore makes use to mark fast scans for overload refill in 'Edit runs'. Consult help for further details!

Help

#### Once you have the data in (click ok through the questions, defaults seem to be ok)

顺 mo\_DBA4AgBiBr8 - CrysAlisPro - RED view: E:\frames\guest\DBA4AgBiBr8\Rigaku training\mo\_DBA4AgBiBr8.par (40.71a 64-bit)



#### Find the peaks and index them



#### Find your unit cell

🜾 mo\_DBA4AgBiBr8 - CrysAlisPro - RED view: E:\frames\guest\DBA4AgBiBr8\Rigaku training\mo\_DBA4AgBiBr8.par (40.71a 64-bit)

- 0 ×



Look at your indexed reflections. Do you index most of them? Refine instrument model (if needed)



These are your indexed peaks. Play around by rotating and using the GUI settings menu

Ewald Explorer (1.0.5)		– 🗆 X
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#### Don't forget to look at the other aspects of projections (stereo and gnomonic are quite instructive)







### Probably a twin (or wrong indexing, less likely). Activate the menu for twinning on the right hand side

🔝 Ew	ald Explorer (1.0.5)			- 🗆 X
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Second lattice found (lucky!). Most of the missing peaks found. The are due to a 180 degree rotations along b-axis

Ewa	ld Explorer (1.0.5)			– 🗆 X
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#### Close the Ewald menu.

#### A new "domain was found. The main domain is ~50% the second 25% and ~20% of reflections overlap

🕼 mo\_DBA4AgBiBr8 - CrysAlisPro - RED view: E:\frames\guest\DBA4AgBiBr8\Rigaku training\mo\_DBA4AgBiBr8.par (40.71a 64-bit)

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- 0 X START/STOP 

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#### Save information and exit.

#### Menus are populated now with the correct parameters. You are ready for data reduction

– 0 × Compost and the second i 4 START/STOP **RED** Ready Crystal RED EXPERIMENT mo\_DBA4AgBiBr8 LATTICE LATICE Current cell (CSD: install) 8.2468(3) 8.1113(3) 9.6913(4) 92.044(3) 101.187(3) 90.390(3) V = 635.49(4) Constrained cell 8.2477(5) 8.1123(5) 9.6887(6) 92.034(5) 101.181(6) 90.381(5) V = 635.49(7) Summatry Symmetry Laue class: 2/m P-lattice • 5 PEAK TABLE UB fit with 14195 obs out of 19632 (total:19632,skipped:0) (72.31%) INSTRUMENT MODEL X-ray wavelength: Mo x-cen: 379.0986 y-cen: 509.7721 distance: 37.0310 beam: 0.0302 Crystals Jana m/Export **Data Collection** Rigaku oxford diffraction CRYSALIS RED -へ の 記 (1)) ENG 5:35 PM 12/7/2020 O 🛱 🔇 😜 🦮 🧊 📕 😓 🚾 🕷 🌖 🚱 🎒 🌺 💿 🖬 🗱 🐲 📔 🕥 **P**2 -

#### Save information and exit.

#### Menus are populated now with the correct parameters. You are ready for data reduction

– 0 × Compost and the second i 4 START/STOP **RED** Ready Crystal RED EXPERIMENT mo\_DBA4AgBiBr8 LATTICE LATICE Current cell (CSD: install) 8.2468(3) 8.1113(3) 9.6913(4) 92.044(3) 101.187(3) 90.390(3) V = 635.49(4) Constrained cell 8.2477(5) 8.1123(5) 9.6887(6) 92.034(5) 101.181(6) 90.381(5) V = 635.49(7) Summatry Symmetry Laue class: 2/m P-lattice • 5 PEAK TABLE UB fit with 14195 obs out of 19632 (total:19632,skipped:0) (72.31%) INSTRUMENT MODEL X-ray wavelength: Mo x-cen: 379.0986 y-cen: 509.7721 distance: 37.0310 beam: 0.0302 Crystals Jana m/Export **Data Collection** Rigaku oxford diffraction CRYSALIS RED -へ の 記 (1)) ENG 5:35 PM 12/7/2020 O 🛱 🔇 😜 🦮 🧊 📕 😓 🚾 🕷 🌖 🚱 🎒 🌺 💿 🖬 🗱 🐲 📔 🕥 **P**2 -

#### Data reduction

#### Press the option to start. This part can also be done automatically. Browse through the options and accept the defaults



#### Integration on the indexed peaks starts. An .hkl file will be generated

CMPR

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Remo\_DBA4AqBiBr8 - CrysAlisPro - RED view: E:\frames\guest\DBA4AqBiBr8\Rigaku traininq\mo\_DBA4AqBiBr8.par (40.71a 64-bit)

#### o × START/STOP RED Background accumulation image 222 of run 1 (image 201 of run 1)... **Data Collection Data Reduction** E.

FRAMES/RUNS In run list: 1523/7, used: 1523/7

3D PROFILE ANALYSIS (twin component #1) Frames done: 151 Reflections tested: 1892, used: 992

**3D INTEGRATION & FITTING** Frames done: 0 Fitted: 0, overflow: 0, hidden: 0 Outliers rejected: 0

> Rigaku oxford diffraction

CRYSALIS

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**P**2

RED -

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DATA REDUCTION OPTIONS 3D profile fitting used

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Crystals

Jana

Once finished menu is populated. Go for the twin analysis to review it and finalize the data.



#### This is where you finalize data reduction to produce your files (corrected hkl and the instruction files) Make all edits here (chemical formula, symmetry preferences, etc)

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顺 mo\_DBA4AgBiBr8 - CrysAlisPro - RED view: E:\frames\guest\DBA4AgBiBr8\Rigaku training\mo\_DBA4AgBiBr8.par (40.71a 64-bit)



#### Choose the correct dataset and finish



- 0 ×



# Select the appropriate software for data solution and refinement (Should appear on the left column as long as Jana2006, Olex2, etc. is already installed in C:\)

顺 mo\_DBA4AgBiBr8 - CrysAlisPro - RED view: E:\frames\guest\DBA4AgBiBr8\Rigaku training\mo\_DBA4AgBiBr8.par (40.71a 64-bit)

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