

MxCuBE Workshop

Soleil, 2012

MAX IV lab status

MAX-lab status

PX Beamlines

BL i911-2

- ◆ Single wavelength
- ◆ Omega rotation

BL i911-3

- ◆ Tuneable
- ◆ MD2 minikappa geometry
- ◆ EDNA pipeline
- ◆ STAC
- ◆ MxCube

MAX-lab status

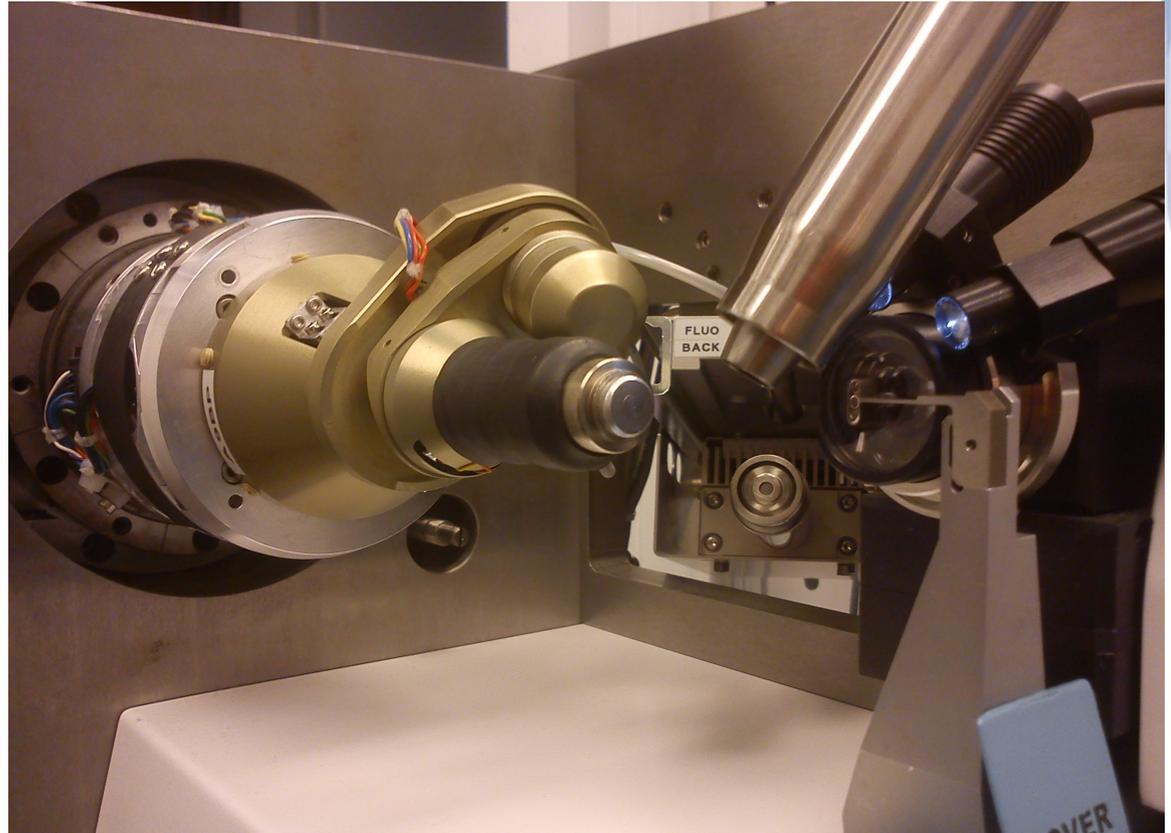
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MAX-lab status

CATS

The screenshot displays the GUI CATS software interface. At the top, the window title is "GUI CATS". The interface is divided into several sections:

- Lid n°1, Lid n°2, Lid n°3:** Each lid section shows "Cassette Standard" and "Spine" status.
- Barcode:** Radio buttons for "Yes" and "No", with "No" selected.
- Actions:** Buttons for "Mount", "Unmount", "Exchange", "Safe", and "Dry Gripper".
- Samples:** Three grids for samples A, B, and C, each with 10 positions (1-10).
- Power:** A red power indicator light and buttons for "ON" and "OFF".
- Control Buttons:** "ABORT", "PANIC", "PAUSE", "RESET ERROR", and "RESUME".
- Command Return:** A text area showing "Unknown" and "OK" button.
- Status/Message:** A text area showing "Auto mode : Yes", "Default : Yes", "Tool : EMBL", "Path name :", "Barcode :", and "Message/Error : doors opened".
- Navigation:** "<< Manual Commands" and "Show/Hide IO" buttons.
- Logo:** "IRELEC" logo at the bottom right.

MAX-lab status

MxCube – Data Collection With EDNA

File Instrumentation Help Expert mode

Hutch Collect Absorption Edge Scan XRF Analysis Element Analysis Beamline Administration

Resolution: _____ Energy: _____
 Current: _____ Energy: _____
 Move to: _____ Å

Wavelength: _____

Parameters Queue EDNA/RADDOSE

Data Collection Parameters

EDNA/RADDOSE

Characterisation: 2 Images

Run N: _____ 1

Prefix: 2 Images prefix _____

Range: _____ +1.00

Exposure: _____ 1.0

Flux: _____ ph/s 100000000000.0

Sample: _____

Dimension: _____ mm: _____ 0.1

z, mm: _____ 0.1

Radiation: _____ 1.0

Diffraction Plan

Account for Radiation Damage: of average protein Crystal

Anomalous: _____

Induce Burn Strategy: _____

Force Space Group: _____ Group

Strategy Complexity: single subwedge

Maximum exposure time per data collection Time(secs): 15000.0

Aimed I over Sigma at highest Resolution: _____ 3.0

Define Aimed Resolution (default - highest possible): _____ Angstroms 3.0

Define Aimed Completeness (default >= 0.99): _____ (0.0-0.99) 0.99

Define Aimed Multiplicity (default - optimized) : _____ 4.0

Collect and Characterise

Characterise with existing images

Directory: _____ Browse

Characterise: _____ Template: _____

Collect and Characterise

Elapsed: 00:00:00 Remaining: 00:00:00

Max-status

MAX current 0

911 Wiggler 2.502

No beam

Free disk space

Collect stage

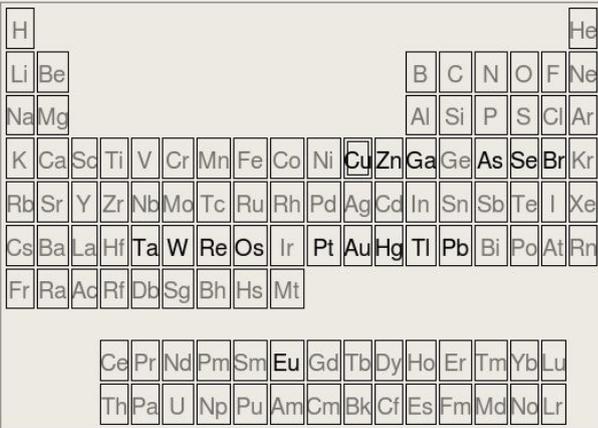
1. Preparing beamline
2. Mounting sample
3. Centring sample
4. Collecting images

MAX-lab status

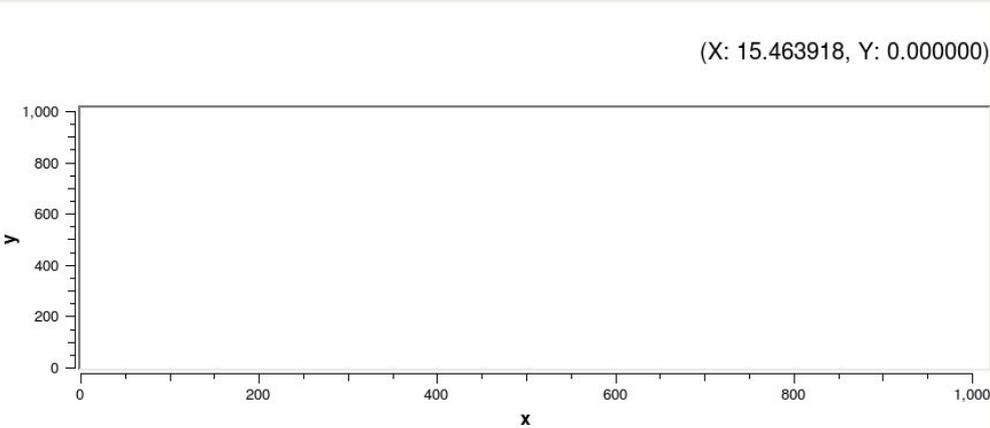
MxCube - Element Absorption Edge Scan

File Instrumentation Help Expert mode

Hutch Collect Absorption Edge Scan XRF Analysis Element Analysis Beamline Administration



Periodic table of elements with Copper (Cu) highlighted in the 11th period, 10th group.



Graph showing X and Y coordinates. X-axis ranges from 0 to 1,000. Y-axis ranges from 0 to 1,000. Current coordinates: (X: 15.463918, Y: 0.000000).

Max-status

MAX current 191.3

911 Wiggler 2.209

Injection

Free disk space

Collect stage

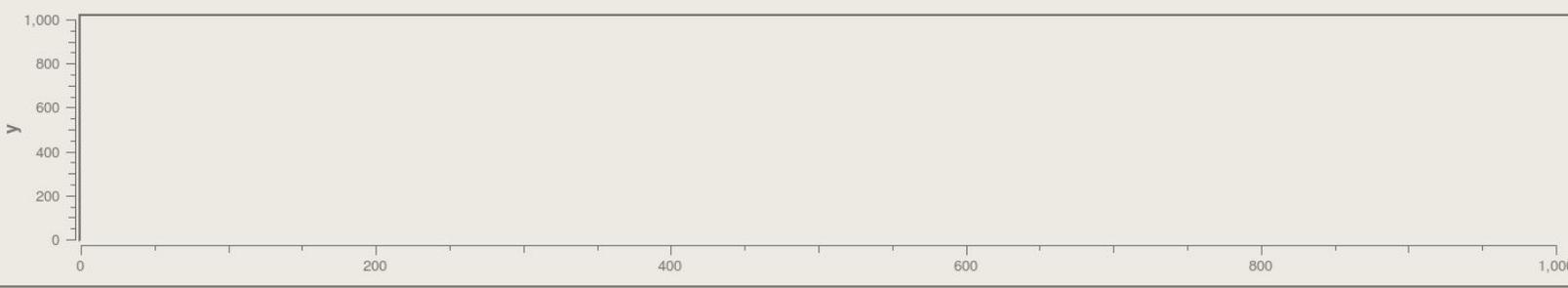
1. Preparing beamline
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Parameters

Prefix: Directory: Browse

Energy scan

Start scan (no element) Peak: (keV) Inflection: (keV) Remote: (keV) 2nd Remote: (keV) ✓ Accept
✗ Reset

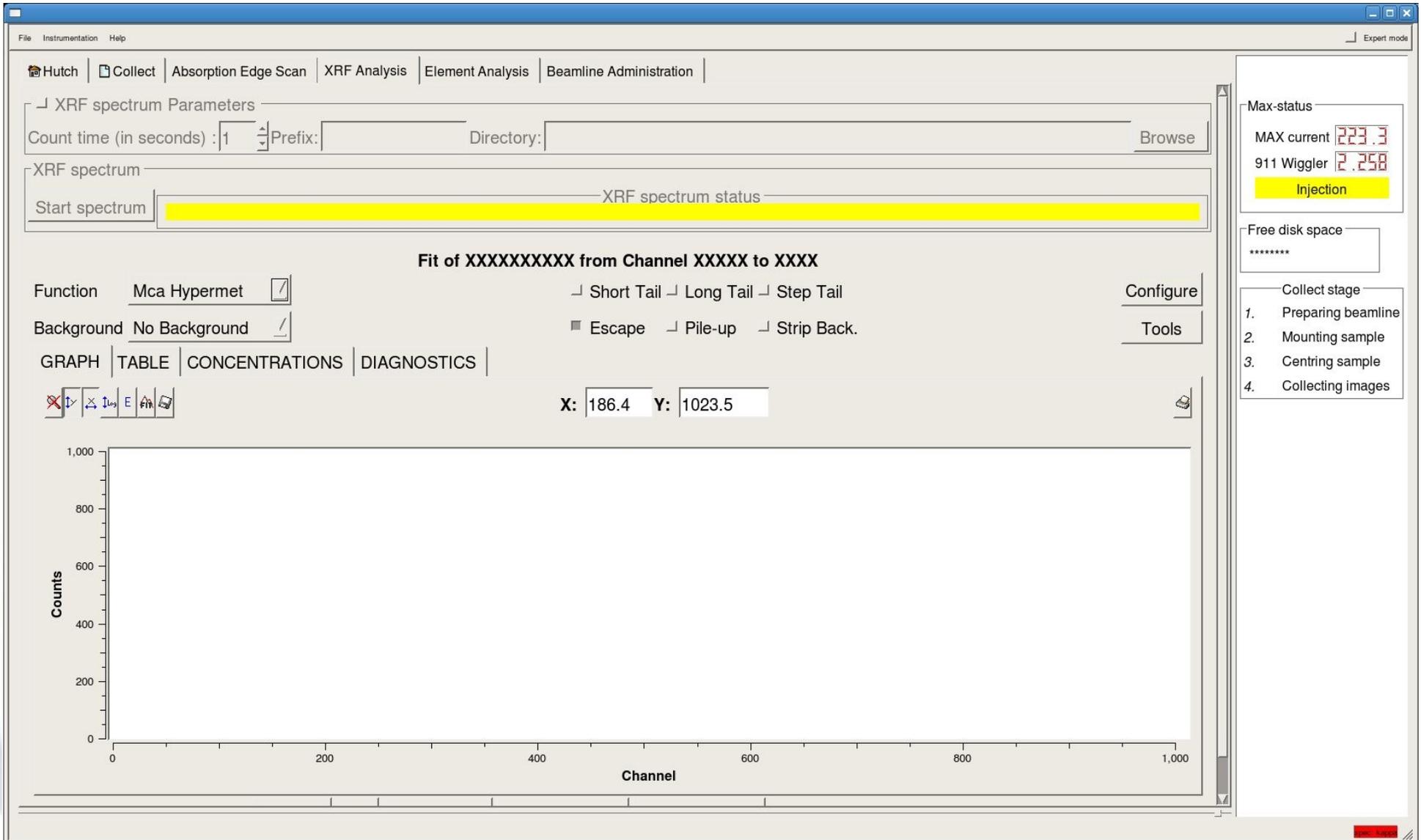


Graph showing X and Y coordinates. X-axis ranges from 0 to 1,000. Y-axis ranges from 0 to 1,000.

MAX-lab

MAX-lab status

MxCube – Fluorescence scan (ESRF)



MAX-lab status

MxCube – Fluorescence Scan (Simplified)

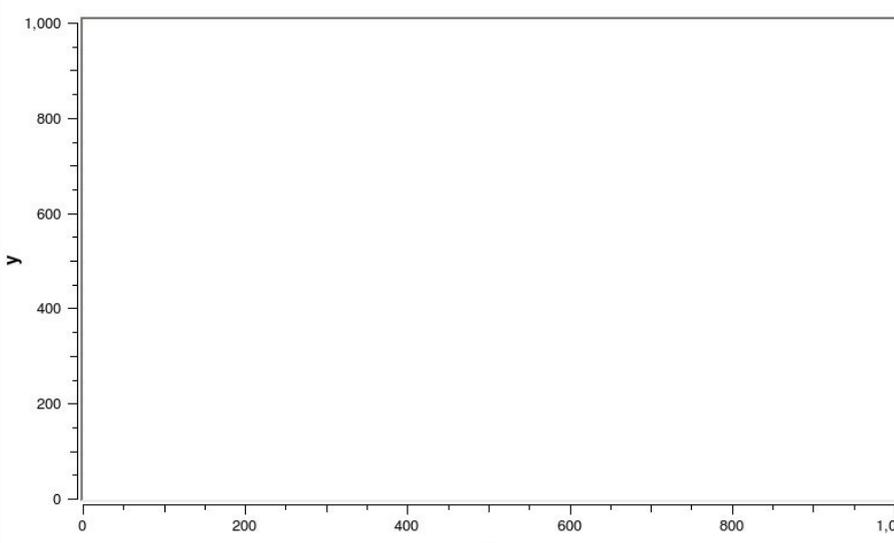
File Instrumentation Help Expert mode

Hutch Collect Absorption Edge Scan XRF Analysis **Element Analysis** Beamline Administration

Element Analysis

(X: 873.937677, Y: 608.695652)

Element	Edge	Energy (keV)



Graph settings

log Y Auto scale Reset scale

Scan parameters

ROI (keV) min/max: / Time (s):

Fluorescence detector:

Start scan: Start

Help Print

Scan files

Max-status

MAX current 243.3

911 Wiggler 2.258

Injection

Free disk space

Collect stage

1. Preparing beamline
2. Mounting sample
3. Centring sample
4. Collecting images

STOP

MAX-lab status

MxCube – Near Future @ MAX IV lab

Include new features:

- MESH scan
- Spiral data collection
- CATS GUI
- MAX IV lab specific features
- ISPyB

Follow updates:

- Data collection strategies, Kappa strategies
- Data processing

MxCube to bli911-2

- Common EDNA pipeline

MAX-lab status

MxCube – Near Future @ MAX IV lab

To be continued...

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MAX-lab status

MxCube

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