



FIZ Karlsruhe

Leibniz Institute for Information Infrastructure

ADVANCING SCIENCE

Searching and Visualising Inorganic Data in the ICSD

25th IUCr congress - Joint Workshop for CSD and ICSD

Dr. Stephan Rühl, FIZ Karlsruhe, August 12, 2021

ICSD at a glance

> 242,000 records

>43,000
Metals/Alloys

>22,000 Metal-organic structures

> 11,000
Minerals

> 19,000
theoretical
structures

>216,000 fully
determined
structures

>26,000
derived
coordinates

> 9,700
structure
Types

>175,000
assigned to
structure
types

Accessing ICSD Web/API

Authentication methods:

■ LoginID/Password

- Single user
- Multiple users (2-4 users)
- API access



FIZ Karlsruhe – Leibniz Institute for Information Infrastructure

Welcome to ICSD Web.

Login

LoginId:

Password:

Login

Lost password? [Get Demo Account](#)

Navigation

[Basic search & retrieve](#)

[Advanced search & retrieve](#)

[Bibliography](#)

[Cell](#)

[Chemistry](#)

[Symmetry](#)

[Crystal Chemistry](#)

[Structure Type](#)

[Experimental Information](#)

[DB Info](#)

[Expert Search](#)

[Query Management](#)

[Manage Queries](#)

[List Combined Queries](#)

[Create Combined Query](#)

[ICSD links](#)

[ICSD News](#)

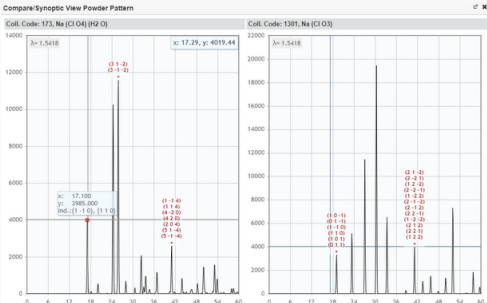
New Features:

- We have added a new search field for the bibliographic search for a DOI. Although not all articles have a DOI stored, at least the vast majority of articles can be found quickly and accurately in this way.
- In the export mask, it is now also possible to run the CIF export not only with the published setting, but also with the standardized setting, which significantly improves the comparability of the structures.
- The ICSD API has been extended so that the content to be used (inorganic structures, organometallic structures, theoretical structures) can now also be selected.

Compare Synoptic View Powder Pattern

Cell Code: 173, Na (Cl O4) (H9 O)

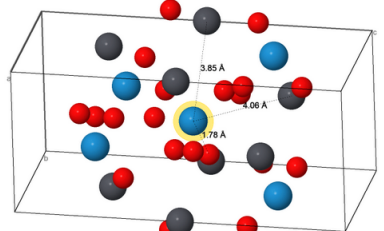
Cell Code: 1391, Na (Cl O3)



Key Features:

- Enhanced search functionality: easy to use and intuitive search interface.
- New and extended information about ICSD including complete Help information.
- Easy analysis of large and complex data sets.
- Simple and powerful query management: load, modify, save and combine queries.
- Personalization/User Profiles for IP access based accounts.
- Visualization of single or multiple crystal structures.
- Generation of simulated powder patterns.
- Content selection (inorganic, metal-organic or theoretical structures).
- Inclusion of abstracts.
- Keywords providing information on Material properties, applications, and methodology.
- Structure types as a sophisticated classification scheme.
- Interactive exploration of atomic environments.
- Customizable display of search results.

Cell Code: 75881, Pb (W O4) - 1994 Xu K-Q...



Accessing ICSD Web/API

Authentication methods:

- IP authentication
 - only for campus/site licenses
- Personalized login/password
 - allows to store private settings

The screenshot displays the ICSD Web interface. At the top, it says 'Welcome to ICSD Web. IP authenticated ([redacted]), Karlsruher Inst fuer Technologie'. The left sidebar contains several sections: 'Login' with fields for 'LoginId' and 'Password', a 'Login Personalized' button, and links for 'Lost password?' and 'Personalize account'; 'Content Selection' with checkboxes for 'Experm. inorganic structures' (checked), 'Experm. metal-organic str.', and 'Theoretical structures'; 'Navigation' with a search icon and a list of categories; 'Advanced search & retrieve' with a search icon and a list of categories; and 'Query Management' with icons and links for 'Manage Queries', 'List Combined Queries', and 'Create Combined Query'. The main content area is titled 'Basic Search & Retrieve' and includes a 'Free Text Search' section with a 'General Attributes' field, a 'Bibliography' section with fields for 'Authors', 'Title of Journal', 'Title of Article', and 'DOI', a 'Chemistry' section with a 'Composition' field and a 'Periodic Table' button, a 'Cell' section with 'Cell Parameters' and 'Cell Volume' fields, a 'Symmetry' section with 'Space Group Symbol', 'Space Group Number', 'Crystal System', and 'Centering' fields, and an 'Exp. Info. & Ref. Data' section with a 'New Data Only' checkbox, 'PDF Number', 'ICSD Collection Code', 'Temperature' (with a unit dropdown set to 'K'), and 'Pressure' (with a unit dropdown set to 'MPa'). On the right side, there is a 'Search Action' section with 'Run Query' and 'Clear Query' buttons, a 'Search Summary' section showing 'Basic Search: -', and a 'Query History' section showing 'Number of queries: 0' and a 'Clear Query History' button. At the bottom of the main content area, there are 'Clear Basic Search' and 'Count Basic Search' buttons.

ICSD - Main interface

Division of the ICSD interface:

- **Header**
- Content selection
 - Basic/Advanced search
 - Query management
- Active search mask
- Query handling
- Results (# of hits)
- Query history (last 30 queries)

The screenshot displays the ICSD web interface. At the top, the header includes the ICSD logo, a welcome message 'Welcome to ICSD Web. Logged in: Ruehl, Stephan', and links for 'FIZ Karlsruhe | Contact', 'Change Password', and 'Logout'.

The main content area is divided into three sections:

- Content Selection:** A sidebar menu with options like 'Experi. inorganic structures', 'Experi. metal-organic str.', 'Theoretical structures', 'Navigation', 'Advanced search & retrieve', 'Bibliography', 'Cell', 'Chemistry', 'Symmetry', 'Crystal Chemistry', 'Structure Type', 'Experimental Information', 'DB Info', 'Expert Search', 'Query Management', 'Manage Queries', 'List Combined Queries', 'Create Combined Query', 'ICSD links', and 'ICSD News'.
- Basic Search & Retrieve:** The central search area with fields for 'Free Text Search', 'Bibliography' (Authors, Title of Journal, Title of Article, DOI), 'Chemistry' (Composition, Periodic Table), 'Cell' (Cell Parameters, Cell Volume, Tolerance), 'Symmetry' (Space Group Symbol, Space Group Number, Crystal System, Centering), and 'Exp. Info. & Ref. Data' (New Data Only, PDF Number, Temperature, ICSD Collection Code, Pressure).
- Search Action:** A sidebar on the right containing 'Run Query', 'Clear Query', 'Search Summary', 'Query History', and a table of recent queries.

The 'Query History' table shows the following data:

Query	Number of hits
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

At the bottom, there are links for 'Legal Notices', 'Privacy Policy', 'Browser Recommendations', and copyright information: '©2021 FIZ Karlsruhe GmbH'. The version number 'Version 4.6.0 (build 20210419-1300) - Data Release 2021.1' is also displayed.

ICSD - Main interface

Division of the ICSD interface:

- Header
- Content selection
- Search mask navigation
 - Basic/Advanced search
 - Query management
- Active search mask
- Query handling
- Results (# of hits)
- Query history (last 30 queries)

The screenshot displays the ICSD web interface. The top header includes the ICSD logo, a welcome message, and user login information. The left sidebar contains navigation links for Content Selection, Navigation, Advanced search & retrieve, Query Management, and ICSD links. The main content area is divided into sections for Basic Search & Retrieve, Bibliography, Chemistry, Cell, Symmetry, and Exp. Info. & Ref. Data. The right sidebar shows Search Action buttons, Search Summary, and Query History.

Content Selection

- ☒ Experm. inorganic structures
- ☒ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Basic search & retrieve
- Advanced search & retrieve
- Bibliography
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info
- Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

Basic Search & Retrieve

Free Text Search

General Attributes

Bibliography

Authors Year of Publication

Title of Journal

Title of Article

DOI

Chemistry

Composition Periodic Table

Cell

Cell Parameters

Cell Volume Tolerance +/- %

Symmetry

Space Group Symbol Space Group Number

Crystal System Centering

Exp. Info. & Ref. Data

New Data Only ☐

PDF Number Temperature K

ICSD Collection Code Pressure MPa

Clear Basic Search Count Basic Search

Search Action

Run Query Clear Query

Search Summary

Basic Search: -

Query History

Number of queries: 3

Clear Query History

2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

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Version 4.6.0 (build 20210419-1300) - Data Release 2021.1

ICSD - Main interface

Division of the ICSD interface:

- Header
- Content selection
- Search mask navigation
 - Basic/Advanced search
 - Query management
- Active search mask
- Query handling
- Results (# of hits)
- Query history (last 30 queries)

The screenshot displays the ICSD web interface. The 'Search mask navigation' section on the left is highlighted with a red box. It includes a 'Content Selection' sidebar with checkboxes for 'Experm. inorganic structures', 'Experm. metal-organic str.', and 'Theoretical structures'. Below this is a 'Navigation' sidebar with links for 'Basic search & retrieve', 'Advanced search & retrieve', 'Bibliography', 'Cell', 'Chemistry', 'Symmetry', 'Crystal Chemistry', 'Structure Type', 'Experimental Information', 'DB Info', and 'Expert Search'. The 'Query Management' section includes 'Manage Queries', 'List Combined Queries', and 'Create Combined Query'. The 'ICSD links' section includes 'ICSD News'. The main content area is titled 'Basic Search & Retrieve' and contains various search fields: 'Free Text Search' (General, Attributes), 'Bibliography' (Authors, Title of Journal, Title of Article, DOI), 'Chemistry' (Composition, Periodic Table), 'Cell' (Cell Parameters, Cell Volume, Tolerance), 'Symmetry' (Space Group Symbol, Space Group Number, Crystal System, Centering), and 'Exp. Info. & Ref. Data' (New Data Only, PDF Number, Temperature, ICSD Collection Code, Pressure). The right sidebar shows 'Search Action' (Run Query, Clear Query), 'Search Summary' (Basic Search: -), 'Query History' (Number of queries: 3, Clear Query History), and a table of recent queries.

Query	Number of hits
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD - Main interface

Division of the ICSD interface:

- Header
- Content selection
- Search mask navigation
 - Basic/Advanced search
 - Query management
- Active search mask
- Query handling
- Results (# of hits)
- Query history (last 30 queries)

The screenshot displays the ICSD web interface. The left sidebar contains navigation menus: 'Content Selection' (with checkboxes for 'Experm. inorganic structures', 'Experm. metal-organic str.', and 'Theoretical structures'), 'Navigation' (with links for 'Basic search & retrieve', 'Bibliography', 'Cell', 'Chemistry', 'Symmetry', 'Crystal Chemistry', 'Structure Type', 'Experimental Information', 'DB Info', and 'Expert Search'), 'Query Management' (with links for 'Manage Queries', 'List Combined Queries', and 'Create Combined Query'), and 'ICSD links' (with a link for 'ICSD News'). The main content area is titled 'Basic Search & Retrieve' and is highlighted with a red box. It contains several search fields: 'Free Text Search' (General Attributes), 'Bibliography' (Authors, Title of Journal, Title of Article, DOI), 'Chemistry' (Composition, Periodic Table, Number of Elements), 'Cell' (Cell Parameters, Cell Volume, Tolerance), 'Symmetry' (Space Group Symbol, Space Group Number, Crystal System, Centering), and 'Exp. Info. & Ref. Data' (New Data Only, PDF Number, Temperature, ICSD Collection Code, Pressure). The bottom of the main area has 'Clear Basic Search' and 'Count Basic Search' buttons. The right sidebar shows 'Search Action' (Run Query, Clear Query), 'Search Summary' (Basic Search: -), and 'Query History' (Number of queries: 3, Clear Query History, and a table of recent queries).

ICSD

Welcome to ICSD Web. Logged in: Ruehl, Stephan

FIZ Karlsruhe | Contact
Change Password | Logout

Content Selection

- ☒ Experm. inorganic structures
- ☒ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Basic search & retrieve
- Bibliography
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info
- Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

Basic Search & Retrieve

Free Text Search

General Attributes

Bibliography

Authors

Title of Journal

Title of Article

DOI

Chemistry

Composition

Periodic Table

Year of Publication

Number of Elements

Cell

Cell Parameters

Cell Volume

Tolerance +/- %

Symmetry

Space Group Symbol

Space Group Number

Crystal System

Centering

Exp. Info. & Ref. Data

New Data Only

PDF Number

Temperature

ICSD Collection Code

Pressure

Clear Basic Search

Count Basic Search

Search Action

Run Query

Clear Query

Search Summary

Basic Search: -

Query History

Number of queries: 3

Clear Query History

2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

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Version 4.6.0 (build 20210419-1300) - Data Release 2021.1

ICSD - Main interface

Division of the ICSD interface:

- Header
- Content selection
- Search mask navigation
 - Basic/Advanced search
 - Query management
- Active search mask
- Query handling
- Results (# of hits)
- Query history (last 30 queries)

The screenshot displays the ICSD web interface. At the top, the header includes the ICSD logo, a welcome message 'Welcome to ICSD Web. Logged in: Ruehl, Stephan', and links for 'FIZ Karlsruhe | Contact', 'Change Password', and 'Logout'. The main content area is divided into several sections:

- Content Selection:** Includes checkboxes for 'Experm. inorganic structures', 'Experm. metal-organic str.', and 'Theoretical structures'.
- Navigation:** A sidebar menu with links for 'Basic search & retrieve', 'Advanced search & retrieve', 'Bibliography', 'Cell', 'Chemistry', 'Symmetry', 'Crystal Chemistry', 'Structure Type', 'Experimental Information', 'DB Info', 'Expert Search', 'Query Management', 'Manage Queries', 'List Combined Queries', 'Create Combined Query', 'ICSD links', and 'ICSD News'.
- Basic Search & Retrieve:** The main search area with fields for 'Free Text Search', 'General Attributes', 'Bibliography' (Authors, Title of Journal, Title of Article, DOI), 'Chemistry' (Composition, Periodic Table), 'Cell' (Cell Parameters, Cell Volume, Tolerance), 'Symmetry' (Space Group Symbol, Space Group Number, Crystal System, Centering), and 'Exp. Info. & Ref. Data' (New Data Only, PDF Number, Temperature, ICSD Collection Code, Pressure).
- Search Action:** A box containing 'Run Query' and 'Clear Query' buttons.
- Search Summary:** A section showing the 'Basic Search' results.
- Query History:** A table showing the last 30 queries with columns for the query time and the number of hits.

At the bottom, there are links for 'Legal Notices', 'Privacy Policy', 'Browser Recommendations', and '©2021 FIZ Karlsruhe GmbH'. The version information 'Version 4.6.0 (build 20210419-1300) - Data Release 2021.1' is also displayed.

Query Time	Number of hits
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD - Main interface

Division of the ICSD interface:

- Header
- Content selection
- Search mask navigation
 - Basic/Advanced search
 - Query management
- Active search mask
- Query handling
- Results (# of hits)
- Query history (last 30 queries)

The screenshot displays the ICSD web interface. The top header includes the ICSD logo, a welcome message, and user information. The left sidebar contains navigation menus for Content Selection, Navigation, Advanced search & retrieve, Query Management, and ICSD links. The main area is titled 'Basic Search & Retrieve' and contains various search fields categorized into Free Text Search, Bibliography, Chemistry, Cell, Symmetry, and Experimental Information & Reference Data. A 'Search Action' panel on the right includes buttons for 'Run Query' and 'Clear Query', a 'Search Summary' box, and a 'Query History' table. The 'Search Summary' box is highlighted with a red border. The 'Query History' table lists the last three queries with their respective hit counts.

Search Summary	
Basic Search:	-

Query History	
Number of queries:	3
Clear Query History	
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD - Main interface

Division of the ICSD interface:

- Header
- Content selection
- Search mask navigation
 - Basic/Advanced search
 - Query management
- Active search mask
- Query handling
- Results (# of hits)
- Query history (last 30 queries)

The screenshot displays the ICSD web interface. The top header includes the ICSD logo, a welcome message, and user information. The left sidebar contains navigation menus for Content Selection, Navigation, Advanced search & retrieve, Query Management, and ICSD links. The main area is titled 'Basic Search & Retrieve' and contains various search fields categorized into Free Text Search, Bibliography, Chemistry, Cell, Symmetry, and Exp. Info. & Ref. Data. On the right, there is a 'Search Action' section with buttons for 'Run Query' and 'Clear Query', a 'Search Summary' section, and a 'Query History' table. The 'Query History' table lists the last three queries with their timestamps and the number of hits.

Query History	
Number of queries:	3
Clear Query History	
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD – Different types of search fields

Different types of search fields:

- Numerical fields
 - Ranges allowed: -, <, >
- Alphanumeric fields
 - Wildcards: *, #
 - Phrase: " "
- Dropdown fields
- Checkboxes
- Command line (Expert search)

The screenshot displays the ICSD (Inorganic Crystal Structure Database) web interface. The top navigation bar includes the ICSD logo, a welcome message, and user information. The main content area is divided into several sections:

- Content Selection:** Includes checkboxes for "Experim. inorganic structures", "Experim. metal-organic str.", and "Theoretical structures".
- Navigation:** A list of search options including "Basic search & retrieve", "Bibliography", "Cell", "Chemistry", "Symmetry", "Crystal Chemistry", "Structure Type", "Experimental Information", "DB Info", and "Expert Search".
- Query Management:** Includes "Manage Queries", "List Combined Queries", and "Create Combined Query".
- ICSD links:** Includes "ICSD News".
- Basic Search & Retrieve:** The main search area with a "Free Text Search" field containing "crystal structure". Below this are sections for "Bibliography", "Chemistry", "Cell", "Symmetry", and "Exp. Info. & Ref. Data".
- Search Action:** Includes "Run Query" and "Clear Query" buttons.
- Search Summary:** Displays the current search criteria and results.
- Query History:** A table showing previous queries and their results.

A dropdown menu is open for the "Title of Journal" field, showing a list of journals including "Journal of Alloy Phase Diagrams".

ICSD – Basic search mask

Basic search mask:

- Mask is handled separately from advanced search masks
- Switching from/to this mask transfers query options
- Covers most frequently used fields from advanced search masks
- „General attributes“ (Search through all text fields in ICSD)
- „Cell parameters“ expects all 6 parameters

ICSD Welcome to ICSD Web. Logged in: Ruehl, Stephan FIZ Karlsruhe | Contact Change Password | Logout

Content Selection

- ☒ Experm. inorganic structures
- ☒ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Basic search & retrieve
- Advanced search & retrieve
- Bibliography
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info
- Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

Basic Search & Retrieve

Free Text Search

General Attributes

Bibliography

Authors Year of Publication

Title of Journal

Title of Article

DOI

Chemistry

Composition Periodic Table

Number of Elements

Cell

Cell Parameters

Cell Volume Tolerance +/- %

Symmetry

Space Group Symbol Space Group Number

Crystal System Centering

Exp. Info. & Ref. Data

New Data Only ☐

PDF Number Temperature K

ICSD Collection Code Pressure MPa

Search Action

Search Summary

Basic Search: -

Query History

Number of queries: 3

2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD – Advanced search mask - Bibliography

- Details of the reference
- Abstracts
 - only for newer entries (≥ 2016)
 - not for all journals
- Keywords
 - only for newer entries (≥ 2017)
 - not the keywords from the publications)

ICSD

Welcome to ICSD Web. Logged in: Ruehl, Stephan

FIZ Karlsruhe | Contact
Change Password | Logout

Content Selection

- ☒ Experm. inorganic structures
- ☒ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Basic search & retrieve
- Advanced search & retrieve**
- Bibliography
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info
- Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

Bibliography Search

Authors: e.g. Jansen

Title of Journal: e.g. Angewandte Chemie

Title of Article: e.g. Super conducting crystals

Year of Publication: e.g. >2008 or 2000-2006 or 2001

Volume: e.g. 10

Page first: e.g. 10

Abstract:

Keywords: e.g. hybrid cage clusters

DOI: e.g. 10.1016/0022-4596(76)90194-8

Search Action

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-

Query History

Number of queries:	3
Clear Query History	
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD – Advanced search mask - Cell

- Cell related search parameter
- Option to reduce the cell parameter
- Cell parameter can be:
 - experimental cell
 - standardized cell
 - reduced cell

The screenshot displays the ICSD Advanced search mask for cell parameters. The interface is divided into several sections:

- Content Selection:** Includes checkboxes for "Experim. inorganic structures", "Experim. metal-organic str.", and "Theoretical structures".
- Navigation:** A sidebar menu with options like "Basic search & retrieve", "Advanced search & retrieve", "Bibliography", "Cell", "Chemistry", "Symmetry", "Crystal Chemistry", "Structure Type", "Experimental Information", "DB Info", "Expert Search", "Query Management", "Manage Queries", "List Combined Queries", "Create Combined Query", "ICSD links", and "ICSD News".
- Cell Search:** The main search area with fields for "Cell Length a", "Cell Length b", "Cell Length c", "Cell Angle α ", "Cell Angle β ", "Cell Angle γ ", "Cell Volume", "Calc. Density" (with units g/cm³), "Global Tolerance +/-" (with a percentage field), "Reduce Cell Parameters" (checkbox), "Centering" (dropdown menu set to "Primitive"), "Units of Length" (dropdown menu set to "Å"), and "Search Cell Data" (dropdown menu set to "Experimental Cell"). There are buttons for "Clear Cell Search" and "Count Cell Search".
- Search Action:** Includes "Run Query" and "Clear Query" buttons.
- Search Summary:** A table showing search results for various categories: Bibliography, Cell, Chemistry, Symmetry, Crystal Chemistry, Structure Types, Experimental Info, DB Info, and Expert.
- Query History:** A table showing the number of queries and the count of results for specific queries.

Category	Count
Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-

Query ID	Number of queries	Count
2021-07-20T12:10	3	736
2021-07-20T11:35		1808
2021-07-20T11:27		941

ICSD – Advanced search mask - Chemistry

- Search fields related to the chemistry
- Composition (periodic table):
 - may contain stoichiometric coefficients and/or oxidation states (e.g. O:3:4:-2:0)
 - Elements in brackets means one of them (OR)
 - Hyphen before an element excludes it (NOT)

ICSD

Welcome to ICSD Web. Logged in: Ruehl, Stephan

FIZ Karlsruhe | Contact
Change Password | Logout

Content Selection

- ☒ Experm. inorganic structures
- ☒ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Q Basic search & retrieve
- Advanced search & retrieve**
- Q Bibliography
- Q Cell
- Q Chemistry
- Q Symmetry
- Q Crystal Chemistry
- Q Structure Type
- Q Experimental Information
- Q DB Info
- Q Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

Chemistry Search

Composition [Periodic Table](#) Number of Elements
e.g. Na Cl

Structural Formula
e.g. Pb (W O4)

Chemical Name

Mineral Name
e.g. Adamite

Mineral Group
e.g. Pyroxene

ANX Formula Number of Formula Units

AB Formula

Formula Weight

[Clear Chemistry Search](#) [Count Chemistry Search](#)

Search Action

[Run Query](#) [Clear Query](#)

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-

Query History

Number of queries:	3
Clear Query History	
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD – Advanced search mask – Chemistry / Periodic Table

- Can be used instead of typing in the composition field. Allows selecting:

- Elements
- Groups (LIG, BEG, SCG, ...)
- Periods (1PE, 2PE, 3PE, ...)
- Special groups like
 - Metals (MET), Transition-Metals (TME), Non-Metals (NME), Lanthanoids (LAN), Actinoids (ACT)

ICSD

Welcome to ICSD Web. Logged in: Ruehl, Stephan

Content Selection

- ☒ Experim. inorganic structures
- ☐ Experim. metal-organic str.
- ☐ Theoretical structures

Navigation

- Q Basic search & retrieve
- Advanced search & retrieve
 - Q Bibliography
 - Q Cell
 - Q Chemistry
 - Q Symmetry
 - Q Crystal Chemistry
 - Q Structure Type
 - Q Experimental Information
 - Q DB Info
 - Q Expert Search
- Query Management
 - Manage Queries
 - List Combined Queries
 - Create Combined Query
- ICSD links
 - ICSD News

Chemistry Search

Composition e.g. Na Cl

Periodic Table

Number of Elements

Search Action

Run Query Clear Query

Search Summary

Bibliography: -

Cell: -

Chemistry: -

Symmetry: -

Crystal Chemistry: -

Structure Types: -

Experimental Info: -

DB Info: -

Expert: -

Query History

Number of queries: 2

Clear Query History

2021-07-21T11:43 1342

2021-07-21T11:42 858

Search Chemistry Visual Search mode

→ H ↓ ↓ He

→ Li Be

→ Na Mg ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ B C N O F Ne

→ K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr

→ Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe

→ Cs Ba Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn

→ Fr Ra Rf Db

→ La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu

→ Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

→ Metals → Transition Metals → Non-Metals

Click on element or select period and/or group.

Number of Elements Units of Coefficients Moles

El.Symb. Co.(min) Co.(max) Ox.(min) Ox.(max)

AND ▼ LIG X

AND ▼ 5PE X

AND ▼ NME X

☐ Restrict total number of elements to selected number of elements

OK Cancel

ICSD – Advanced search mask - Chemistry

- Chemical names are not IUPAC conform, best to use this only to identify groups (e.g. sulfate, phosphate, ...)
- Mineral names are not IMA approved names, but this will be added continuously
- ANX formula and AB formula very similar (AB takes H into account and does not use predefined letters for cations, anions or neutral atom types)

The screenshot displays the ICSD Chemistry Search interface. At the top, it says 'Welcome to ICSD Web. Logged in: Ruehl, Stephan'. The interface is divided into several sections:

- Content Selection:** Includes checkboxes for 'Experim. inorganic structures', 'Experim. metal-organic str.', and 'Theoretical structures'.
- Navigation:** A sidebar with links for 'Basic search & retrieve', 'Advanced search & retrieve', 'Bibliography', 'Cell', 'Chemistry', 'Symmetry', 'Crystal Chemistry', 'Structure Type', 'Experimental Information', 'DB Info', 'Expert Search', 'Query Management', 'Manage Queries', 'List Combined Queries', 'Create Combined Query', 'ICSD links', and 'ICSD News'.
- Chemistry Search:** The main search area with fields for 'Composition' (e.g. Na Cl), 'Structural Formula' (e.g. Pb (W O4)), 'Chemical Name', 'Mineral Name' (e.g. Adamite), 'Mineral Group' (e.g. Pyroxene), 'ANX Formula', 'AB Formula', and 'Formula Weight'. It also includes a 'Periodic Table' button and a 'Number of Elements' field.
- Search Action:** Buttons for 'Run Query' and 'Clear Query'.
- Search Summary:** A table showing search results for 'Bibliography', 'Cell', 'Chemistry', 'Symmetry', 'Crystal Chemistry', 'Structure Types', 'Experimental Info', 'DB Info', and 'Expert'.
- Query History:** A table showing the number of queries and the date/time of the last query.

Search Action	Run Query	Clear Query
Bibliography:	-	-
Cell:	-	-
Chemistry:	-	-
Symmetry:	-	-
Crystal Chemistry:	-	-
Structure Types:	-	-
Experimental Info:	-	-
DB Info:	-	-
Expert:	-	-

Number of queries:	3
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD – Rules to determine ANX formulae

- H is not taken into account, coordinates for all other atoms must be determined.
- Different atom types on the same position are treated as one single atom type (highest site occupation factor SOF). If the SOFs are equal, the first atom type is the relevant atom type.
Exception: anions and cations occupying the same site will not be treated as one atom type.
- All sites occupied by the same atom type are combined unless the oxidation state is different.
- For each atom type the multiplicities are multiplied by the SOFs and the products are added. The sums are rounded and divided by the greatest common divisor. If necessary, all sums are being multiplied by a common factor so that the smallest sum is equal to 1.0.
- Cations are assigned the symbols A–M, neutral atoms N–R and anions are assigned X, Y, Z, S–W.
- The symbols are sorted alphabetically with ascending indices: AB₂X₄, not A₂BX₄.
- All ANX formulae with more than 4 cation symbols, 3 neutral symbols or 3 anion symbols are deleted.

ICSD – Advanced search mask - Symmetry

- Search fields related to the symmetry
- Only experimental cell is covered
- Wyckoff Sequence does not handle a blank as a string separator

The screenshot displays the ICSD Advanced search mask for Symmetry. The interface is divided into several sections:

- Content Selection:** Includes checkboxes for "Experim. inorganic structures", "Experim. metal-organic str.", and "Theoretical structures".
- Navigation:** A list of search categories including Basic search & retrieve, Bibliography, Cell, Chemistry, Symmetry, Crystal Chemistry, Structure Type, Experimental Information, DB Info, and Expert Search.
- Query Management:** Options to Manage Queries, List Combined Queries, and Create Combined Query.
- ICSD links:** A link to ICSD News.
- Symmetry Search:** The main search area with fields for Space Group Symbol (e.g., Fm-3m), Space Group Number (e.g., 1 or 3-120), Crystal System, Crystal Class, Laue Class, Wyckoff Sequence, Pearson Symbol, Polar Axis, Centering, Crystal Class Notation (HM- or Schoenflies-Notation), and Inversion Center. It also includes a "Note: Restrictions apply to Experimental Cell" and buttons for "Clear Symmetry Search" and "Count Symmetry Search".
- Search Action:** Buttons for "Run Query" and "Clear Query".
- Search Summary:** A table showing the results of the search across various categories.
- Query History:** A table showing the number of queries and the date of the search.

Search Summary	
Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-

Query History	
Number of queries:	3
Clear Query History	
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD – Advanced search mask – Crystal Chemistry

- Interatomic distances
 - can include oxidation states
- Minimum distances
 - Similar to interatomic distances, but only the smallest distance is used
- Some classification of entries:
 - Mineral
 - Structure type (assigned)
 - Structure type prototype

The screenshot displays the ICSD web interface for Crystal Chemistry search. The top navigation bar includes the ICSD logo, a welcome message for user 'Ruehl, Stephan', and links for 'FIZ Karlsruhe | Contact', 'Change Password', and 'Logout'.

Content Selection: Includes checkboxes for 'Experim. inorganic structures' (checked), 'Experim. metal-organic str.' (checked), and 'Theoretical structures' (unchecked).

Navigation: A sidebar menu with options: 'Basic search & retrieve', 'Advanced search & retrieve' (selected), 'Bibliography', 'Cell', 'Chemistry', 'Symmetry', 'Crystal Chemistry', 'Structure Type', 'Experimental Information', 'DB Info', and 'Expert Search'.

Query Management: Includes 'Manage Queries', 'List Combined Queries', and 'Create Combined Query'.

ICSD links: Includes 'ICSD News'.

Crystal Chemistry Search: The main search area with three sections:

- Interatomic Distances:** A table with columns for Atom A, Ox. A, Atom B, Ox. B, d_{min}AB, and d_{max}AB. It includes three rows of input fields and 'AND' dropdown menus.
- Minimum Distances:** A section with columns for Atom A, Atom B, d_{min}AB, and d_{max}AB, with input fields for each.
- Crystal Structure is:** A section with checkboxes for 'Polytype Structure', 'Modulated Structure', 'Disordered Structure', 'Order/Disorder Structure', 'Mineral', and 'Prototype Structure Type'. There is also a 'Structure Type' checkbox.

Buttons at the bottom include 'Clear Crystal Search' and 'Count Crystal Search'.

Search Action: Includes 'Run Query' and 'Clear Query' buttons.

Search Summary: A table showing search results for various categories:

Category	Count
Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-

Query History: A table showing the number of queries and the count of results for each query:

Query ID	Number of queries	Count
2021-07-20T12:10	3	736
2021-07-20T11:35	3	1808
2021-07-20T11:27	3	941

ICSD – Advanced search mask – Structure type

- Two ways to search for structure types
 - Direct search for the type
 - Search for the main descriptors for the structure type
 - Space Group
 - Wyckoff Sequence
 - Pearson Symbol
 - ANX formula
- A detailed list of all structure types can be found under the link provided on the search mask.

The screenshot shows the ICSD web interface for a Structure Type search. The page is titled "ICSD" and includes a welcome message: "Welcome to ICSD Web. Logged in: Ruehl, Stephan". The search mask is divided into several sections:

- Content Selection:** Includes checkboxes for "Experim. inorganic structures", "Experim. metal-organic str.", and "Theoretical structures".
- Navigation:** A list of search options: "Basic search & retrieve", "Advanced search & retrieve", "Bibliography", "Cell", "Chemistry", "Symmetry", "Crystal Chemistry", "Structure Type", "Experimental Information", "DB Info", "Expert Search", "Query Management", "Manage Queries", "List Combined Queries", "Create Combined Query", "ICSD links", and "ICSD News".
- Structure Type Search:** The main search area with a "Pre Defined Structure Types" section. It includes a "Structure Type" input field with the example "e.g. Mg2SiO4". Below this is a checkbox for "Search in predefined structure types" and a section for "Structure Type Descriptors" with input fields for "SpaceGrp", "Wyck", "Pearson", and "ANX". At the bottom of this section are buttons for "Clear Structure Search" and "Count Structure Search".
- Search Action:** Includes "Run Query" and "Clear Query" buttons.
- Search Summary:** A table showing search results for various categories: Bibliography, Cell, Chemistry, Symmetry, Crystal Chemistry, Structure Types, Experimental Info, DB Info, and Expert. Each category has a corresponding count.
- Query History:** A table showing the number of queries and the results for each query. The table has columns for the query date and time, and the number of results.

Search Summary	
Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-

Query History	
Number of queries:	3
Clear Query History	
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD – Advanced search mask – Experimental information

- Search fields related to the data collection and refinement
 - Radiation type
 - Sample type
 - Temperature/pressure
 - Other information

The screenshot displays the ICSD Advanced search interface. The top navigation bar includes the ICSD logo, a welcome message for 'Ruehl, Stephan', and links for 'FIZ Karlsruhe | Contact', 'Change Password', and 'Logout'. The left sidebar contains sections for 'Content Selection' (with checkboxes for 'Experim. inorganic structures', 'Experim. metal-organic str.', and 'Theoretical structures'), 'Navigation' (with links for 'Basic search & retrieve' and 'Advanced search & retrieve'), 'Query Management' (with links for 'Manage Queries', 'List Combined Queries', and 'Create Combined Query'), and 'ICSD links' (with a link for 'ICSD News'). The main search area is titled 'Experimental Information Search' and includes input fields for 'Temperature' (with a unit dropdown set to 'K'), 'Pressure' (with a unit dropdown set to 'MPa'), and 'Comments' (with a placeholder 'e.g. stable above'). There are also fields for 'R-Value' and 'Radiation Type' (with checkboxes for 'X-Ray', 'Electrons', 'Neutrons', and 'Synchrotron'). The 'Sample Type' section has checkboxes for 'Powder' and 'Single Crystal'. The 'Additional Properties' section contains two columns of checkboxes for various data types, including 'Twinned Crystal Data', 'Rietveld Refinement employed', 'Anharmonic Temperature Factors given', 'Absolute Configuration determined', 'Experimental PDF number assigned', 'Calculated PDF number assigned', 'NMR Data available', 'Magnetic Structure available', 'Correction of earlier work', 'Temperature Factors available', 'Cell Constants without s.d.', and 'Only Cell and Structure Type determined'. At the bottom of the search area are buttons for 'Clear Experimental Info Search' and 'Count Experimental Info Search'. On the right side, there is a 'Search Action' section with 'Run Query' and 'Clear Query' buttons, a 'Search Summary' section with a list of search criteria and their counts, and a 'Query History' section with a table of previous queries.

Search Summary	
Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-

Query History	
Number of queries:	3
Clear Query History	
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD – Advanced search mask – DB info

- Database-related information
 - Collection code (identifier)
 - Release tag (release version)
 - Recording date
 - Modification date (last mod)

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Content Selection

- ☒ Experm. inorganic structures
- ☒ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Basic search & retrieve
- Advanced search & retrieve**
- Bibliography
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info
- Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

DB Info Search

ICSD Collection Code e.g. 9061 or 90000-95000

PDF Number e.g. 47-1360

Release Tag e.g. 2007.1 or 2005.1-2007.1

Recording Date yyyy-mm-dd, e.g. 1998-06-26

Modification Date yyyy-mm-dd, e.g. 2006-04-01

New Data Only ☐

Search Action

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-

Query History

Number of queries:	3
Clear Query History	
2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

ICSD – Advanced search mask – Expert search

- Command line to search the ICSD (43 search fields are covered)
- Allows combining searches using
 - Boolean operators (AND, OR, NOT)
 - Brackets

ICSD

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Content Selection

- ☒ Experm. inorganic structures
- ☒ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Q Basic search & retrieve
- Advanced search & retrieve
 - Q Bibliography
 - Q Cell
 - Q Chemistry
 - Q Symmetry
 - Q Crystal Chemistry
 - Q Structure Type
 - Q Experimental Information
 - Q DB Info
 - Q Expert Search
- Query Management**
 - Manage Queries
 - List Combined Queries
 - Create Combined Query
- ICSD links**
 - ICSD News

Expert Search

Your Query

e.g. authors: jansen AND publicationyear: 2000-2010

Description of available SearchTerms

SearchTerm	Description	Input Type
AUTHORS	BIBLIOGRAPHY : Authors name for the main (first) reference	Text
ARTICLE	BIBLIOGRAPHY : Title of article for the main (first) reference	Text
PUBLICATIONYEAR	BIBLIOGRAPHY : Year of publication of an article in the reference	Numerical, integer
PAGEFIRST	BIBLIOGRAPHY : First page number of an article in the reference	Numerical, integer
JOURNAL	BIBLIOGRAPHY : Title of journal for the reference	Text
VOLUME	BIBLIOGRAPHY : Volume of the journal in the reference	Numerical, integer
ABSTRACT	BIBLIOGRAPHY : Abstract for the main (first) reference	Text
KEYWORDS	BIBLIOGRAPHY : Keywords for the main (first) reference	Text
DOI	BIBLIOGRAPHY : DOI of the Article	Text
CELLVOLUME	CELL SEARCH : Cell volume	Numerical, floating point
CALCDENSITY	CELL SEARCH : Calculated density	Numerical, floating point
CELLPARAMETERS	CELL SEARCH : Cell lenght a,b,c and angles alpha, beta, gamma separated by whitespace, i.e.: a b c alpha beta gamma, * if any value	Numerical, floating point
SEARCHCELLDATA	CELL SEARCH : Restriction of Cellparameters.	experimental, reduced, standardized
STRUCTUREDFORMULA	CHEMISTRY SEARCH : Search for typical chemical groups	Text
CHEMICALNAME	CHEMISTRY SEARCH : Search for (parts of) the chemical name	Text
MINERALNAME	CHEMISTRY SEARCH : Search for the mineral name	Text
MINERALGROUP	CHEMISTRY SEARCH : Search for the mineral group	Text
ZVALUE	CHEMISTRY SEARCH : Number of formula units per unit cell	Integer
ANXFORMULA	CHEMISTRY SEARCH : Search for the ANX formula	Text
ABFORMULA	CHEMISTRY SEARCH : Search for the AB formula	Text

Search Action

Run Query Clear Query

Search Summary

Bibliography: -
Cell: -
Chemistry: -
Symmetry: -
Crystal Chemistry: -
Structure Types: -
Experimental Info: -
DB Info: -
Expert: -

Query History

Number of queries: 3

Clear Query History

2021-07-20T12:10	736
2021-07-20T11:35	1808
2021-07-20T11:27	941

Clear Expert Search Count Expert Search

ICSD – Query Management – Manage Queries

- Shows the queries from the Query History (last 30 queries) and already stored queries
- Allows to
 - Load query (into the search masks)
 - Run query (first query is loaded into search mask)
 - Save/delete selected queries

ICSD

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Content Selection

- ☒ Experm. inorganic structures
- ☐ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Basic search & retrieve

Advanced search & retrieve

- Bibliography
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info
- Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

	Query Name	Date	Query Type	# of hits	Saved
☐	2021-07-21T11:43	2021-07-21T11:43	Advanced	1342	
☐	2021-07-21T11:42	2021-07-21T11:42	Basic	858	

Query Name:

Release tag: 2021.1

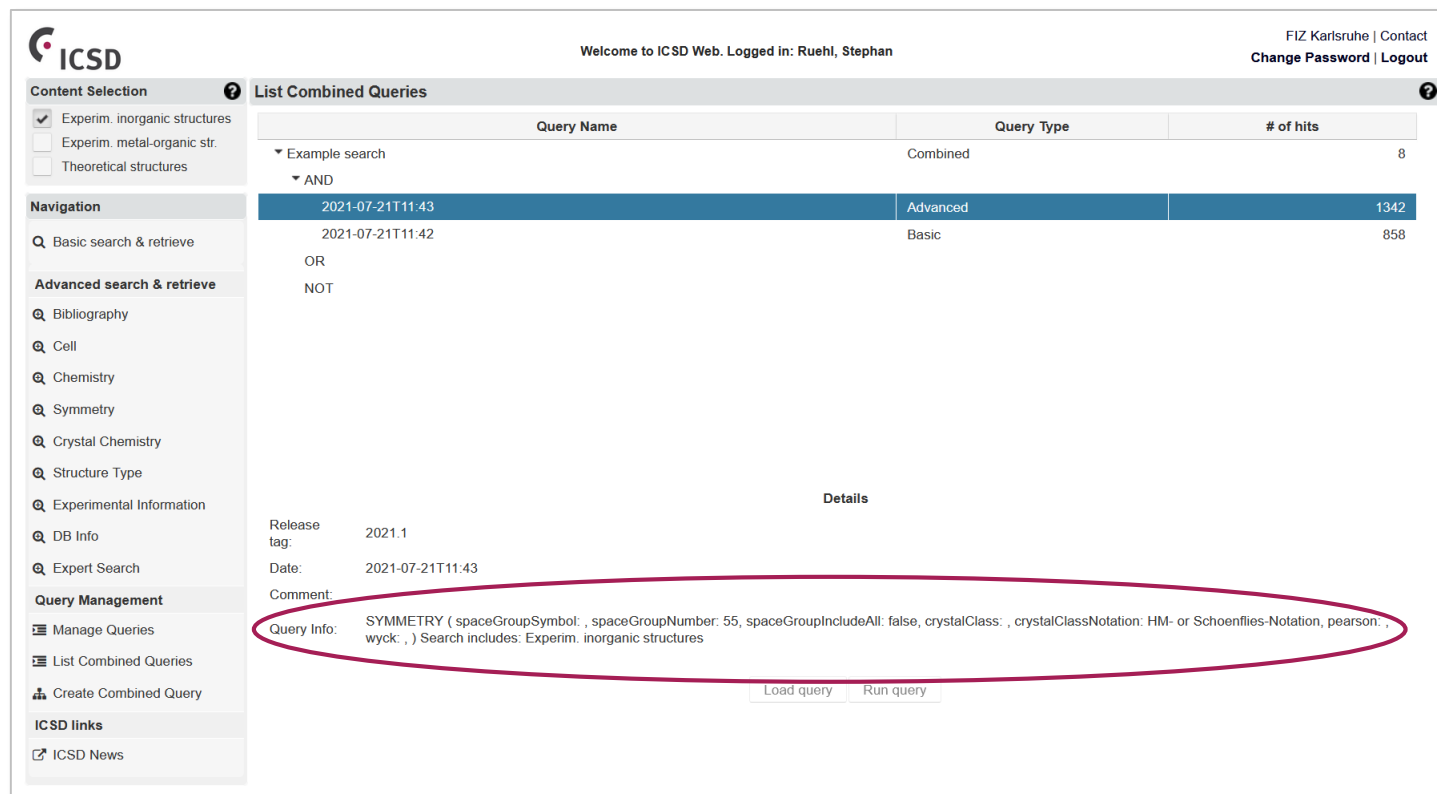
Date: 2021-07-21T11:42

Comment:

Query Info:
CHEMISTRY (pse: [unit of coefficients=Moles, restrictEI=false], composition: , elCount: >2,)
BIBLIOGRAPHY (authorNames: jansen, articleTitle: , journalTitle: , doi: ,)
Search includes: Experm. inorganic structures

ICSD – Query Management – List Combined Queries

- Shows more details on the stored combined queries
- Load/run the query
- Info includes
 - Used queries
 - details for Basic / Advanced
 - Combined queries only provide info on basic and advanced queries used
- Boolean operators used



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Content Selection

- ☒ Experm. inorganic structures
- ☐ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Q Basic search & retrieve

Advanced search & retrieve

- Q Bibliography
- Q Cell
- Q Chemistry
- Q Symmetry
- Q Crystal Chemistry
- Q Structure Type
- Q Experimental Information
- Q DB Info
- Q Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

List Combined Queries

Query Name	Query Type	# of hits
▼ Example search	Combined	8
▼ AND		
2021-07-21T11:43	Advanced	1342
2021-07-21T11:42	Basic	858
OR		
NOT		

Details

Release tag: 2021.1

Date: 2021-07-21T11:43

Comment:

Query Info: SYMMETRY (spaceGroupSymbol: , spaceGroupNumber: 55, spaceGroupIncludeAll: false, crystalClass: , crystalClassNotation: HM- or Schoenflies-Notation, pearson: , wyck: ,) Search includes: Experm. inorganic structures

Load query Run query

ICSD – Query Management – List Combined Queries

- Shows more details on the stored combined queries
- Load/run the query
- Info includes
 - Used queries
 - details for Basic / Advanced
 - Combined queries only provide info on basic and advanced queries used
 - Boolean operators used

ICSD

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Content Selection ?

- ☒ Experim. inorganic structures
- ☐ Experim. metal-organic str.
- ☐ Theoretical structures

Navigation

- Q Basic search & retrieve

Advanced search & retrieve

- Q Bibliography
- Q Cell
- Q Chemistry
- Q Symmetry
- Q Crystal Chemistry
- Q Structure Type
- Q Experimental Information
- Q DB Info
- Q Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

List Combined Queries

Query Name	Query Type	# of hits
Example search	Combined	8
AND		
2021-07-21T11:43	Advanced	1342
2021-07-21T11:42	Basic	858
OR		
NOT		

Details

Release tag: 2021.1

Date: 2021-07-21T11:51

Comment: Author: Jansen, El_Count: >2; Spacegroup: 55

Query Info: AND (2021-07-21T11:43, 2021-07-21T11:42,) OR () NOT () Search includes: Experim. inorganic structures

Load query Run query

ICSD – Query Management – Create Combined Queries

- Easy way to combine queries (point and click)
- Possible boolean operators:
 - AND, OR, NOT
- Basic, advanced and combined queries can be used

Tipp: Provide a meaningful name for combined queries

ICSD

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Content Selection

- ☒ Experim. inorganic structures
- ☐ Experim. metal-organic str.
- ☐ Theoretical structures

Navigation

- Q Basic search & retrieve
- Advanced search & retrieve**
- Q Bibliography
- Q Cell
- Q Chemistry
- Q Symmetry
- Q Crystal Chemistry
- Q Structure Type
- Q Experimental Information
- Q DB Info
- Q Expert Search

Query Management

- Manage Queries
- List Combined Queries
- Create Combined Query

ICSD links

- ICSD News

Create Combined Query

Name:

Comment:

Available Queries:

☐	Query Name	Date	Query Type	# of hits	Saved
☐	2021-07-21T11:43	2021-07-21T11:43	Advanced	1342	
☐	2021-07-21T11:42	2021-07-21T11:42	Basic	858	

Must have (AND):

☐					
☐	2021-07-21T11:43	2021-07-21T11:43	Advanced	1342	
☐	2021-07-21T11:42	2021-07-21T11:42	Basic	858	

Must have at least one of (OR):

No records found.

Must not have (NOT):

No records found.

Run query Count query Clear

ICSD – Example: high temperature superconductors

Interest: high temperature
superconducting ceramics

- First known: $\text{Ba}_2\text{Cu}_3\text{LaO}_7$ (1986)
- Better T_c ($\sim 90\text{k}$): $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ > (1987)



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Content Selection

☒ Experi. inorganic structures

☒ Experi. metal-organic str

☐ Theoretical structures

Navigation

Q Basic search & retrieve

Advanced search & retrieve

Q Bibliography

Q Cell

Q Chemistry

Q Symmetry

Q Crystal Chemistry

Q Structure Type

Q Experimental Information

Q DB Info

Q Expert Search

Query Management

≡ Manage Queries

≡ List Combined Queries

👤 Create Combined Query

ICSD links

🔗 ICSD News

Basic Search & Retrieve

Free Text Search

General Attributes

Bibliography

Authors

Title of Journal

Title of Article

DOI

Chemistry

Composition [Periodic Table](#)

Cell

Cell Parameters

Cell Volume Tolerance +/- %

Symmetry

Space Group Symbol Space Group Number

Crystal System Centering

Exp. Info. & Ref. Data

New Data Only ☐

PDF Number Temperature K

ICSD Collection Code Pressure MPa

Clear Basic Search

Count Basic Search

Search Action

[Run Query](#) [Clear Query](#)

Search Summary

Basic Search: 941

Query History

Number of queries: 0

[Clear Query History](#)

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ICSD – Example: high temperature superconductors - Results

Result list

ICSD

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Results: List View # of Hits: 941

Back to Query Show Detailed View Export Data Print Compare Structures Compare Powder Pattern Column Selection Filter

	Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Cell Parameter	Journal	Publication Year	CCDC
☐	1553	I 41/a m d Z	Hg ₂ .8 (As F6)0.94		A neutron diffraction	Schultz, A.J.; William	7.549(5) 7.549(5) 12	Inorganic Chemistry	1978	↶ ↴
☐	9187	R -3 m H	Ce Ir ₃	NbBe ₃ #ThCo ₃	Celr ₃ : superconducti	Górnicka, Karolina; C	5.280(4) 5.280(4) 26	Superconductor Scie	2019	↶ ↴
☐	11144	I m -3 m	Ba _{0.54} K _{0.46} Bi O ₃		Hydrothermal synthe	Saiduzzaman, Md; Y	8.5207(2) 8.5207(2)	Inorganic Chemistry	2019	↶ ↴
☐	11418	R 3 2 H	Na ₃ Pt ₁₀ Si ₅		Na ₃ Pt ₁₀ Si ₅ . A non-c	Yamada, Takahiro; F	10.1305(5) 10.1305(	Inorganic Chemistry	2019	↶ ↴
☐	11419	R 3 2 H	Na ₃ Pt ₁₀ Si ₅		Na ₃ Pt ₁₀ Si ₅ . A non-c	Yamada, Takahiro; F	10.1536(3) 10.1536(	Inorganic Chemistry	2019	↶ ↴
☐	11420	R 3 2 H	Na ₃ Pt ₁₀ Si ₅		Na ₃ Pt ₁₀ Si ₅ . A non-c	Yamada, Takahiro; F	10.1345(5) 10.1345(	Inorganic Chemistry	2019	↶ ↴
☐	11421	R 3 2 H	Na ₃ Pt ₁₀ Si ₅		Na ₃ Pt ₁₀ Si ₅ . A non-c	Yamada, Takahiro; F	10.1478(3) 10.1478(	Inorganic Chemistry	2019	↶ ↴
☐	11422	R 3 2 H	Na ₃ Pt ₁₀ Si ₅		Na ₃ Pt ₁₀ Si ₅ . A non-c	Yamada, Takahiro; F	10.1421(4) 10.1421(	Inorganic Chemistry	2019	↶ ↴
☐	11514	P 4/m m m	Fe Sr ₂ Y Cu ₂ O ₇ .83 (Ba _{1.5} La _{0.5})Cu ₃ La		Soft magnetic switch	López-Paz, Sara A.;	3.8145(3) 3.8145(3)	Inorganic Chemistry	2019	↶ ↴
☐	11980	I 4/m	Mo ₄ Ga _{18.69} Sn _{1.8}		Endohedral cluster s	Verchenko, Valeriy Y	12.8118(6) 12.8118(	Inorganic Chemistry	2019	↶ ↴

(1 of 95) 1 2 3 4 5 6 7 8 9 10 10

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Version 4.6.0 (build 20210419-1300) - Data Release 2021.1

Buildnumber 8bcae72c5d1a30b4303d5c9b05126084e32c4706

ICSD – Example: high temperature superconductors - Results

Result list:

Sorted by
publication
year



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Results: List View

of Hits: 941

Back to Query

Show Detailed View

Export Data

Print

Compare Structures

Compare Powder Pattern

Column Selection

Filter

☐	☐	Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Cell Parameter	Journal	Publication Year	CCDC	
☐		58853	P n m a	Bi3 Rh	RhBi3	X-ray analysis of the	Kuz'min, R.N. (Kuzn	9.027(6) 4.24(2) 11.5	Kristallografiya	1960		
☐		23930	P m -3 m	Rh17 S15	Pd17Se15	The crystal structure	Geller, S.	9.911(1) 9.911(1) 9.5	Acta Crystallographi	1962		
☐		108629	P m -3 m	Nb3 Si	Auricupride#AuCu3	Nb3 Si, a supercond	Galasso, F.; Pyle, J.	4.211 4.211 4.211 90	Acta Crystallographi	1963		
☐		108633	I m -3 m	(Nb Ti Zr)0.333	bcc#W	Study of Nb-Zr-Ti ph	Doi, Toshio; Ishida, T	3.38 3.38 3.38 90. 91	Nippon Kinzoku Gak	1966		
☐		645571	I m -3 m	Nb Zr	bcc#W	Study of Nb-Zr-Ti ph	Doi, Toshio; Ishida, T	3.44 3.44 3.44 90.0	Nippon Kinzoku Gak	1966		
☐		199126	I 4/m m m	(Y0.7 Th0.3) C2	CaC2(tl6)	High-pressure synth	Krupka, M.C.; Giorgi	3.7088(9) 3.7088(9)	Journal of the Less-C	1969		
☐		611658	I -4 3 d	(Y1.8 Au0.2) C2.6		High-pressure synth	Krupka, M.C.; Giorgi	8.2503(6) 8.2503(6)	Journal of the Less-C	1969		
☐		616530	I -4 3 d	(Y1.8 Bi0.2) C2.9	Pu2C3#Rb4O6	High-pressure synth	Krupka, M.C.; Giorgi	8.2396(4) 8.2396(4)	Journal of the Less-C	1969		
☐		617561	I -4 3 d	(Y1.8 Cr0.2) C2.9	Pu2C3#Rb4O6	High-pressure synth	Krupka, M.C.; Giorgi	8.2384(10) 8.2384(1	Journal of the Less-C	1969		
☐		617983	I -4 3 d	(Y1.8 Ge0.2) C2.7	Pu2C3#Rb4O6	High-pressure synth	Krupka, M.C.; Giorgi	8.286(5) 8.286(5) 8.	Journal of the Less-C	1969		

(1 of 95)12345678910>>>10

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Buildnumber 8bcae72c5d1a30b4303d5c9b05126084e32c4706

ICSD – Example: high temperature superconductors - Results

Result list:

Column
selection

ICSD

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Results: List View # of Hits: 941

Back to Query Show Detailed View Export Data Print Compare Structures Compare Powder Pattern

Column Selection Filter

☐	☒	Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Cell Parameter	Temperature	Pressure
☐	☒	58853	P n m a	Bi3 Rh	RhBi3	X-ray analysis of t	Kuz'min, R.N. (Ku	9.027(6) 4.24(2) 1	293.00	0.101325
☐	☐	23930	P m -3 m	Rh17 S15	Pd17Se15	The crystal structu	Geller, S.	9.911(1) 9.911(1) S	293.00	0.101325
☐	☐	108629	P m -3 m	Nb3 Si	Auricupride#AuCu	Nb3 Si, a supercon	Galasso, F.; Pyle,	4.211 4.211 4.211	293.00	0.101325
☐	☐	108633	I m -3 m	(Nb Ti Zr)0.333	bcc#W	Study of Nb-Zr-Ti	Doi, Toshio; Ishida	3.38 3.38 3.38 90.	293.00	0.101325
☐	☐	645571	I m -3 m	Nb Zr	bcc#W	Study of Nb-Zr-Ti	Doi, Toshio; Ishida	3.44 3.44 3.44 90.	293.00	0.101325
☐	☐	199126	I 4/m m m	(Y0.7 Th0.3) C2	CaC2(II6)	High-pressure syn	Krupka, M.C.; Gio	3.7088(9) 3.7088(9	293.00	0.101325
☐	☐	616530	I -4 3 d	(Y1.8 Bi0.2) C2.9	Pu2C3#Rb4O6	High-pressure syn	Krupka, M.C.; Gio	8.2396(4) 8.2396(4	293.00	0.101325
☐	☐	617561	I -4 3 d	(Y1.8 Cr0.2) C2.9	Pu2C3#Rb4O6	High-pressure syn	Krupka, M.C.; Gio	8.2384(10) 8.2384	293.00	0.101325
☐	☐	617983	I -4 3 d	(Y1.8 Ge0.2) C2.7	Pu2C3#Rb4O6	High-pressure syn	Krupka, M.C.; Gio	8.286(5) 8.286(5)	293.00	0.101325
☐	☐	618369	I -4 3 d	(Y1.8 Mo0.2) C2.9	Pu2C3#Rb4O6	High-pressure syn	Krupka, M.C.; Gio	8.239(1) 8.239(1)	293.00	0.101325

(1 of 95) 1 2 3 4 5 6 7 8 9 10

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Version 4.6.0 (build 20210419-1300) - Data Release 2021.1

Buildnumber 8bcae72c5d1a30b4303d5c9b05126084e32c4706

Formula Units Per Cell
Formula Weight
Temperature
Pressure
R-Value
Sum Formula

ICSD – Example: high temperature superconductors - Results

Result list:

Filter options


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Results: List View
of Hits: 941

Back to Query
Show Detailed View
Export Data
Print
Compare Structures
Compare Powder Pattern
Column Selection
Filter [905 / 941]

☐	Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Cell Parameter	Temperature	Pressure	Publica
☐	58853	P n m a	Bi3 Rh	RhBi3	X-ray analysis of tl	Kuz'min, R.N. (Ku	9.027(6) 4.24(2) 1	293.00	0.101325	1960
☐	23930	P m -3 m	Rh17 S15	Pd17Se15	The crystal structu	Geller, S.	9.911(1) 9.911(1) 9	293.00	0.101325	1962
☐	108629	P m -3 m	Nb3 Si	Auricupride#AuCu	Nb3 Si, a superco	Galasso, F.; Pyle,	4.211 4.211 4.211	293.00	0.101325	1963
☐	108633	I m -3 m	(Nb Ti Zr)0.333	bcc#W	Study of Nb-Zr-Ti	Doi, Toshio; Ishida	3.38 3.38 3.38 90.	293.00	0.101325	1966
☐	645571	I m -3 m	Nb Zr	bcc#W	Study of Nb-Zr-Ti	Doi, Toshio; Ishida	3.44 3.44 3.44 90.	293.00	0.101325	1966
☐	199126	I 4/m m m	(Y0.7 Th0.3) C2	CaC2(tl6)	High-pressure syn	Krupka, M.C.; Gio	3.7088(9) 3.7088(9)	293.00	0.101325	1969
☐	611658	I -4 3 d	(Y1.8 Au0.2) C2.6		High-pressure syn	Krupka, M.C.; Gio	8.2503(6) 8.2503(6)	293.00	0.101325	1969
☐	616530	I -4 3 d	(Y1.8 Bi0.2) C2.9	Pu2C3#Rb4O6	High-pressure syn	Krupka, M.C.; Gio	8.2396(4) 8.2396(4)	293.00	0.101325	1969
☐	617561	I -4 3 d	(Y1.8 Cr0.2) C2.9	Pu2C3#Rb4O6	High-pressure syn	Krupka, M.C.; Gio	8.2384(10) 8.2384	293.00	0.101325	1969
☐	617983	I -4 3 d	(Y1.8 Ge0.2) C2.7	Pu2C3#Rb4O6	High-pressure syn	Krupka, M.C.; Gio	8.286(5) 8.286(5)	293.00	0.101325	1969

(1 of 91)
1 2 3 4 5 6 7 8 9 10

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Quality Filter

Radiation Type

Sample Type

R-value

Experimental Conditions

Reset Filter

ICSD – Example: high temperature superconductors - Results

Result list:

Export data

-> CSV file

ICSD

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Results: List View # of Hits: 941 (905 selected)

Back to Query Show Detailed View Export Data Print Compare Structures Compare Powder Pattern Column Selection Filter [905 / 941]

☒	☒	Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Cell Parameter	Temperature	Pressure	Publication Year	CCDC	
☒	☒	160366	P 4/m m m	Fe Sr2 (Y0.5 Nd0.5)Cu3L	(Ba1.5La0.5)Cu3L	Substitution of ne	Wuernisha, T.; Ha	3.8455(6) 3.8455(	293.00	0.101325	2008		
☒	☒	160367	P 4/m m m	Fe Sr2 (Y0.25 Nd0.75)Cu3L	(Ba1.5La0.5)Cu3L	Substitution of ne	Wuernisha, T.; Ha	3.8498(4) 3.8498(	293.00	0.101325	2008		
☒	☒	167169	P 4/m m m	Nb Sr2 Y Cu2 O7	(Ba1.5La0.5)Cu3L	Comparative study	Kumar, S.; Dogra,	3.863(1) 3.863(1)	293.00	0.101325	2010		
☒	☒	167170	P 4/m m m	Nb Sr2 Eu Cu2 O7	(Ba1.5La0.5)Cu3L					0.101325	2010		
☒	☒	167171	P 4/m m m	Fe Sr2 Y Cu2 O7	(Ba1.5La0.5)Cu3L					0.101325	2010		
☒	☒	167172	P 4/m m m	Al Sr2 Y Cu2 O7	(Ba1.5La0.5)Cu3L					0.101325	2010		
☒	☒	167173	P 4/m m m	Ru Sr2 Eu Cu2 O7	(Ba1.5La0.5)Cu3L					0.101325	2010		
☒	☒	11514	P 4/m m m	Fe Sr2 Y Cu2 O7	(Ba1.5La0.5)Cu3L					0.101325	2019		
☒	☒	83113	P 4/m m m	(Hg0.78 Bi0.22)Cu3L	(Ba1.5La0.5)Cu3L					0.101325	1996		
☒	☒	87250	P 4/m m m	(Hg0.53 Cr0.47)Cu3L	(Ba1.5La0.5)Cu3L					0.101325	1996		

Export Data

Custom File Name

Export Celltype

Remaining CIF downloads this session: 10000

Remaining CIF downloads this year: 999999

Remaining LongView downloads this session: 10000

Remaining LongView downloads this year: 999999

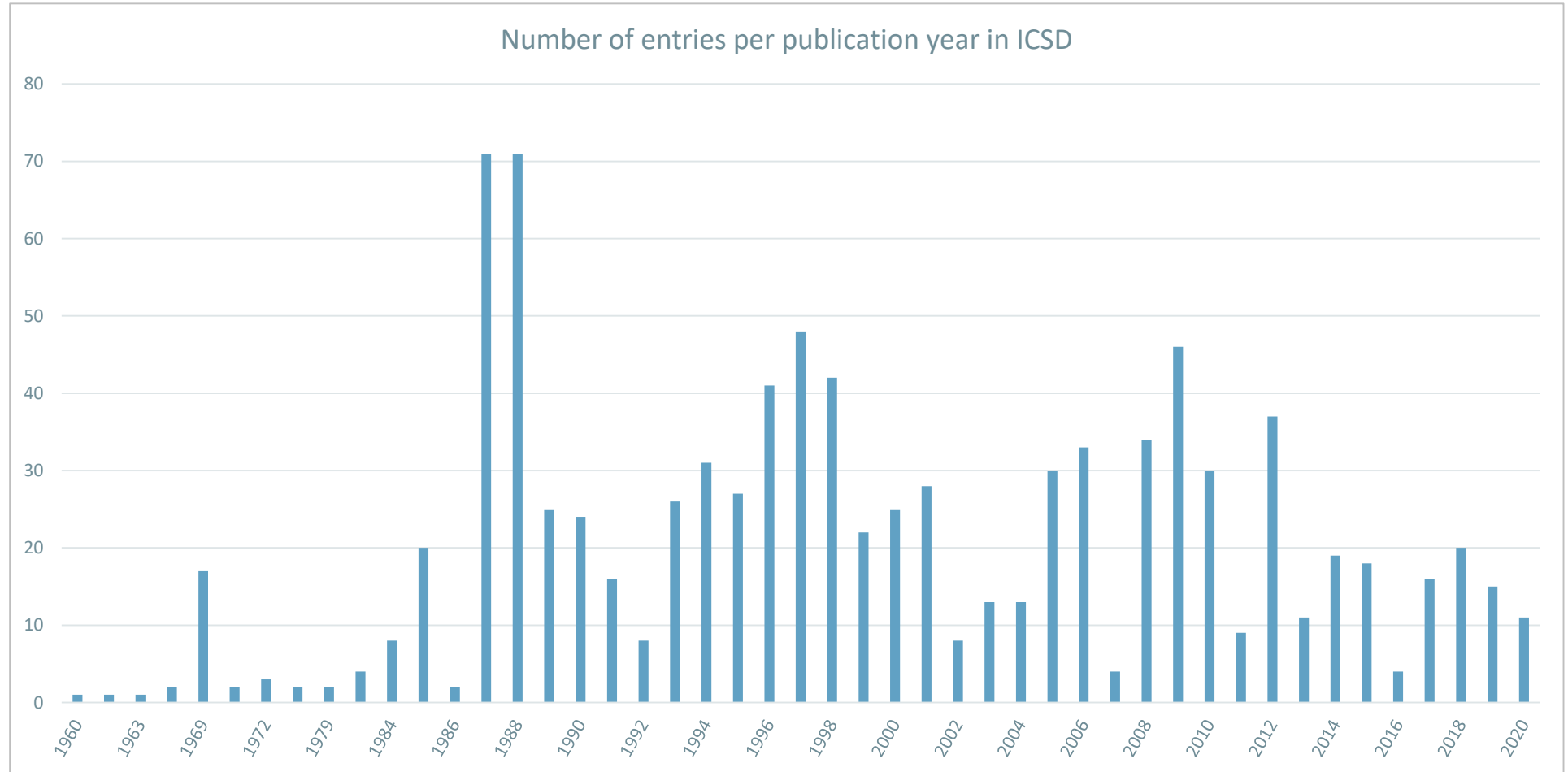
Remaining CSV downloads this session: 10000

Please note: Your selected export size may take up to 30 seconds!

Buildnumber 6bcae72c5d1a30b4303d5c9b05126084e32c4705

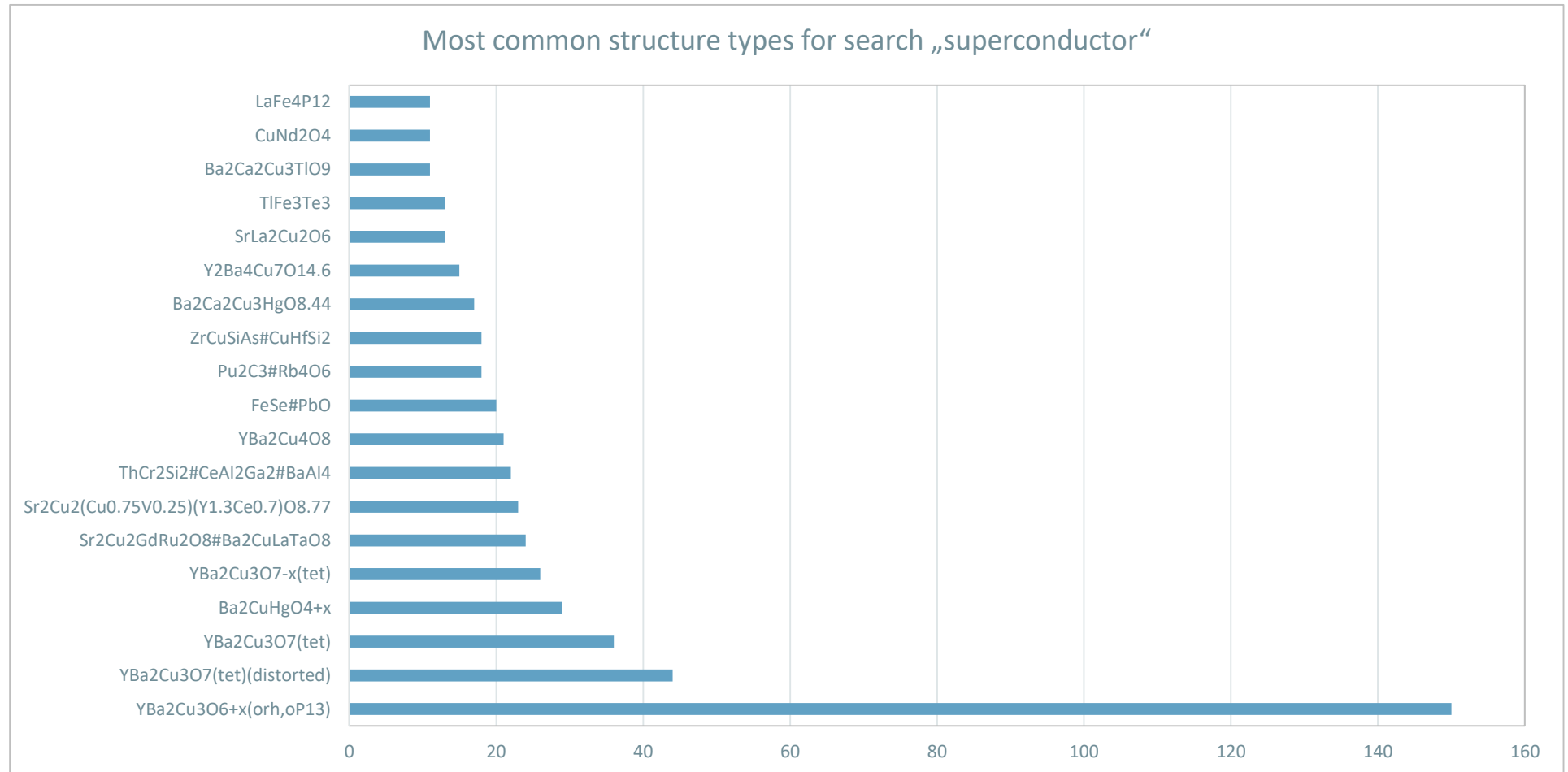
ICSD – Example: high temperature superconductors – External analysis

Information
about super-
conductors
in ICSD



ICSD – Example: high temperature superconductors – External analysis

125 structure types with less than 10 entries left out



ICSD – Example: high temperature superconductors - Results

Result list:

Sorted by
structure
type

ICSD

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Results: List View # of Hits: 941 (2 selected) ?

Back to Query Show Detailed View Export Data Print Compare Structures Compare Powder Pattern Column Selection Filter [905 / 941]

	Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Cell Parameter	Temperature	Pressure	Publication Year	CCDC	
☐	94376	P m m m	Gd0.499 Pr0.298	YBa2Cu3O6+x(orthorhombic)	Investigation of structure	Shakeripour, H.; A	3.8725 3.8942 11.	293.00	0.101325	2001		↶ ⬇
☐	94377	P m m m	Pr Ba2 Cu3 O7	YBa2Cu3O6+x(orthorhombic)	Crystallographic, r	Lisboa-Filho, P.N.;	3.90574(3) 3.9057	293.00	0.101325	2001		↶ ⬇
☐	97066	P m m m	Y Ba2 Cu3 O6.97	YBa2Cu3O6+x(orthorhombic)	Study of the struct	Ahmed, F.U.; Azac	3.8163(6) 3.8659(	293.00	0.101325	2002		↶ ⬇
☐	151637	P m m m	(Y0.8 Ca0.2) Sr Ba	YBa2Cu3O6+x(orthorhombic)	Preparation and cl	Barinotto C., V.H.;	3.826 3.861 11.56	293.00	0.101325	2004		↶ ⬇
☐	151640	P m m m	Ho Ba2 Cu3 O6.9	YBa2Cu3O6+x(orthorhombic)	The influence of T	Golosova, N.; Mirr	3.81400(7) 3.8799	293.00	0.101325	2004		↶ ⬇
☐	151641	P m m m	(Ho0.948 Th0.052	YBa2Cu3O6+x(orthorhombic)	The influence of T	Golosova, N.; Mirr	3.8210(1) 3.8808(	293.00	0.101325	2004		↶ ⬇
☐	151642	P m m m	(Ho0.9 Th0.1) Ba2	YBa2Cu3O6+x(orthorhombic)	The influence of T	Golosova, N.; Mirr	3.8242(1) 3.8809(	293.00	0.101325	2004		↶ ⬇
☐	151676	P m m m	Ca0.6 La0.6 Ba1.6	YBa2Cu3O6+x(orthorhombic)	Preparation and cl	De Los Santos V. I	3.849 3.880 11.63	293.00	0.101325	2004		↶ ⬇
☒	290508	P m m m	La (La0.15 Ba0.85	YBa2Cu3O6+x(orthorhombic)	Synthesis of the s	Valerio, C.Marlon;	3.9060 3.9192 11.	293.00	0.101325	2012		↶ ⬇
☒	65389	P 4/m m m	Ba1.8 Nd1.2 Cu3	YBa2Cu3O7(tetragonal)	Crystal structure o	Izumi, F.; Takekaw	3.8919(3) 3.8919(	293.00	0.101325	1987		↶ ⬇

(64 of 91) 59 60 61 62 63 64 65 66 67 68 10

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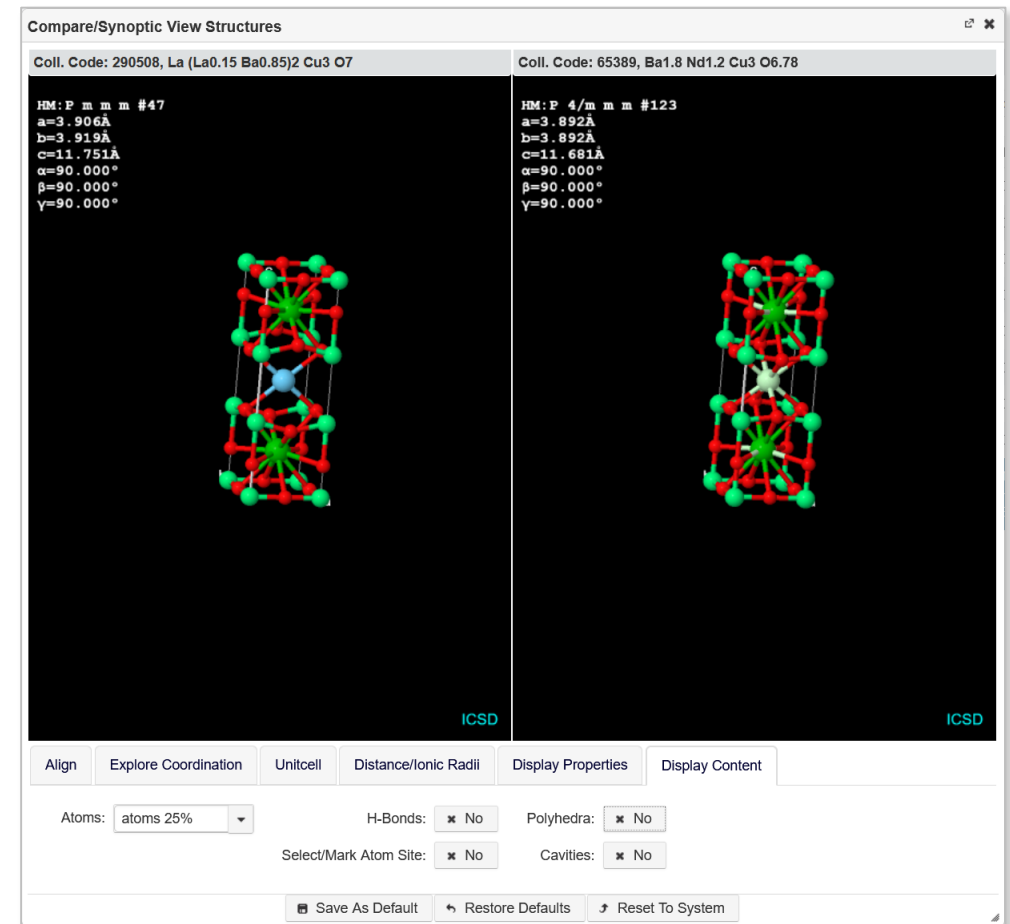
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ICSD – Example: high temperature superconductors - Results

Comparison of two structures
(with different structure types):

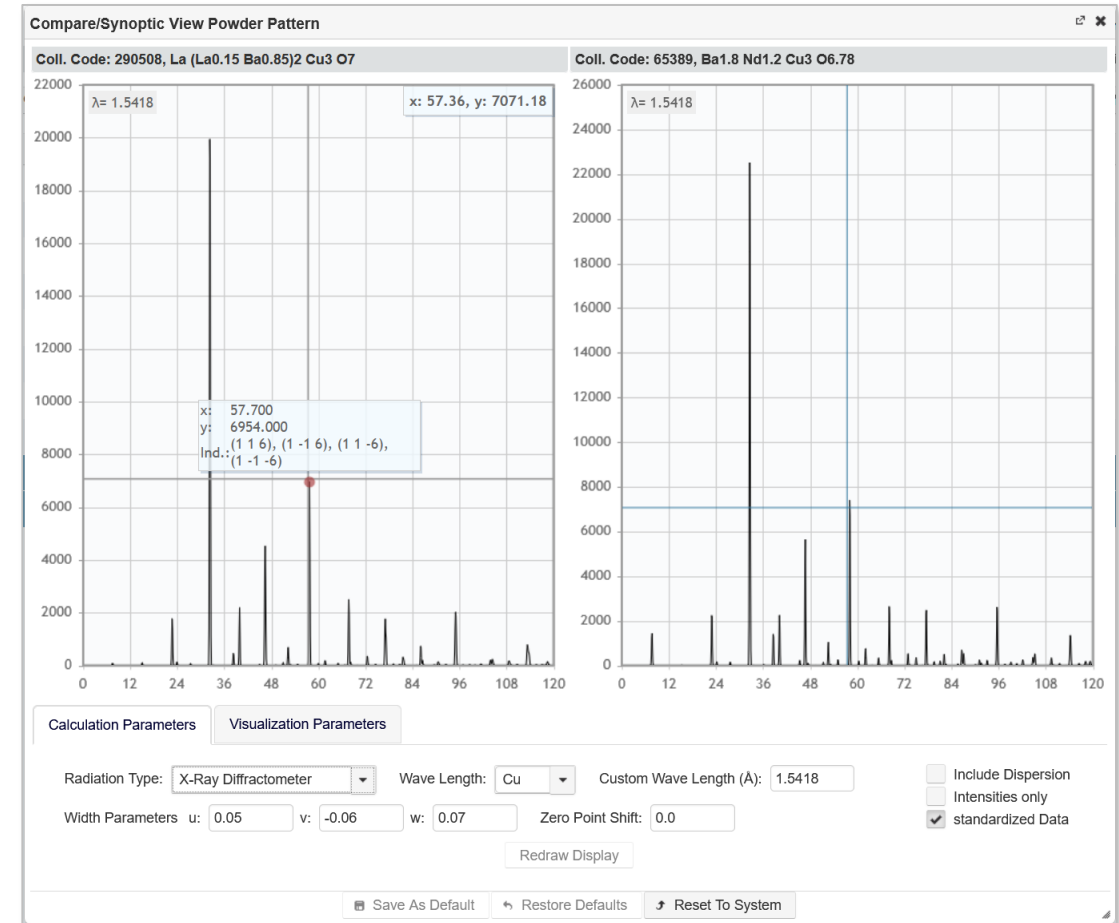
- Pmmm:
Alternating O position below and above the plane of 4 Cu atoms -> 2-fold symmetry
- P4/mmm:
All 4 O atoms above/below the plane of 4 Cu atoms -> 4-fold symmetry



ICSD – Example: high temperature superconductors - Results

Comparison of the two simulated powder patterns for the structures

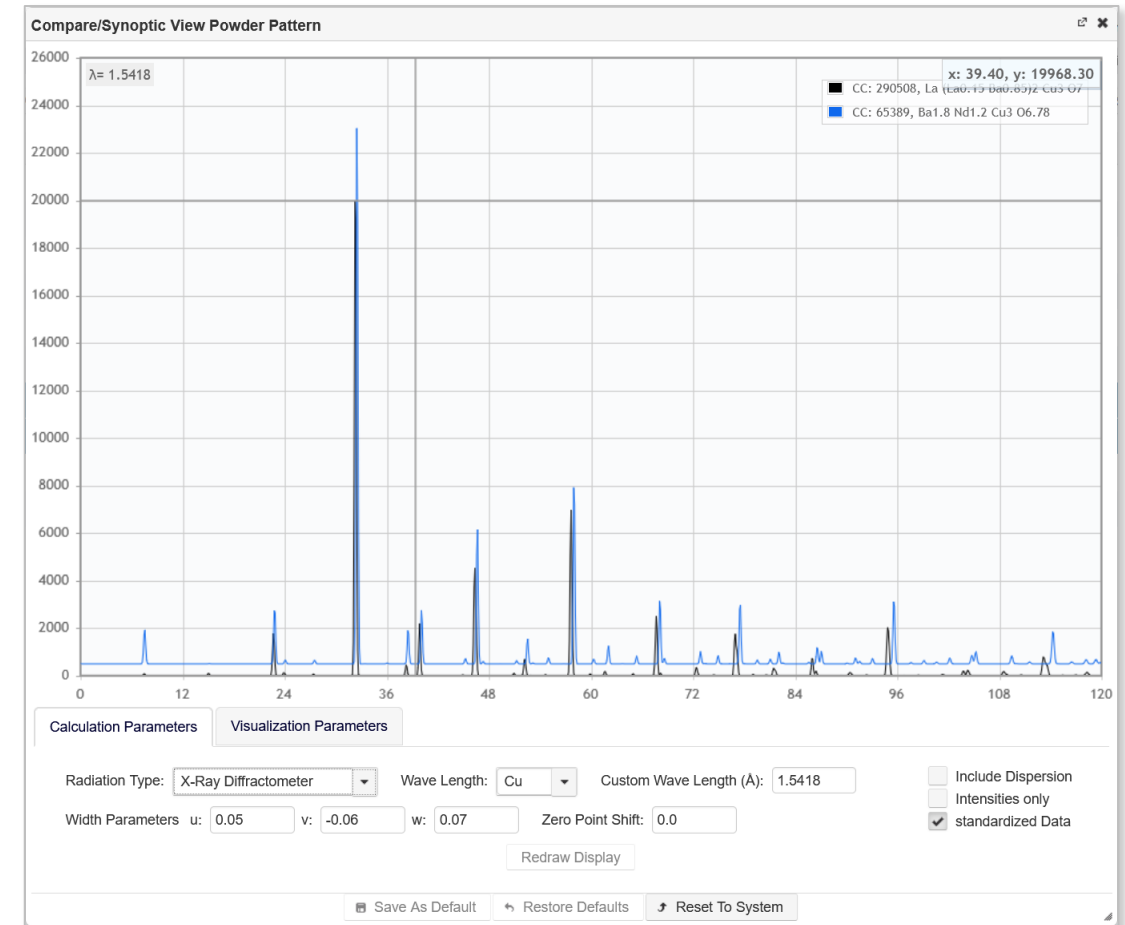
- side-by-side view



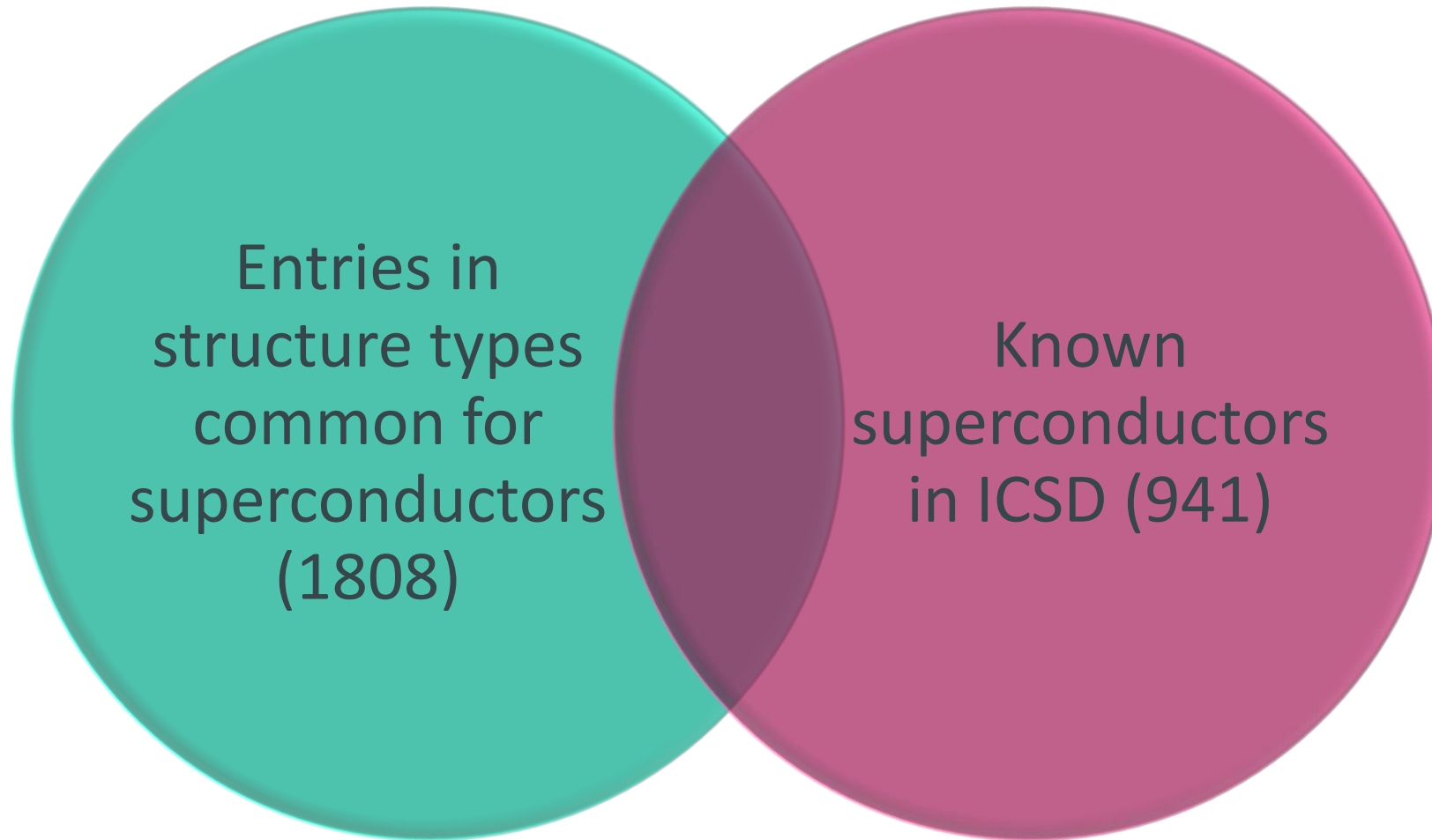
ICSD – Example: high temperature superconductors - Results

Comparison of the two simulated powder patterns for the structures

- staggered view



ICSD – Example: high temperature superconductors



ICSD – Example: high temperature superconductors – New search

Structure type search for YBaCu*
(most common structure types
for superconductors)

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Content Selection

- ☒ Experim. inorganic structures
- ☒ Experim. metal-organic str.
- ☐ Theoretical structures

Navigation

- Basic search & retrieve
- Advanced search & retrieve**
- Bibliography
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info
- Expert Search
- Query Management**
- Manage Queries
- List Combined Queries
- Create Combined Query
- ICSD links**
- ICSD News

Structure Type Search

Pre Defined Structure Types

Structure Type e.g. Mg2SiO4

☒ Search in predefined structure types

Structure Type Descriptors

☐	SpaceGrp	☐	Wyck	☐	Pearson	☐	ANX
--------------------------	----------	--------------------------	------	--------------------------	---------	--------------------------	-----

Structure type definitions

Search Action

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	1808
Experimental Info:	-
DB Info:	-
Expert:	-
Combined Results:	1808

Query History

Number of queries:	1
--------------------	---

2021-07-20T11:27	941
------------------	-----

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ICSD – Example: high temperature superconductors – Combine searches

Manage Queries shows the two queries from the Query History

The screenshot displays the ICSD web interface. The top navigation bar includes the ICSD logo, a welcome message "Welcome to ICSD Web. Logged in: Ruehl, Stephan", and links for "FIZ Karlsruhe | Contact", "Change Password", and "Logout".

The main content area is titled "Manage Queries" and features a table with the following columns: "Query Name", "Date", "Query Type", "# of hits", and "Saved". The table contains two entries:

		Query Name	Date	Query Type	# of hits	Saved
☐	☐	2021-07-20T11:35	2021-07-20T11:35	Advanced	1808	
☐	☒	2021-07-20T11:27	2021-07-20T11:27	Basic	941	

Below the table, there is a form for editing the selected query (2021-07-20T11:27). The form includes fields for "Query Name", "Release tag", "Date", and "Comment". The "Query Info" section shows the search criteria: "SIMPLE (searchTerm: superconductor,)" and "Search includes: Experim. metal-organic str., Experim. inorganic structures".

At the bottom of the form, there are buttons for "Load query", "Run query", "Save selected queries", and "Delete selected queries".

The left sidebar contains the following sections:

- Content Selection**:
 - ☒ Experim. inorganic structures
 - ☒ Experim. metal-organic str.
 - ☐ Theoretical structures
- Navigation**:
 - Basic search & retrieve
 - Advanced search & retrieve
 - Bibliography
 - Cell
 - Chemistry
 - Symmetry
 - Crystal Chemistry
 - Structure Type
 - Experimental Information
 - DB Info
 - Expert Search
- Query Management**:
 - Manage Queries
 - List Combined Queries
 - Create Combined Query
- ICSD links**:
 - ICSD News

ICSD – Example: high temperature superconductors – Combine searches

Combining previous two queries to get the entries that are potential superconductors:

Note: The first query can either be moved to the AND or the OR area, because there is only one query to used.

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Content Selection

- ☒ Exprim. inorganic structures
- ☒ Exprim. metal-organic str.
- ☐ Theoretical structures

Navigation

- Basic search & retrieve
- Advanced search & retrieve
 - Bibliography
 - Cell
 - Chemistry
 - Symmetry
 - Crystal Chemistry
 - Structure Type
 - Experimental Information
 - DB Info
 - Expert Search
- Query Management
 - Manage Queries
 - List Combined Queries
 - Create Combined Query
- ICSD links
 - ICSD News

Create Combined Query

Name: Structure Types for superconductors - known superconductors

Comment: Most common structure types for superconductors - excluding the already known superconductors

Available Queries:

	Query Name	Date	Query Type	# of hits	Saved
☒	2021-07-20T11:35	2021-07-20T11:35	Advanced	1808	
☐	2021-07-20T11:27	2021-07-20T11:27	Basic	941	

Must have (AND):

+ add AND operation

Must have at least one of (OR):

+ -

Must not have (NOT):

+ -

Run query Count query Clear

ICSD – Example: high temperature superconductors – Combine searches

Combining previous two queries to get the entries that are potential superconductors:

The second query must be added to the NOT area.

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Change Password Number of hits : 1529

Content Selection

- ☒ Experm. Inorganic structures
- ☒ Experm. metal-organic str.
- ☐ Theoretical structures

Navigation

- Q Basic search & retrieve
- Advanced search & retrieve
 - Q Bibliography
 - Q Cell
 - Q Chemistry
 - Q Symmetry
 - Q Crystal Chemistry
 - Q Structure Type
 - Q Experimental Information
 - Q DB Info
 - Q Expert Search
- Query Management**
 - Manage Queries
 - List Combined Queries
 - Create Combined Query
- ICSD links**
 - ICSD News

Create Combined Query

Name: Structure Types for superconductors - known superconductors

Comment: Most common structure types for superconductors - excluding the already known superconductors

Available Queries:

☐	Query Name	Date	Query Type	# of hits	Saved
☐	2021-07-20T11:35	2021-07-20T11:35	Advanced	1808	
☐	2021-07-20T11:27	2021-07-20T11:27	Basic	941	

Must have (AND):

☐	2021-07-20T11:35	2021-07-20T11:35	Advanced	1808	
--------------------------	------------------	------------------	----------	------	--

Must have at least one of (OR):

No records found.

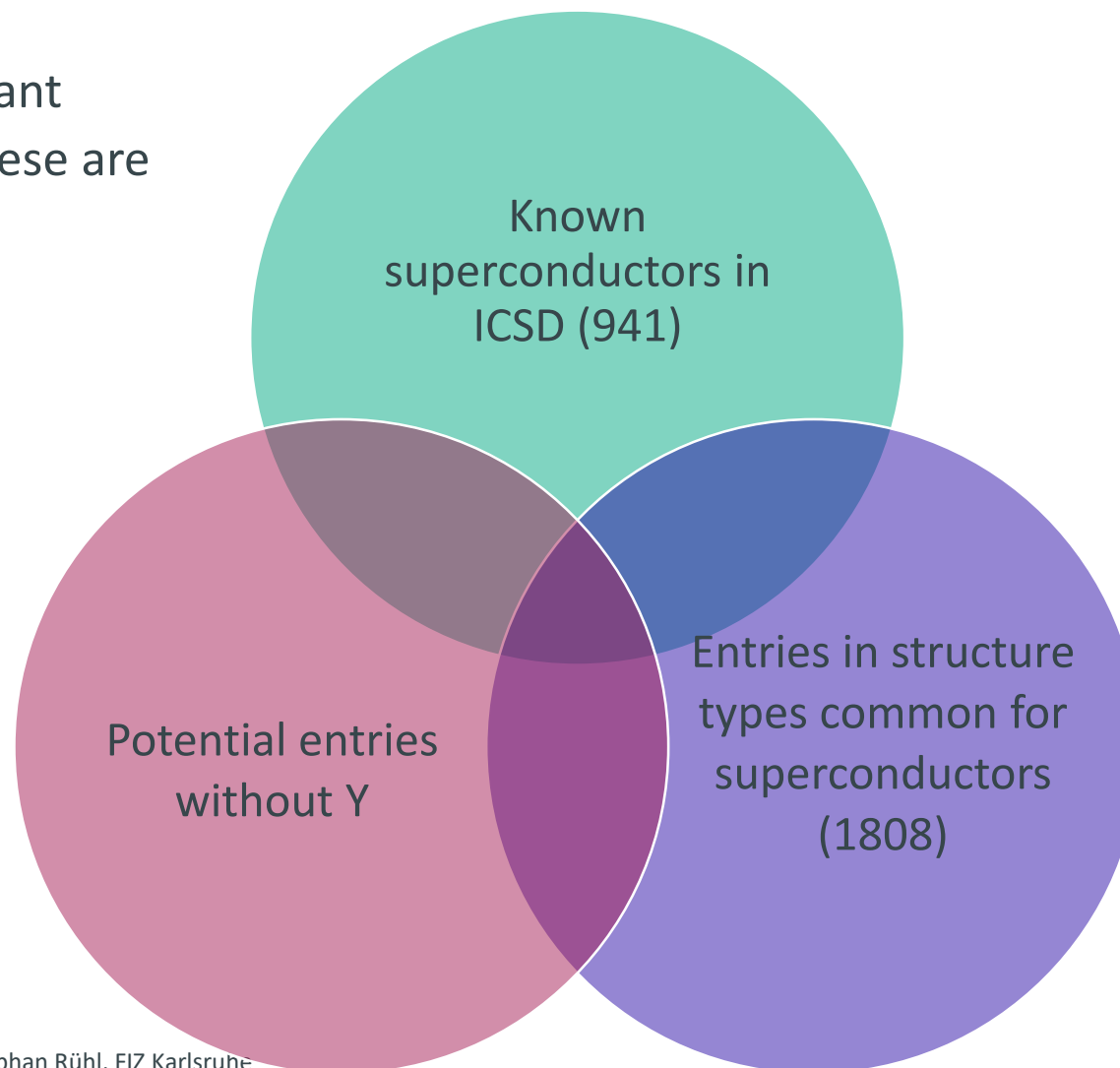
Must not have (NOT):

☐	2021-07-20T11:27	2021-07-20T11:27	Basic	941	
--------------------------	------------------	------------------	-------	-----	--

Run query Count query Clear

ICSD – Example: high temperature superconductors – Exclude Y

Now let's suppose we do not want compounds with Yttrium, as these are already well studied



ICSD – Example: high temperature superconductors – Expert Search

Using the Expert Search Mask

Note: This search is also available for the ICSD API

ICSD

Content Selection

☒ Experm. inorganic structures
☒ Experm. metal-organic str.
☐ Theoretical structures

Navigation

[Basic search & retrieve](#)
[Advanced search & retrieve](#)
[Bibliography](#)
[Cell](#)
[Chemistry](#)
[Symmetry](#)
[Crystal Chemistry](#)
[Structure Type](#)
[Experimental Information](#)
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[Query Management](#)
[Manage Queries](#)
[List Combined Queries](#)
[Create Combined Query](#)
[ICSD links](#)
[ICSD News](#)

Expert Search

Your Query

structuretype: YBa2Cu* not (article: superconductor or abstract: superconductor or keywords: superconductor or comment: superconductor or journal: superconductor or composition: Y)
e.g. authors: jansen AND publicationyear: 2000-2010

Description of available SearchTerms

SearchTerm	Description	Input Type
COLLECTIONCODE	DB INFO : ICSD collection code	Numerical, integer
PDFNUMBER	DB INFO : PDF number as assigned by ICDD	Text
RELEASE	DB INFO : Release tag	Numerical, integer, special format
RECORDINGDATE	DB INFO : Recording date of an ICSD entry	Numerical, integer, special format
MODIFICATIONDATE	DB INFO : Modification date of an ICSD entry	Numerical, integer, special format
COMMENT	EXPERIMENTAL SEARCH : Search for a comment	Text
RVALUE	EXPERIMENTAL SEARCH : R-value of the refinement (0.00 ... 1.00)	Numerical, floating point
TEMPERATURE	EXPERIMENTAL SEARCH : Temperature of the measurement	Numerical, floating point
PRESSURE	EXPERIMENTAL SEARCH : Pressure during the measurement	Numerical, floating point
STRUCTURETYPE	STRUCTURE TYPE : Search for predefined structure types directly	Select one
SPACEGROUPSYMBOL	SYMMETRY : Search for the space group symbol	Text
SPACEGROUPNUMBER	SYMMETRY : Search for the space group number	Numerical, integer
BRAVAISLATTICE	SYMMETRY : Select One: Primitive, a-centered, b-centered, c-centered, Body-centered, Rhombohedral, Face-centered	Select one
CRYSTALSYSTEM	SYMMETRY : Crystal system	Select one
CRYSTALCLASS	SYMMETRY : Search for the crystal class	Text
LAUECLASS	SYMMETRY : Search for predefined laueclass: -1, -3, -3m, 2/m, 4/m, 4/mmm, 6/m 6/mmm, m-3, m-3m, mmm	Select one
WYCKOFFSEQUENCE	SYMMETRY : Search for the Wyckoff sequence	Text
PEARSONSYMBOL	SYMMETRY : Search for the Pearson symbol	Text
INVERSIONCENTER	SYMMETRY : Should inversion center be included?	TRUE or FALSE
POLARAXIS	SYMMETRY : Should polar axis be included?	TRUE or FALSE

Search Action

[Run Query](#) [Clear Query](#)

Search Summary

Bibliography:

-

Cell:

-

Chemistry:

-

Symmetry:

-

Crystal Chemistry:

-

Structure Types:

-

Experimental Info:

-

DB Info:

-

Expert:

736

Combined Results:

736

Query History

Number of queries:

2

[Clear Query History](#)

2021-07-20T11:35

1808

2021-07-20T11:27

941

48

25th IUCr congress: Joint Workshop for CSD and ICSD, Dr. Stephan Rühl, FIZ Karlsruhe

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ICSD – Example: high temperature superconductors – Final result

Result list

ICSD

Welcome to ICSD Web. Logged in: Ruehl, Stephan

FIZ Karlsruhe | Contact
Change Password | Logout

Results: List View # of Hits: 736

[Back to Query](#) [Show Detailed View](#) [Export Data](#) [Print](#) [Compare Structures](#) [Compare Powder Pattern](#) [Column Selection](#) [Filter](#)

☐	☐	Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Cell Parameter	Temperature	Pressure	Publication Year	CCDC	
☐		39265	P 4/m m m	Pr Ba2 Cu2 (Cu0.1	YBa2Cu3O7(tet)	X-ray and KR-spe	Bush, A.A.; Ivanov	3.9056(6) 3.9056(	293.00	0.101325	1990	↗	⬇
☐		39477	P 4/m m m	Sm (Ba1.715 Sm0	YBa2Cu3O7-x(tet)	Preparation of sin	Belokoneva, E.L.;	3.896(4) 3.896(4)	293.00	0.101325	1991	↗	⬇
☐		39670	P 4/m m m	Tl Ba2 La Cu2 O7	YBa2Cu3O7(tet)(c	Non-superconduct	Tamazyan, R.A.; M	3.944(1) 3.944(1)	293.00	0.101325	1992	↗	⬇
☐		41564	P m m m	Pr Ba2 Cu3 O6.95	YBa2Cu3O6+x(ori	Structural, magnet	Malik, S.K.; Jhans	3.8640(4) 3.9250(	293.00	0.101325	1995	↗	⬇
☐		41565	P m m m	Pr Ba2 (Cu.9 Zn.1	YBa2Cu3O6+x(ori	Structural, magnet	Malik, S.K.; Jhans	3.8825(7) 3.9175(	293.00	0.101325	1995	↗	⬇
☐		41566	P 4/m m m	Pr Ba2 (Cu.9 Ga.1	YBa2Cu3O7(tet)	Structural, magnet	Malik, S.K.; Jhans	3.9014(2) 3.9014(	293.00	0.101325	1995	↗	⬇
☐		41695	P 4/m m m	Tl0.98 Sr2 (Lu0.81	YBa2Cu3O7(tet)(c	Underdoped, optin	Shimakawa, Y.; Jo	3.79633(2) 3.7963	293.00	0.101325	1995	↗	⬇
☐		41696	P 4/m m m	Tl0.97 Sr2 (Lu0.75	YBa2Cu3O7(tet)(c	Underdoped, optin	Shimakawa, Y.; Jo	3.79322(2) 3.7932	293.00	0.101325	1995	↗	⬇
☐		41697	P 4/m m m	Tl0.97 Sr2 (Lu0.65	YBa2Cu3O7(tet)(c	Underdoped, optin	Shimakawa, Y.; Jo	3.79896(3) 3.7989	293.00	0.101325	1995	↗	⬇
☐		41698	P 4/m m m	Tl0.97 Sr2 (Lu0.6	YBa2Cu3O7(tet)(c	Underdoped, optin	Shimakawa, Y.; Jo	3.79601(3) 3.7960	293.00	0.101325	1995	↗	⬇

(1 of 74) 1 2 3 4 5 6 7 8 9 10 10

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Version 4.6.0 (build 20210419-1300) - Data Release 2021.1

ICSD – Detailed View - Summary

Detailed Information for an entry:

- Summary
- Visualization
- Published/Standardized Crystal Structure Data
- Distances and Angles
- Bibliography
- Experimental information
- Additional information
- Compare Publ./Standard. Structure

The screenshot shows the ICSD (Inorganic Crystal Structure Database) web interface. At the top, it says "Welcome to ICSD Web. Logged in: Ruehl, Stephan" and "FIZ Karlsruhe | Contact Change Password | Logout". The page title is "Detailed View" and it shows "Entry 1 of 736". Below the title, there are navigation buttons: "Back to Query", "Back to List", and "CCDC", "Export Cif", "Print", "Feedback to Editor". The main content area is divided into two sections: "Summary" and "Details". The "Summary" section contains a table with the following data:

Summary	
Struct. formula	Pr Ba ₂ Cu ₂ (Cu _{0.83} Al _{0.17}) O _{6.55}
Cell parameter	3.9056(6) 3.9056(6) 11.634(2) 90. 90. 90.
Cell volume	177.46 [Å ³]
Temperature	room temperature
Data quality	High quality
Author	Bush, A.A.; Ivanov, S.A.; Zavodnik, V.E.; Goncharuk, I.N.; Limonov, M.F.; Markov, Yu.F.
Reference	Sverkhprovodimost: Fizika, Khimiya, Tekhnika (1990) 3, (5) Article ID * (p. 819-823)

The "Details" section contains a list of expandable/collapsible items:

- Visualization
- Chemistry
- Published Crystal Structure Data
- Standardized Crystal Structure Data
- Distances and Angles
- Bibliography
- Experimental information
- Additional information
- Compare Published and Standardized Structure

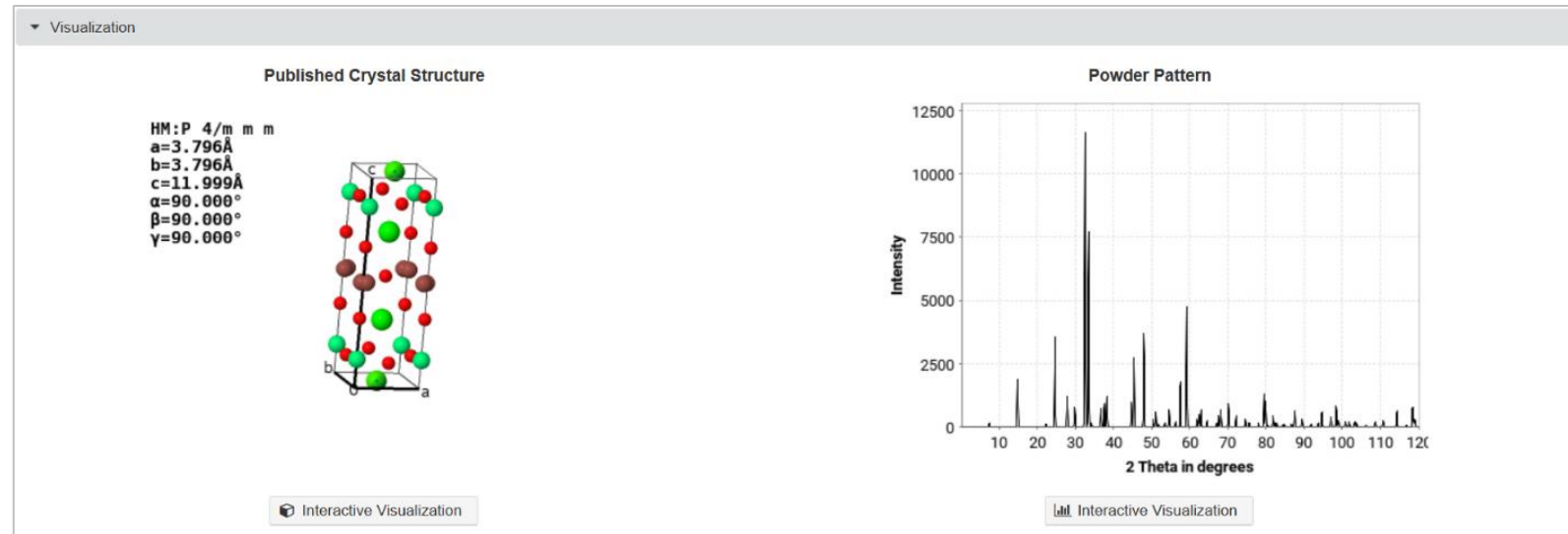
At the bottom of the page, there is a footer with "Legal Notices | Privacy Policy | Browser Recommendations | ©2021 FIZ Karlsruhe GmbH" and "Version 4.6.0 (build 20210419-1300) - Data Release 2021.1".

ICSD – Detailed View - Visualization

Pictures of:

- Crystal structure
- Simulated powder pattern

Interactive Visualization available
with many options to customize it



ICSD – Detailed View - Chemistry

Information on the Chemistry:

- Structured formula provides the formula split up into cations and anions
- Mineral name/group information may be found here
- Chemical names are not necessarily IUPAC names - can be used to search for complex anions

Chemistry			
Sum. formula	Ca0.19 Cu2 Lu0.81 O6.96 Sr2 Ti0.98	Struct. formula	Ti0.98 Sr2 (Lu0.81 Ca0.19) Cu2 O6.96
Molecular weight	763.3165 [u]	Z	1
ANX formula	ABC2D2X7	AB formula	ABC2D2E7
Chemical name	Thallium strontium lutetium calcium copper oxide (0.98/2/0.81/0.19/2/6.96)		

ICSD – Detailed View – Published structure

Crystallographic information for the published structure

Additional information:

- Pearson Symbol
- Wyckoff Sequence
- Axis ratios
- Structure type

Published Crystal Structure Data

Cell parameter	3.79633(2) 3.79633(2) 11.9986(1) 90. 90. 90.	Space group	P 4/m m m (123)		
Cell volume	172.93 Å³	Z	1		
Crystal system	tetragonal	Crystal class	4/mmm		
Laue class	4/mmm				
Structure type	YBa2Cu3O7(tet)(distorted)				
Pearson symbol	tP13				
Wyckoff sequence	m i h g2 d c	Axis ratios	a/b	b/c	c/a
Calc. density	7.33 [g/cm³]		1.0000	0.3164	3.1606

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	B
Tl	1	+3.00	4 m	0.0643(7)	0	0.5	0.245000	0.91(6)
Sr	1	+2.00	2 h	0.5	0.5	0.2898(1)	1	0.77(2)
Lu	1	+3.00	1 c	0.5	0.5	0	0.810000	0.36(4)
Ca	1	+2.00	1 c	0.5	0.5	0	0.190000	0.36(4)
Cu	1	+2.08	2 g	0	0	0.1356(1)	1	
O	1	-2.00	4 i	0	0.5	0.1203(1)	1	
O	2	-2.00	2 g	0	0	0.3291(1)	1	
O	3	-2.00	1 d	0.5	0.5	0.5	0.960000	

EL	Lbl	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Cu	1	0.0032(3)	0.0032(3)	0.0087(5)	0	0	0
O	1	0.0112(5)	0.0040(4)	0.0179(6)	0	0	0
O	2	0.0172(6)	0.0172(6)	0.0060(6)	0	0	0
O	3	0.051(1)	0.051(1)	0.010(1)	0	0	0

ICSD – Detailed View – Distances and Angles

Option to calculate distances and angles:

- Based on elements
- Based on atomic positions

Distances and Angles

Select pairs of elements Select from atom position

Atom A

☐	Ca
☐	Cu
☐	Lu
☐	O

✓ (un)select all

Atom B

☐	Ca
☐	Cu
☐	Lu
☐	O

✓ (un)select all

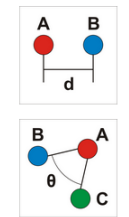
Atom C

☐	Ca
☐	Cu
☐	Lu
☐	O

✓ (un)select all

Histograms

Calculate



Histograms for distances across the whole database

Select pairs of elements Select from atom position

Atom A

	El	Lbl	Ox	Wyck
☐	Ca	1	+2.00	1c
☐	Sr	1	+2.00	2h
☐	Cu	1	+2.08	2g
☐	Lu	1	+3.00	1c

✓ (un)select all

Atom B

	El	Lbl	Ox	Wyck
☐	Ca	1	+2.00	1c
☐	Sr	1	+2.00	2h
☐	Cu	1	+2.08	2g
☐	Lu	1	+3.00	1c

✓ (un)select all

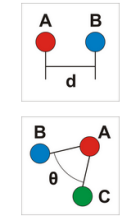
Atom C

	El	Lbl	Ox	Wyck
☐	Ca	1	+2.00	1c
☐	Sr	1	+2.00	2h
☐	Cu	1	+2.08	2g
☐	Lu	1	+3.00	1c

✓ (un)select all

Histograms

Calculate



ICSD – Detailed View – Bibliography, Experimental/Additional Information

Bibliographic information may include abstracts for newer entries (since 2016)

PDF numbers only available for a small amount of entries

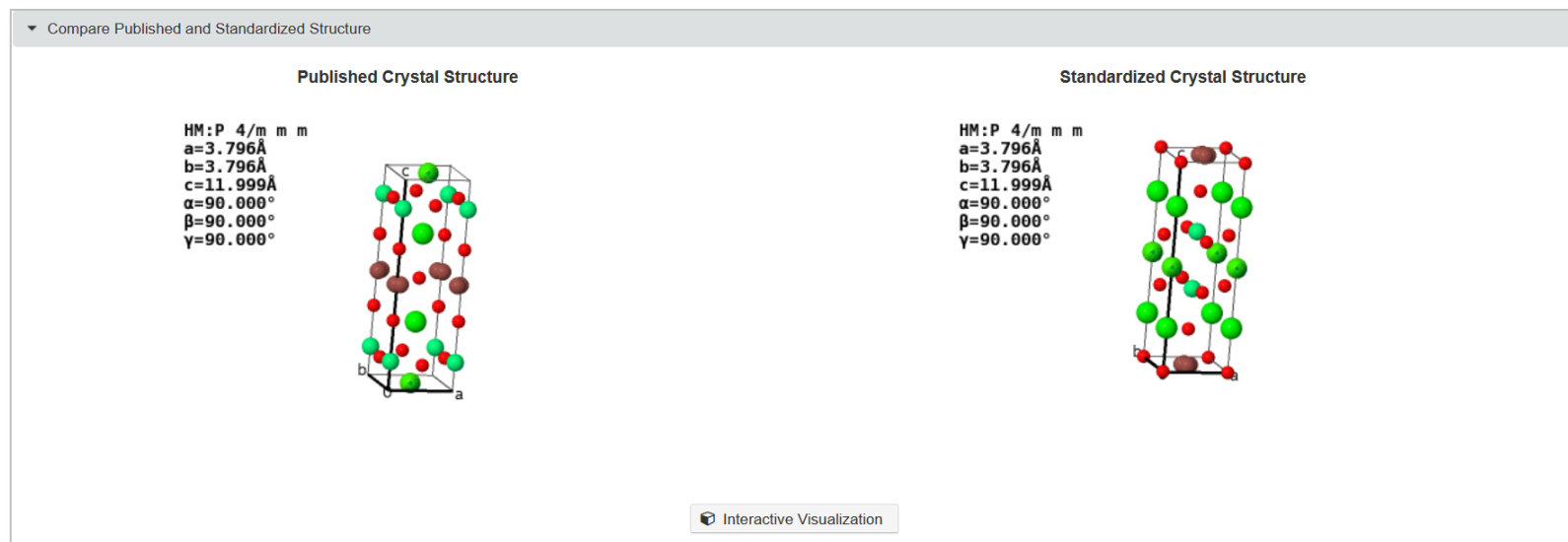
Remarks/Comments can contain valuable additional information

▼ Bibliography			
Author	Shimakawa, Y.; Jorgensen, J.D.; Shaked, H.; Hitterman, R.L.; Kondo, T.; Manako, T.; Kubo, Y.	Title	Underdoped, optimally doped, and overdoped superconductors Tl Sr ₂ (R _{1-x} Cax) Cu ₂ O _{7-d} (R=Lu or Tl)
Reference	Physical Review B: Condensed Matter and Materials Physics (1995) 51, (*) Article ID * (p. 568-575)	DOI	10.1103/PhysRevB.51.568
Get full text	by Google Scholar		
▼ Experimental information			
Temperature	room temperature	Pressure	atmospheric
Radiation type	Neutron	Sample type	Powder data
R-value	0.0492		
PDF calc.	01-089-0010		
Remarks	Rietveld profile refinement applied	Remarks	Temperature factors available
▼ Additional information			
Comments	Underdoped, T _c = 50 K		

ICSD – Detailed View – Compare published/standardized structure

Pictures of the published and the standardized structure

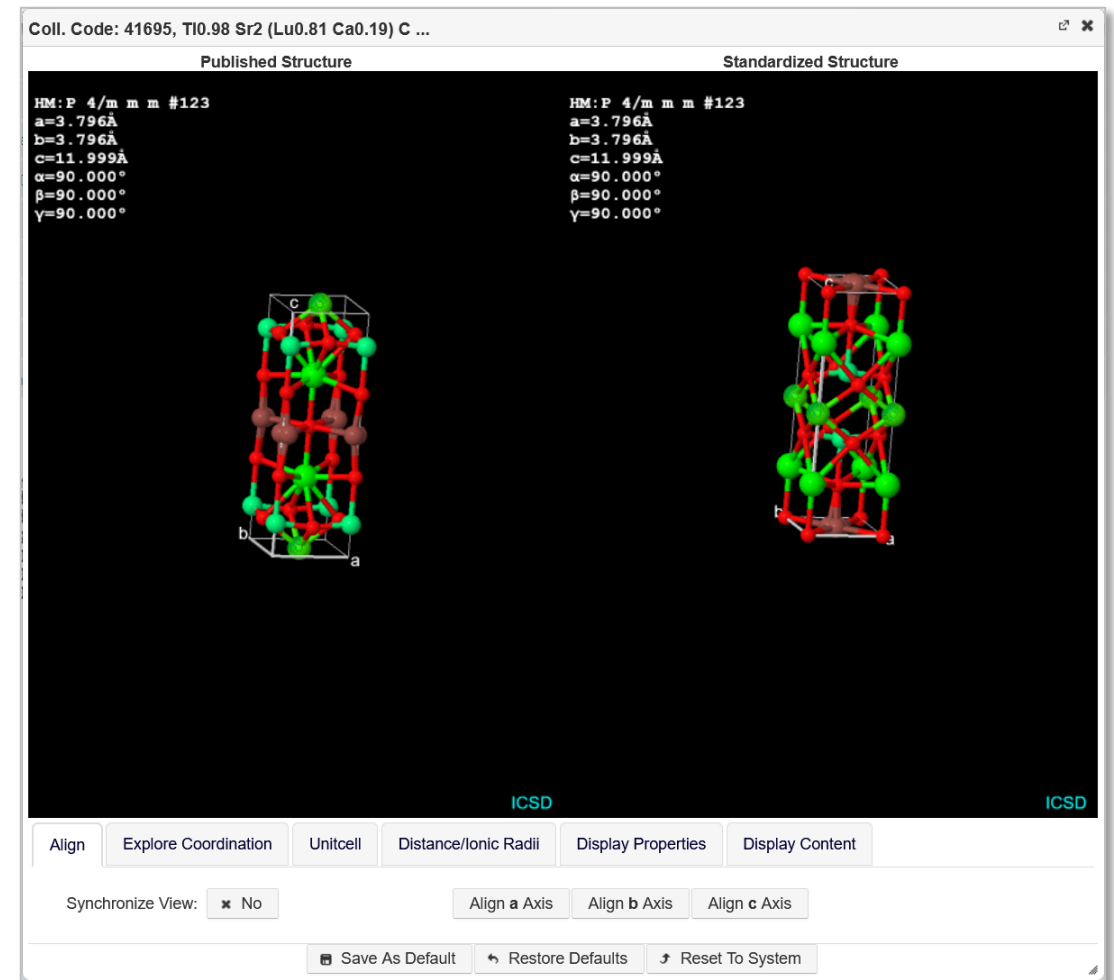
Interactive view is also available



ICSD – Detailed View – Compare published/standardized structure

Interactive view of the published and standardized structure

Visualization can be adjusted as for single structures



ICSD – API (documentation/test)

Intended for projects that require large amounts of data (no limit to CIFdownload).

Can/Should be accessed via client application. E.g. Rigaku is currently working on integrating it into their software.

Python clients:

<https://github.com/Ircfmd/ICSDClient>

https://github.com/simonverret/materials_data_api_scripts

ICSD Rest API V4.3.0
[Base URL: icsd.fiz-karlsruhe.de/ws]
<https://icsd.fiz-karlsruhe.de/ws/swagger.json>

This is the API documentation for the RestFul http web services that you can use to **programmatically access** ICSD search results and resources.
Please note: The use of this API is limited to authorized users! Please contact the helpdesk at icsd@fiz-karlsruhe.de to obtain permission.
[More about ICSD](#)

Schemes
HTTPS

authentication methods to perform login or logout

- POST** `/auth/login` Perform an authentication.
- GET** `/auth/ip` Perform an IP-based authentication.
- GET** `/auth/logout` Invalidates an authenticated session.

search search methods on ICSD database

- GET** `/search/simple` Performs a simple search on any attributes of icsd.
- POST** `/search/simple` Performs a simple search on any attributes of icsd.
- GET** `/search/expert` Performs an 'expert' search for all icsd attributes using search expressions.
- POST** `/search/expert` Performs an 'expert' search for all icsd attributes using search expressions.

CIF methods to get CIF content from database identifiers

- GET** `/cif/multiple` Get crystallographic data in CIF format
- GET** `/cif/{idnum}` Get crystallographic data in CIF format

ICSD – API (Authentication)

Authentication via
login/password to get a token

Searching/downloading is than
handle using the token

authentication methods to perform login or logout

POST /auth/login Perform an authentication.

Currently, there are 2 different authentication methods supported:

- LoginID & Password
- IP-based

Depending on the supplied subject data, the system tries the above listed options in the given order. If the **LoginID** or **Password** are missing, an **IP-based authentication** will be performed

Successfully authenticated users are assigned an authorization token to access the system. This token is returned as part of the HTTP response headers 'ICSD-Auth-Token', and should live as long as the user session on the client side. **Subsequent requests** to any 'non login' resources/methods **should assign this authorization token** in 'ICSD-Auth-Token' http header value. If **client requests are inactive for more than 1 hour**, the **authorization token will be invalidated**. Subsequent requests to any 'non login' resources/methods will be rejected with status code 401 and a **new login** request must be performed.

Parameters Cancel

Name	Description
loginid string (FormData)	The login ID/username of the ICSD account. If this parameter is not set, an IP-based authentication will be performed.
password string (FormData)	The password of the ICSD account. If this parameter is not set, an IP-based authentication will be performed.

Execute

Responses Response content type text/plain

ICSD – API (Authentication)

Authentication via
login/password to get a token

Searching/downloading is then
handled using the token

Execute Clear

Responses Response content type text/plain

Curl

```
curl -X POST "https://icsd.fiz-karlsruhe.de/ws/auth/login" -H "accept: text/plain" -H "Content-Type: application/x-www-form-urlencoded" -d "loginid=loginid&password=yourt20password"
```

Request URL

```
https://icsd.fiz-karlsruhe.de/ws/auth/login
```

Server response

Code	Details
200	Response body Already authenticated. Download Response headers <pre>connection: keep-alive content-length: 22 content-type: text/plain date: Wed, 28 Jul 2021 09:32:05 GMT icsd-auth-token: 69DC33FEB27BCDCCE8A7A5EA3390E0CD keep-alive: timeout=20 strict-transport-security: max-age=31536000, includeSubDomains</pre>

ICSD – API (Search)

Search uses the Expert Mask syntax

Results are a list of idnums
(internal ID for entries not always identical to collection codes)

The screenshot shows the ICSD API search interface. A red oval highlights the search parameters section, which includes:

- query** (required): string (query). The input field contains "authors: jansen".
- content type**: array[string] (query). A dropdown menu is open, showing "EXPERIMENTAL_INORGANIC" (selected), "EXPERIMENTAL_METALORGANIC", and "THERORETICAL_STRUCTURES".
- ICSD-Auth-Token** (required): string (header). The input field contains "69DC33FEB27BCDCCEE8A7A5EA3390E0CC".

Below the input fields are "Execute" and "Clear" buttons. The "Responses" section shows the "Response content type" set to "application/xml". The "Curl" section displays the generated curl command. The "Request URL" section shows the full API endpoint. The "Server response" section shows a 200 status code and the XML response body, which is a list of idnums.

Curl

```
curl -X GET "https://icsd.fiz-karlsruhe.de/ws/search/expert?query=authors%3A%20jansen&content%20type=EXPERIMENTAL_INORGANIC" -H "accept: application/xml" -H "ICSD-Auth-Token: 69DC33FEB27BCDCCEE8A7A5EA3390E0CC"
```

Request URL

```
https://icsd.fiz-karlsruhe.de/ws/search/expert?query=authors%3A%20jansen&content%20type=EXPERIMENTAL_INORGANIC
```

Server response

Code	Details
200	Response body <pre><?xml version="1.0" encoding="UTF-8" standalone="yes"?> <hits> <idnums>208906 208919 208918 38936 700434 208922 208921 700432 86042 208920 700433 208931 800813 208933 208932 915493 915494 12335 12336 919608 36920 405566 919607 405564 405565 923701 84028 405563 84030 208967 919626 208966 208965 407628 208968 84049 802908 919638 919636 919637 919634 919635 919632 919633 73837 20591 73838 417910 417911 417908 417909 4216 417916 417914 417915 417912 417913 22656 22657 200842 39052 39053 49294 49295 2198 2199 49305 49306 155 49307 809130 432302 26793 26794 170 26795 26796 26797 26802 84146 10423 913591 913590 250044 4289 32964 100553 100555 100554 100556 911583 911582 809196 84195 911584 950527 35067 803059 950534 434444 434443 950531 16659 2329 35097 702754 702755 104747 4396 4397 47405 104748 4398 702756 702757 104759 928056 47424 2396 964944 964945 407910 407911 35172 29032 86378 991587 205166 407912 205171 205170 420215 205169 205168 8564 422256 35191 24953 16764 209279 209278 209277 41343 209276 209280 31109 201093 436608 436609 47499 47501 47502 20882 803225 803220 86427 86429 86428 82335 86431 63903 82334 86430 82337 86433 86432 86435 82338 86434 86437 37285 86436 86438 16808 47529 86454 65979 86458 43452 807372 807373 104899 807374 104900 807370 807371 100811 100810 209352 70101 805336 805328 100831 70110 16866 418276 33252 704994 704995 704993 498 805375 74228 418302 975350 45561 20986 418300 20987 63995 418301 63996 805360 938482 63997 418299 59902 100863 100864 702987 301568 100868 803332 803333 805376 803331 805379 703002 29202 703000 29203 703001 703007 6683 100897 954925 100896 954927 408100 954924 100898 250400 954925 408099 209450 703008 25139 25140 25141 25142 31288 37435 37436 111165 809520 809521 809522 954928 47679 705091 705089 705092</pre>

Thank you for your attention

Contact

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ADVANCING SCIENCE

Theoretical structures, practical examples and data mining

25th IUCr congress - Joint Workshop for CSD and ICSD

Dr. Dejan Zagorac, "Vinča" Institute of Nuclear Sciences
Belgrade, Serbia

Theoretical structures in the ICSD database

The major problem of theoretical structures is that a huge amount of calculations exists in a broad variety of quality. We have three major criteria for the selection:

- 1. the structure should be published in a peer-reviewed journal*
- 2. the structures have a low $E(\text{tot})$ (close to the equilibrium structure)*
- 3. we choose the method which delivers data that are closest to comparable experimental results*

Theoretical crystal structures are clearly separated from experimental structures in the ICSD so that you can choose to search only experimental inorganic structures, or experimental metal-organic structures, only theoretical inorganic structures, or any combination of these three options. Furthermore we have categorized all theoretical structures by the following 13 methods used for the theoretical calculation listed below.

Theoretical structures in the ICSD database

 **Journal of Applied Crystallography**

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 RESEARCH PAPERS

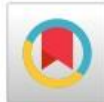
J. Appl. Cryst. (2019). **52**, 918–925
<https://doi.org/10.1107/S160057671900997X>
Cited by **46**



Recent developments in the Inorganic Crystal Structure Database: theoretical crystal structure data and related features

D. Zagorac, H. Müller, S. Ruehl, J. Zagorac and S. Rehme

The Inorganic Crystal Structure Database (ICSD) is the world's largest database of fully evaluated and published crystal structure data, mostly obtained from experimental results. However, the purely experimental approach is no longer the only route to discover new compounds and structures. In the past few decades, numerous computational methods for simulating and predicting structures of inorganic solids have emerged, creating large numbers of theoretical crystal data. In order to take account of these new developments the scope of the ICSD was extended in 2017 to include theoretical structures which are published in peer-reviewed journals. Each theoretical structure has been carefully evaluated, and the resulting CIF has been extended and standardized. Furthermore, a first classification of theoretical data in the ICSD is presented, including additional categories used for comparison of experimental and theoretical information.



Keywords: Inorganic Crystal Structure Database; ICSD; theoretical structures; standardization; classification.

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Theoretical structures in the ICSD database

Table 2

Summary of theoretical categories in the ICSD.

Theoretical category in the ICSD	References†
<i>Ab initio</i> optimization	Zagorac <i>et al.</i> (2014a); Mayo <i>et al.</i> (2016)
Empirical and semi-empirical potential	Fan <i>et al.</i> (2015); Yoo <i>et al.</i> (2016)
Geometric modelling	Zagorac <i>et al.</i> (2014b); George <i>et al.</i> (2015)
Monte Carlo simulation	Hao <i>et al.</i> (2014); Mena <i>et al.</i> (2016)
Molecular dynamics	Schmidt <i>et al.</i> (2015); Paściak <i>et al.</i> (2015)
Plane waves method	Weerasinghe <i>et al.</i> (2015); Goncharov <i>et al.</i> (2016)
FP(L) augmented plane-wave method (+lo)	Mukadam <i>et al.</i> (2016); Čebela <i>et al.</i> (2017)
Projector augmented wave method	Zurek & Yao (2015); Buckeridge <i>et al.</i> (2016)
Linear combination of atomic orbitals method	Zagorac <i>et al.</i> (2011); Larbi <i>et al.</i> (2016)
(FP) linear muffin-tin orbital (ASA)	Uba <i>et al.</i> (2016); Mishra & Ganguli (2016)
Hartree–Fock method	Shimazaki & Nakajima (2015); Zagorac <i>et al.</i> (2017a)
Density functional theory	Civalleri <i>et al.</i> (2007); Schönecker <i>et al.</i> (2015)
Hybrid functionals	Lee <i>et al.</i> (2015); Sluydts <i>et al.</i> (2017)
Predicted (non-existing) crystal structure	Doll <i>et al.</i> (2008); Luković <i>et al.</i> (2017)
Optimized (existing) crystal structure	Olsson <i>et al.</i> (2015); Erba <i>et al.</i> (2015)
Combination of theoretical and experimental structure	Retuerto <i>et al.</i> (2016); Cvijović-Alagić <i>et al.</i> (2019)

† References to example theoretical structures found using that theoretical method and already searchable in the ICSD.

Upgrade of the theoretical CIF file

the ICSD provides additional computational information used in the calculation of the respective theoretical crystal structures. This computational information provides details about the code, search algorithm, method, basis set information and technical details of the calculation (e.g. cutoff energy, K-point mesh etc.), providing information on reproducibility and quality of computations.

In addition we provide comments on the tolerances in energy, forces etc. used in calculations if present (which are similar to the experimental structure criteria R factors, FOMs etc.). Examples will follow.

How to search for new (not-yet synthesized) structures or materials

- Maybe one of the most important examples for the experimental CSD/ICSD users is the use of the theoretical category: predicted (non-existing) crystal structure. As crystal structure predictions become more and more reliable, this category can be an excellent tool for synthesis planning.

ICSD

Welcome to ICSD-Desktop.

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Content Selection

☐ Experm. inorganic structures

☐ Experm. metal-organic str.

☒ Theoretical structures

Navigation

Basic search & retrieve

Advanced search & retrieve

Bibliography

Cell

Chemistry

Symmetry

Crystal Chemistry

Structure Type

Experimental Information

DB Info

Expert Search

Experimental Information Search

Temperature K

Pressure MPa

Comments

e.g. stable above

Calculation Methods

Predicted (non-existing) crystal structure

Clear Experimental Info Search

Count Experimental Info Search

Search Action

Run Query

Clear Query

Search Summary

Bibliography: -

Cell: -

Chemistry: -

Symmetry: -

Crystal Chemistry: -

Structure Types: -

Experimental Info: 3860

DB Info: -

Expert: -

Combined Results: 3860

Query History

Number of queries: 7

Clear Query History

2020-04-03T23:24 404

How to search for new (not-yet synthesized) structures or materials

- Obtaining information on predicted not-synthesized unknown compounds, or/and not-synthesized modifications of known compounds, could be an important advantage for CSD/ICSD users with numerous scientific, technological and industrial applications.
- Search for new predicted (non-existing) structures or materials can be more precise if the user combines search with standardized keywords in the ICSD.

Theoretical category in the ICSD	No. of CIF files
Predicted (non-existing) crystal structure	3860
Optimized (existing) crystal structure	2461
Combination of theoretical and experimental structure	1368

Table 1. Number of theoretical crystal structures (CIF files) in the ICSD Desktop (2019.2)

Search for parameters for method development and future calculations



- Optimized (or existing) crystal structures are theoretically calculated structures of existing experimental crystal structures in the ICSD until the year of publication.
- In experimental materials science and related sciences, they can be used as an excellent tool for industrial and technological applications where it is very important to fine-tune materials, because slight deviations between the calculation and experiment can lead to different properties of the material. [1]
- In computational materials science and related sciences, optimized structures can be used for method development and to generate parameters for future calculations.
- In the following text we show one such example.

[1] D. Zagorac, H. Müller, S. Ruehl, J. Zagorac and S. Rehme, J. Appl. Cryst. (2019) 52, 918-925.

Search for parameters for method development and future calculations

ICSD

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Content Selection

- ☐ Experim. inorganic structures
- ☐ Experim. metal-organic str.
- ☒ Theoretical structures

Navigation

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- Advanced search & retrieve**
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- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information**
- DB Info
- Expert Search

Experimental Information Search

Temperature: K

Pressure: MPa

Comments: e.g. stable above

Calculation Methods: Optimized existing crystal structure

Clear Experimental Info Search

Count Experimental Info Search

Search Action

Run Query

Clear Query

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	2461
DB Info:	-
Expert:	-
Combined Results:	2461

Query History

Number of queries: 0

Clear Query History

Search for parameters for method development and future calculations

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Content Selection

- ☐ Experim. inorganic structures
- ☐ Experim. metal-organic str.
- ☒ Theoretical structures

Navigation

- Basic search & retrieve
- Advanced search & retrieve**
- Bibliography
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information**
- DB Info
- Expert Search

Experimental Information Search

Temperature: K

Pressure: MPa

Comments:

e.g. stable above

Calculation Methods

Projector augmented wave method, Optimized existing crystal structure

- ☒ Projector augmented wave method
- ☐ Linear combination of atomic orbitals method
- ☐ Density functional theory
- ☐ Hartree-Fock method
- ☐ Post-Hartree-Fock method
- ☐ Hybrid functionals
- ☐ Predicted (non-existing) crystal structure
- ☒ Optimized existing crystal structure

Count Experimental Info Search

Search Action

Run Query Clear Query

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	2461
DB Info:	-
Expert:	-
Combined Results:	2461

Query History

Number of queries:	0
--------------------	---

Clear Query History

Search for parameters for method development and future calculations

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Content Selection

☐ Experi. inorganic structures

☐ Experi. metal-organic str.

☒ Theoretical structures

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Symmetry

Crystal Chemistry

Structure Type

Experimental Information

DB Info

Expert Search

Experimental Information Search

Temperature K

Pressure MPa

Comments

e.g. stable above

Calculation Methods

Clear Experimental Info Search

Count Experimental Info Search

Search Action

Run Query

Clear Query

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	1324
DB Info:	-
Expert:	-
Combined Results:	1324

Query History

Number of queries:	0
--------------------	---

Clear Query History

Search for parameters for method development and future calculations

ICSD

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Content Selection

☐ Exprim. inorganic structures

☐ Exprim. metal-organic str.

☒ Theoretical structures

Navigation

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Cell

Chemistry

Symmetry

Crystal Chemistry

Structure Type

Experimental Information

Experimental Information Search

Temperature K

Pressure MPa

Comments
e.g. stable above

Calculation Methods

Clear Experimental Info Search

Count Experimental Info Search

Search Action

Run Query

Clear Query

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	182
DB Info:	-
Expert:	-
Combined Results:	182

Query History

Number of queries:	0
--------------------	---

How to search ICSD for experimental and theoretical data on nanostructures

- Optimized structures are excellent tool for various applications, and maybe one of the most interesting is combination of optimized structures with standardized keywords.
- This searches can involve properties of materials (electronic, magnetic, optical, etc), or the use of keywords combined with, for example, chemical (elements) search, or structural (structure types) information easily enables searches for special materials like superconductors or piezoelectric materials, or technical applications like solar cells or solid electrolytes. [1,2]
- Search for nanostructures can be even further examined by including experimental nanostructures. This can be performed by using theoretical category: combination of theoretical and experimental structure (Table 1).
- If such data exist in the manuscript they are highly valuable to all materials scientists with a great variety of possible applications, owing to the high precision of the published data.
- In the following examples we will show how to search the ICSD for nanostructures.

[1] D. Zagorac, H. Müller, S. Ruehl, J. Zagorac and S. Rehme, J. Appl. Cryst. (2019) 52, 918-925.

[2] <https://icsd.products.fiz-karlsruhe.de/en/howuse/using-keywords-perform-very-specific-searches-icsd>

How to search ICSD for experimental and theoretical data on nanostructures

ICSD

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Content Selection

☐ Experm. inorganic structures
☐ Experm. metal-organic str.
☒ Theoretical structures

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[Crystal Chemistry](#)
[Structure Type](#)
[Experimental Information](#)
[DB Info](#)
[Expert Search](#)

Query Management

Bibliography Search

Authors
e.g. Jansen

Title of Journal
e.g. Angewandte Chemie

Title of Article
e.g. Super conducting crystals

Year of Publication
e.g. >2008 or 2000-2006 or 2001

Volume
e.g. 10

Page first
e.g. 10

Abstract
e.g. hybrid cage clusters

Keywords
Nano
e.g. Polymorphism

Clear Bibliography Search

Count Bibliography Search

Search Action

Run Query

Clear Query

Search Summary

Bibliography: 625

Cell: -

Chemistry: -

Symmetry: -

Crystal Chemistry: -

Structure Types: -

Experimental Info: 1368

DB Info: -

Expert: -

Combined Results: 96

Query History

Number of queries: 7

Clear Query History

2020-04-03T23:24404

2020-04-03T02:032

Figure 4a. Example on how to search the ICSD for theoretical nanostructures (ICSD Desktop 2019.2)

How to search ICSD for experimental and theoretical data on nanostructures: Example with Organic-Inorganic Hybrid Material

ICSD Welcome to ICSD-Desktop. FIZ Karlsruhe | Contact

Results: List View # of Hits: 96 (1 selected)

Back to Query Show Detailed View Export Data Print Visualize Structure Visualize Powder Pattern Column Selection Filter

	Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Reference	
☒	670885	P 42/m n m	Ti O ₂	Rutile-TiO ₂	Density functional theory a	Zhang, Tianshi; Wojtal, Pat	RSC Advances (2015) 5, (	
☐	670886	P 63 m c	Zn O	Wurtzite-ZnS(2H)	Density functional theory a	Zhang, Tianshi; Wojtal, Pat	RSC Advances (2015) 5, (	
☐	671246	F m -3 m	Cd S	NaCl	Co effect on zinc blende-rc	Zhao, Rui; Wang, Pan; Yac	RSC Advances (2015) 5, (	
☐	671247	F -4 3 m	Cd S	Sphalerite-ZnS(cF8)	Co effect on zinc blende-rc	Zhao, Rui; Wang, Pan; Yac	RSC Advances (2015) 5, (	
☐	671334	F m -3 m	Ni ₃ Sn	Heusler-AlCu ₂ Mn	Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
☐	671335	F m -3 m	Ni	fcc(ccp)-Cu	Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
☐	671336	I 41/a m d Z	Ni		Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
☐	671337	P 63/m m c	Ni ₃ Sn ₂	Ni ₃ SnP-Co _{1.75} Ge	Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
☐	671338	F m -3 m	Sn	fcc(ccp)-Cu	Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
☐	671339	I 41/a m d Z	Sn		Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	

(1 of 10) 1 2 3 4 5 6 7 8 9 10

Density functional theory and experimental studies of caffeic acid adsorption on zinc oxide and titanium dioxide nanoparticles

Tianshi Zhang,^a Patrick Wojtal,^a Oleg Rubel^a and Igor Zhitomirsky^{a,*}

Author affiliations
<https://doi.org/10.1039/C5RA21511K>

Abstract

The outstanding adsorption properties of proteins, containing catecholic amino acid, L-3,4-dihydroxyphenylalanine (DOPA), and recent advances in nanoparticle functionalization using molecules from the catechol family have generated interest in the investigation of catechol adsorption and applications of catecholates in nanotechnology. Caffeic acid (CA) is the closest molecular analogue of DOPA. Density functional theory has been applied for the modelling of CA adsorption on the surface of ZnO and TiO₂. Different adsorption modes have been investigated and corresponding adsorption energies were evaluated. According to the calculated energies, the adsorption of CA is energetically favourable at both surfaces with a stronger affinity to TiO₂. The results of theoretical studies were supported by experimental investigations of CA adsorption. The use of CA as a dispersant for hydrothermal synthesis of ZnO allowed for the fabrication of ZnO nanorods with reduced size and increased aspect ratio. The CA, adsorbed during the hydrothermal synthesis on ZnO nanorods, allowed for their electrostatic dispersion and the electrophoretic deposition (EPD) of ZnO films from stable colloidal suspensions. In another strategy, CA was added as a dispersant for the dispersion of TiO₂ nanorods and the EPD of TiO₂ films. The advantages of catecholates for the synthesis of nanoparticles and fabrication of thin films are discussed.

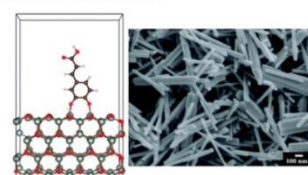


Figure 4b. Example on how to search the ICSD for combined theoretical and experimental nanostructures (ICSD Desktop 2019.2); Example with Organic-Inorganic Hybrid Material(Zhang et al.)

How to search ICSD for experimental and theoretical data on nanostructures

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Detailed View Entry 1 of 1 ?

[Back to Query](#) [Back to List](#) [Previous](#) [Next](#) [Export Cif](#) [Print](#) [Feedback to Editor](#)

Summary Collection Code 670886

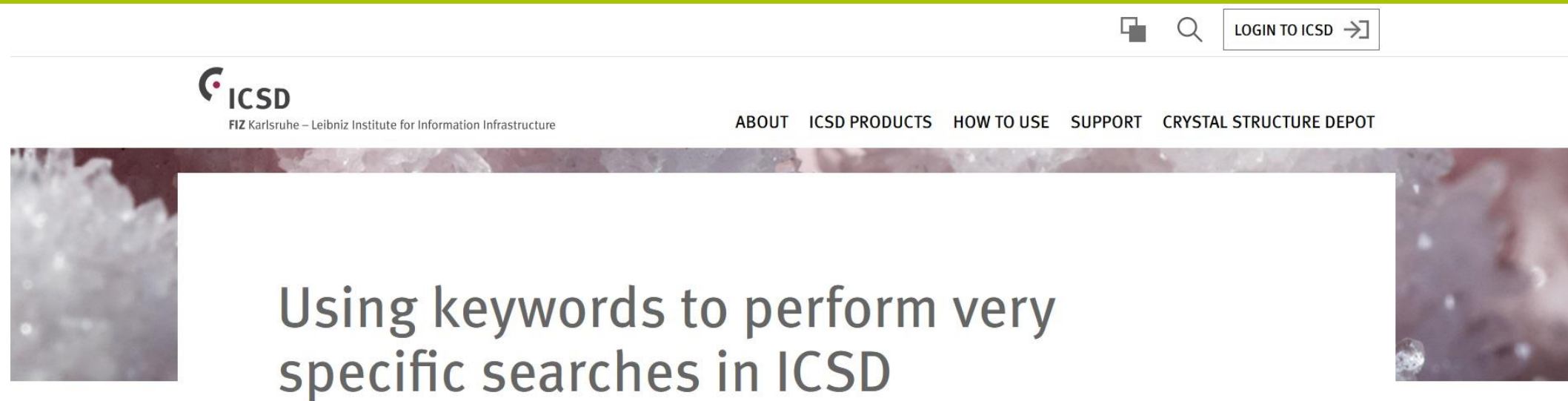
Struct. formula	Zn O	Structure type	Wurtzite-ZnS(2H)
Cell parameter	3.273 3.273 5.333 9 9 12	Space group	P 63 m c (186)
Cell volume	49.47 [Å³]	Z	2
Temperature	room temperature	Pressure	atmospheric
Data quality	Calculated structure		
Author	Zhang, Tianshi; Wojtal, Patrick; Rubel, Oleg; Zhitomirsky, Igor	Title	Density functional theory and experimental studies of caffeic acid adsorption on zinc oxide and titanium dioxide nanoparticles
Reference	RSC Advances (2015) 5, (129) p106877-p106885	DOI	10.1039/c5ra21511k

Details Expand all Collapse all ?

- Visualization
- Chemistry
- Published Crystal Structure Data
- Standardized Crystal Structure Data
- Distances and Angles
- Bibliography
- Theoretical information

Temperature	room temperature	Pressure	atmospheric
Calculation method	Ab initio optimization	Calculation method	Projector augmented wave method
Calculation method	Density functional theory		
Remarks	Optimized existing crystal structure	Remarks	Combination of theoretical and experimental structure

How to search ICSD using keywords



In the context of the ever-increasing demand for energy, batteries play a decisive role as storage devices for excess energy and as "mobile" energy suppliers for applications such as those in the automotive industry. At present, batteries based on lithium ions or lead accumulators are mainly used. But whether these concepts can satisfy the constantly growing demand is questionable. For example, lithium-ion batteries also require other rare elements such as cobalt, so that economic and environmental aspects must also be taken into account. The toxicity of lead has been known for a long time and thus limits possible applications.

<https://icsd.products.fiz-karlsruhe.de/en/howuse/using-keywords-perform-very-specific-searches-icsd>
<https://icsd.products.fiz-karlsruhe.de/sites/default/files/ICSD/documents/use-cases/ICSD-Keywords-2019.pdf>

How to search ICSD for crystal structures using Data Mining methods: Example binary AX system

ICSD

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Expert Search

Chemistry Search

Composition [Periodic Table](#)
e.g. Na Cl

Structural Formula
e.g. Pb (W O4)

Chemical Name

Mineral Name
e.g. Adamite

Mineral Group
e.g. Pyroxene

ANX Formula

AB Formula

Formula Weight

Number of Elements

Number of Formula Units

[Clear Chemistry Search](#) [Count Chemistry Search](#)

Search Action

[Run Query](#) [Clear Query](#)

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	33750
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-
Combined Results:	33750

Query History

Number of queries: 0

[Clear Query History](#)

No records found.

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Chemistry Search

Composition [Periodic Table](#)

e.g. Na Cl

Number of Elements

Structural Formula

e.g. Pb (W O4)

Chemical Name

Mineral Name

e.g. Adamite

Mineral Group

e.g. Pyroxene

ANX Formula

Number of Formula Units

AB Formula

Formula Weight

[Clear Chemistry Search](#)

[Count Chemistry Search](#)

Search Action

[Run Query](#) [Clear Query](#)

Search Summary

Bibliography: -

Cell: -

Chemistry: 41819

Symmetry: -

Crystal Chemistry: -

Structure Types: -

Experimental Info: -

DB Info: -

Expert: -

Combined Results: 41819

Query History

Number of queries: 30

[Clear Query History](#)

2021-08-01T15:39 140

How to search ICSD for crystal structures using Data Mining methods: Example binary AX system

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 - Structure Type**
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- Query Management**
 - Manage Queries
 - List Combined Queries
 - Create Combined Query

Structure Type Search

Pre Defined Structure Types

Structure Type

☐ Search in predefined structure types

Structure Type Descriptors

SpaceGrp	Wyck	Pearson	ANX
☐ A112/m	☐ a	☐ aP16	☐ ax
☐ Aba2	☐ a10	☐ aP2	☒ AX
☐ Ama2	☐ a108	☐ aP4	
☐ Amm2	☐ a12	☐ aP8	
☐ B112/m	☐ a14	☐ cF11	
☐ B2mm	☐ a16	☐ cF12	
☐ Bbmm	☐ a17	☐ cF16	
☐ Bmmb	☐ a18	☐ cF20	

(1 of 18) (1 of 29) (1 of 19)

Clear Structure Search Count Structure Search

Search Action

Run Query Clear Query

Search Summary

- Bibliography: -
- Cell: -
- Chemistry: 41819**
- Symmetry: -
- Crystal Chemistry: -
- Structure Types: 7206**
- Experimental Info: -
- DB Info: -
- Expert: -
- Combined Results: 4732**

Query History

Number of queries: 30

Clear Query History

2021-08-01T15:39	140
2021-06-25T10:41	3
2021-06-25T10:32	3
2021-06-16T13:56	6
2021-06-16T13:46	19

How to search ICSD for crystal structures using Data Mining methods: Example binary AX system

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Query Management

Crystal Chemistry Search

Interatomic Distances

	Atom A	Ox. A		Atom B	Ox. B	$d_{\min}AB$	$d_{\max}AB$
			-				
AND			-				
AND			-				
AND			-				

Minimum Distances

Atom A	Atom B	$d_{\min}AB$	$d_{\max}AB$

Crystal Structure is

☐ Polytype Structure
☐ Modulated Structure
☐ Disordered Structure
☐ Order/Disorder Structure
☐ Mineral
☒ Prototype Structure Type
☐ Structure Type

[Clear Crystal Search](#)[Count Crystal Search](#)[Clear Check Boxes](#)

Search Action

[Run Query](#)[Clear Query](#)

Search Summary

Bibliography:	-
Cell:	-
Chemistry:	41819
Symmetry:	-
Crystal Chemistry:	9490
Structure Types:	7206
Experimental Info:	-
DB Info:	-
Expert:	-
Combined Results:	140

Query History

Number of queries:	30
Clear Query History	
2021-08-01T15:39	140
2021-06-25T10:41	3
2021-06-25T10:38	2

How to search ICSD for crystal structures using Data Mining methods: Example binary AX system

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Results: List View # of Hits: 140 ?

☐	Coll. Code ▲	HMS ⇅	Struct. Form. ⇅	Struct. Type ⇅	Title ⇅	Authors ⇅	Reference ⇅	☆ ▼	
☐	59	P 63/m m c	Ga S	InSe(beta)#GaS	Refinement of the 2h (GaS	Kuhn, A.; Chevy, A.; Chev	Acta Crystallographica, Se	☆	
☐	109	P -1	Te I	Tel	Zur Kenntnis der Subhalog	Kniep, R.; Mootz, D.; Rabe	Zeitschrift fuer Anorganiscl	☆	
☐	1558	C 1 2/m 1	Bi I	Bil(mS32)	Wismutmonojodid Bi J, ein	von Schnering, H.G.; von E	Zeitschrift fuer Anorganiscl	☆	
☐	1559	C 1 2/m 1	Bi I	Bil(mS16)	Wismutmonojodid Bi J, ein	von Schnering, H.G.; von E	Zeitschrift fuer Anorganiscl	☆	
☐	1621	P n a m	Ge S	GeS	Verfeinerung der Struktur v	Bissert, G.; Hesse, K.F.	Acta Crystallographica, Se	☆	
☐	2304	P 1 21/n 1	S4 N4	S4N4	Crystal structure of tetrasu	de Lucia, M.L.; Coppens, F	Inorganic Chemistry (1978	☆	
☐	2429	P 21 3	In Cl	InCl	The structures of yellow an	van der Vorst, C.P.J.M.; Ve	Acta Crystallographica, Se	☆	
☐	2626	P 1 21/n 1	As4 Se4	AsS	Tetra-arsenic tetraselenide	Smail, E.J.; Sheldrick, G.M	Acta Crystallographica, Se	☆	
☐	14009	P 21 21 21	Na P	NaP	Darstellung, Struktur und E	von Schnering, H.G.; Hoen	Zeitschrift fuer Anorganiscl	☆	
☐	15065	P n a 21	Co As	CoAs	Structural and magnetic pr	Selte, K.; Kjekshus, A.	Acta Chemica Scandinavic	☆	

(1 of 14)   1 2 3 4 5 6 7 8 9 10   10 ▼

How to search ICSD for crystal structures using Data Mining methods: Example binary AX system



CrystEngComm

PAPER

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[View Journal](#)



Cite this: DOI: 10.1039/c7ce01039g

Structure prediction of aluminum nitride combining data mining and quantum mechanics†

J. Zagorac, ^{id}*^a D. Zagorac,^a M. Rosić,^a J. C. Schön^b and B. Matović^a

Aluminum nitride (AlN) is a compound with wide technological applications from optics to electronics. At ambient pressure and temperature, AlN has a hexagonal wurtzite type of structure, while the zinc blende (ZnS) type of structure is found in very thin films. At high pressures, a first-order phase transformation from the wurtzite structure to a rock salt type structure has been observed. This study covers the experimentally observed modifications of AlN, investigates their relations and searches for new possible modifications. Therefore, data mining of over 140 000 structure candidates has been performed, followed by local optimizations at the *ab initio* level with Hartree–Fock, LDA, and B3LYP functionals. Finally, twelve structure candidates have proven to be the most promising ones. These include the novel metastable AlN polytypes and the 5-5-type as a possible high pressure candidate of AlN.

Received 2nd June 2017,
Accepted 1st August 2017

DOI: 10.1039/c7ce01039g

rsc.li/crystengcomm

How to search ICSD for crystal structures using Data Mining methods: Example binary AX system- AlN compound

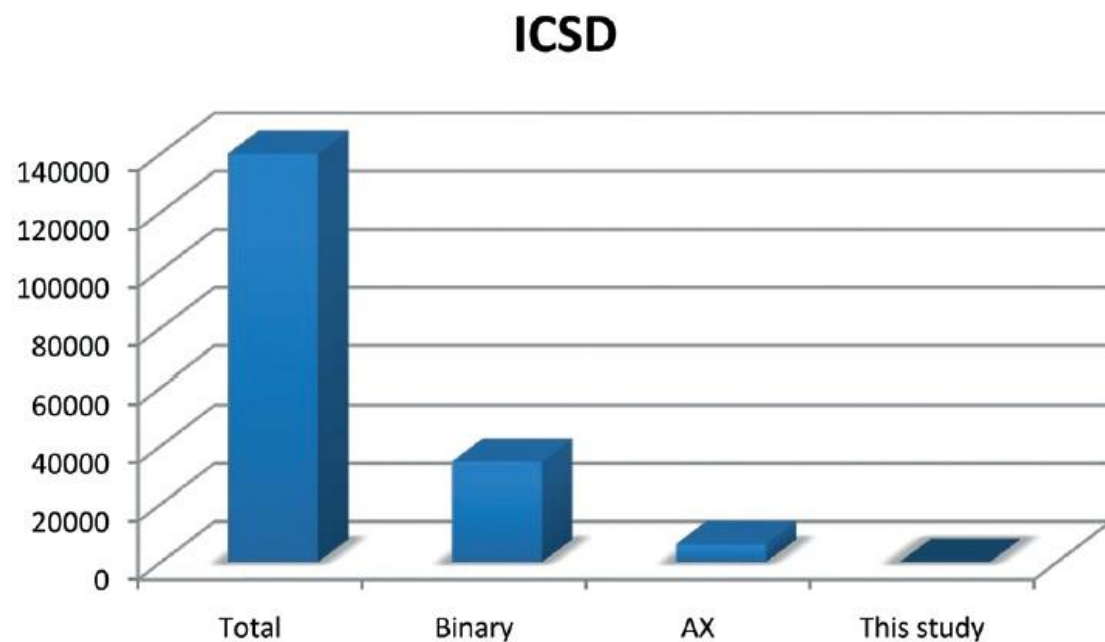


Fig. 2 Statistical analysis of the data mining *ab initio* approach. The figure depicts drastic reduction of possible structure candidates from this study to the total amount of structures listed in the ICSD database, saving time and computational cost.

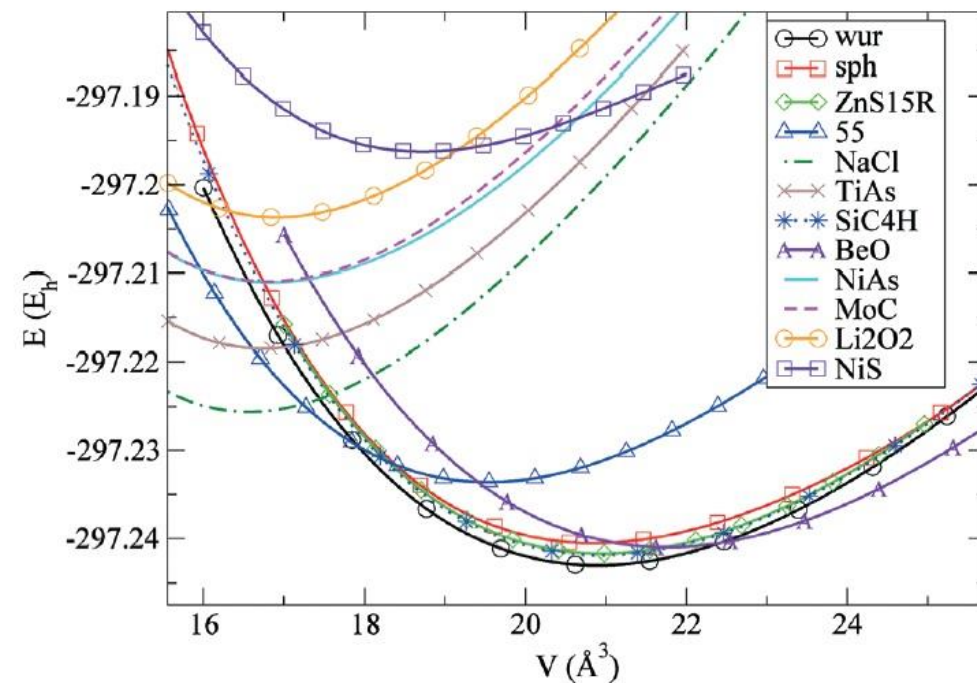


Fig. 3 Calculated $E(V)$ curves for the optimized AlN structure types obtained using the B3LYP functional. Energies per formula unit are given in hartrees (E_h).

How to search ICSD for crystal structures using Data Mining methods: Further examples

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Modelling and Simulation in Materials Science and Engineering

PAPER

Structure prediction, high pressure effect and properties investigation of superhard B₆O

J Zagorac^{1,2} , D Jovanović^{1,3}, T Volkov-Husović⁴, B Matović^{1,2} and D Zagorac^{1,2}

Published 4 February 2020 • © 2020 IOP Publishing Ltd

[Modelling and Simulation in Materials Science and Engineering](#), Volume 28, Number 3

Citation J Zagorac et al 2020 *Modelling Simul. Mater. Sci. Eng.* **28** 035004

Springer Link

Open Access | Published: 06 July 2020

Predicting Feasible Modifications of Ce₂ON₂ Using a Combination of Global Optimization and Data Mining

J. Zagorac, J. C. Schön , B. Matović, T. Škundrić & D. Zagorac

[Journal of Phase Equilibria and Diffusion](#) **41**, 538–549 (2020) | [Cite this article](#)

25th IUCr congress: Joint Workshop for CSD and ICSD, Dr. Dejan Zagorac, Vinča Institute of Nuclear Sciences

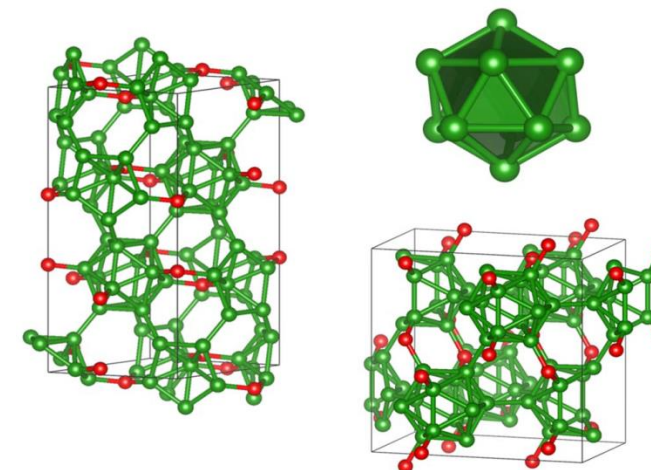
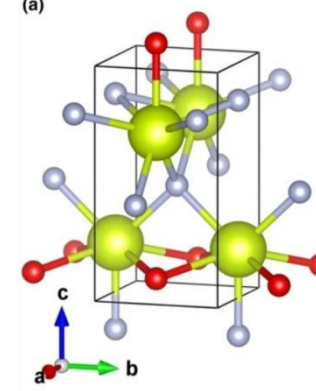
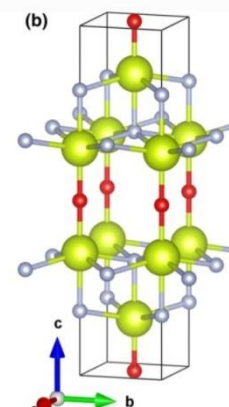


Fig. 2
(a)



(b)



Summary and Perspectives

- Theoretical background on the ICSD database
- How to search for:
 - new predicted (not-yet synthesized) structures or materials
 - optimized (experimentally observed) inorganic structures
 - parameters for method development and future calculations
 - experimental and theoretical data on nanostructures
- Data mining based searches with examples - searches for group of structures/data with common descriptors
- Reliable databases (such as CSD and ICSD), and crystal structure data of high quality can serve as an excellent tool in pandemic situation worldwide with less possibilities for performing experiments



Thank you for your attention and stay healthy!

Your comments and suggestions are welcome as well as theoretical CIF files which you can send to: crysddata@fiz-karlsruhe.de

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