



*High Data-Rate Macromolecular Crystallography
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Contributions to Metadata Discussion

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Introduction

It is a long standing practice in MX to use a wide variety of data and metadata formats. As we move to higher data rates and multimodal experiments combining data from multiple institutions, and demands for longer term archiving are being imposed to support more accurate journal referring and to facilitate reprocessing of data from archives, more common agreement in metadata would be very helpful.

NIAC and COMCIFS have been working since 2012 on interoperation of NeXus and CIF formats and metadata. DECTRIS has adopted NeXus/HDF5 for the Eiger.

Now, in order to achieve maximal interoperability and maximal range of processing options, it would be helpful to agree on a minimal set of metadata that would be available for all MX images.



Current Metadata Practices

Some applications do not require any metadata with images and draw their metadata from separate control files.

Some applications require metadata just sufficient to process the data as a single axis rotation experiment or as stills, e.g. using a small set of minicbf or equivalent set of NeXus tags:

```
# Detector: Dectris Eiger 16M, S/N E-32-0101
# Pixel_size 75e-6 m x 75e-6 m
# Silicon sensor, thickness 0.450000 m
# Exposure_time 0.049990 s
# Exposure_period 0.050000 s
# Count_cutoff 125019 counts
# Wavelength 0.978943 A
# Detector_distance 0.180001 m
# Beam_xy (2012, 2420) pixels
# Start_angle 0.800000 deg.
# Angle_increment 0.100000 deg.
```

Some applications require much more complete metadata, especially to describe complex axis configurations.



New Opportunity with Eiger Data

The adoption of NeXus for the Eiger presents us with a new opportunity to avoid some of the difficulties over the past decade with multiple approaches to the metadata issue. The Eiger NeXus/HDF5 master file is a container into which different metadata sources can pour what useful information they may have.

The DECTRIS hardware and software can provide the initial framework of metadata known to it and store that in the master file.

The beamline controls software can merge additional metadata known to the beamline into the master file, without having to rewrite the master file.

Users and archives can continue the process of annotating the collection without the need for rewrites of files.

Each application can then use as much or as little metadata as it needs.



Where to Find Useful HDRMX Metadata

See <http://www.hdrmx.medsbio.org/> at the Eiger Data Tags tab

Eiger Data Tags

- In this space we will be providing information on the data and metadata tags used in handling Eiger images. There is a gradually evolving set of documents available on the Dectris website www.dectris.com. Dectris given permission for us to consolidate and summarize some of that information here for convenience. This is a work in progress. [\[more/less ...\]](#)

This is a table of the Dectris Software Releases of "EIGER Detector HDF5 NeXus Format" through release 1.3.0. Partial information from the NeXus NXmx application definition has been added. You may sort on by clicking on the heading. Please report comments and corrections to the [hdrmx-bb](#) list.

Version	NeXus Path	Name	Type	Units	Description	Full CBF	mini CE
< 1.2.0	/(entry):NXentry /(instrument):NXinstrument /(beam):NXbeam/wavelength	wavelength	NX_FLOAT	A	wavelength of the beam in the case of monochromatic beam	_diffn_radiation_wavelength.wavelength 0.7085	Wavelength 0.7085 A
< 1.2.0	/(entry):NXentry /(instrument):NXinstrument /(detector):NXdetector/geometry /orientation	orientation	NX_FLOAT		To be described by Dectris		
< 1.2.0	/(entry):NXentry /(instrument):NXinstrument /(detector):NXdetector/geometry /translation	translation	NX_FLOAT		To be described by Dectris		
≥ 1.2.0	/(entry):NXentry /(instrument):NXinstrument /(beam):NXbeam /incident_wavelength	incident_wavelength	NX_FLOAT	A	Wavelength of the beam in the case of monochromatic beam	_diffn_radiation_wavelength.wavelength	Wavelength
	/(entry):NXentry	beam_center_x	NX_FLOAT		Beam center in x in pixels.	_diffn_detector_element.reference_center_fast	Beam_x

See

<http://download.nexusformat.org/sphinx/classes/applications/NXmx.html>

and especially

http://download.nexusformat.org/sphinx/classes/base_classes/NXtransformations.html

Think about what is there and what else is needed for **your** experiments.

