

Dictionary of XAS Data Interchange Metadata

XDI Working Group

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1 Overview

This is **version 1.0** of the dictionary of metadata to be used with the XAS Data Interchange (XDI) format. Each item definition includes:

1. The name representing the datum
2. The meaning of the datum
3. Thw units of the datum
4. The format for representing its value

Words used to signify the requirements in the specification **shall** follow the practice of [RFC 2119](#).

A use of this dictionary is not compliant if it fails to satisfy one or more of the **must** or **required** level requirements presented herein.

1.1 The meaning of metadata

The purpose of this dictionary is to identify a set of metadata to be encoded in the specification of the *XDI* format and to assign names to each meaningful concept. This effort must take a broad view, capturing metadata concepts as broadly as they are used in the community. This effort must also be open ended in that there must be a mechanism for providing new forms of metadata not considered up front. This effort is intended to serve as the XAS metadata dictionary for other data format types, for instance a database format for libraries of XAS spectra or a hierarchical format for multi-spectral datasets.

1.2 The *XDI* syntax

This dictionary has been developed along with the [*XDI* specification](#). All examples given in this dictionary use all recommendations of the *XDI* syntax. The metadata name consists of the capitalized namespace, followed by a dot, followed by a tag. Here is an example: `Element.symbol`. When appearing in an *XDI* file to convey a metadata value, the line begins with a comment token and end with an end-of-line token. A colon is the delimiting token between the metadata name and its value. Here is an example:

```
# Element.symbol: Cu
```

1.3 The format of the value

Some of the tags in this dictionary have formatted values as part of their definitions.

- *string*: A string is specifically an ASCII string representable by characters in the the lower 128 of the ASCII set. This **must** the English-language representation of the value. For example, the string representing `Facility.name` for the Thai synchrotron **must** be `SLRI` rather than a sequence of characters in the Thai script.

- *free-format string*: This is a string which can contain any character (save end-of-line characters) in any encoding system. A free-format string need not be ASCII and need not be English. Because applications using *XDI* may not be capable of handling some encoding systems, it is **recommended** that free-format strings be ASCII.
- *string + units*: This is a string as defined above, followed by white space, followed by a string denoting the units of the previous string. As an example, a value for `Column.1` might be `energy eV`, which identifies the contents of the first column in the data table as containing energy values expressed in electron volt units. The selection of possible units for a tag is given in the definition of the tag.
- *float*: A float is a string which is interpretable as a floating-point number in the C programming language. An integer is permissible. Values of `NaN`, `sNaN`, `qNaN`, `inf`, `+inf`, and `-inf` are not allowed in *XDI*. That is, a float in *XDI* **must** be a finite number. See [IEEE 754-2008](#).
- *float + units*: This is a float as defined above, followed by white space, followed by a string identifying the units of the number. For example, a value for `Sample.temperature`, which identifies the temperature at which an XAS measurement is made, might be `500 K`, identifying the temperature of the measurements in Kelvin temperature units. The selection of possible units for a tag is given in the definition of the tag.
- *chemical formulas*: `Sample.stoichiometry` is intended to represent the elemental composition of the sample. To allow interpretation of chemical formulas by computer, this field and extension fields which represent chemical information **must** use the [IUCr definition of a chemical formula](#).
- *time*: Because of the wide variability of cultural standards in the representation of time, *XDI* defines a strict standard for time stamps in *XDI* files. `Scan.start_time`, `Scan.end_time`, and any extension fields dealing in time **must** use the [ISO 8601 specification for combined dates and times](#)
- *element symbols*: `Element.symbol`, `Element.reference`, and any extension fields identifying specific elements **must** use one of the recognized 1, 2, or 3 letter symbols given in Sec. 2.10
- *edge symbols*: `Element.edge`, `Element.ref_edge`, and any extension fields identifying specific absorption edges **must** use one of the recognized 1 or 2 letter symbols given in Sec. 2.10. Note that the subscript is represented as an Arabic numeral and not as a Roman numeral.

Some additional comments:

- Locale is **not** respected when interpreting floating point numbers. The decimal mark **must** be a dot (`.`, ASCII 46). The decimal mark **must not** be a comma (`,`, ASCII 44).
- A tag which is in a defined family but which is not defined in this dictionary **must** be interpreted as have a free-format string as its value.
- A tag which is present in an *XDI* file but which has no value or only white space as its value (i.e. the colon is followed by zero or more spaces tokens then by an end-of-line token) **must** be interpreted as a zero-length string or as the value 0, as appropriate to the value type.
- Strings identifying facilities and beamlines **must** use whatever convention is in use at the beamline. In the case where a beamline is known both by a designation and a name (for example, beamline 13ID at the Advanced Photon Source is also known by its name, "GSECARS"), the designation is **recommended**.

76 2 The dictionary

77 2.1 Name spaces

78 The purpose of namespaces is to provide sensible, widely understood, semantic groupings of defined
 79 metadata tags. All tags associated with conveying information about sample preparation and the
 80 measurement environment of the sample belong in the *Sample* namespace, all tags associated with
 81 the configuration of the beamline optics belong in the *Beamline* namespace, and so on.

82 Namespaces are strings composed of a subset of the ASCII character set. The first character **must**
 83 be a letter. The remaining characters **must** be letters, numbers, underscores, or dashes. Letters are
 84 ASCII 65 through 90 (`A-Z`) and ASCII 97-122 (`a-z`). Numbers are ASCII 48-57 (`0-9`). Underscore
 85 (`_`) is ASCII 95 and dash (`-`) is ASCII 45. The namespace **must** be interpreted as case insensitive.

86 Here is a list of all defined semantic groupings:

- 87 1. `Facility`: Tags related to the synchrotron or other facility at which the measurement was
 made
- 88 2. `Beamline`: Tags related to the structure of the beamline and its photon delivery system
- 89 3. `Mono`: Tags related to the monochromator
- 90 4. `Detector`: Tags related to the details of the photon detection system
- 91 5. `Sample`: Tags related to the details of sample preparation and measurement
- 92 6. `Scan`: Tags related to the parameters of the scan
- 93 7. `Element`: Tags related to the absorbing atom
- 94 8. `Column`: Tags used for identifying the data columns and their units

96 Below, specific members of these namespaces are defined. The definitions are not exclusive. Other
 97 metadata can be placed in these namespaces as needed. Of course, undefined metadata are un-
 98 likely to be interpreted correctly by applications using this dictionary. Metadata added to a defined
 99 namespace **must not** use a defined tag. The defined namespaces and tags **shall** be interpreted
 100 without sensitivity to case.

101 When defined metadata are present, the units and formatting specified below **must** be observed.

102 2.2 Tags

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

104 Tags are strings composed of a subset of the ASCII character set. All characters **must** be letters
 105 (ASCII 65 through 90, `A-Z`) and ASCII 97-122, (`a-z`), numbers (ASCII 48-57, `0-9`), underscore
 106 (ASCII 95, `_`), or dash (ASCII 45, `-`).

107 The tag **must** be interpreted as case insensitive.

108 2.3 Required metadata

109 Three items are essential to the interchange and successful interpretation of XAS data. These are
 110 **required** in all files using the [XDI specification](#).

- 111 • `Element.symbol`: The element of the absorbing atom. The periodic table is replete with exam-
 ples 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. Without identification
 of the species of the absorbing atom and of the absorption edge measured, some data cannot
 be unambiguously identified.

- 116 • `Element.edge`: The absorption edge measured. See above.
- 117 • `Mono.d_spacing`: The d-spacing of the monochromator. This is **required** when the abscissa is
118 expressed in angle or encoder steps. It is required to convert that abscissa into energy. Also
119 a correction to the energy axis of measured data, which may be required in the case of a mis-
120 calibration due to inaccuracies in the translation from angular position of the monochromator
121 to energy, would need the d-spacing.

122 Most other metadata definitions that follow are **optional** for use with *XDI*. Some are **recommended**
123 for use with all *XDI* files. The **recommended** metadata convey information that is of substantive
124 value to the interpretation of the data.

125 2.4 Defined items in the Facility namespace

- 126 • **Namespace:** `Facility` – **Tag:** `name`
 - 127 – *Description*: The name of synchrotron or other X-ray facility. This is **recommended** for
128 use in all *XDI* files.
 - 129 – *Units*: none
 - 130 – *Format*: string
- 131 • **Namespace:** `Facility` – **Tag:** `energy`
 - 132 – *Description*: The energy of the current in the storage ring.
 - 133 – *Units*: GeV, MeV
 - 134 – *Format*: float + units
- 135 • **Namespace:** `Facility` – **Tag:** `current`
 - 136 – *Description*: The amount of stored current in the storage ring at the beginning of the
137 scan.
 - 138 – *Units*: mA, A
 - 139 – *Format*: float + units
- 140 • **Namespace:** `Facility` – **Tag:** `source`
 - 141 – *Description*: A string identifying the source of the X-rays, such as “bend magnet”, “undu-
142 lator”, or “rotating copper anode”. This is **recommended** for use in all *XDI* files.
 - 143 – *Units*: none
 - 144 – *Format*: string

145 2.5 Defined items in the Beamline namespace

- 146 • **Namespace:** `Beamline` – **Tag:** `name`
 - 147 – *Description*: The name by which the beamline is known. This is **recommended** for use
148 in all *XDI* files.
 - 149 – *Units*: none
 - 150 – *Format*: free-format string
- 151 • **Namespace:** `Beamline` – **Tag:** `collimation`
 - 152 – *Description*: A concise statement of how beam collimation is provided
 - 153 – *Units*: none
 - 154 – *Format*: free-format string
- 155 • **Namespace:** `Beamline` – **Tag:** `focusing`

-
- 156 – *Description*: A concise statement about how beam focusing is provided
 157 – *Units*: none
 158 – *Format*: free-format string
- 159 • **Namespace:** Beamline – **Tag:** harmonic_rejection
 160 – *Description*: A concise statement about how harmonic rejection is accomplished
 161 – *Units*: none
 162 – *Format*: free-format string

163 2.6 Defined items in the Mono namespace

- 164 • **Namespace:** Mono – **Tag:** name
 165 – *Description*: A string identifying the material and diffracting plane or grating spacing of
 the monochromator
 166 – *Units*: none
 167 – *Format*: free-format string
- 168 • **Namespace:** Mono – **Tag:** d_spacing
 169 – *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.
 170 – *Units*: Å
 171 – *Format*: float

175 This is the appropriate namespace for parameters of an energy dispersive polychromator. Such
 176 parameters may be defined in future versions of this dictionary.

177 2.7 Defined items in the Detector namespace

- 178 • **Namespace:** Detector – **Tag:** i0
 179 – *Description*: A description of how the incident flux was measured
 180 – *Units*: none
 181 – *Format*: free-format string
- 182 • **Namespace:** Detector – **Tag:** it
 183 – *Description*: A description of how the transmission flux was measured
 184 – *Units*: none
 185 – *Format*: free-format string
- 186 • **Namespace:** Detector – **Tag:** if
 187 – *Description*: A description of how the fluorescence flux was measured
 188 – *Units*: none
 189 – *Format*: free-format string
- 190 • **Namespace:** Detector – **Tag:** ir
 191 – *Description*: A description of how the reference flux was measured
 192 – *Units*: none
 193 – *Format*: free-format string

2.8 Defined items in the Sample namespace

- **Namespace:** `Sample` – **Tag:** `name`
 - *Description:* A string identifying the measured sample
 - *Units:* none
 - *Format:* free-format string
- **Namespace:** `Sample` – **Tag:** `id`
 - *Description:* A number or string uniquely identifying the measured sample. This is intended for interoperation with a database or with laboratory management software.
 - *Units:* none
 - *Format:* free-format string
- **Namespace:** `Sample` – **Tag:** `stoichiometry`
 - *Description:* The stoichiometric formula of the measured sample
 - *Units:* none
 - *Format:* see [the IUCr definition of chemical_formula](#)
- **Namespace:** `Sample` – **Tag:** `prep`
 - *Description:* A string summarizing the method of sample preparation
 - *Units:* none
 - *Format:* free-format string
- **Namespace:** `Sample` – **Tag:** `experimenters`
 - *Description:* The names of the experimenters present for the measurement
 - *Units:* none
 - *Format:* free-format string
- **Namespace:** `Sample` – **Tag:** `temperature`
 - *Description:* The temperature at which the sample was measured
 - *Units:* degrees K, degrees C
 - *Format:* float + units

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.

Here are some other possible tags denoting extrinsic parameters of the experiment along the line of `Sample.temperature`. These may be added as defined fields in future versions of the *XDI* specification.

- `Sample.pressure`
- `Sample.ph`
- `Sample.eh`
- `Sample.volume`
- `Sample.porosity`
- `Sample.density`
- `Sample.concentration`
- `Sample.resistivity`
- `Sample.viscosity`

-
- ```

235 • Sample.electric_field
236 • Sample.magnetic_field
237 • Sample.magnetic_moment
238 • Sample.crystal_structure
239 • Sample.opacity
240 • Sample.electrochemical_potential

```

241 Almost all of these examples **should** take a float+units as values.

## 2.9 Defined items in the Scan namespace

- ```

243 • Namespace: Scan - Tag: start_time
244   - Description: The beginning time of the scan. This is recommended for use with XDI.
245   - Units: time
246   - Format: ISO 8601 specification for combined dates and times

247 • Namespace: Scan - Tag: end_time
248   - Description: The beginning time of the scan.
249   - Units: time
250   - Format: ISO 8601 specification for combined dates and times

251 • Namespace: Scan - Tag: edge_energy
252   - Description: The absorption edge as used in the data acquisition software.
253   - Units: eV (recommended), keV, inverse Å
254   - Format: float + units

```

255 This is the appropriate namespace for any parameters associated with scan parameters, such as
256 integration times, monochromator speed, scan boundaries, or step sizes.

257 An example of a combined date and time representation is 2007-04-05T14:30, which means 2:30 in
258 the afternoon on the day of April 5th in the year 2007.

2.10 Defined items in the Element namespace

- ```

260 • Namespace: Element - Tag: symbol
261 - Description: The measured absorption edge. This is a required parameter for use with
262 XDI.
263 - Units: none
264 - Format: one of these 118 1, 2, or 3 character strings for the standard atomic symbols
265 (not case sensitive):

```

```

266 H He Li Be B C N O F Ne Na Mg Al Si P S
267 Cl Ar K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge
268 As Se Br Kr Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd
269 In Sn Sb Te I Xe Cs Ba La Ce Pr Nd Pm Sm Eu Gd
270 Tb Dy Ho Er Tm Yb Lu Hf Ta W Re Os Ir Pt Au Hg
271 Tl Pb Bi Po At Rn Fr Ra Ac Th Pa U Np Pu Am Cm
272 Bk Cf Es Fm Md No Lr Rf Db Sg Bh Hs Mt Ds Rg Cn
273 Uut Fl Uup Lv Uus Uuo

```

274 See [Wikipedia's list of element symbols](#).

275 • **Namespace:** `Element` – **Tag:** `edge`

276 – *Description:* The measured absorption edge. This is a **required** parameter for use with  
 277 *XDI*.

278 – *Units:* none

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

280     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

281 See table 10.10 at [IUPAC notation for X-ray absorption edges](#) for further explanation. The  
 282 use of the generic edges *L*, *M*, *N*, and *O* is **not recommended**, but **may** be used for spectra  
 283 spanning multiple edges.

284 • **Namespace:** `Element` – **Tag:** `reference`

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

287 – *Units:* none

288 – *Format:* same as `Element.symbol`

289 • **Namespace:** `Element` – **Tag:** `ref_edge`

290 – *Description:* The measured edge of the reference spectrum. This is a **recommended**  
 291 parameter for use in an *XDI* file containing a reference spectrum.

292 – *Units:* none

293 – *Format:* same as `Element.edge`

## 2.11 Defined items in the Column namespace

295 Items in the Column namespace describe single columns of the data table. The first column **must**  
 296 be the energy.

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

298 • **Namespace:** `Column` – **Tag:** `1`

299 – *Description:* A description of the abscissa array for the measured data. This is **recom-**  
 300 **mended** for use in an *XDI* file.

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

302 – *Format:* word + units

303 • **Namespace:** `Column` – **Tag:** `N`

304 – *Description:* A description of the *N*th column (where *N* is an integer) of the measured  
 305 data. This is **recommended** for use in an *XDI* file.

306 – *Units:* as needed

307 – *Format:* word (+ units)

308 The following labels are defined for common array types. `Column.N` items **must** use these labels  
 309 when appropriate. The array label line at the beginning of the data section of the *XDI* file also **must**  
 310 use these labels when those columns are present.

| Column label        | Meaning     | choice of units (if required) |
|---------------------|-------------|-------------------------------|
| <code>energy</code> | mono energy | eV / keV / pixel              |

| Column label           | Meaning                              | choice of units (if required) |
|------------------------|--------------------------------------|-------------------------------|
| <code>angle</code>     | mono angle                           | degrees / radians / steps     |
| <code>i0</code>        | monitor intensity                    |                               |
| <code>itrans</code>    | transmission intensity               |                               |
| <code>ifluor</code>    | fluorescence intensity               |                               |
| <code>irefer</code>    | reference intensity                  |                               |
| <code>mutrans</code>   | mu transmission                      |                               |
| <code>mufluor</code>   | mu fluorescence                      |                               |
| <code>murefer</code>   | mu reference                         |                               |
| <code>normtrans</code> | normalized mu transmission           |                               |
| <code>normfluor</code> | normalized mu fluorescence           |                               |
| <code>normrefer</code> | normalized mu reference              |                               |
| <code>k</code>         | wavenumber                           |                               |
| <code>chi</code>       | EXAFS                                |                               |
| <code>chi_mag</code>   | magnitude of Filtered $\chi(k)$      |                               |
| <code>chi_ph</code>    | phase of Filtered $\chi(k)$          |                               |
| <code>chi_re</code>    | real part of Filtered $\chi(k)$      |                               |
| <code>chi_im</code>    | imaginary part of Filtered $\chi(k)$ |                               |
| <code>r</code>         | radial distance                      |                               |
| <code>chir_mag</code>  | magnitude of FT[ $\chi(k)$ ]         |                               |
| <code>chir_ph</code>   | phase of FT[ $\chi(k)$ ]             |                               |
| <code>chir_re</code>   | real part of FT[ $\chi(k)$ ]         |                               |
| <code>chir_im</code>   | imaginary part of FT[ $\chi(k)$ ]    |                               |

311 A column containing some other measurement **must** be identified with units when appropriate. For  
 312 example, a column counting time since the `Scan.start_time` timestamp might be labeled as

313    # Column.N: elapsed\_time seconds

314 while a column containing an ongoing measure of temperature as a voltage on a thermocouple might  
 315 be labeled as

316    # Column.N: thermocouple millivolts

---

## 317 2.12 Extension fields

318 Metadata tags carry syntax and may carry semantics. That is, it is possible to have syntactically  
319 correct tags that have no definition. Such tags could carry information considered useful by the  
320 user or the author of software that, at some point, touches the data.

321 Such a tag could be an extension within an existing namespace. This has already been discussed in  
322 the context of the `Sample` and `Scan` namespaces.

323 Such a tag could also be part of a new namespace. One application of a new namespace would be to  
324 tie a group of metadata tags to a particular application. For example, the data processing program  
325 Athena might attach tags associated with the parameters for normalizing the data. That might look  
326 something like this:

```
327 # Athena.pre1: -150
 328 # Athena.pre2: -30
 329 # Athena.nor1: 150
 330 # Athena.nor2: 800
```

331 These define the boundaries of the pre- and post-edge lines used to determine the edge step of the  
332  $\mu(E)$  spectrum.

333 The use of such extension tags is encouraged for authors of controls, data acquisition, data analysis,  
334 and data archiving software.

335 If an extension tag is not understood due its lack of defined semantics, the **recommended** behavior  
336 for software touching the data is to silently preserve the metadata.