3.3.2.26. NXxas

SMR 2025-08-14, include notes for mapping to CDIF schema.org. See proposed NXxas update in 3.3.2.27. NXxas\_new

Downloaded from https://manual.nexusformat.org/classes/applications/NXxas.html

# **Status**:

application definition, extends [NXobject](https://manual.nexusformat.org/classes/base_classes/NXobject.html#nxobject)

# **Description**:

This is an application definition for raw data from an X-ray absorption spectroscopy experiment. This is essentially a scan on energy versus incoming/ absorbed beam.

# **Symbols**:

The symbol(s) listed here will be used below to coordinate datasets with the same shape.

**nP**: Number of points

# **Groups cited**:

[NXdata](https://manual.nexusformat.org/classes/base_classes/NXdata.html#nxdata), [NXdetector](https://manual.nexusformat.org/classes/base_classes/NXdetector.html#nxdetector), [NXentry](https://manual.nexusformat.org/classes/base_classes/NXentry.html#nxentry), [NXinstrument](https://manual.nexusformat.org/classes/base_classes/NXinstrument.html#nxinstrument), [NXmonitor](https://manual.nexusformat.org/classes/base_classes/NXmonitor.html#nxmonitor), [NXmonochromator](https://manual.nexusformat.org/classes/base_classes/NXmonochromator.html#nxmonochromator), [NXsample](https://manual.nexusformat.org/classes/base_classes/NXsample.html#nxsample), [NXsource](https://manual.nexusformat.org/classes/base_classes/NXsource.html#nxsource)

# **Structure**:

## ENTRY:

(required) [NXentry](https://manual.nexusformat.org/classes/base_classes/NXentry.html#nxentry)

### **@entry**:

(required) [NX\_CHAR](https://manual.nexusformat.org/nxdl-types.html#nx-char)

NeXus convention is to use “entry1”, “entry2”, … for analysis software to locate each entry.

Use this to create @id for the JSON-LD

### **title**:

(required) [NX\_CHAR](https://manual.nexusformat.org/nxdl-types.html#nx-char) [⤆](https://manual.nexusformat.org/classes/base_classes/NXentry.html#nxentry-title-field)

schema:name

### **start\_time**:

(required) [NX\_DATE\_TIME](https://manual.nexusformat.org/nxdl-types.html#nx-date-time) [⤆](https://manual.nexusformat.org/classes/base_classes/NXentry.html#nxentry-start-time-field)

prov:wasGeneratedBy: {

"@type": ["Event","nx:analysisEvent" ],

schema:startDate

### **definition**:

(required) [NX\_CHAR](https://manual.nexusformat.org/nxdl-types.html#nx-char) [⤆](https://manual.nexusformat.org/classes/base_classes/NXentry.html#nxentry-definition-field)

Official NeXus NXDL schema to which this file conforms

Obligatory value: **NXxas**

schema:additionalType

## **INSTRUMENT**: (required) [NXinstrument](https://manual.nexusformat.org/classes/base_classes/NXinstrument.html#nxinstrument) [⤆](https://manual.nexusformat.org/classes/base_classes/NXentry.html#nxentry-instrument-group)

Instrument is represented as an array, either with one single instrument description, or a list of components.

prov:wasGeneratedBy: {

"@type": ["Event","nx:analysisEvent" ],

nx:instrument {"@type","Thing", "schema:additionalType": use to type components of the instrument…}

### **source**: (required) [NXsource](https://manual.nexusformat.org/classes/base_classes/NXsource.html#nxsource) [⤆](https://manual.nexusformat.org/classes/base_classes/NXinstrument.html#nxinstrument-source-group)

An instrument component

nx:instrument: [{ "schema:additionalType": xas:Source

#### type:

(required) [NX\_CHAR](https://manual.nexusformat.org/nxdl-types.html#nx-char) [⤆](https://manual.nexusformat.org/classes/base_classes/NXsource.html#nxsource-type-field)

nx:instrument: [ {

"schema:additionalType": xas:Source: {

"schema:additionalProperty": [

{ "schema:propertyID": "xas:type",

"schema:value": … } … }

#### name:

(required) [NX\_CHAR](https://manual.nexusformat.org/nxdl-types.html#nx-char) [⤆](https://manual.nexusformat.org/classes/base_classes/NXsource.html#nxsource-name-field)

nx:instrument: [ {

"schema:additionalType": xas:Source: {

"schema:name": … }

#### probe:

(required) [NX\_CHAR](https://manual.nexusformat.org/nxdl-types.html#nx-char) [⤆](https://manual.nexusformat.org/classes/base_classes/NXsource.html#nxsource-probe-field)

Obligatory value: **x-ray**

nx:instrument: [ {

"schema:additionalType": xas:Source: {

"schema:additionalProperty": [

{ "schema:propertyID": "xas:probe",

"schema:value": "x-ray" } … }

### **monochromator**:

**An instrument component**

(required) [NXmonochromator](https://manual.nexusformat.org/classes/base_classes/NXmonochromator.html#nxmonochromator) [⤆](https://manual.nexusformat.org/classes/base_classes/NXinstrument.html#nxinstrument-monochromator-group)

#### energy:

(required) [NX\_FLOAT](https://manual.nexusformat.org/nxdl-types.html#nx-float) (Rank: 1, Dimensions: [nP]) [⤆](https://manual.nexusformat.org/classes/base_classes/NXmonochromator.html#nxmonochromator-energy-field)

This is a dimension, instance variable is monochromator/energy; the energy of the incident beam directed at the sample in eV (???)

"schema:variableMeasured": [ {

"@type": [ "InstanceVariable", "schema:PropertyValue" ],

"schema:name": " monochromator.energy "

schema:alternateName

schema:unitText

Rank and dimension[nP] should be in component description.

cdi:physicalDataType

cdi:name

cdi:displayLabel

cdi:simpleUnitOfMeasure

### **incoming\_beam**:

(required) [NXdetector](https://manual.nexusformat.org/classes/base_classes/NXdetector.html#nxdetector) [⤆](https://manual.nexusformat.org/classes/base_classes/NXinstrument.html#nxinstrument-detector-group)

#### data:

(required) [NX\_NUMBER](https://manual.nexusformat.org/nxdl-types.html#nx-number) (Rank: 1, Dimensions: [nP]) [⤆](https://manual.nexusformat.org/classes/base_classes/NXdetector.html#nxdetector-data-field)

This is a dimension, instance variable is incoming\_beam; counts at the monitor fo the incident beam (????)

"schema:variableMeasured": [ {

"@type": [ "InstanceVariable", "schema:PropertyValue" ],

"schema:name": "incoming\_beam"

Rank and dimension[nP] should be in component description.

schema:alternateName

schema:unitText: counts

cdi:physicalDataType : positive integer?

cdi:name

cdi:displayLabel

cdi:simpleUnitOfMeasure count

### **absorbed\_beam**: (required) [NXdetector](https://manual.nexusformat.org/classes/base_classes/NXdetector.html#nxdetector) [⤆](https://manual.nexusformat.org/classes/base_classes/NXinstrument.html#nxinstrument-detector-group)

#### data:

(required) [NX\_NUMBER](https://manual.nexusformat.org/nxdl-types.html#nx-number) (Rank: 1, Dimensions: [nP]) [⤆](https://manual.nexusformat.org/classes/base_classes/NXdetector.html#nxdetector-data-field)

This data corresponds to the sample signal.

This is a dimension, instance variable is absorbed\_beam; counts at the detector for the x-ray passing through sample (????)

"schema:variableMeasured": [ {

"@type": [ "InstanceVariable", "schema:PropertyValue" ],

"schema:name": "absorbed\_beam"

Rank and dimension[nP] should be in component description.

schema:alternateName

schema:unitText: counts

cdi:physicalDataType : positive integer?

cdi:name

cdi:displayLabel

cdi:simpleUnitOfMeasure count

### **SAMPLE**: (required) [NXsample](https://manual.nexusformat.org/classes/base_classes/NXsample.html#nxsample) [⤆](https://manual.nexusformat.org/classes/base_classes/NXentry.html#nxentry-sample-group)

#### name:

(required) [NX\_CHAR](https://manual.nexusformat.org/nxdl-types.html#nx-char) [⤆](https://manual.nexusformat.org/classes/base_classes/NXsample.html#nxsample-name-field)

Descriptive name of sample

prov: wasGeneratedBy: {

"@type": ["Event","nx:analysisEvent" ],

…..

{"schema:mainEntity": {  
 "@type": "schema:Thing",  
 "schema:additionalType": "MaterialSample",  
 "schema:name": "…",

### **MONITOR**: (required) [NXmonitor](https://manual.nexusformat.org/classes/base_classes/NXmonitor.html#nxmonitor) [⤆](https://manual.nexusformat.org/classes/base_classes/NXentry.html#nxentry-monitor-group)

#### mode:

(required) [NX\_CHAR](https://manual.nexusformat.org/nxdl-types.html#nx-char) [⤆](https://manual.nexusformat.org/classes/base_classes/NXmonitor.html#nxmonitor-mode-field)

Count to a preset value based on either clock time (timer) or received monitor counts (monitor). Any of these values: monitor | timer

"prov:wasGeneratedBy": {  
 "@type": [ "Event", "xas:analysisEvent" ],  
 "schema:additionalProperty": [  
 { "@type": "schema:PropertyValue",  
 "schema:propertyID": "monitor.mode",

"schema:value": "monitor" or "timer"

cdi:physicalDataType : string

#### preset:

(required) [NX\_FLOAT](https://manual.nexusformat.org/nxdl-types.html#nx-float)

preset value for time or monitor

"schema:additionalProperty": [  
 { "@type": "schema:PropertyValue",  
 "schema:propertyID": "monitor.preset",

"schema:value": "monitor" or "timer"

cdi:physicalDataType : float

#### data:

(required) [NX\_NUMBER](https://manual.nexusformat.org/nxdl-types.html#nx-number) (Rank: 1, Dimensions: [nP]) [⤆](https://manual.nexusformat.org/classes/base_classes/NXmonitor.html#nxmonitor-data-field)

This field could be a link to /NXentry/NXinstrument/incoming\_beam:NXdetector/data

If mode is timer, this should be the same as incoming\_beam dimension; if mode is monitor, then is should be a constant = to the preset value ??

### **DATA**: (required) [NXdata](https://manual.nexusformat.org/classes/base_classes/NXdata.html#nxdata) [⤆](https://manual.nexusformat.org/classes/base_classes/NXentry.html#nxentry-data-group)

This provides two dimensions for standard plot of data, but links to data arrays in other places..

#### mode: (required) [NX\_CHAR](https://manual.nexusformat.org/nxdl-types.html#nx-char)

Detection method used for observing the sample absorption (pick one from the enumerated list and spell exactly)

Any of these values:

* Total Electron Yield
* Partial Electron Yield
* Auger Electron Yield
* Fluorescence Yield
* Transmission

"schema:keywords": [  
 {  
 "@type": "schema:DefinedTerm",  
 "schema:name": "[term]",  
 "schema:termCode": "…",  
 "schema:identifier": "https://xas.org/vocab/detectionmode/{term}",  
 "schema:inDefinedTermSet": "https://xas.org/vocab/detectionmode "  
 },

#### energy:

[link](https://manual.nexusformat.org/design.html#design-links) (suggested target:

/NXentry/NXinstrument/monochromator:NXmonochromator/energy)

/nx:displayplot:{

nx:display\_x: "link to instance variable, or component—need path to access data"

}

#### absorbed\_beam:

[link](https://manual.nexusformat.org/design.html#design-links) (suggested target:

/NXentry/NXinstrument/absorbed\_beam:NXdetector/data)

/nx:displayplot:{

nx:display\_y: "link to instance variable"

}

See example JSON-LD for description of dimension data structure using CDI-DDI

# **Hypertext Anchors**

List of hypertext anchors for all groups, fields, attributes, and links defined in this class.

* [/NXxas/ENTRY-group](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-group)
* [/NXxas/ENTRY/DATA-group](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-data-group)
* [/NXxas/ENTRY/DATA/absorbed\_beam-link](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-data-absorbed-beam-link)
* [/NXxas/ENTRY/DATA/energy-link](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-data-energy-link)
* [/NXxas/ENTRY/DATA/mode-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-data-mode-field)
* [/NXxas/ENTRY/definition-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-definition-field)
* [/NXxas/ENTRY/INSTRUMENT-group](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-group)
* [/NXxas/ENTRY/INSTRUMENT/absorbed\_beam-group](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-absorbed-beam-group)
* [/NXxas/ENTRY/INSTRUMENT/absorbed\_beam/data-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-absorbed-beam-data-field)
* [/NXxas/ENTRY/INSTRUMENT/incoming\_beam-group](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-incoming-beam-group)
* [/NXxas/ENTRY/INSTRUMENT/incoming\_beam/data-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-incoming-beam-data-field)
* [/NXxas/ENTRY/INSTRUMENT/monochromator-group](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-monochromator-group)
* [/NXxas/ENTRY/INSTRUMENT/monochromator/energy-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-monochromator-energy-field)
* [/NXxas/ENTRY/INSTRUMENT/SOURCE-group](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-source-group)
* [/NXxas/ENTRY/INSTRUMENT/SOURCE/name-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-source-name-field)
* [/NXxas/ENTRY/INSTRUMENT/SOURCE/probe-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-source-probe-field)
* [/NXxas/ENTRY/INSTRUMENT/SOURCE/type-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-instrument-source-type-field)
* [/NXxas/ENTRY/MONITOR-group](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-monitor-group)
* [/NXxas/ENTRY/MONITOR/data-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-monitor-data-field)
* [/NXxas/ENTRY/MONITOR/mode-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-monitor-mode-field)
* [/NXxas/ENTRY/MONITOR/preset-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-monitor-preset-field)
* [/NXxas/ENTRY/SAMPLE-group](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-sample-group)
* [/NXxas/ENTRY/SAMPLE/name-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-sample-name-field)
* [/NXxas/ENTRY/start\_time-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-start-time-field)
* [/NXxas/ENTRY/title-field](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-title-field)
* [/NXxas/ENTRY@entry-attribute](https://manual.nexusformat.org/classes/applications/NXxas.html#nxxas-entry-entry-attribute)

**NXDL Source**:

<https://github.com/nexusformat/definitions/blob/main/applications/NXxas.nxdl.xml>