



Metadata for raw data from X-ray diffraction and other structural techniques

A Satellite Workshop to the 29th European
Crystallographic Meeting

Practical session: 1. Catalogue of metadata standards



DDDWG Work Plan

Metadata

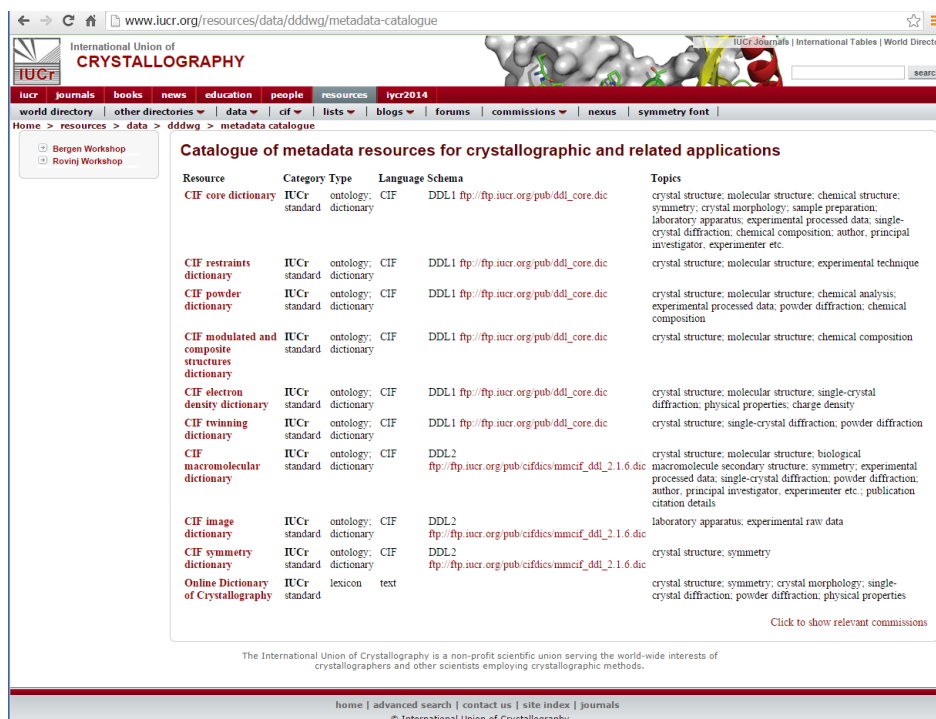
DDDWG Triennial Report 2011-2014

- In the Madrid Congress the **Commissions were charged** at the DDD inaugural meeting **to define the metadata that should accompany their raw data ...**
- While each IUCr Commission needs to specify 'technical' metadata - *i.e.* those specific to their experimental raw data - there is also a need to review 'generic' metadata – *e.g.* who 'owns' a data set, details of research grants, embargo periods etc. A higher-level classification of the domain of study may be needed. *E.g.* a synchrotron facility might need to define different data storage policies for, say, X-ray diffraction images *versus* X-ray tomography images. Such policies could be automatically implemented if data sets had characteristics identifying what sort of scientific study they represent.

DDDWG Work Plan

Commissions were charged at the DDD inaugural meeting to define the metadata

Metadata Catalogue



The screenshot shows the IUCr Metadata Catalogue website. The header includes the IUCr logo and navigation links for journals, books, news, education, people, resources, and Iucr2014. The main content area is titled 'Catalogue of metadata resources for crystallographic and related applications' and contains a table of resources. The table has four columns: Resource, Category Type, Language Schema, and Topics. The resources listed include CIF core dictionary, CIF restraints dictionary, CIF powder dictionary, CIF modulated and composite structures dictionary, CIF electron density dictionary, CIF twinning dictionary, CIF macromolecular dictionary, CIF image dictionary, CIF symmetry dictionary, and Online Dictionary of Crystallography. Each resource entry provides details on its category, type, language, schema, and a list of topics it covers. A link to show relevant commissions is provided at the bottom of the table.

Resource	Category Type	Language Schema	Topics	
CIF core dictionary	IUCr standard	ontology; CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical structure; symmetry; crystal morphology; sample preparation; laboratory apparatus; experimental processed data; single-crystal diffraction; chemical composition; author; principal investigator; experimenter etc.
CIF restraints dictionary	IUCr standard	ontology; CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; experimental technique
CIF powder dictionary	IUCr standard	ontology; CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical analysis; experimental processed data; powder diffraction; chemical composition
CIF modulated and composite structures dictionary	IUCr standard	ontology; CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical composition
CIF electron density dictionary	IUCr standard	ontology; CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; single-crystal diffraction; physical properties; charge density
CIF twinning dictionary	IUCr standard	ontology; CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; single-crystal diffraction; powder diffraction
CIF macromolecular dictionary	IUCr standard	ontology; CIF dictionary	DDL2 ftp://ftp.iucr.org/pub/cifdics/mmCIF_ddl_2.1.6.dic	crystal structure; molecular structure; biological macromolecule secondary structure; symmetry; experimental processed data; single-crystal diffraction; powder diffraction; author; principal investigator, experimenter etc.; publication citation details
CIF image dictionary	IUCr standard	ontology; CIF dictionary	DDL2 ftp://ftp.iucr.org/pub/cifdics/mmCIF_ddl_2.1.6.dic	laboratory apparatus; experimental raw data
CIF symmetry dictionary	IUCr standard	ontology; CIF dictionary	DDL2 ftp://ftp.iucr.org/pub/cifdics/mmCIF_ddl_2.1.6.dic	crystal structure; symmetry
Online Dictionary of Crystallography	IUCr standard	lexicon text		crystal structure; symmetry; crystal morphology; single-crystal diffraction; powder diffraction; physical properties

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<http://www.iucr.org/resources/data/dddwg/metadata-catalogue>

Metadata catalogue

← → ↻ 🏠 www.iucr.org/resources/data/dddwg/metadata-catalogue ☆ ☰

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[Bergen Workshop](#)
[Rovinj Workshop](#)

Catalogue of metadata resources for crystallographic and related applications

Resource	Category	Type	Language	Schema	Topics
CIF core dictionary	IUCr standard	ontology; dictionary	CIF	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical structure; symmetry; crystal morphology; sample preparation; laboratory apparatus; experimental processed data; single-crystal diffraction; chemical composition; author, principal investigator, experimenter etc.
CIF restraints dictionary	IUCr standard	ontology; dictionary	CIF	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; experimental technique
CIF powder dictionary	IUCr standard	ontology; dictionary	CIF	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical analysis; experimental processed data; powder diffraction; chemical composition
CIF modulated and composite structures dictionary	IUCr standard	ontology; dictionary	CIF	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical composition
CIF electron density dictionary	IUCr standard	ontology; dictionary	CIF	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; single-crystal diffraction; physical properties; charge density
CIF twinning dictionary	IUCr standard	ontology; dictionary	CIF	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; single-crystal diffraction; powder diffraction
CIF macromolecular dictionary	IUCr standard	ontology; dictionary	CIF	DDL2 ftp://ftp.iucr.org/pub/cifdics/mmCIF_ddl_2.1.6.dic	crystal structure; molecular structure; biological macromolecule secondary structure; symmetry; experimental processed data; single-crystal diffraction; powder diffraction; author, principal investigator, experimenter etc.; publication citation details
CIF image dictionary	IUCr standard	ontology; dictionary	CIF	DDL2 ftp://ftp.iucr.org/pub/cifdics/mmCIF_ddl_2.1.6.dic	laboratory apparatus; experimental raw data
CIF symmetry dictionary	IUCr standard	ontology; dictionary	CIF	DDL2 ftp://ftp.iucr.org/pub/cifdics/mmCIF_ddl_2.1.6.dic	crystal structure; symmetry
Online Dictionary of Crystallography	IUCr standard	lexicon	text		crystal structure; symmetry; crystal morphology; single-crystal diffraction; powder diffraction; physical properties

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Metadata catalogue

← → ↻ 🏠 www.iucr.org/resources/data/dddwg/metadata-catalogue#nul ☆ ☰

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world directory | **other directories** | **data** | **cif** | **lists** | **blogs** | **forums** | **commissions** | **nexus** | **symmetry font**

Home > resources > data > dddwg > metadata catalogue

⊕ Bergen Workshop
⊕ Rovinj Workshop

Catalogue of metadata resources for crystallographic and related applications

Resource	Category	Type	Language	Schema	Topics
CIF core dictionary	IUCr	ontology; standard	CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical structure; symmetry; crystal morphology; sample preparation; laboratory apparatus; experimental processed data; single-crystal diffraction; chemical composition; author, principal investigator, experimenter etc.
<i>Commission on Aperiodic Crystals; Commission on Crystal Growth and Characterization of Materials; Commission on Crystallographic Computing; Ad Interim Commission on Crystallography of Materials; Commission on Electron Diffraction; Commission on High Pressure; Commission on Inorganic and Mineral Structures; Commission on Magnetic Structures; Commission on Mathematical and Theoretical Crystallography; Commission on Neutron Scattering; Commission on NMR Crystallography and Related Methods; Commission on Powder Diffraction; Commission on Structural Chemistry</i>					
CIF restraints dictionary	IUCr	ontology; standard	CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; experimental technique
<i>Commission on Crystallographic Computing; Commission on Structural Chemistry</i>					
CIF powder dictionary	IUCr	ontology; standard	CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical analysis; experimental processed data; powder diffraction; chemical composition
<i>Commission on Crystallographic Computing; Commission on Neutron Scattering; Commission on Powder Diffraction; Commission on Structural Chemistry</i>					
CIF modulated and composite structures dictionary	IUCr	ontology; standard	CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical composition
<i>Commission on Aperiodic Crystals; Commission on Structural Chemistry</i>					
CIF electron density dictionary	IUCr	ontology; standard	CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; single-crystal diffraction; physical properties; charge density
<i>Commission on Charge; Commission on Electron Diffraction; Commission on Structural Chemistry</i>					
CIF twinning dictionary	IUCr	ontology; standard	CIF dictionary	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; single-crystal diffraction; powder diffraction
<i>Commission on Crystal Growth and Characterization of Materials; Commission on Mathematical and Theoretical Crystallography; Commission on Structural Chemistry</i>					
CIF macromolecular dictionary	IUCr	ontology; standard	CIF dictionary	DDL2 ftp://ftp.iucr.org/pub/cifdics/mmCIF_ddl_2.1.6.dic	crystal structure; molecular structure; biological macromolecule secondary structure; symmetry; experimental processed data; single-crystal diffraction; powder diffraction; author, principal investigator, experimenter etc.; publication citation details

Metadata catalogue - detail

Catalogue of metadata resources for crystallographic and related applications

Resource	Category	Type	Language	Schema	Topics
CIF core dictionary	IUCr standard	ontology; dictionary	CIF	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical structure; symmetry; crystal morphology; sample preparation; laboratory apparatus; experimental processed data; single-crystal diffraction; chemical composition; author, principal investigator, experimenter etc.
<i>Commission on Aperiodic Crystals; Commission on Crystal Growth and Characterization of Materials; Commission on Crystallographic Computing; Ad Interim Commission on Crystallography of Materials; Commission on Electron Diffraction; Commission on High Pressure; Commission on Inorganic and Mineral Structures; Commission on Magnetic Structures; Commission on Mathematical and Theoretical Crystallography; Commission on Neutron Scattering; Commission on NMR Crystallography and Related Methods; Commission on Powder Diffraction; Commission on Structural Chemistry</i>					

Metadata catalogue – more detail

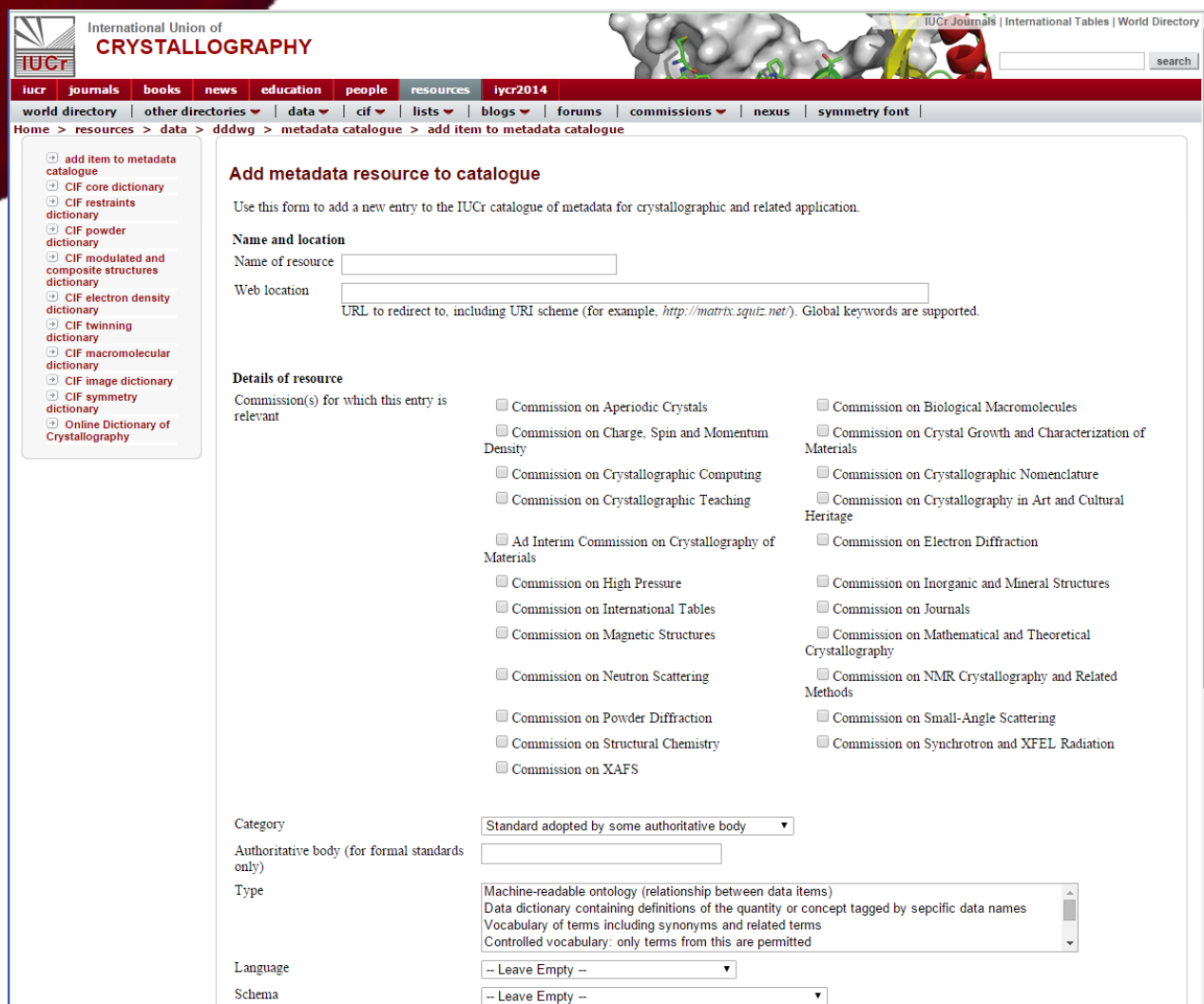
Name of property	Example	Comments
Resource name	CIF core dictionary	
Resource URI	ftp://ftp.iucr.org/pub/cif_core.dic	Link to resource itself? Documentation?
Category	standard	Controlled vocabulary
Authority	IUCr	
Type	ontology; dictionary	Controlled vocabulary
Language	CIF	Controlled vocabulary
Schema	DDL1	Controlled vocabulary
Schema URI	ftp://ftp.iucr.org/pub/ddl_core.dic	
Topics	crystal structure; molecular structure; chemical structure; symmetry; ...	Controlled vocabulary
Commissions	<i>Commission on Aperiodic Crystals; Commission on ...</i>	Controlled vocabulary for IUCr Commissions. Other stakeholders?

Metadata catalogue - detail

Catalogue of metadata resources for crystallographic and related applications

Resource	Category	Type	Language	Schema	Topics
CIF core dictionary	IUCr standard	ontology; dictionary	CIF	DDL1 ftp://ftp.iucr.org/pub/ddl_core.dic	crystal structure; molecular structure; chemical structure; symmetry; crystal morphology; sample preparation; laboratory apparatus; experimental processed data; single-crystal diffraction; chemical composition; author, principal investigator, experimenter etc.
<i>Commission on Aperiodic Crystals; Commission on Crystal Growth and Characterization of Materials; Commission on Crystallographic Computing; Ad Interim Commission on Crystallography of Materials; Commission on Electron Diffraction; Commission on High Pressure; Commission on Inorganic and Mineral Structures; Commission on Magnetic Structures; Commission on Mathematical and Theoretical Crystallography; Commission on Neutron Scattering; Commission on NMR Crystallography and Related Methods; Commission on Powder Diffraction; Commission on Structural Chemistry</i>					
CIF image dictionary	IUCr standard	ontology; dictionary	CIF	DDL2 ftp://ftp.iucr.org/pub/cifdics/mmCIF_ddl_2.1.6.dic	laboratory apparatus; experimental raw data
<i>Commission on Biological Macromolecules; Commission on Crystallographic Computing; Commission on Powder Diffraction; Commission on Structural Chemistry</i>					
Online Dictionary of Crystallography	IUCr standard	lexicon	text		crystal structure; symmetry; crystal morphology; single-crystal diffraction; powder diffraction; physical properties
<i>Commission on Aperiodic Crystals; Commission on Biological Macromolecules; Commission on Charge, Spin and Momentum Density; Commission on Crystal Growth and Characterization of Materials; Commission on Crystallographic Computing; Commission on Crystallographic Nomenclature; Commission on Crystallographic Teaching; Commission on Crystallography in Art and Cultural Heritage; Ad Interim Commission on Crystallography of Materials; Commission on Electron Diffraction; Commission on High Pressure; Commission on Inorganic and Mineral Structures; Commission on International Tables; Commission on Journals; Commission on Magnetic Structures; Commission on Mathematical and Theoretical Crystallography; Commission on Neutron Scattering; Commission on NMR Crystallography and Related Methods; Commission on Powder Diffraction; Commission on Small-Angle Scattering; Commission on Structural Chemistry; Commission on Synchrotron and XFEL Radiation; Commission on XAFS</i>					

Metadata catalogue - populating



The screenshot shows the 'Add item to metadata catalogue' form on the IUCr website. The page has a red header with the IUCr logo and navigation links. A sidebar on the left lists various dictionaries. The main form area is titled 'Add metadata resource to catalogue' and includes fields for 'Name and location', 'Details of resource' (a grid of checkboxes for different IUCr commissions), 'Category', 'Authoritative body', 'Type', 'Language', and 'Schema'.

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Home > resources > data > dddwg > metadata catalogue > add item to metadata catalogue

Add metadata resource to catalogue

Use this form to add a new entry to the IUCr catalogue of metadata for crystallographic and related application.

Name and location

Name of resource

Web location

URL to redirect to, including URI scheme (for example, <http://matrix.squiz.net/>). Global keywords are supported.

Details of resource

Commission(s) for which this entry is relevant

<input type="checkbox"/> Commission on Aperiodic Crystals	<input type="checkbox"/> Commission on Biological Macromolecules
<input type="checkbox"/> Commission on Charge, Spin and Momentum Density	<input type="checkbox"/> Commission on Crystal Growth and Characterization of Materials
<input type="checkbox"/> Commission on Crystallographic Computing	<input type="checkbox"/> Commission on Crystallographic Nomenclature
<input type="checkbox"/> Commission on Crystallographic Teaching	<input type="checkbox"/> Commission on Crystallography in Art and Cultural Heritage
<input type="checkbox"/> Ad Interim Commission on Crystallography of Materials	<input type="checkbox"/> Commission on Electron Diffraction
<input type="checkbox"/> Commission on High Pressure	<input type="checkbox"/> Commission on Inorganic and Mineral Structures
<input type="checkbox"/> Commission on International Tables	<input type="checkbox"/> Commission on Journals
<input type="checkbox"/> Commission on Magnetic Structures	<input type="checkbox"/> Commission on Mathematical and Theoretical Crystallography
<input type="checkbox"/> Commission on Neutron Scattering	<input type="checkbox"/> Commission on NMR Crystallography and Related Methods
<input type="checkbox"/> Commission on Powder Diffraction	<input type="checkbox"/> Commission on Small-Angle Scattering
<input type="checkbox"/> Commission on Structural Chemistry	<input type="checkbox"/> Commission on Synchrotron and XFEL Radiation
<input type="checkbox"/> Commission on XAFS	

Category

Authoritative body (for formal standards only)

Type
Data dictionary containing definitions of the quantity or concept tagged by sepcific data names
Vocabulary of terms including synonyms and related terms
Controlled vocabulary: only terms from this are permitted

Language

Schema

<http://www.iucr.org/resources/data/dddwg/metadata-catalogue/add-item>

Metadata catalogue - identification

- Should the web location refer to the machine-readable resource itself, or to a documentation / home page?
- Should there be separate entries for separate versions?

Add metadata resource to catalogue

Use this form to add a new entry to the IUCr catalogue of metadata for crystallographic and related application.

Name and location

Name of
resource

CIF core dictionary

Web location

ftp://ftp.iucr.org/pub/cif_core.dic

URL to redirect to, including URI scheme (for example, *http://matrix.squiz.net/*).

Metadata catalogue - stakeholders

- Very IUCr specific
- Remove from public form?
- Add other categories of stakeholder?

Details of resource

Commission(s)
for which this
entry is relevant

- | | |
|--|---|
| <input type="checkbox"/> Commission on Aperiodic Crystals | <input type="checkbox"/> Commission on Biological Macromolecules |
| <input type="checkbox"/> Commission on Charge, Spin and Momentum Density | <input type="checkbox"/> Commission on Crystal Growth and Characterization of Materials |
| <input type="checkbox"/> Commission on Crystallographic Computing | <input type="checkbox"/> Commission on Crystallographic Nomenclature |
| <input type="checkbox"/> Commission on Crystallographic Teaching | <input type="checkbox"/> Commission on Crystallography in Art and Cultural Heritage |
| <input type="checkbox"/> Ad Interim Commission on Crystallography of Materials | <input type="checkbox"/> Commission on Electron Diffraction |
| <input type="checkbox"/> Commission on High Pressure | <input type="checkbox"/> Commission on Inorganic and Mineral Structures |
| <input type="checkbox"/> Commission on International Tables | <input type="checkbox"/> Commission on Journals |
| <input type="checkbox"/> Commission on Magnetic Structures | <input type="checkbox"/> Commission on Mathematical and Theoretical Crystallography |
| <input type="checkbox"/> Commission on Neutron Scattering | <input type="checkbox"/> Commission on NMR Crystallography and Related Methods |
| <input type="checkbox"/> Commission on Powder Diffraction | <input type="checkbox"/> Commission on Small-Angle Scattering |
| <input type="checkbox"/> Commission on Structural Chemistry | <input type="checkbox"/> Commission on Synchrotron and XFEL Radiation |
| <input type="checkbox"/> Commission on XAFS | |

Metadata catalogue - category

- Only one allowed
- Additional categories?
- “Authority” can be relatively informal
- Should we require documentation for the authority?

Category

▼

Standard adopted by some authoritative body

De facto standard arising from widespread use

Draft or proposed standard

Working system in local use (e.g. within a facility)

Other

Authoritative
body (for formal
standards only)

Metadata catalogue – type and language

- Multiple “type” allowed
- Only one language / schema

Type

Machine-readable ontology (relationship between data items)
Data dictionary containing definitions of the quantity or concept tagged by sepcific data names
Vocabulary of terms including synonyms and related terms
Controlled vocabulary: only terms from this are permitted
List of keywords (differs from controlled vocabulary in that additional terms may be inserted by user)
Other
Lexicographic dictionary of terminology

Language

▼
Crystallographic Information Framework
W3C Web Ontology Language
XML schema
Unstructured text

Schema

▼
Dictionary Definition Language version 1
Dictionary Definition Language version 2
Dublin Core
METS (Metadata Encoding and Transmission Standard)

URI of schema

Metadata catalogue – topics

- Multiple choice
- Community critique / suggestions especially welcomed

Topics covered by resource

<input type="checkbox"/> crystal structure	<input type="checkbox"/> molecular structure	<input type="checkbox"/> biological macromolecule secondary structure	<input type="checkbox"/> chemical structure
<input type="checkbox"/> symmetry	<input type="checkbox"/> crystal morphology	<input type="checkbox"/> sample preparation	<input type="checkbox"/> chemical analysis
<input type="checkbox"/> chemical reaction	<input type="checkbox"/> laboratory apparatus	<input type="checkbox"/> safety hazard, toxicity etc.	<input type="checkbox"/> experimental raw data
<input type="checkbox"/> experimental processed data	<input type="checkbox"/> single-crystal diffraction	<input type="checkbox"/> powder diffraction	<input type="checkbox"/> physical properties
<input type="checkbox"/> chemical composition	<input type="checkbox"/> charge density	<input type="checkbox"/> experimental technique	<input type="checkbox"/> author, principal investigator, experimenter etc.
<input type="checkbox"/> funding body, grant number etc.	<input type="checkbox"/> publication citation details		