



CONNECTING RESEARCH,
ADVANCING KNOWLEDGE

FAIR Facilities and Instruments in DataCite Services

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FAIR Facilities and Instruments Workshop

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About me

Current work

- DataCite: Director of Strategic Programs & Partnerships
- ROR (Research Organization Registry): Director

Prior work

- California Digital Library / EZID
- UC Berkeley Library
- PLOS

Other relevant affiliations & activities

- Make Data Count Advisory Group
- NISO US National PID Strategy WG
- OpenAlex Advisory Board



Roadmap

- Introduction to DataCite
- Overview of facility and instrument use cases at DataCite
- Reflections on workshop recommendations
- Requests for community input and involvement



DataCite at a glance

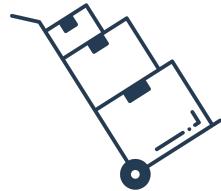


- Global non-profit **membership organization & community of practice**
 - Libraries, repositories, publishers, government agencies, research facilities and other research organizations
- **DOI registration service for outputs, resources, and activities**
 - Publications, datasets, software, samples and specimens, instruments, projects, data management plans, awards, and more
- Open tools and services for **connecting, querying, discovering, analyzing, and integrating DOI and PID metadata**
 - PID graph, REST API, OAI-PMH, data dump, search and dashboard UIs
- **Standard, extensible, interoperable metadata schema**
 - Developed and maintained with user and community input, and aligned to other schemas

DataCite metadata: Powering discovery



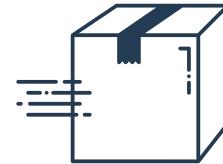
Research organizations provide metadata to DataCite and register a DOI for diverse types of outputs and activities that they produce and manage



DataCite stores the metadata and establishes connections across outputs and activities using PIDs



Metadata is made openly available through DataCite APIs, data files, and interfaces



Metadata is discovered and harvested by users and systems to track and analyze outputs or integrate in other systems

DataCite use cases and benefits



- **Create DOIs** for research outputs, resources, and activities
- Elevate **visibility and discoverability** of research
- **Index and harvest metadata** about research outputs, resources, and activities
- **Uncover connections, trends, and insights** across research outputs and activities
- **Create efficiencies** in research management, tracking, and reporting
- **Align with recommended practices and policies** for FAIR data, open science, public access, and more

DataCite key themes and takeaways



A global, dynamic community for everyone

- **Community-led non-profit open infrastructure**
- Metadata, services, and practices **always evolving alongside community needs**

An expansive and interoperable metadata store

- **More than data**
- A metadata store; **not a content repository**
- DataCite schema can **co-exist with local metadata schemes**
- Schema **designed to support citation & discovery**

One layer of a rich research landscape

- DataCite metadata **underpins many other systems**
- DataCite metadata becomes **more useful when it includes other PIDs**
- **Collaboration and coordination** are key

DataCite for facilities and instruments



Facilities and instruments in DataCite: multiple pathways and approaches



- Resource and output **identification**
- **Attribution and relationships** via metadata schema and PID connections
 - Creator and contributor attribution
 - Institutional attribution (as creator, contributor, publisher, or funder)
 - Funder and funding acknowledgment
 - Related works and identifiers
 - Multiple relationship types
- **Metadata interoperability** via crosswalks/mappings
- **Tracking, reporting, and analysis** via APIs and discovery tools

Resource and output identification

* Resource Type General

The general type of the resource.

Select Resource Type General

Image

Instrument

Interactive resource

Journal

Journal article

Model

Output management

Preprint

E2 - Flat-Cone Diffractometer

<https://doi.org/10.5442/ni000001>

Description

Creators

Contributors

Registration

A 3-dimensional part of the reciprocal space can be scanned in less than five steps by combining the "off-plane E flat-cone layer concept while using a new computer-controlled tilting axis of the detector bank. Parasitic scatter from furnace walls is reduced by an oscillating "radial" collimator. The datasets and all connected information is stored in NeXus file format for each measurement and can be easily archived. The software package TVneXus deals with the transformed physical spaces and the usual data analysis tools (e.g. MatLab). TVneXus can convert to various data formats: diffractograms, linear detector projections, rotation crystal pictures or the 2D/3D reciprocal space.

BER II Beamline published 2019 in Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Instrument

 <https://doi.org/10.5442/ni000001>

Resource and output identification

A screenshot of a web page titled 'DataCite Metadata Schema'. The page features a dark header with the DataCite logo and version '4.6'. Below the header is a search bar labeled 'Search docs'. The main content area includes sections for 'Introduction', 'DataCite Metadata Properties', and 'Appendices'. Under 'Appendices', there is a section for 'Appendix 1: Controlled List Definitions' which lists 'contributorType', 'dateType', and 'resourceTypeGeneral'.

Example: <https://api.datacite.org/dois/application/vnd.datacite.datacite+xml/10.6083/m4qn65c5>

Suggested Dublin Core Mapping: Image

Instrument

Description: A device, tool or apparatus used to obtain, measure and/or analyze data.

Examples and Usage Notes: Note that this is meant to be the instrument instance, e.g., the individual physical device, not the digital description or design of an instrument.

Example:

```
<resourceType resourceTypeGeneral="Instrument">Reflectometer</resourceType>
```

Suggested Dublin Core Mapping: N/A

Metadata schema: Attribution



```
▼ "creators": [
  ▼ {
    "name": "Helmholtz-Zentrum Berlin Für Materialien Und Energie",
    "nameType": "Organizational",
    "affiliation": [],
    ▼ "nameIdentifiers": [
      ▼ {
        "schemeUri": "https://ror.org",
        "nameIdentifier": "https://ror.org/02aj13c28",
        "nameIdentifierScheme": "ROR"
      }
    ]
  }
]
```

Instrument DOI metadata attributes research facility and references facility ROR ID

Metadata schema: Relationships



```
"relatedIdentifiers": [
```

```
    {
```

```
        "relationType": "IsDescribedBy",  
        "relatedIdentifier": "10.17815/jlsrf-4-110",  
        "relatedIdentifierType": "DOI"
```

Instrument DOI metadata references
published article



Journal of large-scale
research facilities

Journal of large-scale research facilities, 4, A129 (2018) <http://dx.doi.org/10.17815/jlsrf-4-110>

Published: 19.03.2018

E2: The Flat-Cone Diffractometer at BER II

Helmholtz-Zentrum Berlin für Materialien und Energie *

Instrument Scientists:

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- Dr. M. Reehuis, Helmholtz-Zentrum Berlin für Materialien und Energie,
Department Quantum Phenomena in Novel Materials,
phone: +49(0)30 8062-42692, e-mail: reehuis@helmholtz-berlin.de

Abstract: The flat-cone diffractometer E2 at the research reactor BER II is a thermal neutron single-crystal diffractometer for 3D reciprocal space mapping by using four delay-line area detectors (300 ×

Metadata schema: Relationships



Neutron study of the topological flux model of hydrogen ions in water ice

CC0 https://doi.org/10.5442/nd000001

Description Creators Registration

The familiarity of water ice means we often overlook its non-trivial character illustrated, for example, by the many snowflake morphologies resulting from disordered combinations of covalent and hydrogen bonds between hydrogen atoms in ice's most common phase (Ih) that keep the H₂O molecular character. Using neutron diffraction on the BER-II, Helmholtz-Zentrum Berlin, we probe the atomic scale configuration in the Ih phase of water ice in a "disordered" state as exhibiting a form of topological order characterized by an emergent gauge field. This is between low-temperature experiment and analytical theory, which even allows us to estimate the density of the emergent gauge field. The development of quantitative models of water ice paves the way for further studies of atomic-scale understanding of this most commonplace of solids. The merged untransformed datasets E2 at the neutron source BER II is given in the Nexus/HDF5 file format. The calculated reciprocal space is given in HDF5 files.

Dataset published 2018 in Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Dataset

https://doi.org/10.5442/nd000001

Dataset DOI metadata references instrument and published article, asserting precise relation types

```
"relatedIdentifiers": [
  {
    "relationType": "IsCitedBy",
    "relatedIdentifier": "10.1103/physrevb.99.174111",
    "relatedIdentifierType": "DOI"
  },
  {
    "relationType": "References",
    "relatedIdentifier": "10.17815/jlsrf-4-110",
    "relatedIdentifierType": "DOI"
  },
  {
    "relationType": "IsCollectedBy",
    "relatedIdentifier": "10.5442/ni000001",
    "relatedIdentifierType": "DOI"
  }
]
```

Published article

Instrument

Metadata schema: Relationships



E2 - Flat-Cone Diffractometer <https://doi.org/10.5442/ni000001>

Description Creators Contributors Registration

A 3-dimensional part of the reciprocal space can be scanned in less than five steps by combining the “off-plane Bragg-scattering” and the flat-cone layer concept while using a new computer-controlled tilting axis of the detector bank. Parasitic scattering from crystal or furnace walls is reduced by an oscillating “radial” collimator. The datasets and all connected information is stored in one independent NeXus file format for each measurement and can be easily archived. The software package TVnexus deals with the raw data sets, the transformed physical spaces and the usual data analysis tools (e.g. MatLab). TVnexus can convert to various data sets e.g. into powder diffractograms, linear detector projections, rotation crystal pictures or the 2D/3D reciprocal space.

BER II Beamline published 2019 in Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Instrument <https://doi.org/10.5442/ni000001>

Connections

```
graph TD; Instrument[Instrument 1] --- Text[Text 1]; Instrument[Instrument 1] --- Dataset[Dataset 1];
```

Related Works

Publication Year

Year	Count
2019	2

Work Types

Type	Percentage
Dataset	50%
Text	50%

Licenses

License	Percentage
Unknown	50%
CC-BY-SA	50%

Neutron study of the topological flux model of hydrogen ions in water ice

J.-U. Hoffmann, K. Siemensmeyer, S. Isakov, D. J. P. Morris, B. Kleimke, I. Glavatsky, K. Seiffert, D. A. Tennant, S. Sondhi & R. Moessner

Dataset published 2018 in Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

The familiarity of water ice means we often overlook its non-trivial character illustrated, for example, by the many snowflake morphologies resulting from disordered combinations of covalent and hydrogen bonds between hydrogen and oxygen atoms in water ice's most common phase (Ih) that keep the H₂O molecular character. Using neutron diffraction on the flat-cone diffractometer E2 at BER-II, Helmholtz-Zentrum Berlin, we probe the atomic scale configuration in the Ih phase of water ice to test theories that describe this “disordered” state as exhibiting a form of topological order characterized by an emergent gauge field. We find excellent agreement between low-temperature experiment and analytical theory, which even allows us to estimate the density of defects charged under this emergent gauge field. The development of quantitative models of water ice paves the way for further studies to develop a comprehensive atomic-scale understanding of this most commonplace of solids. The merged untransformed datasets from the flat-cone diffractometer E2 at the neutron source BER II is given in the Nexus/HDF5 file format. The calculated reciprocal space and the simulation are stored as HDF5 files.

DOI registered March 6, 2018 via DataCite.

Dataset <https://doi.org/10.5442/nd000001>

E2: The Flat-Cone Diffractometer at BER II

Jens-Uwe Hoffmann & Manfred Reehuis

Journal Article published 2018 in Journal of large-scale research facilities JLSRF

The flat-cone diffractometer E2 at the research reactor BER II is a thermal neutron single-crystal diffractometer for 3D reciprocal space mapping by using four delay-line area detectors (300 × 300 mm²). Alternatively it is suitable for powder measurements with medium resolution and broad 2-theta scattering range.

Other Identifiers

Publisher ID: A129

DOI registered via Crossref.

3 Citations

Journal Article <https://doi.org/10.17815/jlsrf-4-110>

Relationships exposed in DataCite Commons discovery interface

Metadata schema: Crosswalks



[☰](#) [DataCite Metadata Schema](#)

[Home](#) / [Mappings](#) / PIDINST Schema Mapping

PIDINST Schema ¹ Mapping

Table 7: PIDINST to DataCite Mapping

PIDINST Property	DataCite v. 4.5	Comments
Identifier	1. Identifier	
identifierType	1.a identifierType "DOI"	
Name	3. Title	May be the title of a dataset, the name of a piece of software or instrument.
Owner	7. Contributor with 7.a contributorType: HostingInstitution	Can be used for the owner of an instrument, i.e. the institution responsible for the management of the instrument. This may include the legal owner, the operator, or an institute providing access to the instrument. Use the contributorType "HostingInstitution". The instrument owner may also be included in 4. Publisher . ²
ownerName	7.1 contributorName	
ownerIdentifier	7.4 namelIdentifier	
ownerIdentifierType	7.4.a namelIdentifierSche me	

Tracking and reporting: analysis



Helmholtz-Zentrum Berlin für Materialien und Energie <https://ror.org/02aj13c28>

430 Works 159 Citations ⓘ 645 Views ⓘ 844 Downloads ⓘ

Founded 2009

Links
Homepage
Wikipedia

Other Identifiers
GRID grid.424048.e
Crossref Funder ID [10.13039/100013110](https://doi.org/10.13039/100013110)
ISNI 0000000110903682
Wikidata Q314578
Wikidata Q316122

Geolocation
52° 31' 27.732" N, 13° 24' 37.908" W

Germany Facility Funder

<https://ror.org/02aj13c28>

430 Works

Publication Year

Work Types

Licenses

Other

Software

Text

Instrument

Journal Article

Dataset

Other

Unknown

CC-BY-4.0

CC-BY-NC-4.0

CC-0-1.0

Apache-2.0

Facility-based tracking and reporting in DataCite Commons discovery interface

Tracking and reporting: citations



NSF/NCAR Hercules C130 Aircraft <https://doi.org/10.5065/d6wm1bg0>

288 Citations

Description Creators Contributors Registration

The C-130 is a versatile and capable research platform that carries a wide variety of scientific payloads. The C-130 has a 10-hour flight endurance, a 2,900 nautical mile range at up to 27,000 ft, and a payload capacity of up to 13,000 lbs. In addition to standard thermodynamic, microphysics and radiation sensors, the C-130 has a roomy fuselage payload area (414 ft²) and many versatile inlets and optical ports. The aircraft carries instruments and sensors in pods and pylons on both wings. The C-130 can carry advanced EOL and community instrumentation.

Aircraft For Earth Observations Research published 1994 in [Earth Observing Laboratory](#)

Physical Object

<https://doi.org/10.5065/d6wm1bg0>

Connections

?

Physical Object

Dataset
444

Citations reporting in DataCite Commons discovery interface

DataCite alignment with workshop recommendations



Use cases and recommendations: themes and reflections



- **DataCite is already well equipped** to support the use cases and align with recommendations
- **Multiple pathways for alignment** via DataCite services and metadata schema
 - DOI registration
 - Metadata properties
 - Connection metadata
 - Metadata crosswalks/mappings
 - DataCite APIs and discovery interfaces
- **Metadata quality and completeness** is a collective challenge and responsibility!

Use cases

as supported by DataCite



Use case	DataCite support
Traceability	<ul style="list-style-type: none">- “Instrument” resource type- Connection metadata to assert relationships and citations- Citations and usage data
Equity	<ul style="list-style-type: none">- Metadata openly available via APIs, DataCite Commons, public data file- Metadata harvested by downstream discovery services
Attribution	<ul style="list-style-type: none">- Metadata about people and organizations associated with facilities and instruments- Citations and usage data
Reproducibility	<ul style="list-style-type: none">- Citation of specific instruments in metadata
Provenance	<ul style="list-style-type: none">- Connection metadata to assert relationships and citations- Related identifiers

Granularity recommendations as supported by DataCite



Use case	Recommendation	DataCite support
Traceability	Less granular PID assignment (e.g. a small number of PIDs assigned at to high-level entities, such as facilities or instruments as a whole)	<ul style="list-style-type: none">- Resource type for "Instrument"
Equity		<ul style="list-style-type: none">- Openly available metadata
Attribution		<ul style="list-style-type: none">- Metadata properties for creator, affiliation, and funder metadata
Reproducibility	More granular PID assignment (e.g. more PIDs assigned to specific low-level instruments, and potentially to particular instrument configurations, with versioning of PIDs and instruments)	<ul style="list-style-type: none">- Related identifiers
Provenance		<ul style="list-style-type: none">- Connection metadata to assert relationships and citations- Related identifiers

Metadata recommendations as supported by DataCite



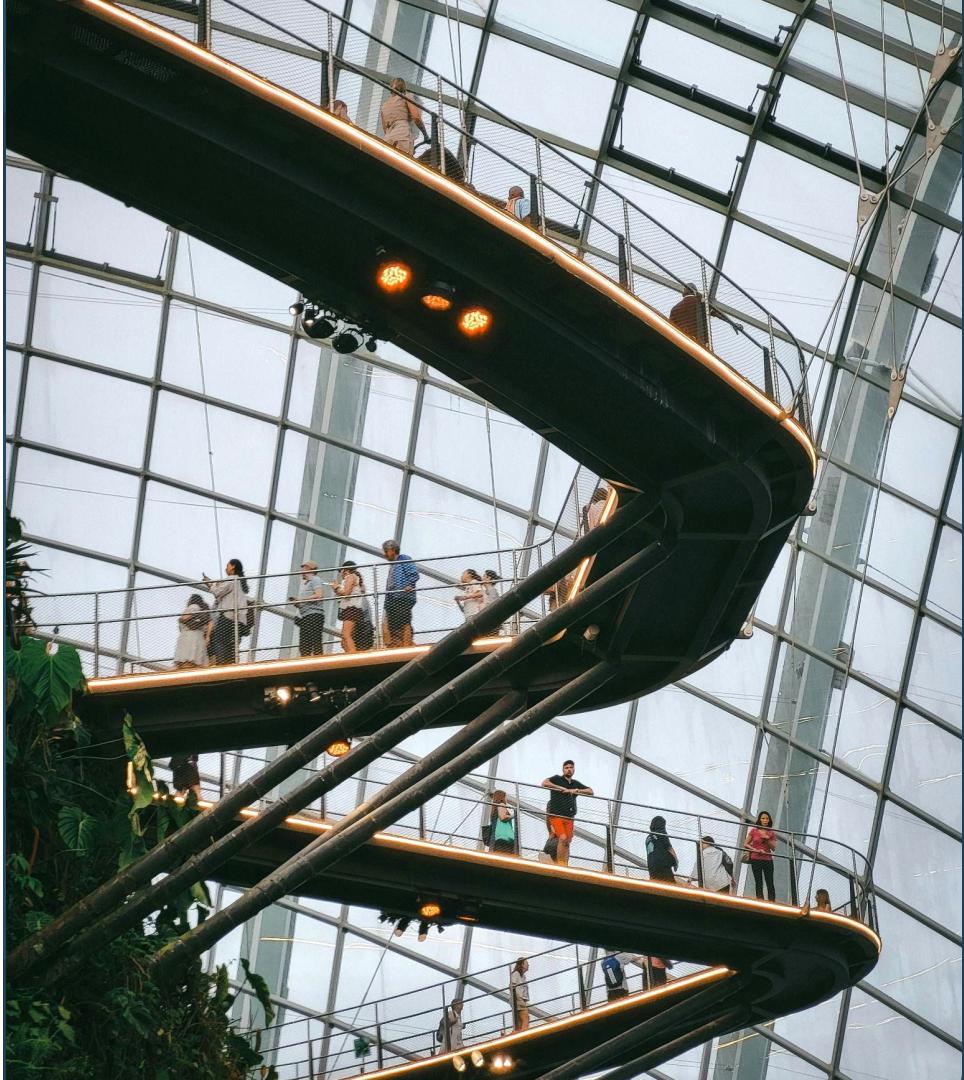
Recommendation	DataCite support
PID metadata should align with the PIDINST metadata guidelines	PIDINST schema mapping
High-level metadata for the Traceability, Equity, & Attribution use cases	“Instrument” resource type
For the Reproducibility & Provenance use cases, more detailed platform/instrument metadata is necessary to include in PID and associated metadata (e.g., protocols, dataset metadata)	More detailed metadata (beyond the scope of the DataCite Metadata Schema) can always be linked using a RelatedIdentifier with relationType="HasMetadata"
Associated metadata beyond what can be included in PID metadata, this should be provided by the responsible party and be made available at (or linked from) the PID landing page	More detailed metadata (beyond the scope of the DataCite Metadata Schema) can always be linked using a RelatedIdentifier with relationType="HasMetadata"
Connections between related PIDs should be included in PID metadata whenever they exist.	relatedIdentifiers metadata property supports multiple types of identifiers, including RRIDs

PID provider recommendations as supported by DataCite



Recommendation	DataCite support
Ensure interoperability among facility/instrument PID systems	<ul style="list-style-type: none">- PIDINST mapping- Related identifier and connection metadata
Develop services that promote use and tracking of PIDs facilities/instruments	<ul style="list-style-type: none">- Citations and metrics
Provide PID metadata options that align with the PIDINST metadata guidelines	<ul style="list-style-type: none">- PIDINST mapping
Provide PID metadata options and/or guidance to enable machine-actionable identification of the type of entity to which the PID refers	<ul style="list-style-type: none">- Controlled list of resource types- PID metadata in specific properties (ORCID, ROR, related identifiers)

**Share your
thoughts & get
involved**



What you can do



- If you're registering DOIs with DataCite: optimize metadata quality and completeness upon registration or update DOIs post-registration
- Share how you're already using DataCite for instrument and facility use cases
- Let us know how DataCite can (better) support your use cases for instruments and facilities?
- Work with us as we explore innovative pathways to metadata enrichments
- Join our community if you're not part of it already!



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