XDI specification

From <https://github.com/XraySpectroscopy/XAS-Data-Interchange/blob/master/specification/dictionary.md#the-dictionary> 2025-08-11

1. `Facility`: Tags related to the synchrotron or other facility at which the measurement was made

1. `Beamline`: Tags related to the structure of the beamline and its photon delivery system

1. `Mono`: Tags related to the monochromator

1. `Detector`: Tags related to the details of the photon detection system

1. `Sample`: Tags related to the details of sample preparation and measurement

1. `Scan`: Tags related to the parameters of the scan

1. `Element`: Tags related to the absorbing atom

1. `Column`: Tags used for identifying the data columns and their units

Below, specific members of these namespaces are defined. The

definitons are not exclusive. Other metadata can be placed in these

namespaces as needed. Of course, undefined metadata are unlikely to

be interpreted correctly by applications using this dictionary.

Metadata added to a defined namespace \*\*must not\*\* use a defined

tag. The defined namespaces and tags \*\*shall\*\* be interpreted

without sensitivity to case.

When defined metadata are present, the units and formatting specified

below \*\*must\*\* be observed.

## Tags

Tags are the words used to denote a specific entry in a namespace.

Tags are strings composed of a subset of the ASCII character set. All

characters \*\*must\*\* be letters (ASCII 65 through 90, `A-Z` and ASCII

97-122, `a-z`), numbers (ASCII 48-57, `0-9`), underscore (ASCII 95,

`\_`), or dash (ASCII 45, `-`).

The tag \*\*must\*\* be interpreted as case insentitive.

## **Required metadata**

Three items are essential to the interchange and successful

interpretation of XAS data. These are \*\*required\*\* for a file to be a

compliant XDI file.

\* `Element.symbol`: The element of the absorbing atom. The periodic

table is replete with examples of atoms that have absorption edges

with very similar edge energies. For example, the tabulated values

of the Cr K edge and the Ba L1 edge are both 5989 eV, while Se K

and Tl L3 are both at 12658. Without identification of the species

of the absorbing atom and of the absorption edge measured, some

data cannot cannot be unambiguously identified.

\* `Element.edge`: The absorption edge measured. See above.

\* `Mono.d\_spacing`: The d-spacing of the monochromator. It is

required to convert an abscissa represented as monochromator angle

or encoder step count into energy. Also a correction to the energy

axis of measured data, which may be required in the case of a

miscalibration due to inaccuracies in the translation from angular

position of the monochromator to energy, would need the d-spacing.

Most other metadata definitions that follow are \*\*optional\*\* for use

with XDI. Some are \*\*recommended\*\* for use with all XDI files. The

\*\*recommended\*\* metadata convey information that is of substantive

value to the interpretation of the data.

# ## Recommeneded metadata

The current list of recommended metadata, i.e. metadata which

constitutes best practice when writing any data file, is

\* `Facility.name`

\* `Facility.xray\_source`

\* `Beamline.name`

\* `Scan.start\_time`

\* `Column.1`

# ## Facility

## \* `name`

\* Description: The name of synchrotron or other X-ray facility.

This is \*\***recommended**\*\* for use in all XDI files.

\* Units: none

\* Format: string

\* CDIF: contributor/{roleName:"Facility", contributor/name:[name],@type:ResearchOrganization }

## \* `energy`

\* Description: The energy of the stored current in the storage ring. [is this a constant for a facility, or is it context for this experiment?]

\* Units: GeV, MeV

\* Format: float + units

\* CDIF XAS extension: facility.\_energy #/prov:wasGeneratedBy/schema:additionalProperty/../schema:propertyID

## \* `current`

\* Description: The amount of stored current in the storage ring at

the beginning of the scan. [is this a constant for a facility, or is it context for this experiment? NXxas has /instrument/source/facility\_ring\_current, is that the same thing?]

\* Units: mA, A

\* Format: float + units

\* CDIF XAS extension: facility.current. #/prov:wasGeneratedBy/schema:additionalProperty/../schema:propertyID

## \* `xray\_source`

\* Description: A string identifying the source of the X-rays,

such as "bend magnet", "undulator", or "rotating copper

anode". This is \*\***recommended**\*\* for use in all XDI files. [is this a constant for a facility, or is it context for this experiment?]

\* Units: none

\* Format: string

\* CDIF XAS extension: facility.xray\_source. #/prov:wasGeneratedBy/schema:location/schema:additionalProperty/1/schema:propertyID

# ## Beamline namespace

## \* `name`

\* Description: The name by which the beamline is known. This is

\*\***recommended**\*\* for use in all XDI files. For a beamline with a

facility designation and a common name (such as 13-BM-B at the

APS, also known as GSECARS), the designation is preferred.

\* Units: none

\* Format: free-format string

\* CDIF XAS extension: analysisEvent/instrument::child[additionalType = xas:Beamline]/name:{name}

## \* `collimation`

\* Description: A concise statement of how beam collimation is provided

\* Units: none

\* Format: free-format string

\* CDIF XAS extension: analysisEvent//instrument::child[additionalType = xas:Beamline]/additionalProperty::child[propertID = collimation]/value:{collimation statement}

\* CDIF XAS extension: beamline.collimation [not in NXxas]

## \* `focusing`

\* Description: A concise statement about how beam focusing is provided

\* Units: none

\* Format: free-format string

\* CDIF XAS extension: analysisEvent//instrument::child[additionalType = xas:Beamline]/additionalProperty::child[propertID = focusing]/value:{focusing statement}

\* CDIF XAS extension: beamline.focusing [not in NXxas]

## \* `harmonic\_rejection`

\* Description: A concise statement about how harmonic rejection is accomplished

\* Units: none

\* Format: free-format string

\* CDIF XAS extension: analysisEvent//instrument::child[additionalType = xas:Beamline]/additionalProperty::child[propertID = harmonic\_rejection]/value:{statement}

\* CDIF XAS extension: beamline.harmonic\_rejection

# ## Mono namespace

CDIF XAS extension: analysisEvent//instrument::child[additionalType = xas:Monochromator]

## \* `name`

\* Description: A string identifying the material and diffracting

plane or grating spacing of the monochromator. Example data has

‘Si 111’

\* Units: none

\* Format: free-format string

\* CDIF XAS extension: …/name:””

\* CDIF XAS extension: mono.name

\* NXxas separates Element and Reflector; reflector is a array dim[3].

## \* `d\_spacing`

\* Description: The known d-spacing of the monochromator under

operating conditions. This is a \*\***required**\*\* parameter for use

with XDI when data are specified as a function of angle or step

count.

\* Units: &Aring;

\* Format: float

\* CDIF XAS extension: additionalProperty/child::[propertyID = d\_spacing]/value:{d\_spacing}

\* CDIF XAS extension: mono.d\_spacing

# ## Detector namespace

## \* `i0`

\* Description: A description of how the incident flux was measured.

Values in example data are ‘10cm N2’

\* Units: none

\* Format: free-format string

\* "xas:instrument": [{

"@type": "schema:Thing",  
 "schema:additionalType": "xas:Detector",

"schema:additionalProperty": [ {  
 "@type": "schema:PropertyValue",  
 "schema:propertyID": "xas:FluxMeasureMethod",  
 "schema:name": "i0", ….

\* NXxas might be NXdetector/type ?.

## \* `it`

\* Description: A description of how the tranmission flux was

measured

\* Units: none

\* Format: free-format string

\* … see above

## \* `if`

\* Description: A description of how the fluorescence flux was

measured

\* Units: none

\* Format: free-format string

\* … see above

## \* `ir`

\* Description: A description of how the reference flux was

measured

\* Units: none

\* Format: free-format string

\* … see above

# ## Sample namespace

## \* `name`

\* Description: A string identifying the measured sample

\* Units: none

\* Format: free-format string

\* CDIF: schema.org: {mainEntity/@type:Thing,additionalType:’MaterialSample’, title:[name].

\* CDIF XAS extension: sample.name

## \* `id`

\* Description: A number or string uniquely identifying the

measured sample. This is intended for interoperation with a

database or laboratory management software. It could be, for

example, a bar code number.

\* Units: none

\* Format: free-format string

\* CDIF: schema.org: {mainEntity/@type:Thing,additionalType:’MaterialSample’, identifier:[id] }.

\* CDIF XAS extension: sample.id

## \* `stoichiometry`

\* Description: The stoichiometric formula of the measured sample

\* Units: none

\* Format: see [the IUCr definition of chemical\_formula](http://www.iucr.org/\_\_data/iucr/cifdic\_html/1/cif\_core.dic/Cchemical\_formula.html)

\* CDIF XAS extension:: schema.org: {mainEntity/@type:Thing,additionalType:’MaterialSample’,xas:stoichiometry:[stoichiometry]}.

\* CDIF XAS extension: sample.stoichiometry

## \* `prep`

\* Description: A string summarizing the method of sample preparation

\* Units: none

\* Format: free-format string

\* CDIF XAS extension:: schema.org: {mainEntity/@type:Thing,additionalType:’MaterialSample’,xas:sample.prep:[prep]}.

\* CDIF XAS extension: sample.prep

## \* `experimenters`

\* Description: The names of the experimenters present for the measurement

\* Units: none

\* Format: free-format string

\* CDIF XAS extension:: schema.org: {creator:[@type:Person, name:””….]}. ?use role with role=experimenter?]

\* CDIF XAS extension: experimenters:[“”,””,….]

## \* `temperature`

\* Description: The temperature at which the sample was measured

\* Units: degrees K, degrees C

\* Format: float + units

\* CDIF XAS extension:: analysisEvent:{temperature:””,….}

\* CDIF XAS extension: sample.temperature

## Other properties

The Sample namespace is rather open-ended. It is probably impossible

to anticipate all the kinds of sample-related metadata that may be

useful to attach to data. That said, it would be useful to suggest

tags for a number of common kinds of extrinsic parameters along the

line of `Sample.temperature`. These may be added as defined fields in

future versions of the XDI specification.

Pattern, for each of these properties:

\* CDIF XAS extension:: analysisEvent:{-property-:””,….}

\* CDIF XAS extension: sample.-property-

\* `Sample.pressure`

\* `Sample.ph`

\* `Sample.eh`

\* `Sample.volume`

\* `Sample.porosity`

\* `Sample.density`

\* `Sample.concentration`

\* `Sample.resistivity`

\* `Sample.viscosity`

\* `Sample.electric\_field`

\* `Sample.magnetic\_field`

\* `Sample.magnetic\_moment`

\* `Sample.crystal\_structure`

\* `Sample.opacity`

\* `Sample.electrochemical\_potential`

Many of these examples would take a float+units as values.

# ## Scan namespace

## \* `start\_time`

\* Description: The beginning time of the scan. This is \*\***recommended**\*\* for use with XDI.

\* Units: time

\* Format: [ISO 8601 specification for combined dates and times](http://en.wikipedia.org/wiki/ISO\_8601#Combined\_date\_and\_time\_representations)

\* CDIF XAS extension:: analysisEvent:{startDate:””,….}

## \* `end\_time`

\* Description: The ending time of the scan.

\* Units: time

\* Format: [ISO 8601 specification for combined dates and times](http://en.wikipedia.org/wiki/ISO\_8601#Combined\_date\_and\_time\_representations)

\* CDIF XAS extension:: analysisEvent:{endDate:””,….}

## \* `edge\_energy`

\* Description: The absorption edge as used in the data acquisition software. [is this the observation result, or a configuration parameter set a priori?]

\* Units: eV (\*\***recommended**\*\*), keV, inverse &Aring;

\* Format: float + units

\* CDIF XAS extension:: analysisEvent:{additionalProperty:{@type:PropertyValue, propertyID:edge\_energy, value:””}

This is the appropriate namespace for any parameters associated with

scan parameters, such as integration times, monochromator speed, scan

boundaries, or step sizes.

An example of a combined date and time representation is

`2007-04-05T14:30:22`, which means 22 seconds after 2:30 in the

afternoon on the day of April 5th in the year 2007.

# ## Element namespace

## \* `symbol`

\* Description: The measured absorption edge. This is a

\*\***required**\*\* parameter for use with XDI.

\* Units: none

\* Format: one of these 118 1, 2, or 3 character strings for the standard atomic symbols (not case sensitive):

H He Li Be B C N O F Ne Na Mg Al Si P S

Cl Ar K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge

As Se Br Kr Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd

In Sn Sb Te I Xe Cs Ba La Ce Pr Nd Pm Sm Eu Gd

Tb Dy Ho Er Tm Yb Lu Hf Ta W Re Os Ir Pt Au Hg

Tl Pb Bi Po At Rn Fr Ra Ac Th Pa U Np Pu Am Cm

Bk Cf Es Fm Md No Lr Rf Db Sg Bh Hs Mt Ds Rg Cn

Uut Fl Uup Lv Uus Uuo

See [Wikipedia's list of element symbols](http://en.wikipedia.org/wiki/Symbol\_%28chemical\_element%29).

## \* `edge`

\* Description: The measured absorption edge. This is a

\*\***required**\*\* parameter for use with XDI.

\* Units: none

\* Format: one of these 28 1 or 2 character strings (not case sensitive):

K L L1 L2 L3 M M1 M2 M3 M4 M5

N N1 N2 N3 N4 N5 N6 N7 O O1 O2 O3 O4 O5 O6 O7

See table 10.10 at

[IUPAC notation for X-ray absorption edges](http://old.iupac.org/publications/analytical\_compendium/Cha10sec348.pdf)for further explanation. The use of the generic edges \_L\_, \_M\_, \_N\_, and \_O\_ is \*\*not recommended\*\*, but \*\*may\*\* be used for spectra spanning multiple edges.

## \* `reference`

\* Description: The absorption edge of the reference spectrum. This is a \*\*recommended\*\* parameter for use in an XDI file containing a reference spectrum.

\* Units: none

\* Format: same as `Element.symbol`

## \* `ref\_edge`

\* Description: The measured edge of the reference spectrum. This

is a \*\***recommended**\*\* parameter for use in an XDI file containing a

reference spectrum.

\* Units: none

\* Format: same as `Element.edge`

# ## Column namespace

**The data are described as DDI-CDI Wide data. For CDIF Discovery they would need to be also described as variableMeasured.**

Items in the Column namespace describe single columns of the data

table. The first column \*\***must**\*\* be the energy.

All tags in the `Column` namespace \*\*must\*\* be integers.

\* \*\*Namespace:\*\* `Column` -- \*\*Tag:\*\* `1`

\* Description: A description of the abscissa array for the measured

data. This is \*\***recommended**\*\* for use in an XDI file.

\* Units: eV (\*\***recommended**\*\*), keV, pixel, angle in degrees, angle in radians, steps

\* Format: word + units

\* \*\*Namespace:\*\* `Column` -- \*\*Tag:\*\* `N`

\* Description: A description of the Nth column (where `N` is an

integer) of the measured data. This is \*\*recommended\*\* for use

in an XDI file.

\* Units: as needed

\* Format: word (+ units)

The following labels are defined for common array types. `Column.N`

items \*\***must**\*\* use these labels when appropriate. The array label

line at the beginning of the data section of the XDI file also

\*\***must**\*\* use these labels when those columns are present.

**These would all be in schema:variableMeasured typed as both cdi:instanceVariable and schema:PropertyValue**

|  |  |  |
| --- | --- | --- |
| **Column label** | **Meaning** | **choice of units** |
| **cdi:name and schema:name** | **schema:alternateName** | **schama:unitText and cdi:simpleUnitOfMeasure** |
| energy | mono energy | eV / keV / pixel |
| angle | mono angle | degrees / radians / steps |
| i0 | monitor intensity |  |
| itrans | transmission intensity |  |
| ifluor | fluorescence intensity |  |
| irefer | reference intensity |  |
| mutrans | mu transmission |  |
| mufluor | mu fluorescence |  |
| murefer | mu reference |  |
| normtrans | normalized mu transmission |  |
| normfluor | normalized mu fluorescence |  |
| normrefer | normalized mu reference |  |
| k | wavenumber |  |
| chi | EXAFS |  |
| chi\_mag | magnitude of Filtered chi(k) |  |
| chi\_pha | phase of Filtered chi(k) |  |
| chi\_re | real part of Filtered chi(k) |  |
| chi\_im | imaginary part of Filtered chi(k) |  |
| r | radial distance |  |
| chir\_mag | magnitude of FT[chi(k)] |  |
| chir\_pha | phase of FT[chi(k)] |  |
| chir\_re | real part of FT[chi(k)] |  |
| chir\_im | imaginary part of FT[chi(k)] |  |

A column containing some other measurement \*\*must\*\* be identified with

units when appropriate. For example, a column counting time since the

`Scan.start\_time` timestamp might be labeled as

# Column.N: elapsed\_time seconds

while a column containing an ongoing measure of temperature as a

voltage on a themocouple might be labeled as

# Column.N: thermocouple millivolts

## Extension fields

Metadata tags carry syntax and may carry semantics. That is, it is

possible to have syntactically correct tags that have no definition.

Such tags could carry information considered useful by the user or the

author of software that, at some point, touches the data.

Such a tag could be an extension within an existing namespace. This

has already been discussed in the context of the `Sample` and `Scan`

namespaces.

Such a tag could also be part of a new namespace. One application of

a new namespace would be to tie a group of metadata tags to a

particular application. For example, the data processing program

Athena might attach tags associated with the parameters for

normalizing the data. That might look something like this:

# Athena.pre1: -150

# Athena.pre2: -30

# Athena.nor1: 150

# Athena.nor2: 800

These define the boundaries of the pre- and post-edge lines used to

determine the edge step of the mu(E) spectrum.

The use of such extension tags is encouraged for authors of controls,

data acquisition, data analysis, and data archiving software.

If an extension tag is not understood due its lack of defined

semantics, the \*\*recommended\*\* behavior for software touching

the data is to silently preserve the metadata.