

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

A Satellite Workshop to the 29th European Crystallographic Meeting

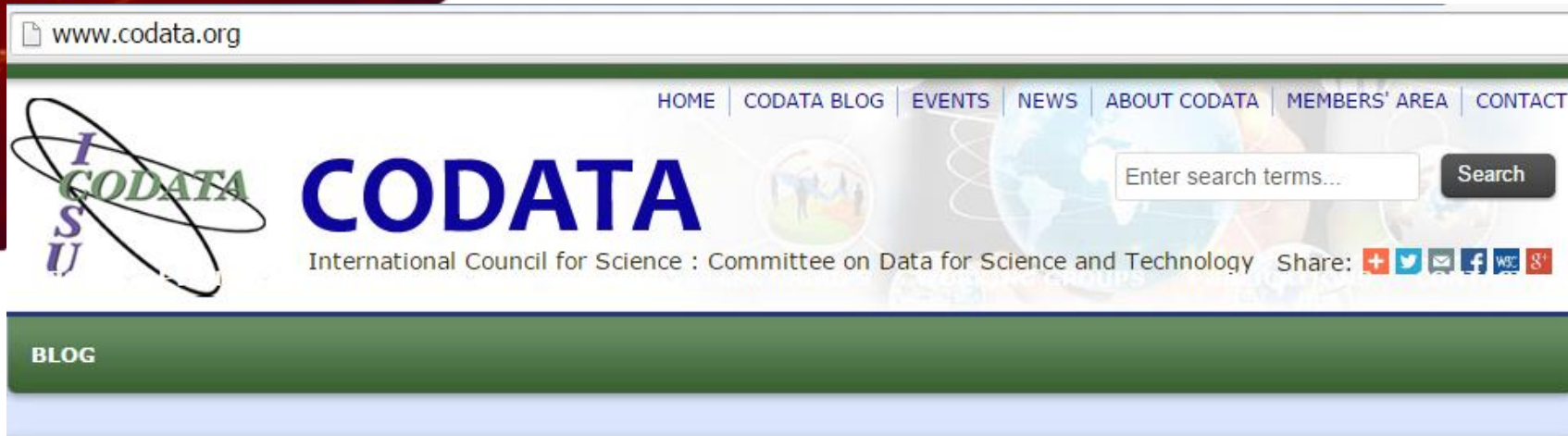
## CODATA and (meta)data characterisation in the wider world

Brian McMahon



International Union of Crystallography  
5 Abbey Square  
Chester CH1 2HU  
UK  
[bm@iucr.org](mailto:bm@iucr.org)

# CODATA – ICSU Committee on Data for Science and Technology



<http://www.codata.org>



# CODATA – ICSU Committee on Data for Science and Technology

## Some facts

- Founded 1966
- Scientific Committee of ICSU
- Mission: to strengthen international science for the benefit of society by promoting improved scientific and technical data management and use.
- Remit: CODATA is concerned with all types of quantitative data from experimental measurements/observations in the physical, biological, geological and astronomical sciences. Particular emphasis is given to data management problems common to different scientific disciplines and to data used outside the field in which they were generated.
- General objectives: improvement of the quality and accessibility of data, as well as the methods by which data are acquired, managed and analysed; facilitation of international cooperation among those collecting, organizing and using data; promotion of an increased awareness in the scientific and technical community of the importance of these activities.



# CODATA – ICSU Committee on Data for Science and Technology

## Some facts

- Headquarters: Paris, France
- Members: National Members, International Scientific Unions, Co-Opted Organizations, Supporting Organizations
- Officers: *President* Geoffrey Boulton (UK); *Secretary General* Sara Graves (USA); *Treasurer* John Broome (Canada)
- Executive Director: Simon Hodson (UK)
- Task Groups (*e.g.* Data Citation Standards and Practices; Interoperable Data Publications; Physical Constants of Nature)
- Working Groups: Description of Nanomaterials (CODATA/VAMAS)
- Biennial CODATA Prize: Syd Hall '*for outstanding achievement in the world of scientific and technical data*'
- IUCr Representatives: J. R. Helliwell (2012- ); B. McMahon (2000-2012)



## CODATA/VAMAS Working Group on Description of Nanomaterials

- Convened 2012 under auspices of CODATA and VAMAS (Versailles Project on Advanced Materials and Standards)
- Chairs: John Rumble (formerly NIST), Steve Freiman, Clayton Teague
- Workshops
  - Paris February 2012 (IUCr: Reinhard Neder)
  - Paris May 2013 (IUCr; Daniel Chateigner)
  - North Carolina
  - Paris April 2014
  - Beijing September 2014
  - Maastricht July 2015
- Uniform Description System for Materials on the Nanoscale v1.0 published February 2015

<http://www.codata.org/nanomaterials>

# CODATA/VAMAS Working Group on Description of Nanomaterials

## IUCr participation in the CODATA / VAMAS Working Group on Nanomaterials

Daniel Chateigner  
CRISMAT-ENSICAEN  
Université de Caen Basse-Normandie  
6 Bd. Maréchal Juin  
14050 Caen, France

daniel.chateigner@ensicaen.fr

John R. Helliwell  
School of Chemistry  
University of Manchester  
Oxford Road  
Manchester M13 9PL, UK

john.helliwell@manchester.ac.uk

Reinhard Neder  
Physics Department  
University of Erlangen  
Staudtstr. 3  
D-91058 Erlangen, Germany

reinhard.neder@krist.uni-erlangen.de



### Introduction

Nanotechnology is moving towards commercialization, yet numerous scientific questions remain unanswered. One of the most critical challenges is that there is no common nomenclature or description system for nanomaterials that is accepted by a single discipline, let alone by all disciplines. The International Union of Crystallography (IUCr) and its Committee for the Maintenance of the CIF Standard (COMCIF) are well matched to help with this task set up under the aegis of CODATA/VAMAS.

IUCr was invited to participate in a CODATA/VAMAS Working Group in 2012. CODATA is the Committee on Data for Science and Technology of ICSU, the International Council for Science (<http://www.codata.org>). VAMAS is the Versailles Project on Advanced Materials and Standards (<http://www.vamas.org>). There have been 3 Workshops so far.

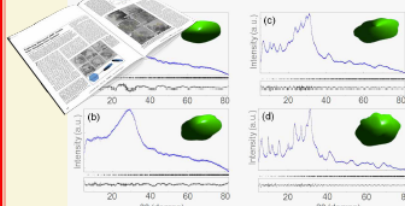
The overall goal is to define the needs of as many scientific disciplines and user communities as possible. This White Paper will be transmitted to ISO Technical Committee 229 on Nanotechnology ([http://www.iso.org/iso/technical\\_committee/committees/229](http://www.iso.org/iso/technical_committee/committees/229)) as well as other international and national standards development bodies and government agencies. Within this Working Group, crystallographers unambiguously define and characterize the structure of nanomaterials.



Furthermore X-ray reflectivity is suitable when the nano character is only expressed along one direction (stacks, films). Compared to other fields of science, Crystallography appears as a potential leader of quantitative nanomaterial descriptors and definitions. We bring different perspectives to the task including the physical and biological sciences relevant to inorganic, organic and bio nanomaterials.

### Capturing Ultrasmall EMT Zeolite from Template-Free Systems

E.-P. Ng, D. Chateigner, T. Bein, V. Valtchev & S. Mintova (2012). *Science*, 335, 70-74



cited in Science Magazine 'Breakthrough of the Year 2011'

### Crystallographic Techniques

**Diffraction** (scattering + interference): X-ray, gamma radiation, neutrons, electrons

**Reflectivity** (specular, off-specular): X-rays and neutrons

**Small-angle scattering**: X-rays (SAXS), neutrons (SANS)

**Tomography** (absorption or phase contrast): X-rays, neutrons, electrons

**Imaging** (HRTEM)

**Spectroscopy**: X-ray (XRF, XANES, EXAFS, DAFS), electrons (EDS), muons ( $\mu$ SR), photoluminescence, dynamic light scattering (DLS)

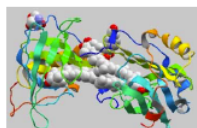
### Crystallographic Information Framework (CIF)

CIF dictionaries provide a formal taxonomy of crystallographic terms and ideas. Dictionary entries are constructed in a structured machine-readable manner that facilitates validation and structuring of data: <http://www.iucr.org/resources/cif/dictionaries>

Dictionaries: Core, Restraints, Powder, Modulated-Composite, Electron Density, Twinning, Macromolecular, Images, Symmetry

Local dictionaries: reflectivity (to come), MPOD (properties), MAUD

Electron, neutron and X-ray scattering and diffraction, at small and wide angles, and imaging techniques offer a physically grounded determination of the coherent size domains (including crystal shape). Our tools can approach the physical state of nanoaggregates.



### Acknowledgement

Brian McIlahon (IUCr, Chester, UK) is thanked for discussions and assistance with this poster.

- Summary of IUCr contributions presented as a poster to the ACA 2014 Annual Meeting

[http://www.ecole.ensicaen.fr/~chateign/danielc/posters/Chateigner\\_poster\\_ACA2014\\_CODATA%20VAMASv3.pdf](http://www.ecole.ensicaen.fr/~chateign/danielc/posters/Chateigner_poster_ACA2014_CODATA%20VAMASv3.pdf)



# CODATA/VAMAS Working Group on Description of Nanomaterials

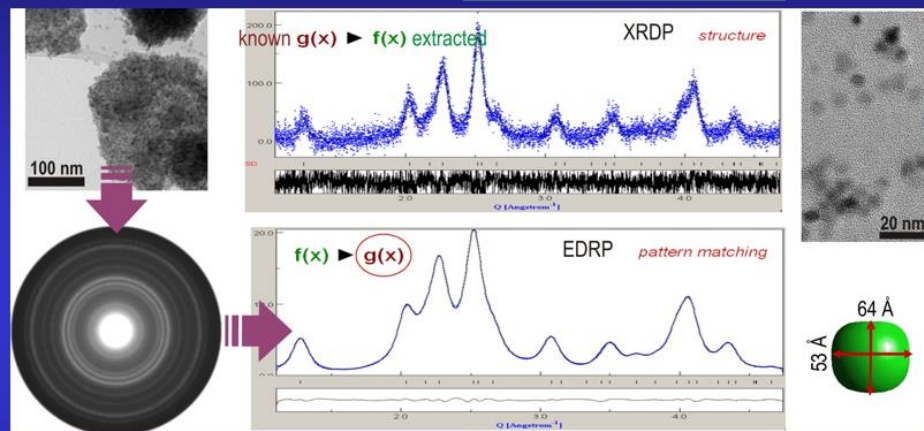
## Crystallography Information File (CIF)

CIF dictionaries provide a formal taxonomy of crystallographic terms and ideas. Dictionary entries are constructed in a structured machine-readable manner that facilitates validation and structuring of data: <http://www.iucr.org/resources/cif/dictionaries>

Dictionaries: Core, Restraints, Powder, Modulated-Composite, Electron density, Twinning, Macromolecular, Images, Symmetry

Local dictionaries: reflectivity (to come), MPOD (Properties), MAUD

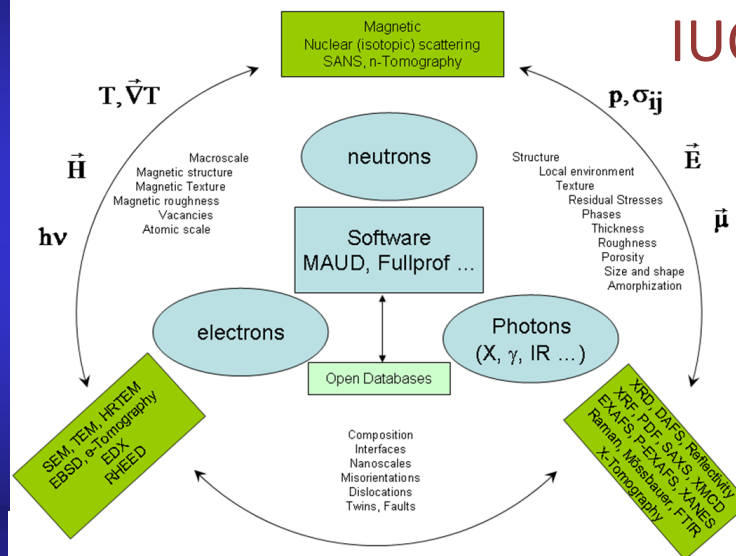
## Reflection for 3h (100mg)



## TEM in seconds (few μg)

$$\langle R_h \rangle = R_0 + R_1 P_2^0(x) + R_2 P_2^1(x) \cos \varphi + R_3 P_2^1(x) \sin \varphi + R_4 P_2^2(x) \cos 2\varphi + R_5 P_2^2(x) \sin 2\varphi + \dots$$

## IUCr input



## Crystallographic Techniques

Diffraction (scattering + interferences): X, γ, n, e<sup>-</sup>

Reflectivity (specular, off-specular): x-rays and neutrons

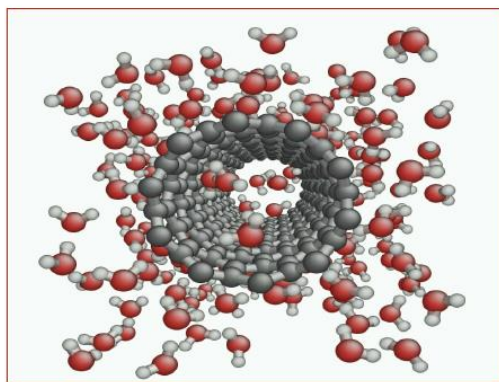
Small-Angles Scattering: x-rays (SAXS), neutrons (SANS)

Tomography (absorption or phase contrasts): x-rays, neutrons, electrons

Spectroscopy: X (XRF, XANES, EXAFS, DAFS)  
e<sup>-</sup> (EDS)  
μ<sup>+</sup> (μSR)

# CODATA/VAMAS Working Group on Description of Nanomaterials

## Uniform Description System for Materials on the Nanoscale



Prepared by the CODATA-VAMAS Working Group  
On the Description of Nanomaterials  
[www.codata.org/nanomaterials](http://www.codata.org/nanomaterials)

Version 1.0  
1 February 2015

UDS for Materials on the Nanoscale, v1.0, 1 February 2015

Table 7. Descriptors for the crystal structure of a nano-object

Descriptors for the Crystal Structure of a Nano-Object	
Descriptor	Definition
<b>Subcategory: Physical Structure Identification</b>	
Physical structure name	Name of the physical structure within the nano-object that is being described by its crystal structure
Physical structure type	Structure type: layer, shell, surface, etc.
Physical structure location	Location of the physical structure within the nano-object
General nano-object type	Metal, polymer, etc.
<b>Subcategory: Unit Cell Information</b>	
Crystal system	The crystal system of the physical structure (one of seven)
Breavais lattice	The Breavais lattice of the physical structure (one of 14)
Space group	The space group
Miller indices	The appropriate Miller indices
<b>Subcategory: Basic Unit Cell Parameters</b>	
Cell length <i>a</i>	Cell length <i>a</i> appropriate for the crystal system value
Cell length <i>b</i>	Cell length <i>b</i> appropriate for the crystal system value
Cell length <i>c</i>	Cell length <i>c</i> appropriate for the crystal system value
Cell angle <i>alpha</i>	Cell angle <i>alpha</i> appropriate for the crystal system value
Cell angle <i>beta</i>	Cell angle <i>beta</i> appropriate for the crystal system value
Cell angle <i>gamma</i>	Cell angle <i>gamma</i> appropriate for the crystal system value
Cell volume	Measured or calculated cell volume
Cell measurement temperature	Temperature at which crystal structure data were measured



# Other organizations with interdisciplinary interest in scientific metadata

## ICSTI – International Council for Scientific and Technical Information



The screenshot shows the ICSTI website homepage. The header features the ICSTI logo with the tagline "Enabling Science and Innovation" and the full name "International Council for Scientific and Technical Information". Navigation links include "Contact", "Site map", "Members' Area", and a search bar. A main menu contains links for "Home", "About Us", "Events", "Partnerships", "Membership", "Reports & Projects", "Archived News", and "Insights".

**HEADLINES**

- SUMMER LEAVE**  
2 Aug 2015 - The Office of ICSTI will be closed for holidays from August 8th to August 23rd, 2015. Happy Summer!
- 2015 GA MEETING : WORKSHOP PRESENTATIONS ARE AVAILABLE**  
8 July 2015 - Slides from the ITOC and TACC workshops held as part of the ICSTI 2015 General Assembly meeting on 4 July in Hannover can now be retrieved for download in the Members' Area of the website. Thanks to all our speakers, workshop chairs, and ICSTI and non-ICSTI delegates who attended and helped to make this informative and enlightening event a great success.
- 2015 GA & WORKSHOPS in HANNOVER - Final Programs Available**  
28 May 2015 - Both ITOC and TACC Workshop programs are now complete and have been posted on the ICSTI Upcoming Events dedicated webpage. The workshops will provide a space for peers to exchange ideas, to build new partnerships, and to hear papers from leading experts from top organisations. We remind you that both are open to ICSTI and non-ICSTI delegates and we encourage you to not only participate in what we believe will be two successful and productive sessions, but also to promote them through your professional networks.  
[Event Schedule and All Information](#)
- ICSTI HANNOVER WORKSHOPS - CONFIRMED SPEAKERS ANNOUNCED**  
10 Apr 2015 - Chairs of the ICSTI committees ITOC and TACC are pleased to unveil the preliminary presenter lists for the two workshops organised as part of our upcoming 4 July 2015 General Assembly meeting. Of particular interest is the discipline diversity of the speakers and the workshop programs are designed to provide exciting debates around the themes of *Open Science and Open Data* and of *Innovation*.  
[The information](#)
- ICSTI INSIGHT SERIES - Issue March 2015**  
5 Mar 2015 - Wendy Warr has authored this new issue of the ICSTI Insight series titled *"Evolution in the Implementation of Peer Review."* The six chapters of the article — Traditional peer review ; Open peer review ; Early alternatives to the traditional process ; Social media and virtual communities ; Evolving models of peer review ; New publishing platforms — provide a focus on the significant experiments and changes in peer review practices and describe the challenges faced by the traditional scholarly publishing models in a context of new types of research data sharing and web-based scientific collaborations.  
[Read the article.](#)

**MEMBER RSS FEEDS**

- 1 - 2015-08-17 : Nouveauté : le Registre de IFLA pour le patrimoine documentaire - (IFLA)
- 1 - 2015-08-17 : Nueva Iniciativa : Registro de la IFLA de Riesgos para el Patrimonio Documental - (IFLA)
- 1 - 2015-08-17 : Gerade gestartet : Das Risikoregister der IFLA für dokumentarisches Erbe - (IFLA)
- 1 - 2015-08-17 : 刚刚发布 : 国际图联文献遗产风险登记表 - (IFLA)
- 1 - 2015-08-17 : Just launched : IFLA Risk Register for documentary heritage - (IFLA)
- 1 - 2015-08-17 : سجل الإقدام لحماية التراث الوثائقي من المخاطر - (IFLA)
- 1 - 2015-08-17 : Запущен новый проект : Реестр Риска IFLA для документального наследия - (IFLA)
- 1 - 2015-08-16 : Allocution inaugurale de la présidente de IFLA Sinikka Sipilä - (IFLA)
- 1 - 2015-08-16 : Eröffnungsrede der IFLA-Präsidentin Sinikka Sipilä - (IFLA)
- 1 - 2015-08-16 : 国际图联主席西尼卡·西皮莱开幕式致辞 - (IFLA)

<http://www.icsti.org>



## Other organizations with interdisciplinary interest in scientific metadata

### ICSTI – International Council for Scientific and Technical Information

- Affiliate of the International Council for Science (ICSU)
- Mission: facilitate cooperation among stakeholders engaged in the scientific communication process with the aim of improving the effectiveness of scientific research
- Task Groups: CODATA/ICSTI Task Group on Data Citation Standards and Practices
- Workshops/Conferences: Goportis Conference 2013 on Non-Textual Information – *Strategy and Innovation Beyond Text*; Winter Workshop 2012 – *Delivering Data in Science*; Winter Workshop 2010 – *Interactive Publications and the Record of Science*; Conference 2009 – *Managing Data for Science*
- ICSTI Insights: *The Living Publication*

# Other organizations with interdisciplinary interest in scientific metadata

## RDA – Research Data Alliance

The screenshot shows the RDA website with a dark red header. The main navigation bar includes links for Home, Organisation, Working and Interest Groups, Plenary Meetings, News & Events, Early Career Programmes, and About. A search bar is located on the right. The RDA logo and tagline 'Research Data Sharing without barriers' are on the left. Social media icons for Facebook, Twitter, LinkedIn, and RSS are on the right. A large banner for the '6TH PLENARY PARIS' is featured, with the dates '23/25 SEPTEMBER 2015' and the theme 'Enterprise engagement'. Below the banner, a navigation bar lists various events and challenges. The main content area is divided into three columns: 'Request for Comments' with a link to 'Practical Policy Recommendations' by Herman Stehouwer; 'RDA Outputs' with a link to 'VIEW ALL' and a 'DOWNLOAD the RDA Outputs booklet' button; and 'Focus' with a link to 'TAB Election 2015 | Call for Nominations'.

REGISTER LOGIN CONTACT US

**RDA** Research Data Sharing without barriers  
RESEARCH DATA ALLIANCE

Share your news with RDA, write to [news@rd-alliance.org](mailto:news@rd-alliance.org)

ALL NEWS f t in RSS

Home Organisation Working and Interest Groups Plenary Meetings News & Events Early Career Programmes About

**6TH PLENARY PARIS** ... CNAM **23/25 SEPTEMBER 2015**

**Enterprise engagement**  
Special focus: Research Data for climate change

Build the social and technical bridges that enable data sharing!

6th PLENARY || REGISTRATION || PROGRAMME || Climate Change Data Challenge || Experimentation Day || Sponsoring ||

**Request for Comments**

**Practical Policy Recommendations**  
By Herman Stehouwer

**RDA Outputs**

RDA group outputs are focused on tangibly accelerate progress for global data sharing and increase data-driven innovation.

[VIEW ALL](#)

[DOWNLOAD the RDA Outputs booklet](#)

**Focus**

**TAB Election 2015 | Call for Nominations**

RDA is now seeking candidates for its annual Technical Advisory Board (TAB) election, which will be held in September 2015. With two current appointed members and two elected members stepping down, four vacancies will be open for election on TAB. Bridget Almas, Chuang Liu, Beth Plale, and Jamie Shiers will be stepping down.

<https://rd-alliance.org>




## Other organizations with interdisciplinary interest in scientific metadata

RDA – Research Data Alliance

- Launched 2013
- Core group: European Commission, US National Science Foundation, US National Institute of Standards and Technology, Australian Government Department of Innovation
- Other agencies, companies, associations and institutions
- Individual membership – 3000 from 102 countries
- Plenary Meetings
- Project-oriented methodology

# Other organizations with interdisciplinary interest in scientific metadata

## DCC – Digital Curation Centre

 **DCC** because good research needs good data

Contact us

Search

Home | Digital curation | About us | News | Events | Resources | Training | Projects | Community | Tailored support




**11th International Digital Curation Conference**  
Amsterdam, 22 - 25 February 2016


Call for Papers | Dates

Latest news


Next events



**DCC, DPC and ULCC launch training needs survey**  
11 August, 2015 | in DCC News



**International Journal of Digital Curation opens Volume 10, Issue 2**  
30 June, 2015 | in Publications



**IDCC16 - Save the Date**  
25 June, 2015 | in DCC News

**How can the DCC help you?**

**About us**

We are a world-leading centre of expertise in digital information curation...

**What is digital curation?**

Digital curation involves maintaining, preserving and adding value to digital research data throughout its lifecycle...

**Working with HEIs**

Under the institutional engagement programme we have been working with HEIs to provide tailored support...

**Editor's choice**

**DCC Institutional Survey 2015**

Make sure your institution is taking part in our annual survey of RDM in UK Higher Education...

**DMPonline roadmap**

Find out about updates to DMPonline and what we have planned for the future...

**Your Data Stories blog**

New blog to share examples of good and 'not-so-good' practice in RDM...

**Recent blog posts**

**Digital Preservation for the Arts, Social Sciences and Humanities - benefits for everyone**

**Jisc research data spring takes its next leap forward**

**Guest blog: Ethics and research data management in arts, humanities and social science research**

**RDMF13: notes from breakout group 3 (roles and training)**

All blog posts >

<http://www.dcc.ac.uk>





## Other organizations with interdisciplinary interest in scientific metadata


### DCC – Digital Curation Centre

- Launched 1 March 2004, following successful response to JISC Circular 6/038 by consortium comprising Universities of Edinburgh and Glasgow (jointly hosting National e-Science Centre), UKOLN at University of Bath, and STFC, which managed Rutherford Appleton and Daresbury Laboratories
- National centre for solving challenges in digital curation that could not be tackled by any single institution or discipline
- Shift from development of curation tools to renewed focus on building capacity, capability and skills for data curation across the UK's higher education research community

# Other organizations with interdisciplinary interest in scientific metadata

## DCC – Disciplinary Metadata

[Contact us](#)

 **D|C|C** because good research needs good data  [Search](#)

[Home](#) [Digital curation](#) [About us](#) [News](#) [Events](#) [Resources](#) [Training](#) [Projects](#) [Community](#) [Tailored support](#)

[Home](#) > [Drupal](#) > [Resources](#) > [Metadata Standards](#)

In this section

[Briefing Papers](#)

[How-to Guides & Checklists](#)

[Developing RDM Services](#)

[Curation Lifecycle Model](#)

[Curation Reference Manual](#)

[Policy and legal](#)

[Data Management Plans](#)

[Tools](#)

[Case studies](#)

[Repository audit and assessment](#)

Standards

Disciplinary Metadata

DIFFUSE

[Publications and presentations](#)

[Roles](#)

[Curation journals](#)

[Informatics research](#)

[External resources](#)

[Online Store](#)


Disciplinary Metadata

While data curators, and increasingly researchers, know that good metadata is key for research data access and re-use, figuring out precisely what metadata to capture and how to capture it is a complex task. Fortunately, many academic disciplines have supported initiatives to formalise the metadata specifications the community deems to be required for data re-use. This page provides links to information about these disciplinary metadata standards, including profiles, tools to implement the standards, and use cases of data repositories currently implementing them.


For those disciplines that have not yet settled on a metadata standard, and for those repositories that work with data across disciplines, the General Research Data section links to information about broader metadata standards that have been adapted to suit the needs of research data.

Please note that a community-maintained version of this directory [@](#) has been set up under the auspices of the Research Data Alliance.


Search by Discipline




Biology




Earth Science



General Research Data



Physical Science



Social Science & Humanities

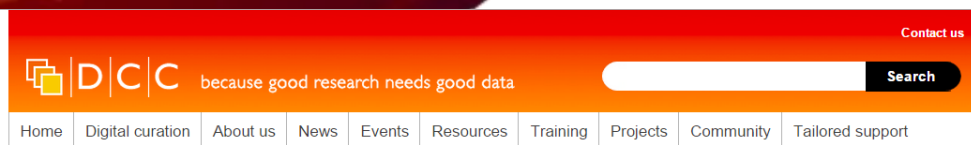
<http://www.dcc.ac.uk/resources/metadata-standards>

## RDA/DCC – Disciplinary Metadata

<http://rd-alliance.github.io/metadata-directory/>

# Other organizations with interdisciplinary interest in scientific metadata

## DCC – Disciplinary Metadata Catalogue



Home > Drupal > Resources > Subject Areas > Physical Science

### Physical Science

Geography Geoscience Space science Chemistry Crystallography Multi-disciplinary Biochemistry Geology Molecular biology Remote Sensing Astronomy Nuclear and Particle Physics Solar physics Bioinformatics Astrophysics Physics Meteorology Materials Science

### Metadata Standards

#### AVM - Astronomy Visualization Metadata

A standard defining discovery metadata for fully rendered astronomical images.

#### CIF - Crystallographic Information Framework

An extensible standard file format and set of protocols structured data.

#### CSMD-CCLRC Core Scientific Metadata Model

A study-data oriented model that captures high-level information about scientific studies and the data that they produce, primarily tailored for the physical sciences.

#### FITS - Flexible Image Transport System

Used by the astronomy community to originally describe standards to describe multi-dimensional data including scaling and distortions that may be present.

#### International Virtual Observatory Alliance Technical Specifications

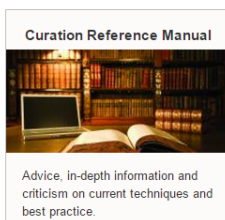
A set of specifications, including metadata standards, that archives into an international virtual observatory.

#### Observations and Measurements

This standard specifies an XML implementation for the (O&M) conceptual model, including a schema for Sami.

#### PDBx/mmCIF – Protein Data Bank Exchange Dictionary and the Macromolecular Crystallographic Information Framework

PDBx/mmCIF is the standard archive format used by the Protein Data Bank (PDB). It provides both metadata and data according to properties defined in the Macromolecular Crystallographic Information Framework (mmCIF).



### CIF - Crystallographic Information Framework

An extensible standard file format and set of protocols for the exchange of crystallographic and related structured data.

### CSMD-CCLRC Core Scientific Metadata Model

A study-data oriented model that captures high-level information about scientific studies and the data that they produce, primarily tailored for the physical sciences.

### PDBx/mmCIF – Protein Data Bank Exchange Dictionary and the Macromolecular Crystallographic Information Framework

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<http://www.dcc.ac.uk/resources/subject-areas/physical-science>



# Other organizations with interdisciplinary interest in scientific metadata

## RDA/DCC – Disciplinary Metadata Catalogue

**Metadata**

RDA | Metadata Directory

Edit this page

Getting Started

View the standards

View the extensions

View the tools

View the use cases

Browse by subject areas

Adding standards

Adding extensions

Adding tools

Adding use cases

github

@twitter

linkedin

facebook

### CIF - Crystallographic Information Framework

A well-established standard file structure for the archiving and distribution of crystallographic information, CIF is in regular use for reporting crystal structure determinations to Acta Crystallographica and other journals.

Sponsored by the International Union of Crystallography, the current standard dates from 1997. As of July 2011, a new version of the CIF standard is under consideration.

#### Summary [Edit](#)

**Standard Website**  
<http://www.iucr.org/resources/cif>

**Specification**  
<http://www.iucr.org/resources/cif/spec>

**Related Vocabularies**  
[IUCr Recommended abbreviations within data names](#)  
[CIF dictionaries](#)

**Subjects**  
[Engineering](#)  
[Physical Sciences & Mathematics](#)

**Disciplines**  
[Chemistry](#)  
[Crystallography](#)  
[Materials Science](#)

#### Extensions [Add](#)

#### Tools [Add](#)

**CIF2Cell** [Edit](#)  
A tool to generate the geometrical setup for various electronic structure codes from a [CIF](#) file.

**IUCr checkCIF** [Edit](#)  
A tool used to check the integrity and consistency of crystal structure encodings in [CIF](#) format.

**Software for CIF** [Edit](#)  
The International Union of Crystallography's list of programs and libraries available for use with [CIF](#) files.

#### Use Cases [Add](#)

**American Mineralogist Crystal Structure Database** [Edit](#)  
A [CIF](#) crystal structure database that includes every structure published in the American Mineralogist, The Canadian Mineralogist, European Journal of Mineralogy and Physics and Chemistry of Minerals, as well as selected datasets from other journals.

**Cambridge Structural Database** [Edit](#)  
A repository of small molecule crystal structures, many with accompanying [CIF](#) files.

**Crystallography Open Database** [Edit](#)  
An open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, many of which are in [CIF](#) form.

<http://rd-alliance.github.io/metadata-directory/standards/cif-crystallographic-information-framework.html>



# IUCr/DDDWG initiative

## Catalogue of metadata resources for crystallography

International Union of  
**CRYSTALLOGRAPHY**

[iucr](#) | [journals](#) | [books](#) | [news](#) | [education](#) | [people](#) | [resources](#) | [iucr2014](#)

[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
<b>CIF core dictionary</b>	IUCr standard	ontology; dictionary	CIF	DDL1 <a href="ftp://ftp.iucr.org/pub/ddl_core.dic">ftp://ftp.iucr.org/pub/ddl_core.dic</a>	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.
<b>CIF restraints dictionary</b>	IUCr standard	ontology; dictionary	CIF	DDL1 <a href="ftp://ftp.iucr.org/pub/ddl_core.dic">ftp://ftp.iucr.org/pub/ddl_core.dic</a>	crystal structure; molecular structure; experimental technique
<b>CIF powder dictionary</b>	IUCr standard	ontology; dictionary	CIF	DDL1 <a href="ftp://ftp.iucr.org/pub/ddl_core.dic">ftp://ftp.iucr.org/pub/ddl_core.dic</a>	crystal structure; molecular structure; chemical analysis; experimental processed data; powder diffraction; chemical composition
<b>CIF modulated and composite structures dictionary</b>	IUCr standard	ontology; dictionary	CIF	DDL1 <a href="ftp://ftp.iucr.org/pub/ddl_core.dic">ftp://ftp.iucr.org/pub/ddl_core.dic</a>	crystal structure; molecular structure; chemical composition
<b>CIF electron density dictionary</b>	IUCr standard	ontology; dictionary	CIF	DDL1 <a href="ftp://ftp.iucr.org/pub/ddl_core.dic">ftp://ftp.iucr.org/pub/ddl_core.dic</a>	crystal structure; molecular structure; single-crystal diffraction; physical properties; charge density
<b>CIF twinning dictionary</b>	IUCr standard	ontology; dictionary	CIF	DDL1 <a href="ftp://ftp.iucr.org/pub/ddl_core.dic">ftp://ftp.iucr.org/pub/ddl_core.dic</a>	crystal structure; single-crystal diffraction; powder diffraction
<b>CIF macromolecular dictionary</b>	IUCr standard	ontology; dictionary	CIF	DDL2 <a href="ftp://ftp.iucr.org/pub/cifdics/mmcif_ddl_2.1.6.dic">ftp://ftp.iucr.org/pub/cifdics/mmcif_ddl_2.1.6.dic</a>	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
<b>CIF image dictionary</b>	IUCr standard	ontology; dictionary	CIF	DDL2 <a href="ftp://ftp.iucr.org/pub/cifdics/mmcif_ddl_2.1.6.dic">ftp://ftp.iucr.org/pub/cifdics/mmcif_ddl_2.1.6.dic</a>	laboratory apparatus; experimental raw data
<b>CIF symmetry dictionary</b>	IUCr standard	ontology; dictionary	CIF	DDL2 <a href="ftp://ftp.iucr.org/pub/cifdics/mmcif_ddl_2.1.6.dic">ftp://ftp.iucr.org/pub/cifdics/mmcif_ddl_2.1.6.dic</a>	crystal structure; symmetry
<b>Online Dictionary of Crystallography</b>	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>



## Other generic metadata systems

- DCMI – Dublin Core Metadata Initiative
- NISO – ISO 23081 Records Management Metadata Standard
- NISO – Z39.87 Data Dictionary: Technical Metadata for Still Images
- PREMIS – Preservation metadata
- METS – Structural metadata regarding objects within a digital library
- TOTEM – Trustworthy Online Technical Environment Metadata Registry



## Concordances

### Relationship between generic and disciplinary metadata formulations

	Generic (DC)	Disciplinary (CIF)
Purpose	Cataloguing; classification; identification; discovery; location; provenance	Reproducibility; provenance; validation; discovery; retrieval
Users	Librarians; digital archivists; repository managers; funders	Scientists; software developers; LIMS developers; data managers; analysts
Granularity	Macro	Micro
Scale	Relatively small (DC: 15 terms)	Relatively large (coreCIF: ~720 terms; pdbx/mmCIF: ~4700 terms)
Stability	Static	Extensible (mmCIF had 4100 terms in 2006)
Semantics	Fluid	Precise

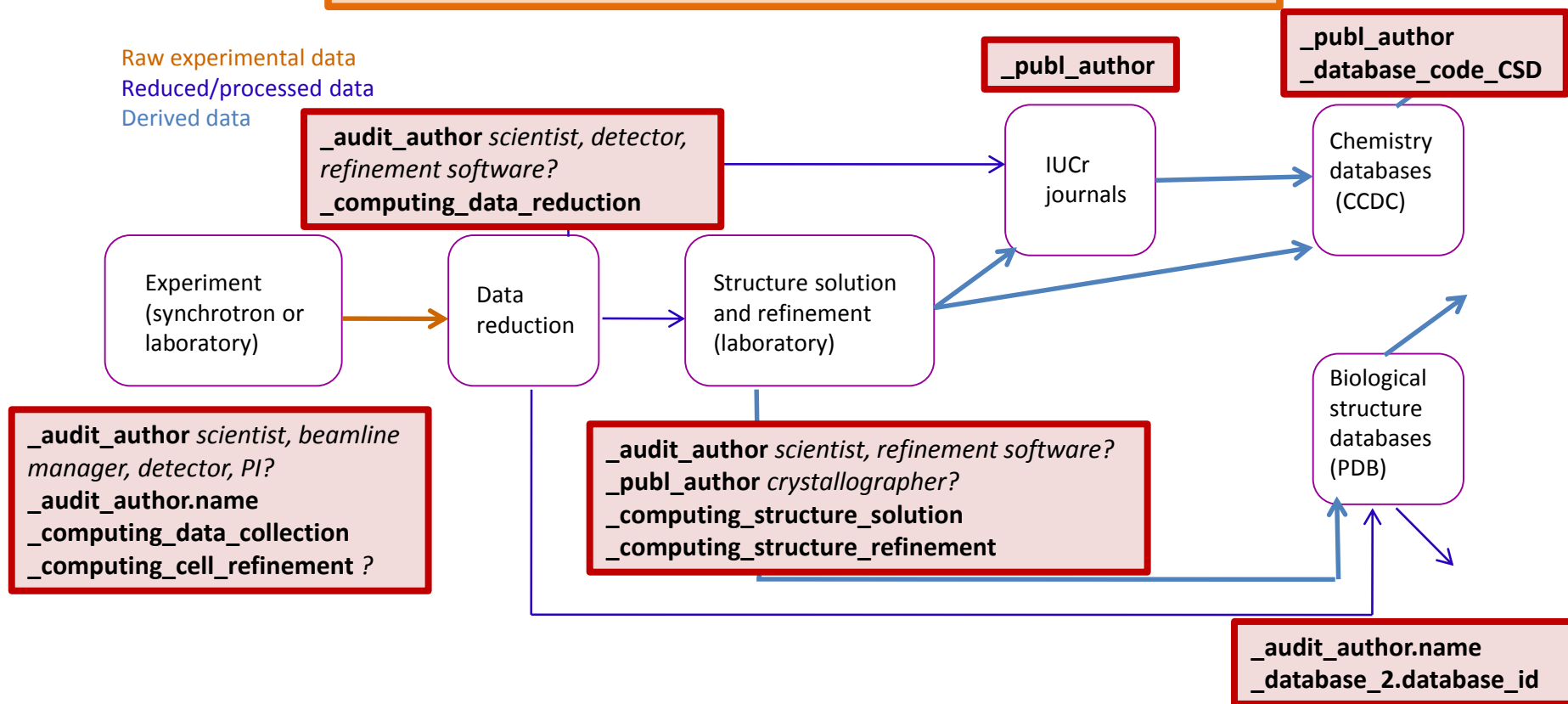
# Concordances

## Contextual significance of a high-level metadata descriptor

### DC: Creator

*An entity primarily responsible for making the resource*

Raw experimental data  
Reduced/processed data  
Derived data





## Middleware

Is there a need for an intermediate ‘glue’ layer of metadata?

	Generic (DC)	<i>Metametadata</i>	Disciplinary (CIF)
Purpose	Cataloguing; classification; identification; discovery; location; provenance	Provenance; classification; purpose; schema; discovery	Reproducibility; provenance; validation; discovery; retrieval
Users	Librarians; digital archivists; repository managers; funders	Repository managers; funders; knowledge base builders; end users	Scientists; software developers; LIMS developers; data managers; analysts
Granularity	Macro	Intermediate	Micro
Scale	Relatively small	As required	Relatively large
Stability	Static	Relatively stable, but extensible	Extensible
Semantics	Fluid	Specific	Precise



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

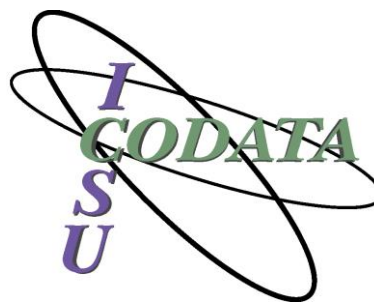
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