Detectors for single-crystal area detector diffractometers

Mathias Meyer
X-ray Group Software Manager
Rigaku, founded in 1951, are well respected for the high performance and stable rotating anodes around the world.

- Our first rotating anode was built in 1952

Oxford Diffraction, in its many guises (Kuma, Varian, Agilent) has always retained they key people responsible for success in software, CCD design and the worlds first dual source systems

- The Gemini was launched at the IUCr in Florence 2004
A NEW BEGINNING

The joining of Rigaku and Oxford opens up a realm of possibilities, the merging of superior hardware, software and expertise will allow for an exciting future in single crystal diffraction. The merging of the two groups is represented in our new logo which takes elements from both.

Expertise from both R&D groups is now shared providing an exciting future for single crystal X-ray diffraction.
Roots PhD at UNIL
1992...
Frustration 1993: incommensurates

Figure 2
Reconstruction of the reciprocal plane \( h\bar{2}l \) in \( \gamma \)-sodium carbonate. The intersections of dotted and solid white lines correspond to main reflections systematically absent as a result of the \( C \) centering. The white circle shows the position of the fifth-order satellite \( 2L1 \). This reflection is visible in the insert showing the corresponding area on a different scale.

Michal Dusok et al., "Sodium carbonate revisited"
Efficiently measure incommensurate samples?

(McIntyre, Neutron News 2, 1992, 15)
Efficiently measure incommensurate samples?

(McIntyre, Neutron News 2, 1992, 15)
A ‘Gedankenexperiment’

- We build an area detector diffractometer
- Have source
- Have goniometer
- Have an ‘ideal detector’
A ‘Gedankenexperiment’

X-ray Source
Provides X-ray Beam

Goniometer:
Crystal Positioning ‘Robot’

X-ray Detector
-Specialist digital camera
- ‘photos’ of X-rays

Rigaku
oxford diffraction
The ‘ideal’ detector
The ‘ideal’ detector

- What should it do?
  - Experiments at Cu, Mo, Ag, synchrotron?
  - Samples 1 μm to 1 mm
  - Fast, precise

- What kind of properties
  - Size
  - Resolution
  - ‘Color’: Energy
  - Detectivity
  - Speed
  - Practical operation
  - Price

Jim Pflugrath once said: "The ideal detector tells you where every photon landed and when."
XtaLAB Synergy S/R with HyPix6000HE

- ACA 2016 launch HyPix 6000

- 100 microns resolution with top-hat PSF
- 100Hz – shutterless with near 0 dead-time
- 10 deg/sec top dc speed, very fast positioning
- PhotonJet sources
- WIT in 17s
- Full mmm data set in ~2min
- P1 = full sphere in <15min
Synergy R and HyPix6000HE:
100µm pixel, 100Hz operation, 10deg/s scans
The ‘real’ detectors SX AD

The ‘real’ detectors SX AD

Charge integrating detectors

Event counters: HPAD, HPC – Hybrid pixel counters

Detecting X-rays with a CCD Integrative detector

- Patented reversible CCD/taper bonding – No risk of catastrophic delamination
- Beryllium Window
- Proprietary SuperPlus™ scintillator converts X-rays to visible light with Very high sensitivity
- Low-loss fibre optic taper
- KAF4320 CCD Chip 2k by 2k pixels
- Peltier cooling to -40°C
  - For ultra-low noise
  - Water block used for high thermal stability

Shutter Closed

Shutter Open
The closest thing to an ideal detector...

Direct Detection of X-rays in silicon sensor
→ Point Spread Function of 1 pixel

Single Photon-counting in CMOS
→ no readout noise & dark current
→ high dynamic range (20 bit)
→ fast readout

CMOS: Complementary metal–oxide–semiconductor
- CMOS is only a production technology
- CMOS based detectors can be very different

adapted from: Dectris
Key Features of HPC Detectors

• Direct detection of X-ray photons – no conversion to light
• Excellent point spread function – top hat

adapted from: Dectris
Key Features of HPC Detectors (Pilatus)

- Excellent signal-to-noise ratio via single photon counting
- Adjustable threshold to suppress fluorescence
- High dynamic range: 1:1,048,576 photons per pixel
- High counting ranges: up to $2 \times 10^6$ photons per second per pixel
- Short readout time: 7 ms
- Frame rate up to 20 images per second
The ‘real’ detectors SX AD

<table>
<thead>
<tr>
<th>Integrative detectors, CPAD’</th>
<th>Event counters, HPAD’</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indirect detection via X-ray scintillator</td>
<td>Direct detection via photo-electric effect</td>
</tr>
<tr>
<td>Light conduction via taper/fiber glass</td>
<td>-</td>
</tr>
<tr>
<td>Light detection, Integrating‘</td>
<td>Charge detection, Photon counting‘</td>
</tr>
<tr>
<td>CCD</td>
<td>CMOS</td>
</tr>
<tr>
<td>FET-&gt;ADC-&gt;memory</td>
<td>Memory</td>
</tr>
<tr>
<td>No energy discrimination</td>
<td>Energy thresholds</td>
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The ‘real’ detectors SX AD

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</tbody>
</table>

- No energy discrimination
- Energy thresholds
What is data quality?

\[
\frac{I}{\sigma} \rightarrow I \rightarrow \left( \sum \frac{I}{\sigma} \right) / \text{time}
\]

\[
\sigma^2 = \sigma^2_{Inet} + 2\sigma^2_{back} + \sigma^2_d + \sigma^2_{sys}
\]
The single crystal diffraction experiment

Inorganic Materials
Absorbing Samples
Mo vs. Cu
Benefits of Cu
Small Crystals
Absolute Configuration

Twinning
Incommensurates
Charge Density
High Pressure
Large Crystals
Diffuse Scatter

Powder Diffraction
Photocrystallography
Novel Applications
Multi-Temperature
Quasi-Crystals
The single crystal diffraction experiment

Small Molecule
3-D structure & connectivity

Accurate bond lengths & angles

120°

Shape and chemical structure (specificity / activity) of active site

3-D structure / folding

Protein
Importance of weak data

- Make a typical experiment
  - Cu radiation
  - Resolution 0.78Ång
  - $(I/sig)_{mean} = 15$ to 0.837Ång (IUCR)
Importance of weak data

- Make a typical experiment
  - Cu radiation
  - Resolution 0.78\text{Ang}
  - $(I/\text{sig})_{\text{mean}} = 15 \text{ to } 0.837\text{Ang}$ (IUCR)
Importance of weak data

Histogram of data

Intensity histogram of an organic non-centrosymmetric sample
Importance of weak data

Histogram of data

Intensity histogram of an organic non-centrosymmetric sample

Number of reflections

Log Intensity (photons)
Importance of weak data

Histogram of data

2/3 of the reflections have counts <1% of the maximum intensity*

Detective Quantum Efficiency (DQE)

\[
DQE = \frac{T_w \eta_{ph}}{1 + \frac{1}{g} + \frac{A(n_r^2 + i_d t)}{IT_w \eta_{ph} g^2}}
\]

Window
Scintillator

Gain

Noise:
Read and dark

DQE: Cu and Mo

DQE vs Intensity (Cu)

DQE vs Intensity (Mo)
Importance of weak data
Comparison of tech
Importance of weak data
Comparison of tech
Importance of weak data
Comparison of tech

<table>
<thead>
<tr>
<th>Tech</th>
<th>((l/sig)_{\text{mean}})</th>
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</thead>
<tbody>
<tr>
<td>Ideal</td>
<td>15</td>
</tr>
<tr>
<td>CCD</td>
<td>13.6</td>
</tr>
<tr>
<td>CMOS</td>
<td>11.3</td>
</tr>
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<td>HPAD</td>
<td>14.2</td>
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![Rigaku Oxford Diffraction logo]
Importance of weak data

Comparison of tech

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</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Tech</th>
<th>Time to reach ideal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ideal</td>
<td>1</td>
</tr>
<tr>
<td>CCD</td>
<td>1.38</td>
</tr>
<tr>
<td>CMOS</td>
<td>4.76</td>
</tr>
<tr>
<td>HPAD</td>
<td>1.11</td>
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</table>
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Comparison of tech

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<td>15</td>
</tr>
<tr>
<td>CCD</td>
<td>13.8</td>
</tr>
<tr>
<td>CMOS</td>
<td>12.8</td>
</tr>
<tr>
<td>HPAD</td>
<td>12.7</td>
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</table>
Importance of weak data
Comparison of tech

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<table>
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<tr>
<th>Tech</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Ideal</td>
<td>1</td>
</tr>
<tr>
<td>CCD</td>
<td>1.23</td>
</tr>
<tr>
<td>CMOS</td>
<td>2.22</td>
</tr>
<tr>
<td>HPAD</td>
<td>1.38</td>
</tr>
</tbody>
</table>
Importance of weak data
Charge density

- Make a typical experiment
  - Mo radiation
  - Resolution 0.45\text{Ang}
  - Diffraction limit set to 0.5\text{Ang} \rightarrow (I/sig)_{\text{mean}} = 2
  - To get this we pump I:
    - $(I/sig)_{\text{mean}} = 35 \text{ to } 0.837\text{Ang}$ (IUCR)
Importance of weak data
Comparison of tech

<table>
<thead>
<tr>
<th>Tech</th>
<th>(l/sig)$_{\text{mean, all}}$, 0.837</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ideal</td>
<td>35.1</td>
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<tr>
<td>CCD</td>
<td>32.4</td>
</tr>
<tr>
<td>CMOS</td>
<td>31.8</td>
</tr>
<tr>
<td>HPAD</td>
<td>29.9</td>
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</table>

<table>
<thead>
<tr>
<th>Tech</th>
<th>(l/sig)$_{\text{mean, all}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ideal</td>
<td>8.6</td>
</tr>
<tr>
<td>CCD</td>
<td>7.8</td>
</tr>
<tr>
<td>CMOS</td>
<td>7.0</td>
</tr>
<tr>
<td>HPAD</td>
<td>7.3</td>
</tr>
</tbody>
</table>
**Importance of weak data**

**Comparison of tech**

<table>
<thead>
<tr>
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<tr>
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<th>Time to reach ideal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ideal</td>
<td>1</td>
</tr>
<tr>
<td>CCD</td>
<td>3.42</td>
</tr>
<tr>
<td>CMOS</td>
<td>59.17</td>
</tr>
<tr>
<td>HPAD</td>
<td>1.38</td>
</tr>
</tbody>
</table>
Importance of weak data

Conclusion

Noise does matter!
Oxford Diffraction R&D have designed, built and tested a CMOS detector of identical internal construction to a commercially available model.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Atlas S2 CCD</th>
<th>APS CMOS (Oxford Diffraction R&amp;D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active area, Taper</td>
<td>100x100mm, taper 2:1</td>
<td>100x100mm, taper 1:1</td>
</tr>
<tr>
<td>Gain [e-/MoKα]</td>
<td>180</td>
<td>261</td>
</tr>
<tr>
<td>Sensor</td>
<td>Truesense* Imaging CCD</td>
<td>Teledyne Dalsa RadEye 100 CMOS</td>
</tr>
<tr>
<td>Noise [MoKα-photons]</td>
<td>~0.05</td>
<td>~0.5 *Formerly Kodak</td>
</tr>
</tbody>
</table>
CCD vs. APS CMOS
Comparative Detectivity Measurements

X-ray source

Filter

X-ray detector
CCD vs. APS CMOS
Comparative Detectivity Measurements

- The filter has been chosen in such a way as to observe single photon events

- In order to visualize signal-to-noise differences 100 images are averaged and scaled so that the noise level is the same for all modes of operation
CCD vs. APS CMOS
Comparative Detectivity Measurements

Exposure time [s] 0.1 0.5 1 5

Atlas CCD

APS CMOS (RadEye100 Chip – Oxford Diffraction R&D)
HW – Detector technology: Key metrics

- Detectivity
- Dynamic range
- Speed
- Size
- Price
S2 CCD Detectors: INTELLIGENT MEASUREMENT SYSTEM

Smart Sensitivity Control (SSC)

- **Self-optimizing** detector amplification based on strength of observed data (similar to ISO settings in digital photography)
- Standard, Medium and High SSC modes
- Maximises dynamic range for strong data
- Improvement in signal-to-noise for weak data
- A unique feature of Rigaku Oxford Diffractions CCD X-ray detectors
S2 CCD Detectors: INTELLIGENT MEASUREMENT SYSTEM

Instant-switching hardware binning:

- **Adjustable** pixel sizes for variable resolution
- Flexibility in dynamic range
- Fast re-measurement of overflowed reflections
- Theta-dependent binning
- Automatic software switches binning modes **instantly**

<table>
<thead>
<tr>
<th>Binning</th>
<th>Combined Pixel Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 x 1</td>
<td>24 μm</td>
</tr>
<tr>
<td>2 x 2</td>
<td>48 μm</td>
</tr>
<tr>
<td>4 x 4</td>
<td>96 μm</td>
</tr>
</tbody>
</table>

Higher spatial resolution
Larger dynamic range
Lower detectivity
Longer processing time
Larger files

Lower spatial resolution
Smaller dynamic range
Higher detectivity
Shorter processing time
Smaller files

Rigaku Oxford Diffraction
# S2 CCD Detectors: INTELLIGENT MEASUREMENT SYSTEM

<table>
<thead>
<tr>
<th>Exposure time</th>
<th>0.5s</th>
<th>1s</th>
<th>2s</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Standard SSC mode</strong></td>
<td>![Standard 0.5s]</td>
<td>![Standard 1s]</td>
<td>![Standard 2s]</td>
</tr>
<tr>
<td><strong>High SSC mode</strong></td>
<td>![High 0.5s]</td>
<td>![High 1s]</td>
<td>![High 2s]</td>
</tr>
</tbody>
</table>

![Graph comparison between Standard and High modes for different exposure times]
# S2 CCD Detectors: INTELLIGENT MEASUREMENT SYSTEM

<table>
<thead>
<tr>
<th>Exposure time</th>
<th>0.5s</th>
<th>1s</th>
<th>2s</th>
<th>5s</th>
</tr>
</thead>
<tbody>
<tr>
<td>2x2</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
</tr>
<tr>
<td>4x4</td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
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</table>
S2 CCD Detectors:
INTELLIGENT MEASUREMENT SYSTEM: IMS

If the user modifies one of the suggested settings, ‘Auto suggest’ link appears, which allows him to re-enable automatic suggestions.
Strategy
Intelligent Measurement System – IMS for CCD

Base binning
Smart sensitivity control
Theta dependent binning
Gonio/scan settings correlation
HPC – Hybrid Pixel Counters:

• HPC detectors deliver excellent data quality due to high dynamic range and superb signal-to-noise
  - No rescans required to correct for overloads or to measure strong data

• Signal threshold reduces noise from fluorescence

• Shutterless data collection
  - Simplifies measurement setup
  - Improves data quality
  - Can dramatically shorten wall time

• Top-hat point spread function means better spatial resolution for reflections
Fine slicing and count rate correction

Wide slicing

HPADs are rate meters!
To integrate they require rate correction!
Simple rate correction requires near constant signal

Rate = counts/time

Optimal fine phi-slicing for single-photon-counting pixel detectors
HPC – IMS: Feature

Feature:

• Strong reflections may be affected by coincidence-loss (dead time correction): rates > 400k/pix.s

• Fine-slicing may be required for more accurate count-rate correction

• Excessive fine slicing may yield photon loss due to (even) short dead or readout time

• In shutterless mode no re-measurement possible

• Pixels exceeding count-rate or absolute counter limit will be treated as overflows
Data quality and count rates
Coincidence loss

Optimal fine phi-slicing for single-photon-counting pixel detectors
Data quality and count rates

Coincidence loss

We have to make a <0.5% integral!

Optimal fine phi-slicing for single-photon-counting pixel detectors
As a rule of thumb we require 7-10 profile steps in a >400k/pix.s peak!
Fine slicing and count rate correction

Rate = counts/time

Important feature: No matter what scan speed we use the local angular rates stay!
Data quality and count rates

Coincidence loss

So we require high readout frequency at fast scan speed and ideally no readout overhead!

New Hybrid Photon Counting Detector
HyPix6000HE – (near) Zero Dead-Time Mode+100Hz
HPC – Hybrid Pixel Counters: IMS

The optimal data collection frequency is suggested from the pre-experiment evaluation and the user selected exposure time.
HPC – IMS

- Detector may operate at higher frequency than CrysAlisPro frame rate
- Accumulation of detector frames (high freq) into final frames (lower frequency) is done in memory at acquisition time
Strategy
Intelligent Measurement System – IMS for HPC

Base scan width
HPAD op mode
IMS HPAD
Rate limits
Counter limits
Generator setting
Advances from where?

- HW – instrumentation
- $\frac{I}{\sigma}$
- Procedure
- Data reduction
- Corrections
HW – Sources

Same sample 0.3mm, normal tubes (2kW, 0.5mm collimator), micro-focus (50W), 007HF (1200W)

<table>
<thead>
<tr>
<th>Source type</th>
<th>Integral intensity relative Enhance Mo</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enhance Mo</td>
<td>1</td>
</tr>
<tr>
<td>Enhance Cu</td>
<td>5</td>
</tr>
<tr>
<td>Ultra Cu</td>
<td>40</td>
</tr>
<tr>
<td>Nova Cu 2\textsuperscript{nd} gen</td>
<td>240</td>
</tr>
<tr>
<td>PhotonJet S Cu</td>
<td>480</td>
</tr>
<tr>
<td>PhotonJet R Cu</td>
<td>Up to 3000</td>
</tr>
</tbody>
</table>
## HW – Fullwell/Dynamic

<table>
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<tr>
<th>Detector generation</th>
<th>Full well $X_{ph}$</th>
<th>Relative</th>
</tr>
</thead>
<tbody>
<tr>
<td>KM4CCD, Sapphire 2x2</td>
<td>10’000</td>
<td>1</td>
</tr>
<tr>
<td>Ruby 2x2</td>
<td>2’500</td>
<td>0.25</td>
</tr>
<tr>
<td>Atlas 2x2</td>
<td>3’000</td>
<td>0.3</td>
</tr>
<tr>
<td>Atlas – S2 4x4</td>
<td>48’000</td>
<td>4.8</td>
</tr>
<tr>
<td>Pilatus 200K</td>
<td>$2^{20}=1’000’000$</td>
<td>100</td>
</tr>
<tr>
<td>HyPix 6000HE</td>
<td>$2^{32}=4’000’000’000$</td>
<td>40000</td>
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# HW – Detector Speed

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<th>FPS</th>
<th>Relative</th>
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<tbody>
<tr>
<td>KM4CCD, Sapphire 512²</td>
<td>0.1</td>
<td>1</td>
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<tr>
<td>Ruby 512²</td>
<td>0.21</td>
<td>2</td>
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<tr>
<td>Atlas 512²</td>
<td>0.7</td>
<td>7</td>
</tr>
<tr>
<td>Atlas – S2 512²</td>
<td>1.4</td>
<td>14</td>
</tr>
<tr>
<td>Pilatus 200K</td>
<td>20</td>
<td>200</td>
</tr>
<tr>
<td>shutterless 86% duty cycle</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HyPix 6000HE</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>shutterless ~100% duty cycle</td>
<td></td>
<td></td>
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</table>
### HW – Detector Size

<table>
<thead>
<tr>
<th>Detector relative size</th>
<th>Unique speed</th>
<th>Observation speed</th>
</tr>
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<tbody>
<tr>
<td>Eos</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Atlas</td>
<td>1.3-1.6</td>
<td>1.6-1.8</td>
</tr>
<tr>
<td>Titan</td>
<td>1.4-1.8</td>
<td>2.0-2.2</td>
</tr>
</tbody>
</table>
‘What is this?’ tool

- Available after screening
- Only requires compound elements
- Uses AutoChem2.1/3.0
- Uses up to 5deg/s (CCD) or 10deg/s (HPAD) scan speed!
What is this? tool: 70s later...
What is this? tool: Connectivity solved! <70s
XtaLAB Synergy: PhotonJet R, HyPix6000HE
XtaLAB Synergy and HyPix6000HE:

100µm pixel, 100Hz operation, 10deg/s scans
Synergy: XtaLAB Synergy

A combination of leading edge components and user-inspired software tied together through a highly parallelized architecture to produce fast, precise data in an intelligent fashion.
Synergy: XtaLAB Synergy

NEW PhotonJet sources – our 3rd generation microfocus X-ray sources

NEW goniometer – with motor speeds which have been doubled

Closer sample to detector distance

The widest range of available detectors to suit. CCD or HPC? Your choice.

Unique telescoping 2θ arm provides total flexibility for your diffraction experiment.

Enhanced kappa goniometer design with symmetrical 2θ positioning
Synergy: XtaLAB Synergy

These results highlight the benefits of the new, faster goniometer, the closer detector distance and increase in source flux of the microfocus source with the Atlas S2 detector.

<table>
<thead>
<tr>
<th>Experiment parameters</th>
<th>SuperNova AS2</th>
<th>XtaLAB Synergy AS2 very fast</th>
<th>XtaLAB Synergy AS2 using extra data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal to detector distance (mm)</td>
<td>50</td>
<td>35.5</td>
<td>35.5</td>
</tr>
<tr>
<td>Completeness to 0.84 Å</td>
<td>99.2</td>
<td>98.6</td>
<td>99.8</td>
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<tr>
<td>Redundancy</td>
<td>2.7</td>
<td>2.1</td>
<td>2.7</td>
</tr>
<tr>
<td>Relative goniometer speed</td>
<td>x1</td>
<td>x2</td>
<td>x2</td>
</tr>
<tr>
<td>I/sigma to 0.84Å</td>
<td>26</td>
<td>39</td>
<td>59</td>
</tr>
<tr>
<td>Experiment time</td>
<td>12 min 48 sec</td>
<td>7 min 38 sec</td>
<td>11 min 17 sec</td>
</tr>
<tr>
<td>Rint</td>
<td>0.036</td>
<td>0.021</td>
<td>0.016</td>
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<tr>
<td>R1 (%)</td>
<td>3.97</td>
<td>3.00</td>
<td>2.54</td>
</tr>
</tbody>
</table>
Synergy: XtaLAB Synergy

Ylid data collection IUCR in minimum time

For comparison: SN Atlas: 52mm = 12mins

<table>
<thead>
<tr>
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<td>35</td>
<td>5</td>
<td>8</td>
<td>338</td>
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<td>679</td>
<td>3</td>
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</tbody>
</table>
Thank you for listening!

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