Meta-data et al

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High Data-Rate Macromolecular Crystallography
MAX-IV, Lumd
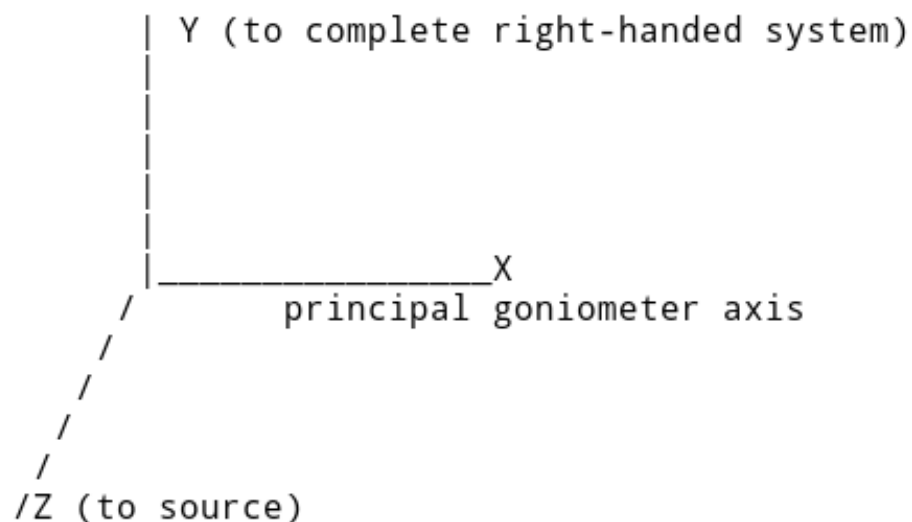15th - 17th March 2017

Importance of correct meta-data

- request from user/customer for autoPROC support of Bruker PHOTON-II detector

- Bruker provided example dataset (Lysozyme, single-sweep)

- CBF file following imgCIF 1.3.2 (http://www.iucr.org/resources/cif/dictionaries/cif_img)

- autoPROC will extract full experiment description from provided information

Importance of correct meta-data

```
| Y (to complete right-handed system)
|
|
|
|
|
|
|_____X
/       principal goniometer axis
/
/
/
/
/Z (to source)
```

imgCIF coordinate system

Axis 1 (X): The X-axis is aligned to the mechanical axis pointing from the sample or specimen along the principal axis of the goniometer.

Axis 2 (Y): The Y-axis completes an orthogonal right-handed system defined by the X-axis and the Z-axis (see below).

Axis 3 (Z): The Z-axis is derived from the source axis which goes from the sample to the source. The Z-axis is the component of the source axis in the direction of the source orthogonal to the X-axis in the plane defined by the X-axis and the source axis.

http://www.iucr.org/__data/iucr/cifdic_html/2/cif_img.dic/Caxis.htm

Goniostat and detector axes

```
loop_
_axis.id
_axis.depends_on
_axis.equipment
_axis.type
_axis.vector[1]
_axis.vector[2]
_axis.vector[3]
_axis.offset[1]
_axis.offset[2]
_axis.offset[3]
OMEGA . goniometer rotation 1 0 0 0 0 0
CHI OMEGA goniometer rotation 0 0 1 0 0 0
PHI CHI goniometer rotation -1 0 0 0 0 0
TWOTHETA . detector rotation 1 0 0 0 0 0
DX TWOTHETA detector translation 0 0 -1 0 0 0
YAW DX detector rotation 1 0 0 0 0 0
PITCH YAW detector rotation 0 -1 0 0 0 0
ROLL PITCH detector rotation 0 0 1 0 0 0
H ROLL detector translation 0 -1 0 0 0 0
V H detector translation -1 0 0 0 0 0
ELEMENT X V detector translation 0 -1 0 -69.12 -51.84 0
ELEMENT Y ELEMENT X detector translation 1 0 0 0 0 0
```

Importance of correct meta-data

```
loop_
_diffrn_scan_frame_axis.axis_id
_diffrn_scan_frame_axis.displacement
_diffrn_scan_frame_axis.angle
DX 60.00154 ?
TWOTHETA ? 9
OMEGA ? 268.0001
PHI ? 155.0003
CHI ? 22.99989
H -0.650700000650699 ?
V -0.107986500107984 ?
PITCH ? -0.07
ROLL ? -0.217
YAW ? 0.059
```

**Goniostat angles and detector angle/distance**

Importance of correct meta-data

```
loop_
_diffrn_scan_axis.axis_id
_diffrn_scan_axis.displacement_start
_diffrn_scan_axis.displacement_increment
_diffrn_scan_axis.displacement_range
_diffrn_scan_axis.angle_start
_diffrn_scan_axis.angle_increment
_diffrn_scan_axis.angle_range
 DX 60.00154 0 0 ? ? ?
 TWOTHETA ? ? ? 9 0 0
 OMEGA ? ? ? 268.0001 0 0
 PHI ? ? ? 155.0003 0.5 0.5
 CHI ? ? ? 22.99989 0 0
 H -0.650700000650699 0 0 ? ? ?
 V -0.107986500107984 0 0 ? ? ?
 PITCH ? ? ? -0.07 0 0
 ROLL ? ? ? -0.217 0 0
 YAW ? ? ? 0.059 0 0
```

Rotation axis and increment

So far so good … but:
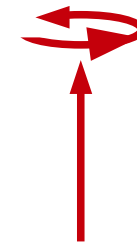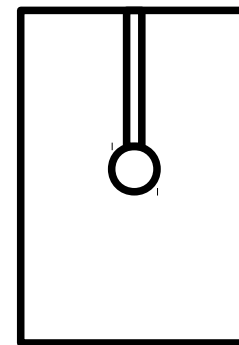
Importance of correct meta-data

X

Y
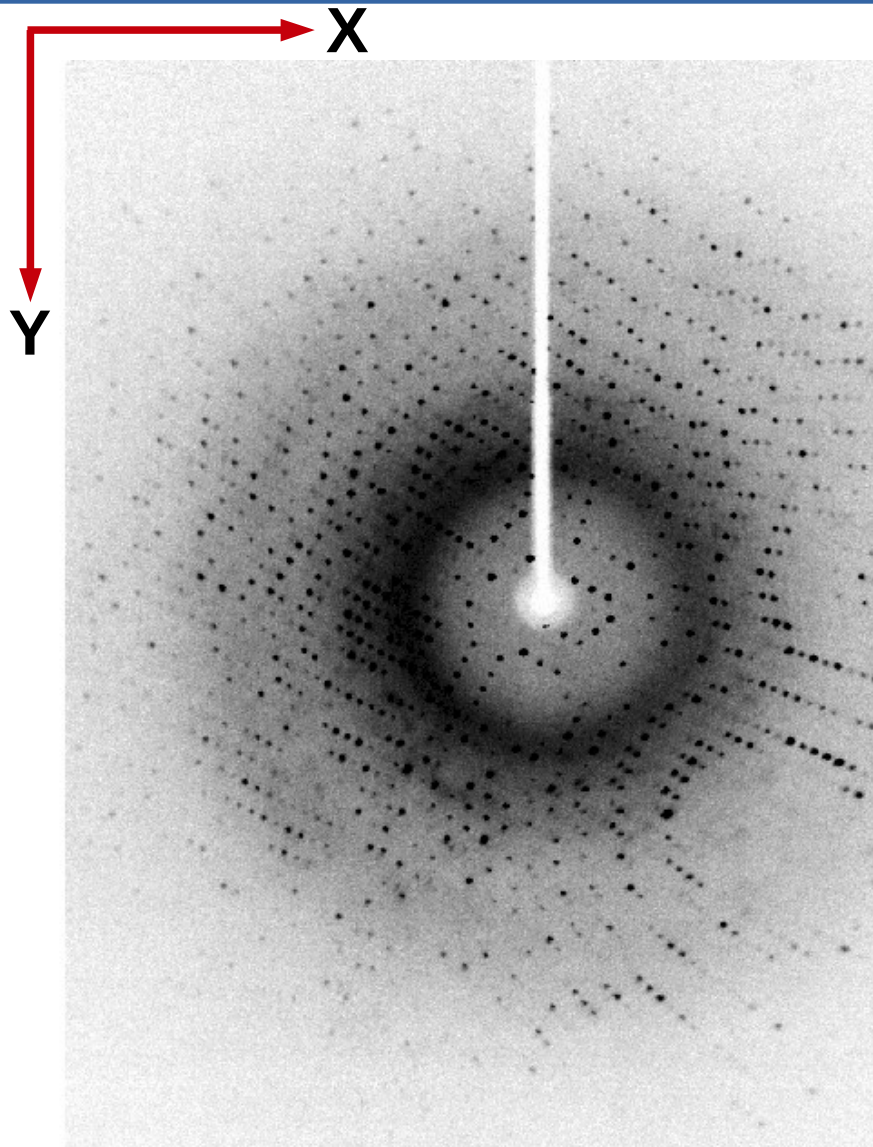
2-theta = +9
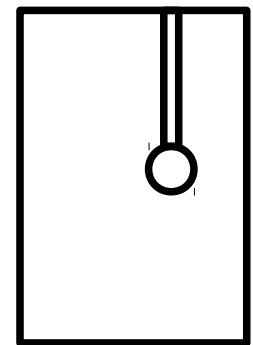
Detector X = 0 -1 0
Detector Y = 1 0 0
2-theta = 1 0 0

2-theta

-1 0 0   **????**

Importance of correct meta-data

- Solution to this conundrum quite easy after very helpful discussions with Bruker (Matt Benning, Jörg Kärcher): ELEMENT_Y was inverted in the header.

[…] the only way he could get other programs (Mosflm, Adxv) to work with the imgCIF format was to invert ELEMENT_Y, it was pointing along -1 0 0 in our original implementation. Certainly not the best solution, you would think since imgCIF was supposed to be a standard format all developers would have supported it as is. [...] we are willing to go back to the proper definition of ELEMENT_Y.
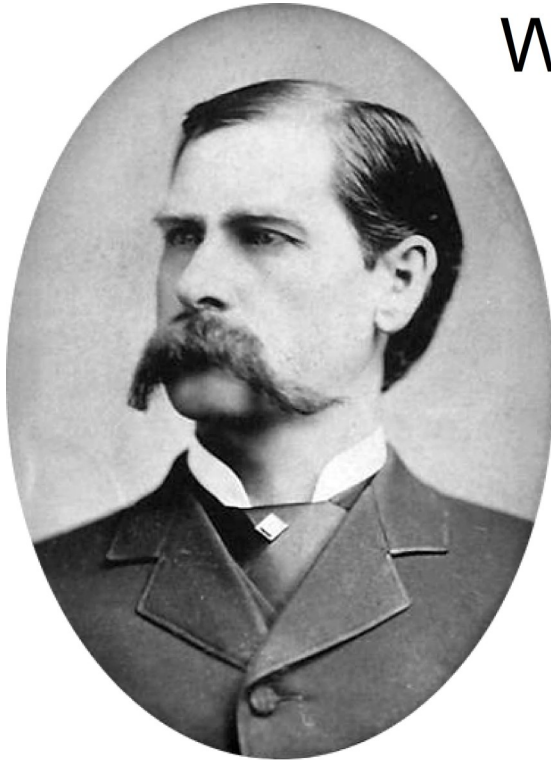
detector → **standard** → **meta-data**

software →

- Dirk Reinert (Boehringer-Ingelheim)

- Matt Benning, Jörg Kärcher (Bruker)

- Herb Bernstein

http://www.globalphasing.com/autoproc/wiki/index.cgi?DataProcessingHdf5
http://www.globalphasing.com/autoproc/wiki/index.cgi?BeamlineSettings

"**Fast is fine, but accuracy is final.**"

Wyatt Earp (1848-1929)

"**If everything seems under control, you're not going fast enough.**"

Mario Andretti (1940-)