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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

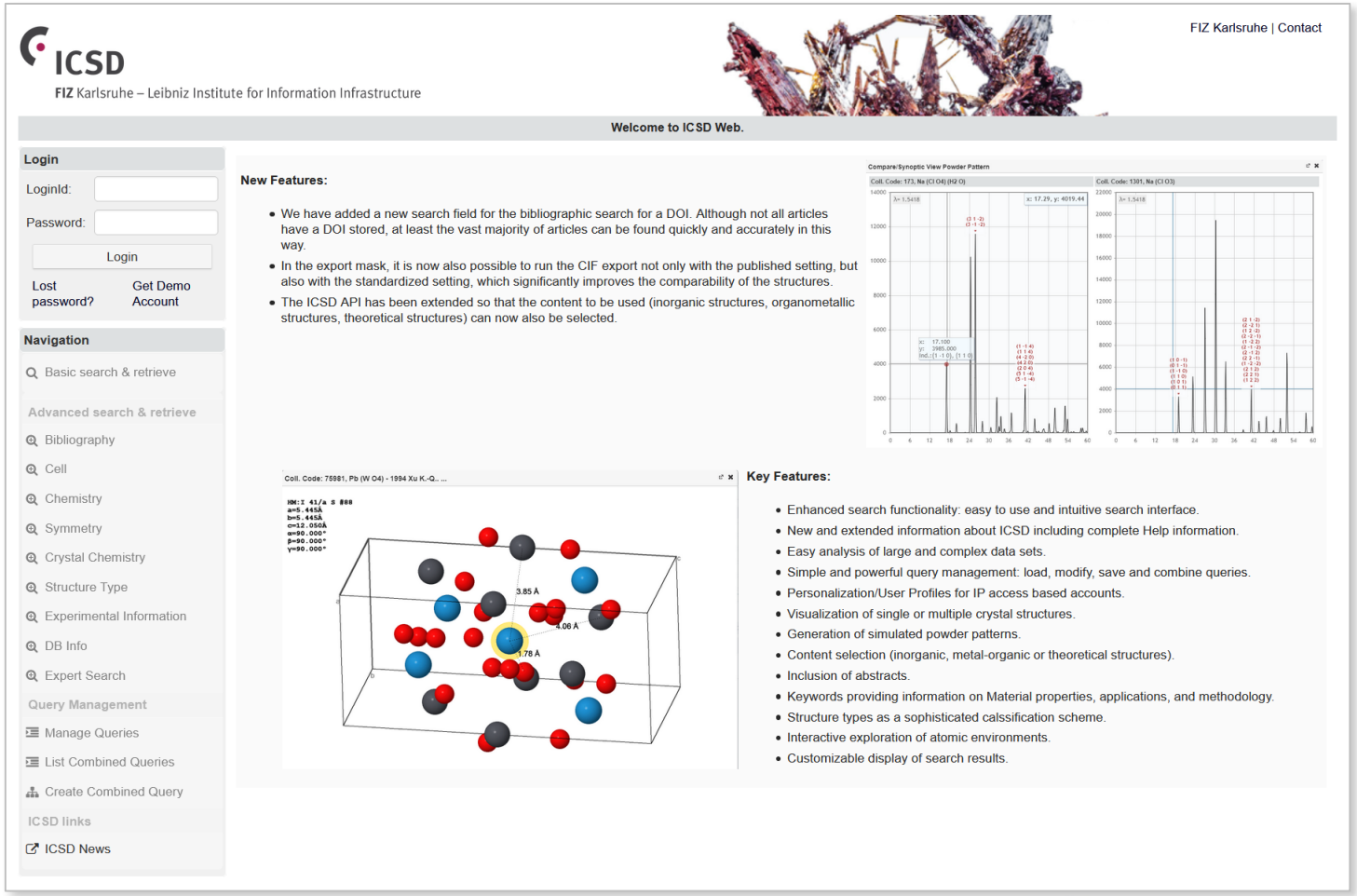
> 9,700 structure Types

>175,000 assigned to structure types

Accessing ICSD Web/API

Authentication methods:

- LoginID/Password
  - Single user
  - Multiple users (2-4 users)
  - API access



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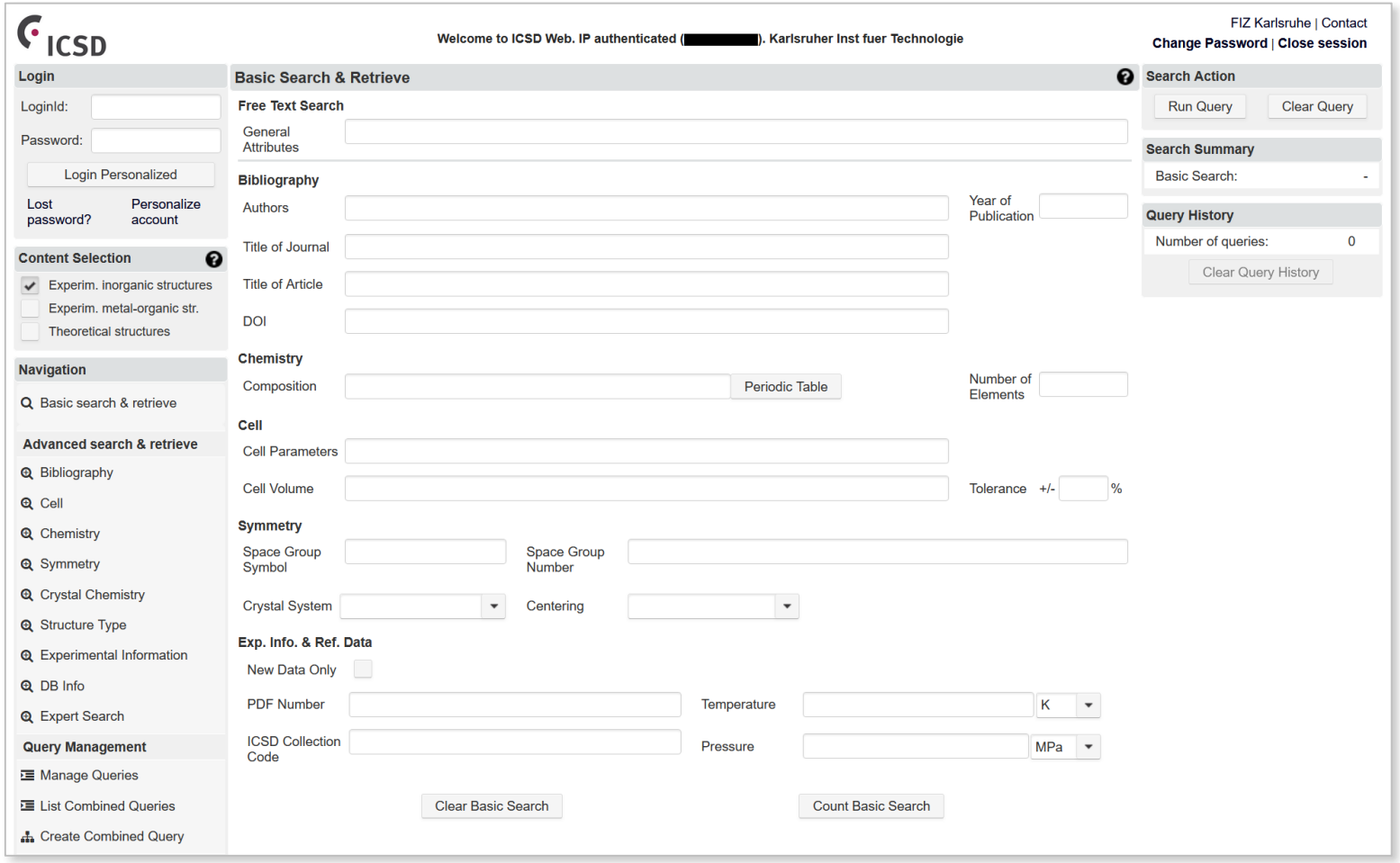
Accessing ICSD Web/API

Authentication methods:

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



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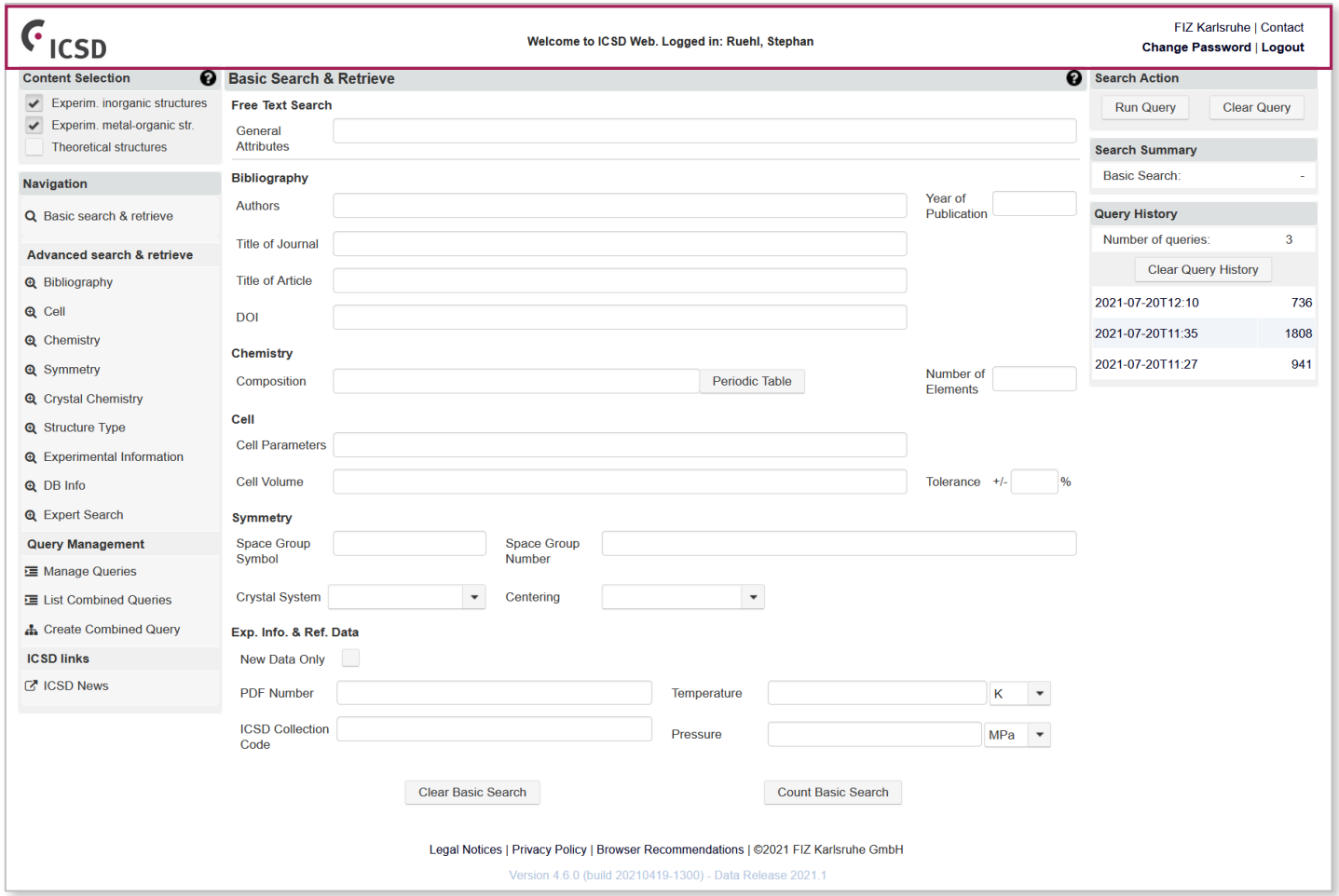
ICSD - Main interface

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)



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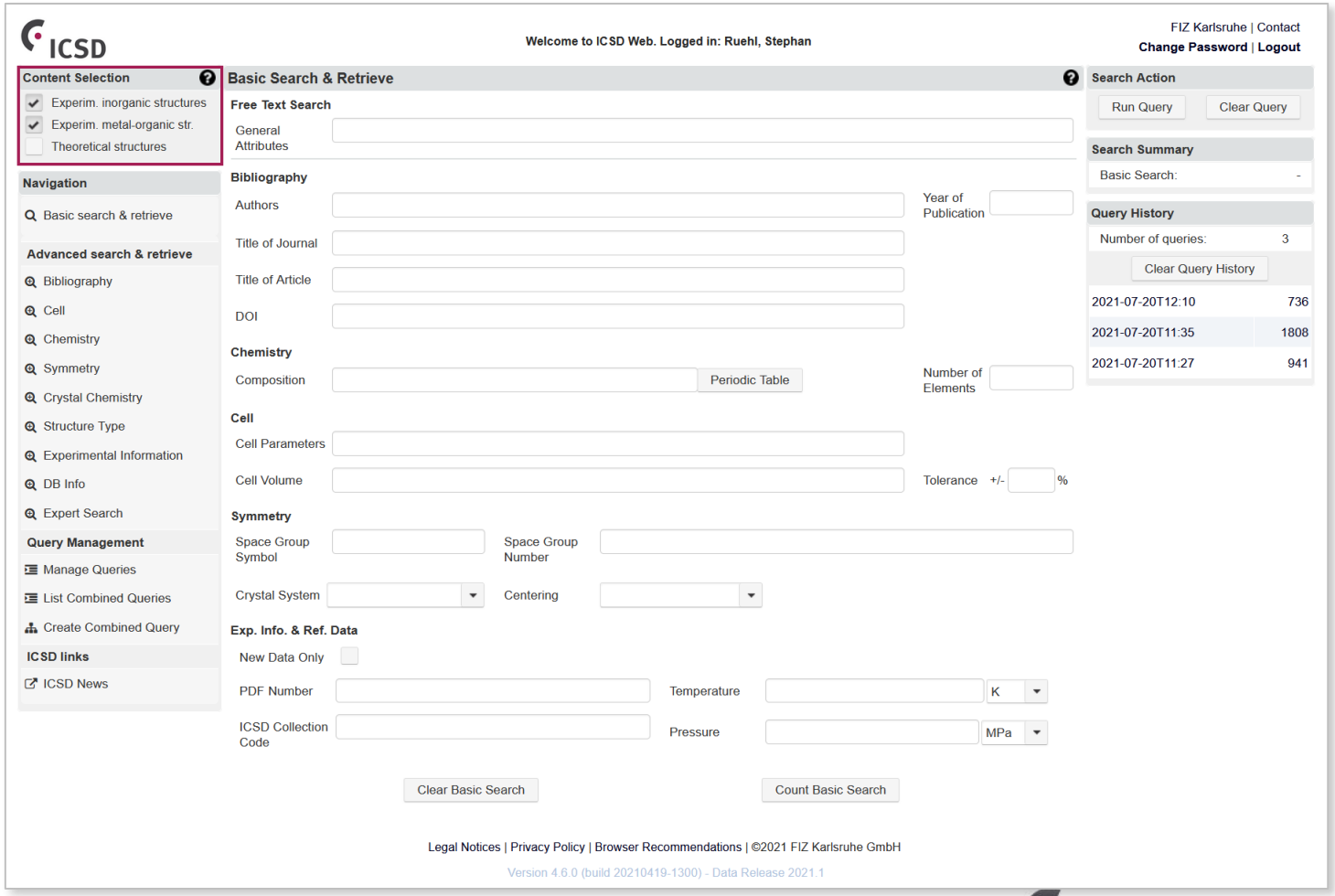

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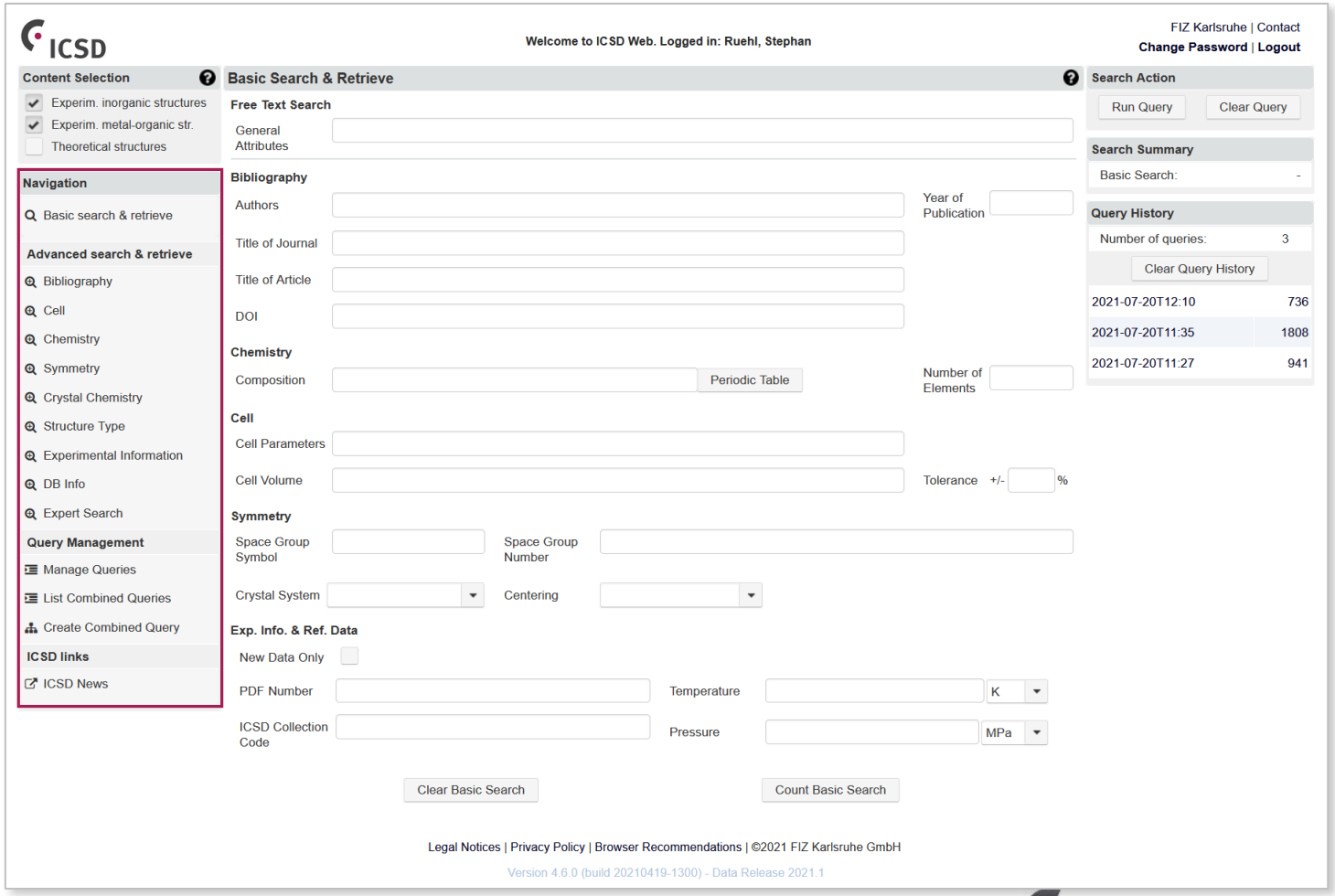

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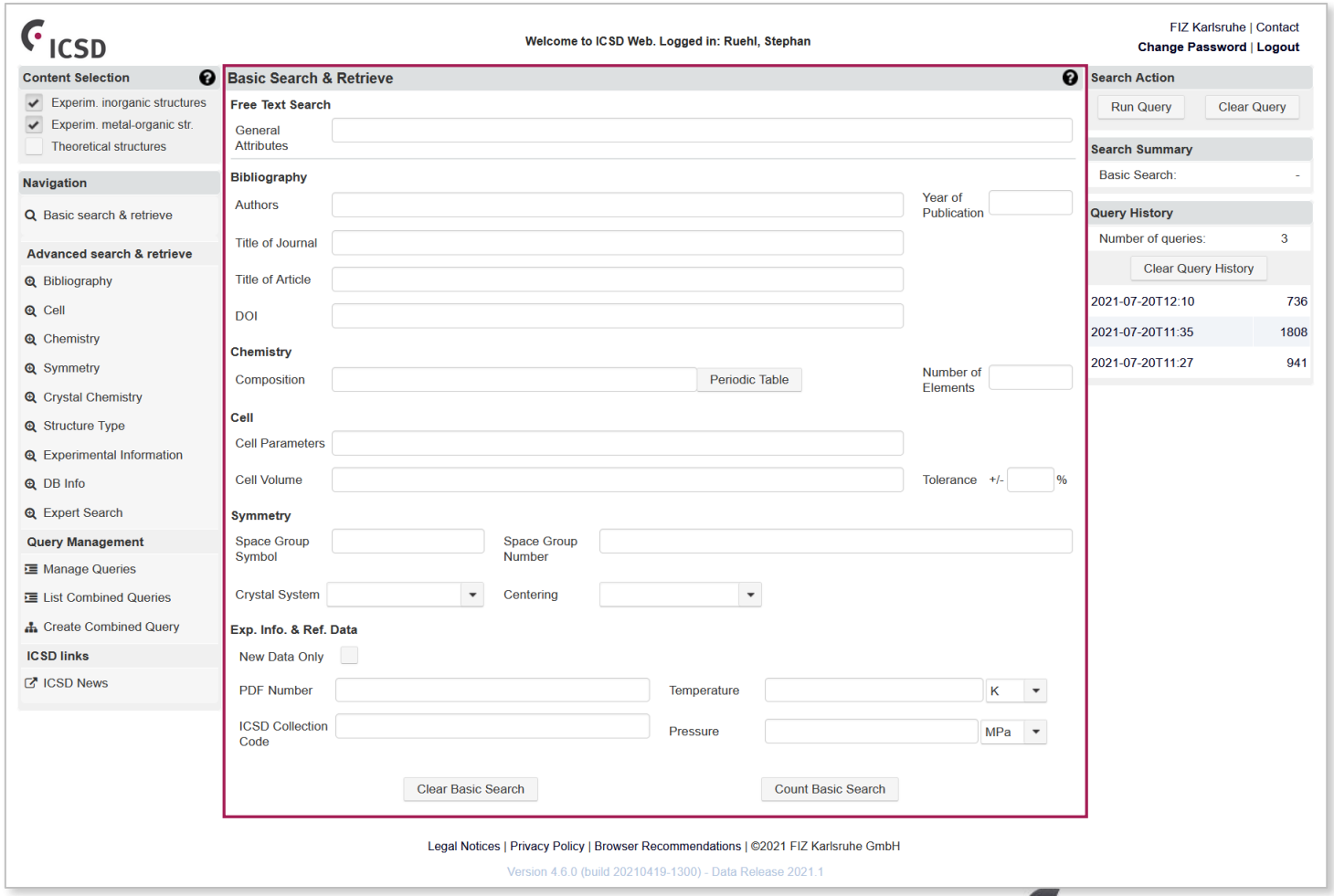

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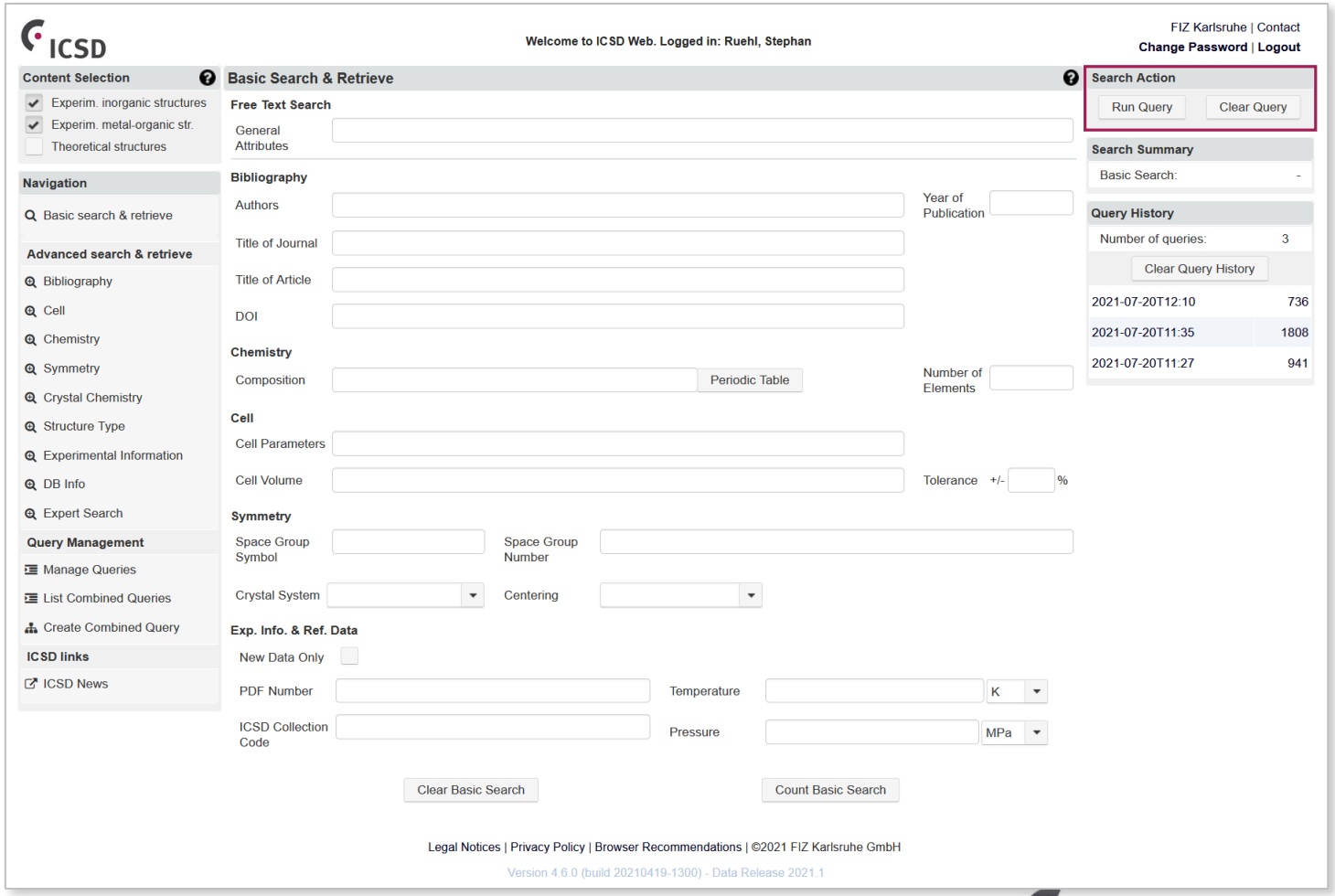

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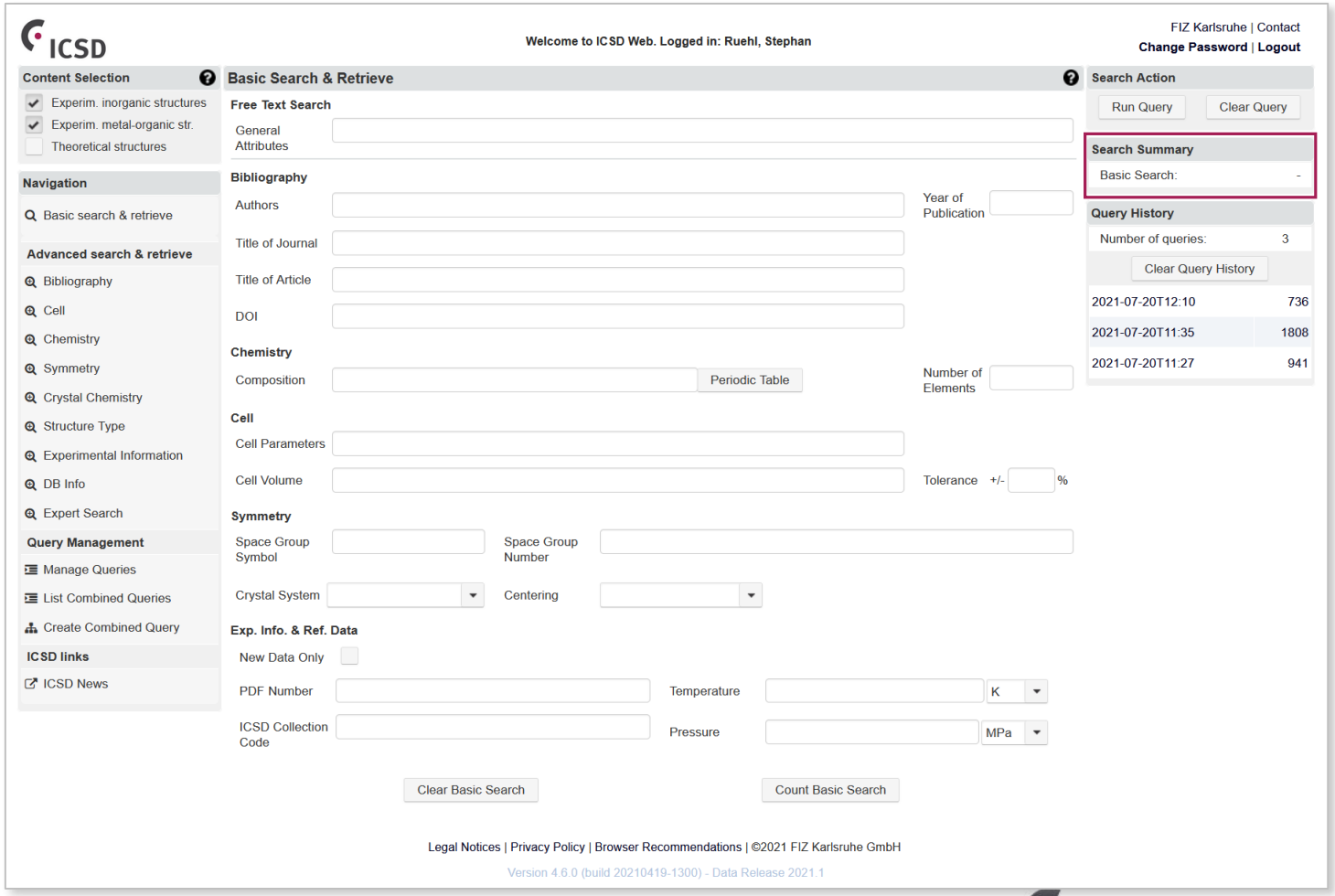

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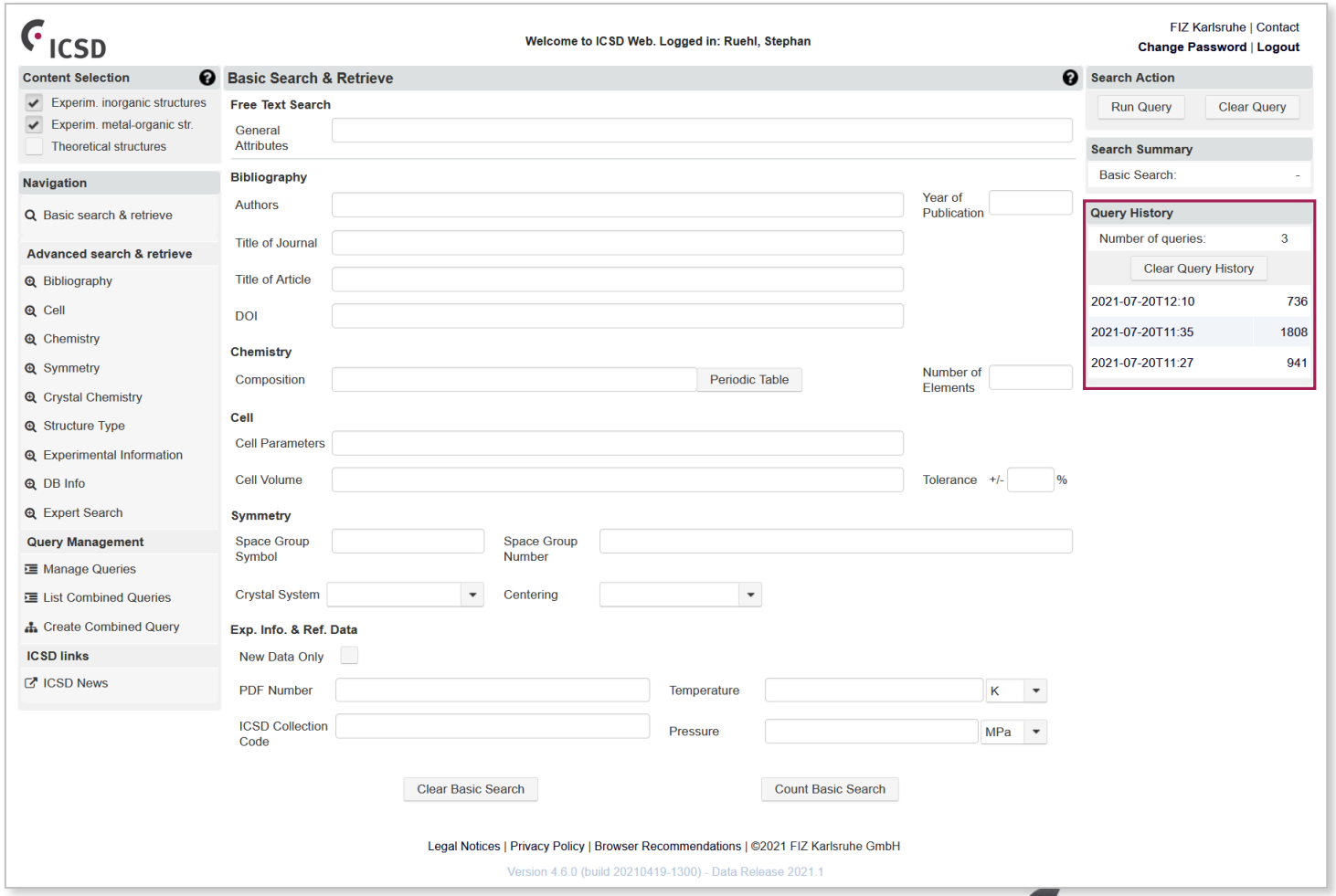

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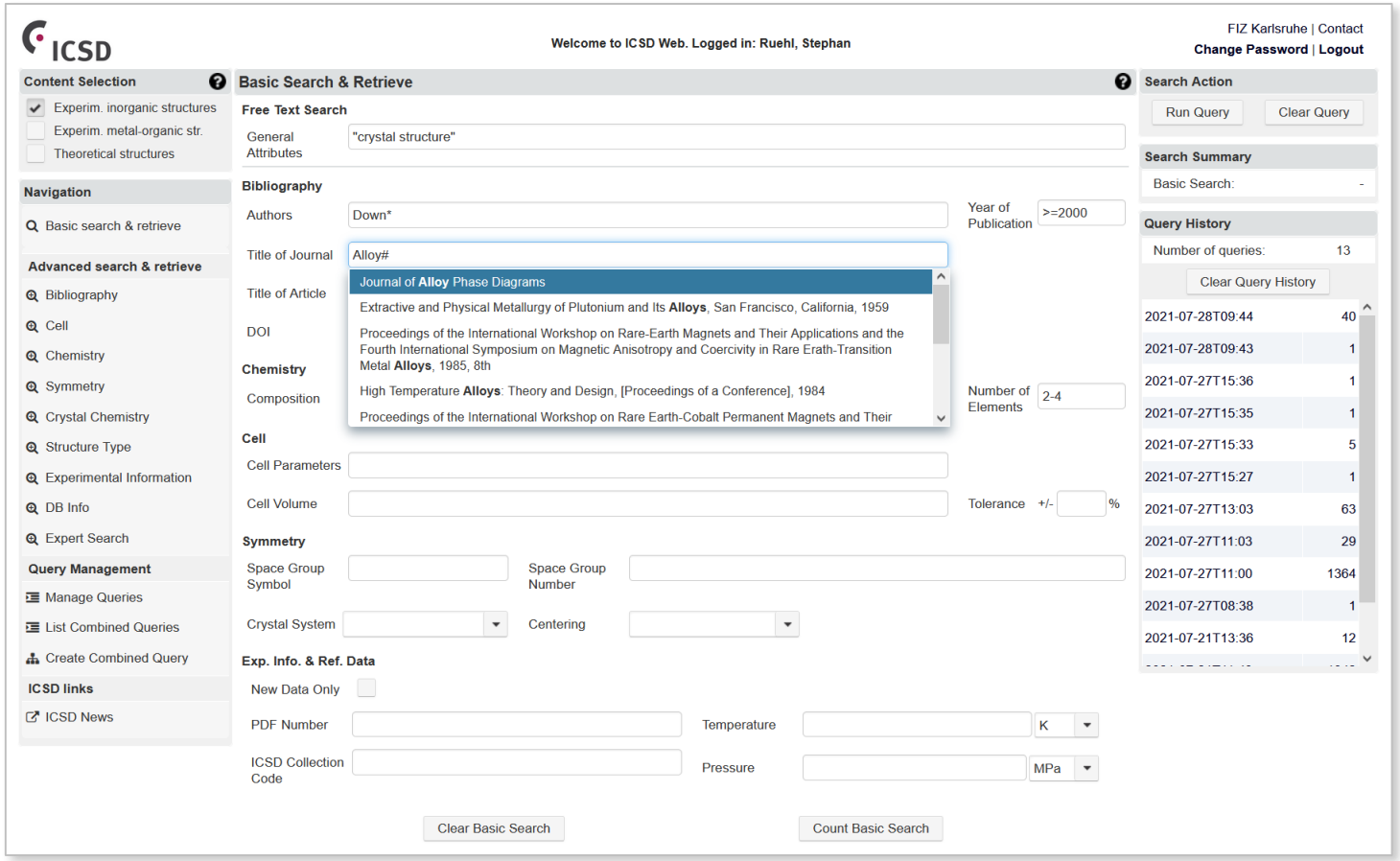
ICSD – Different types of search fields

Different types of search fields:

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



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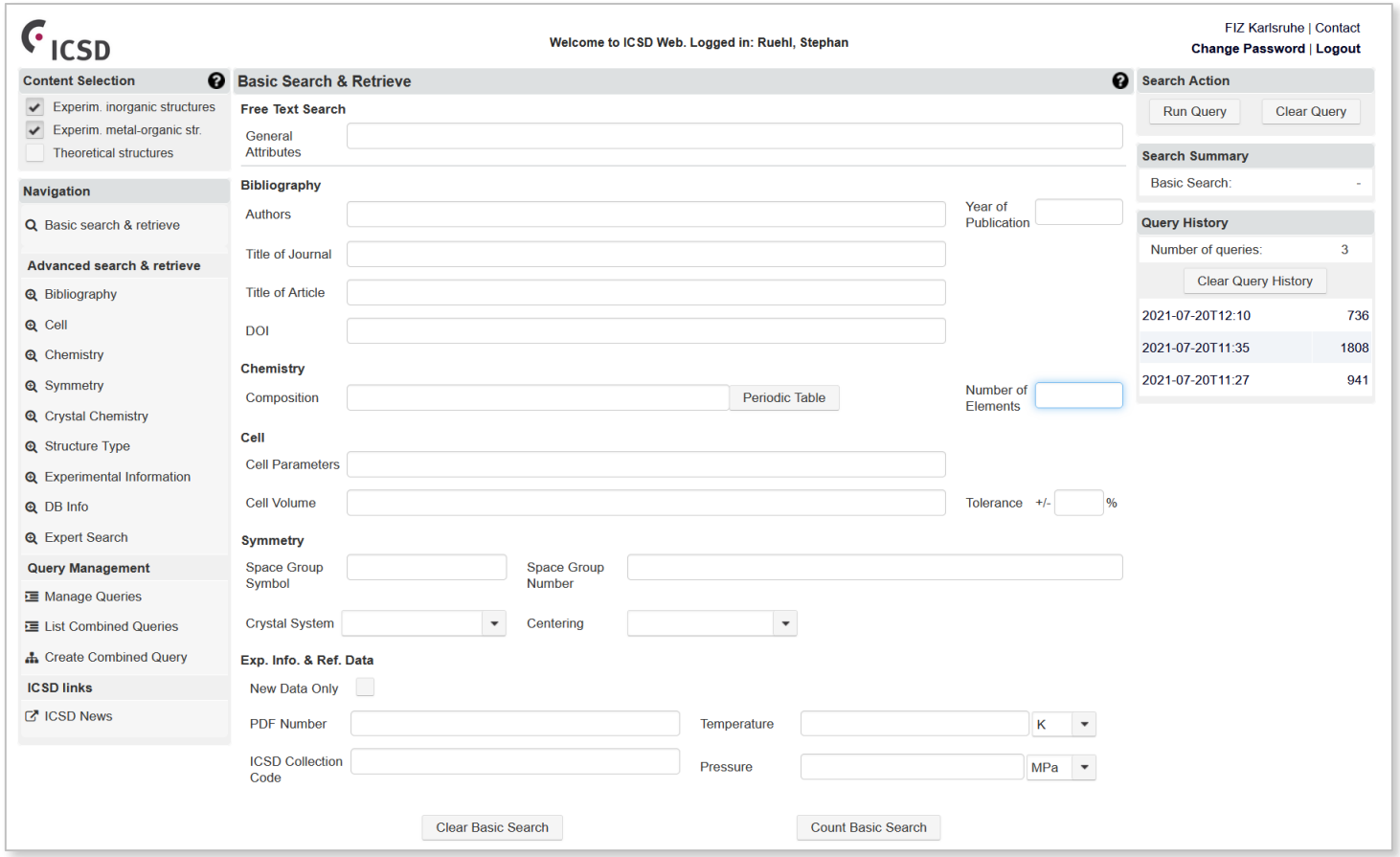
ICSD – Basic search mask

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



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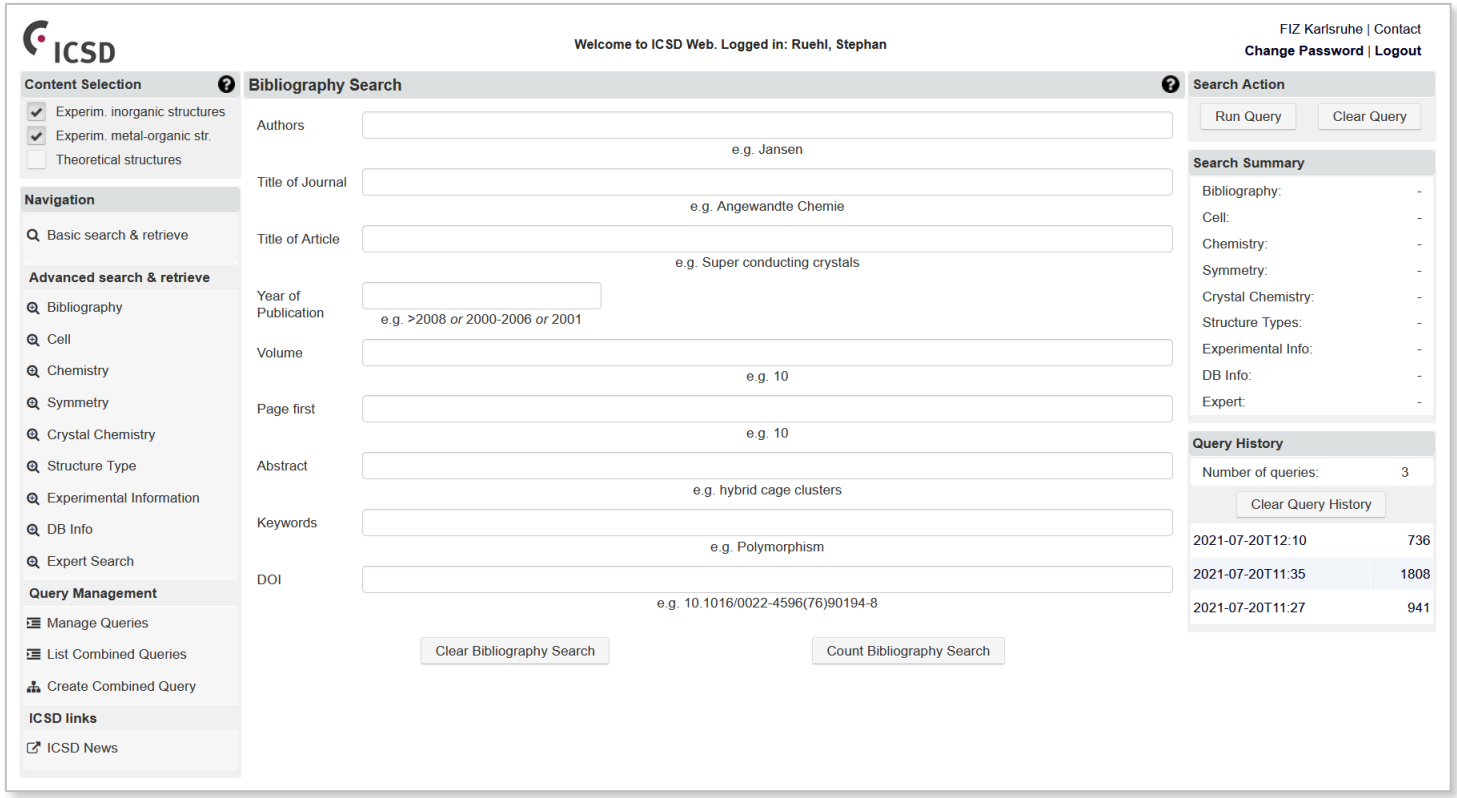
ICSD – Advanced search mask - Bibliography

- 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)



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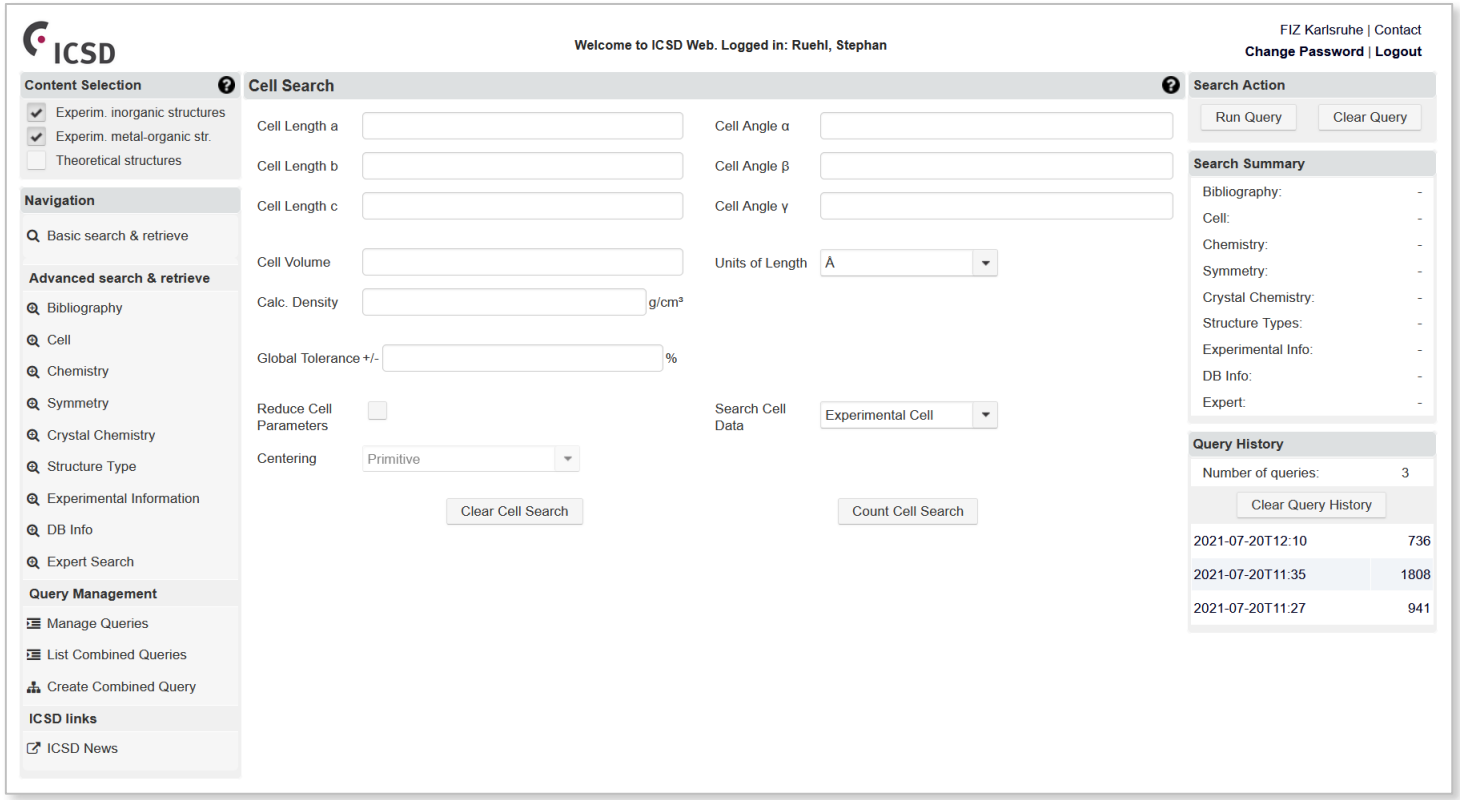
ICSD – Advanced search mask - Cell

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



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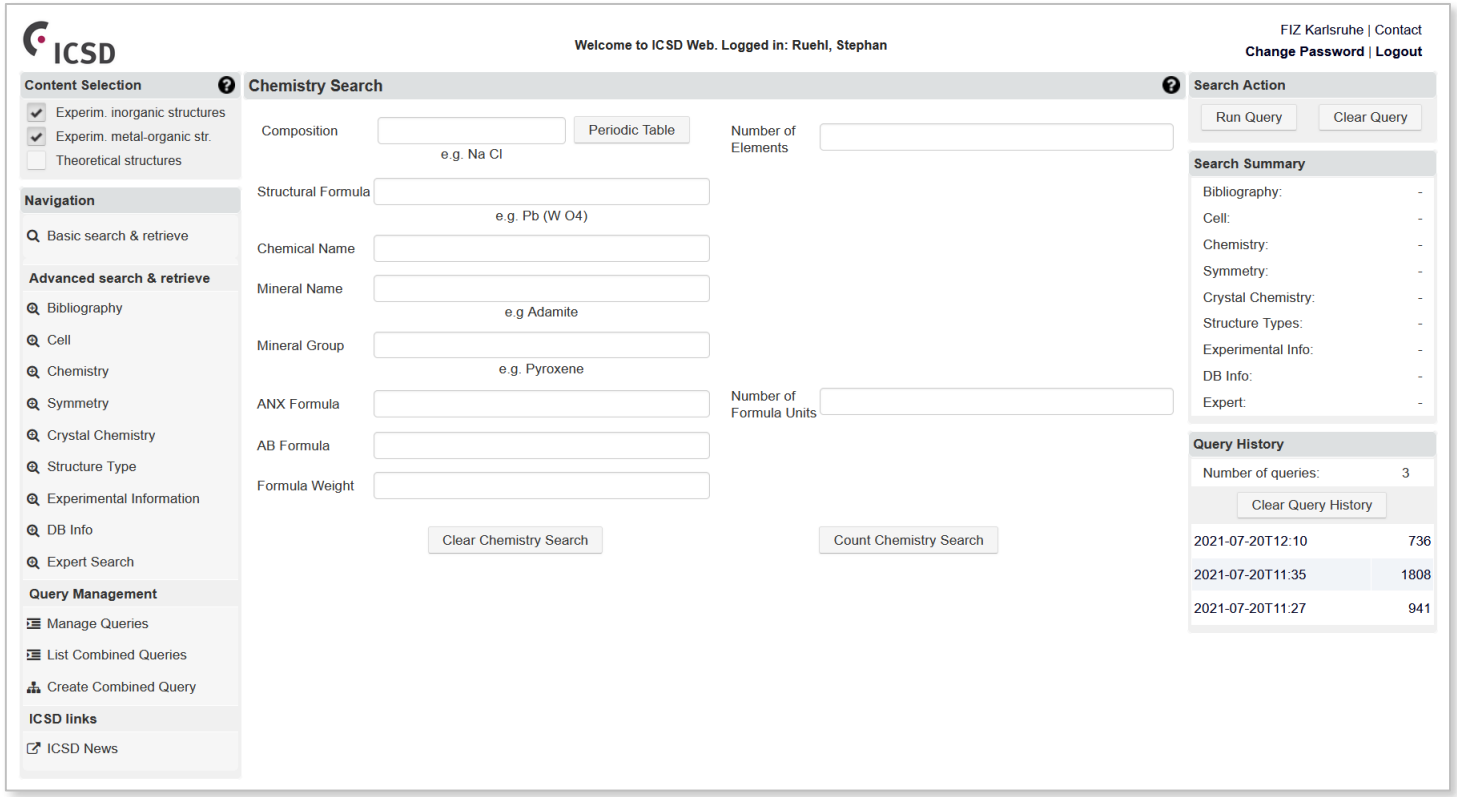
ICSD – Advanced search mask - Chemistry

- 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)



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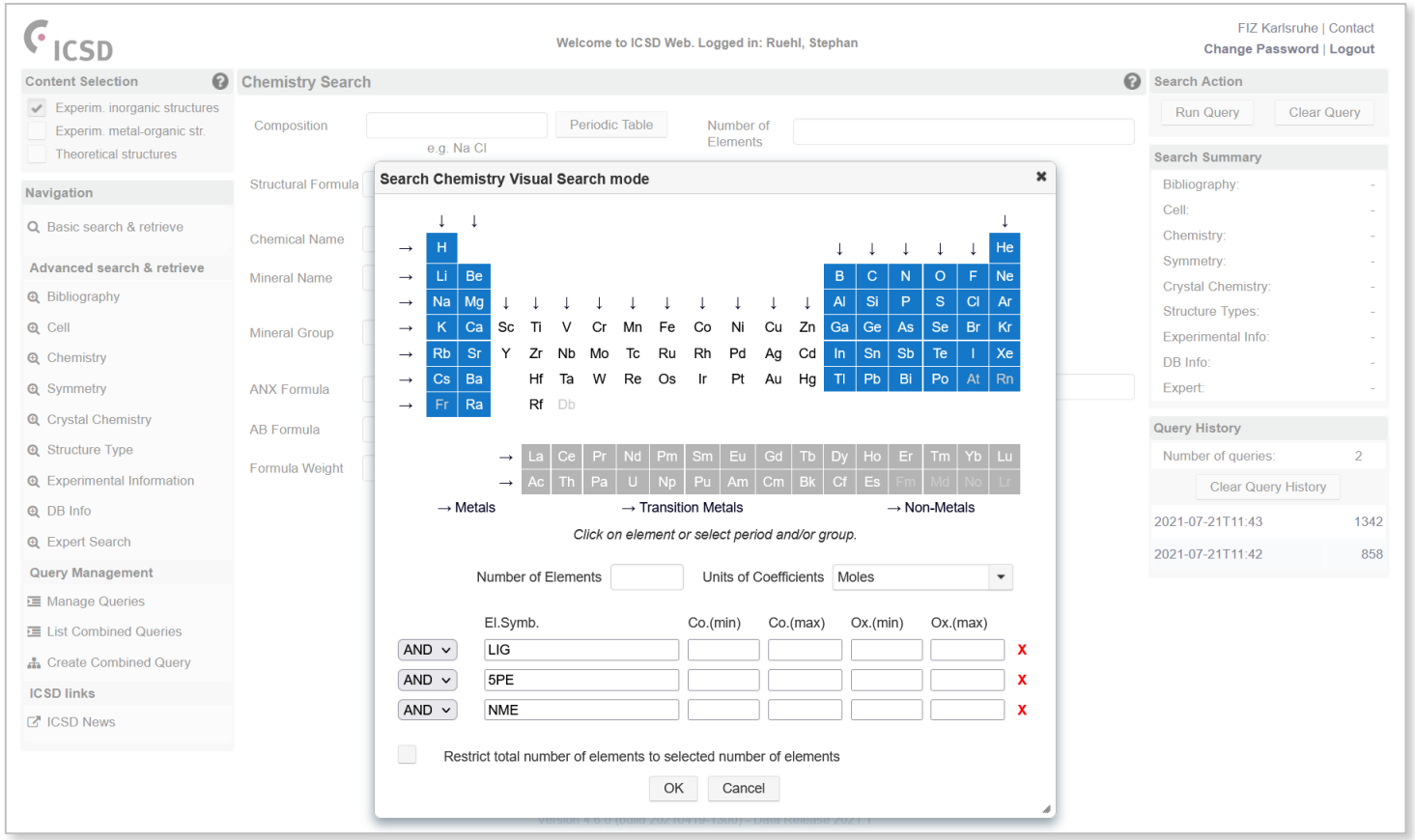
ICSD – Advanced search mask – Chemistry / Periodic Table

- 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), Actiniods (ACT)



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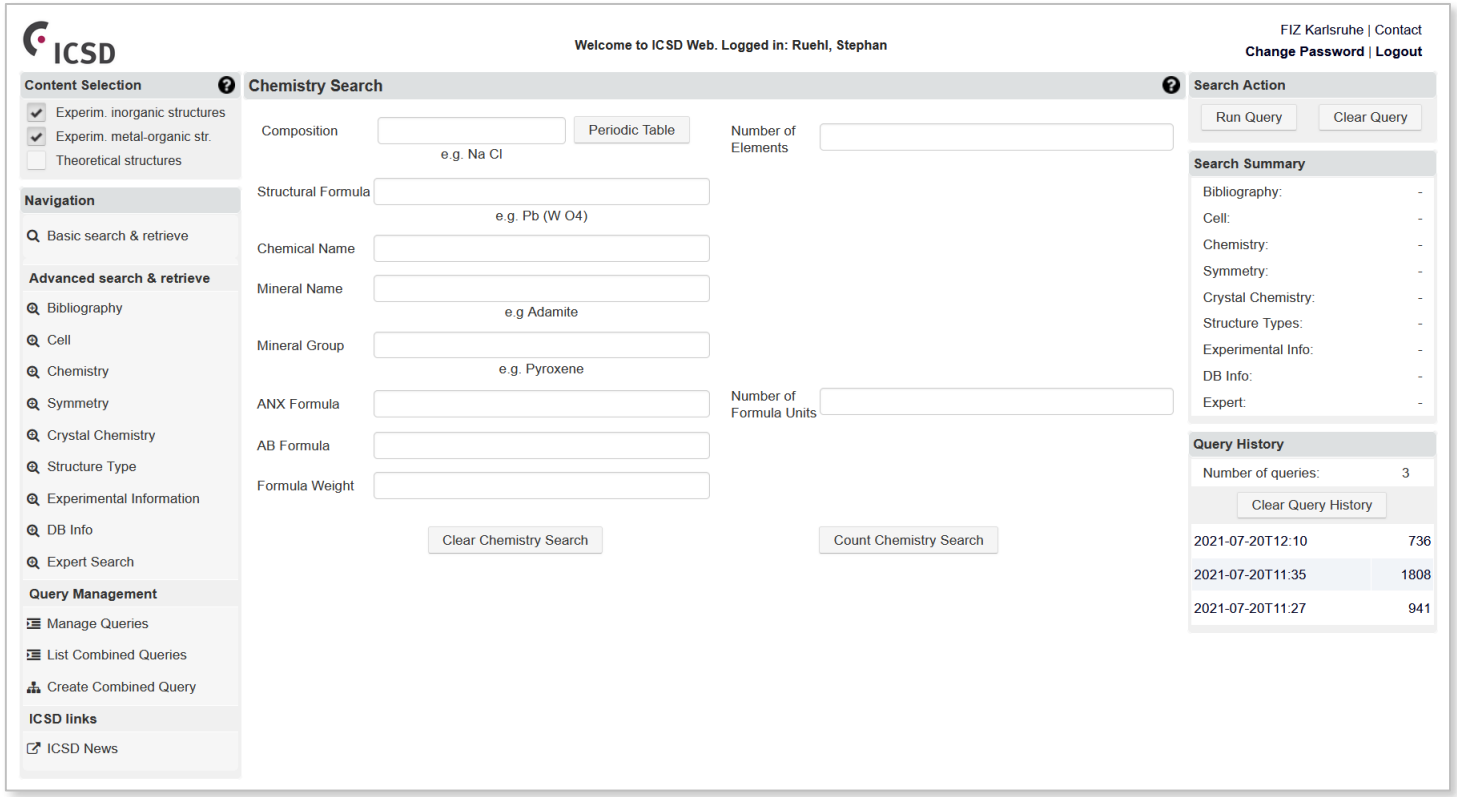
ICSD – Advanced search mask - Chemistry

- 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)



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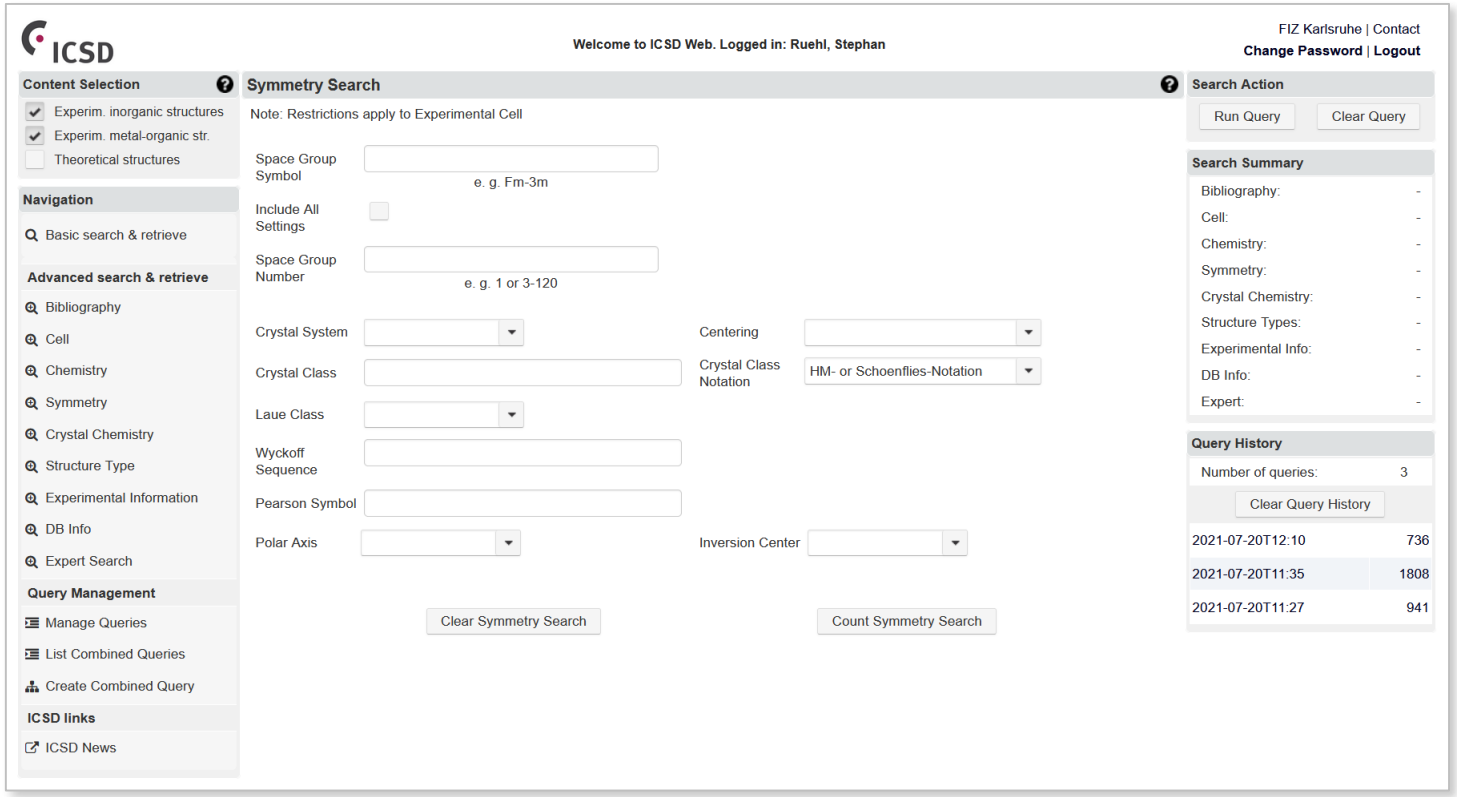
ICSD – Rules to determine ANX formulae

- 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



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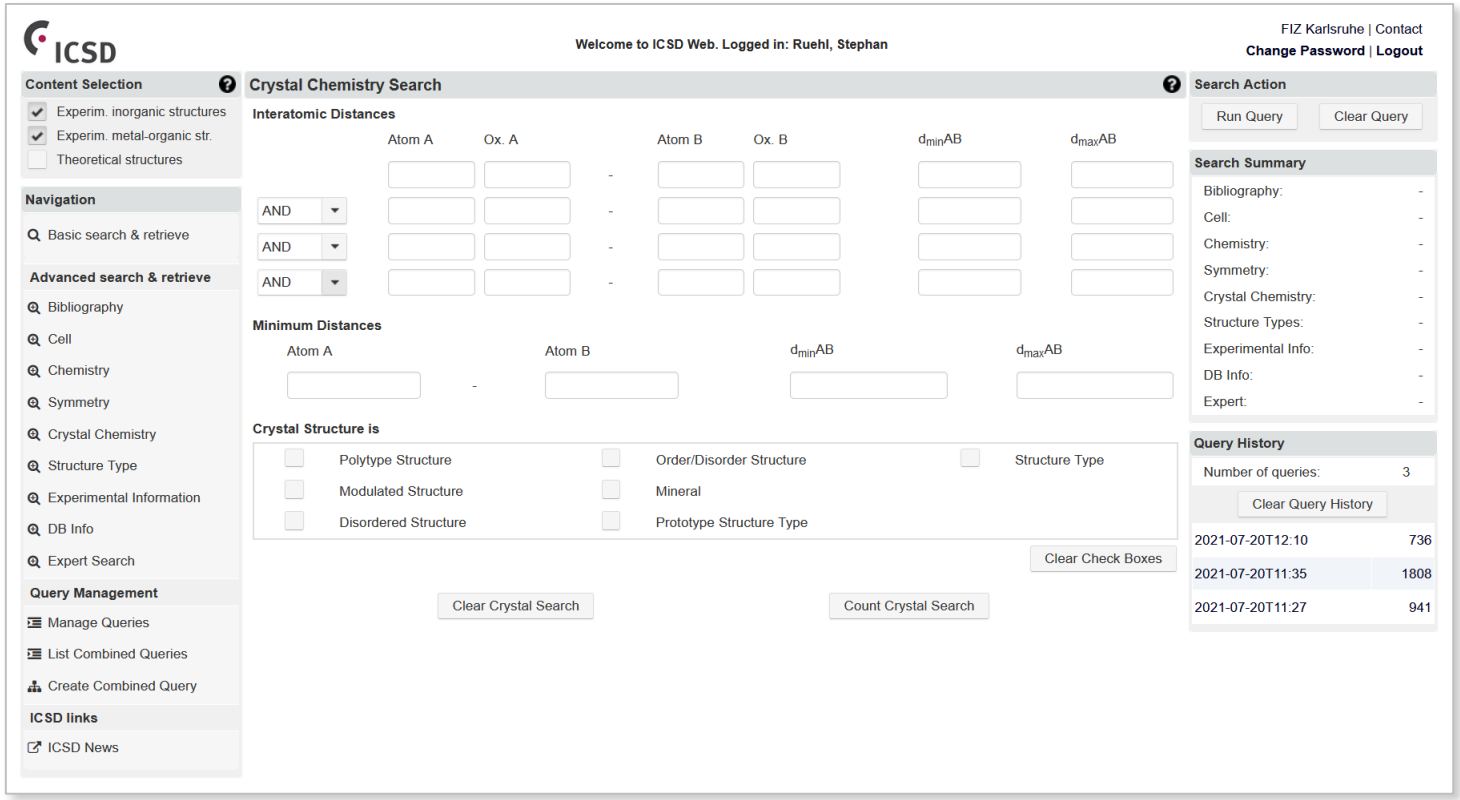
ICSD – Advanced search mask – Crystal Chemistry

- 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



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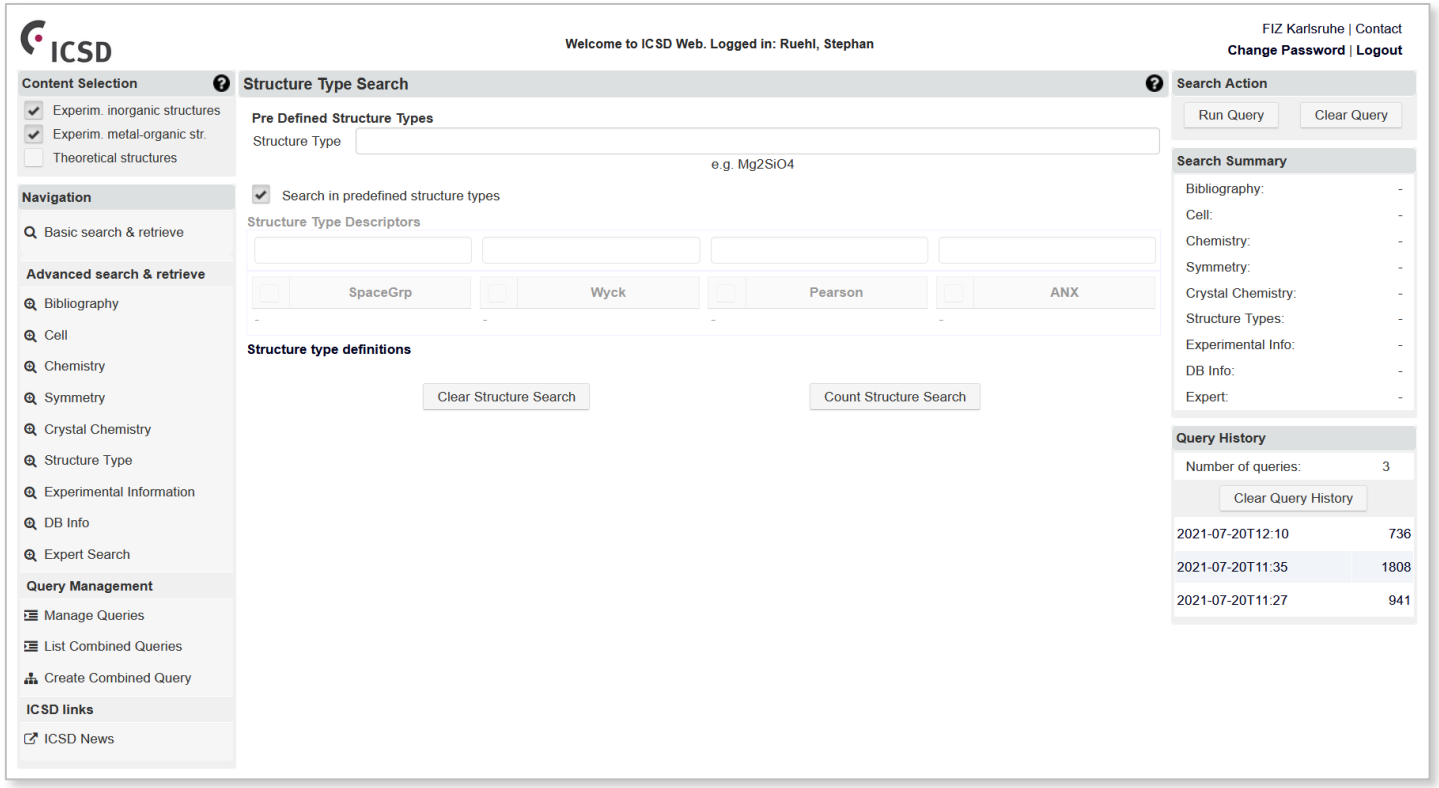
ICSD – Advanced search mask – Structure type

- 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.



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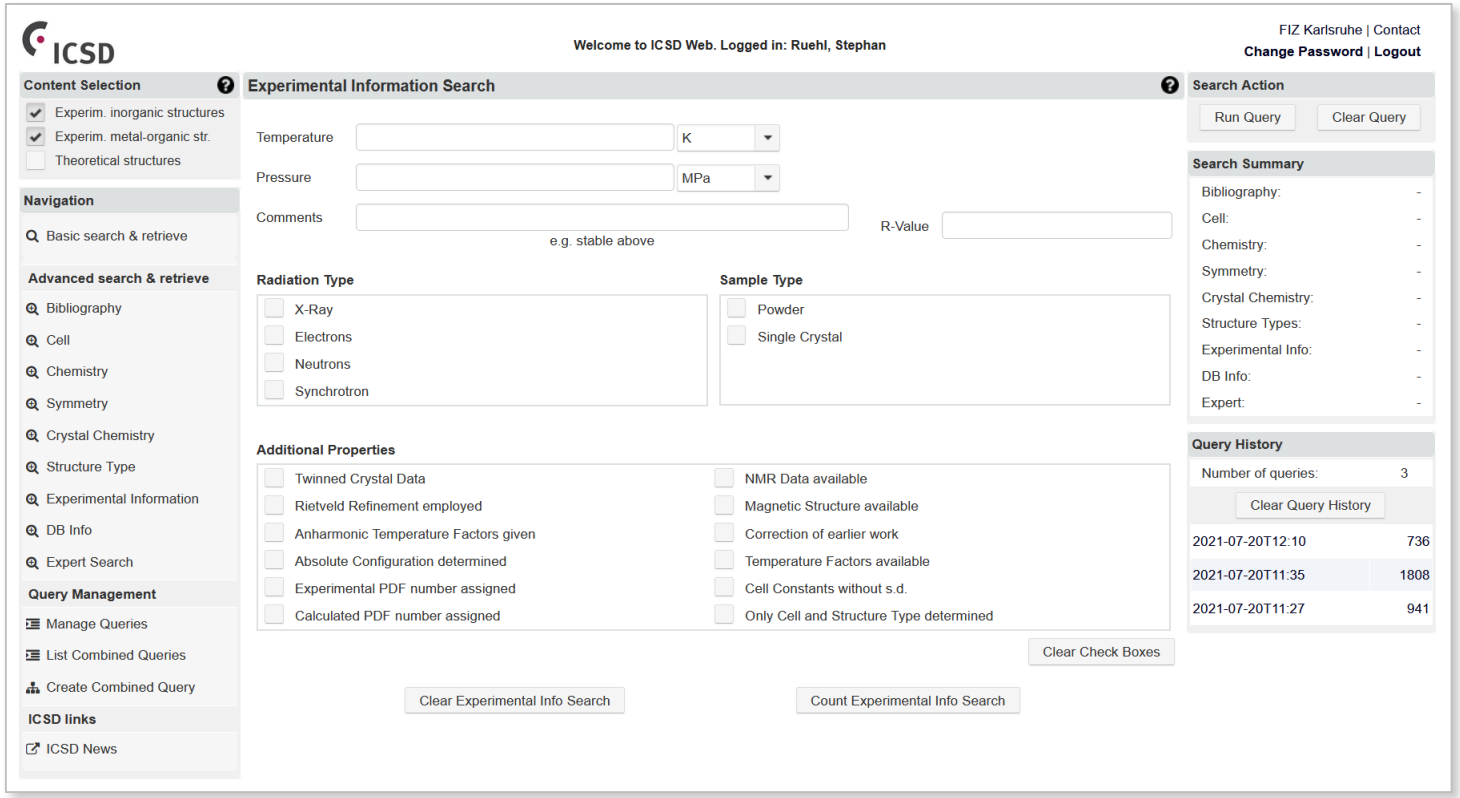
ICSD – Advanced search mask – Experimental information

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



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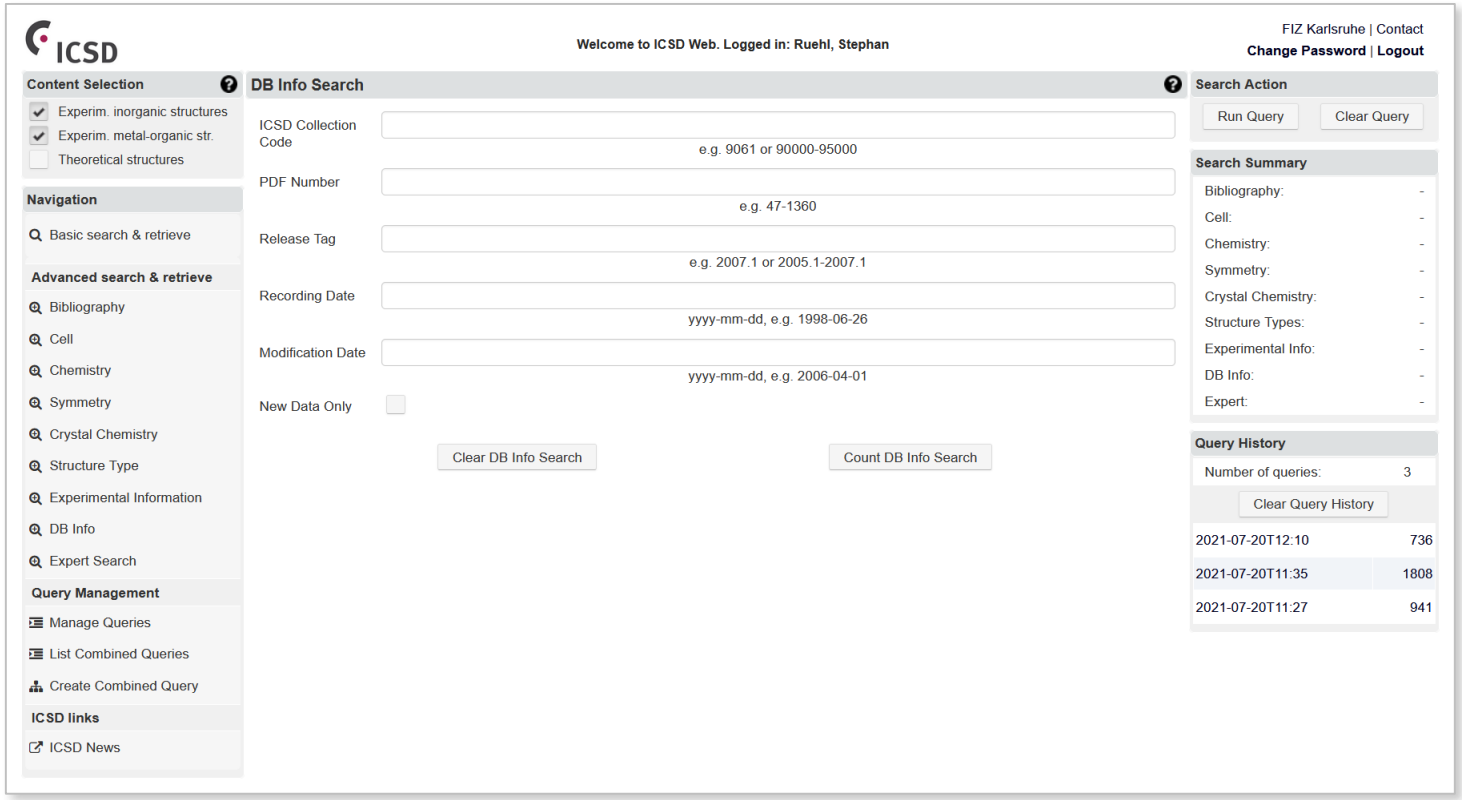
ICSD – Advanced search mask – DB info

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



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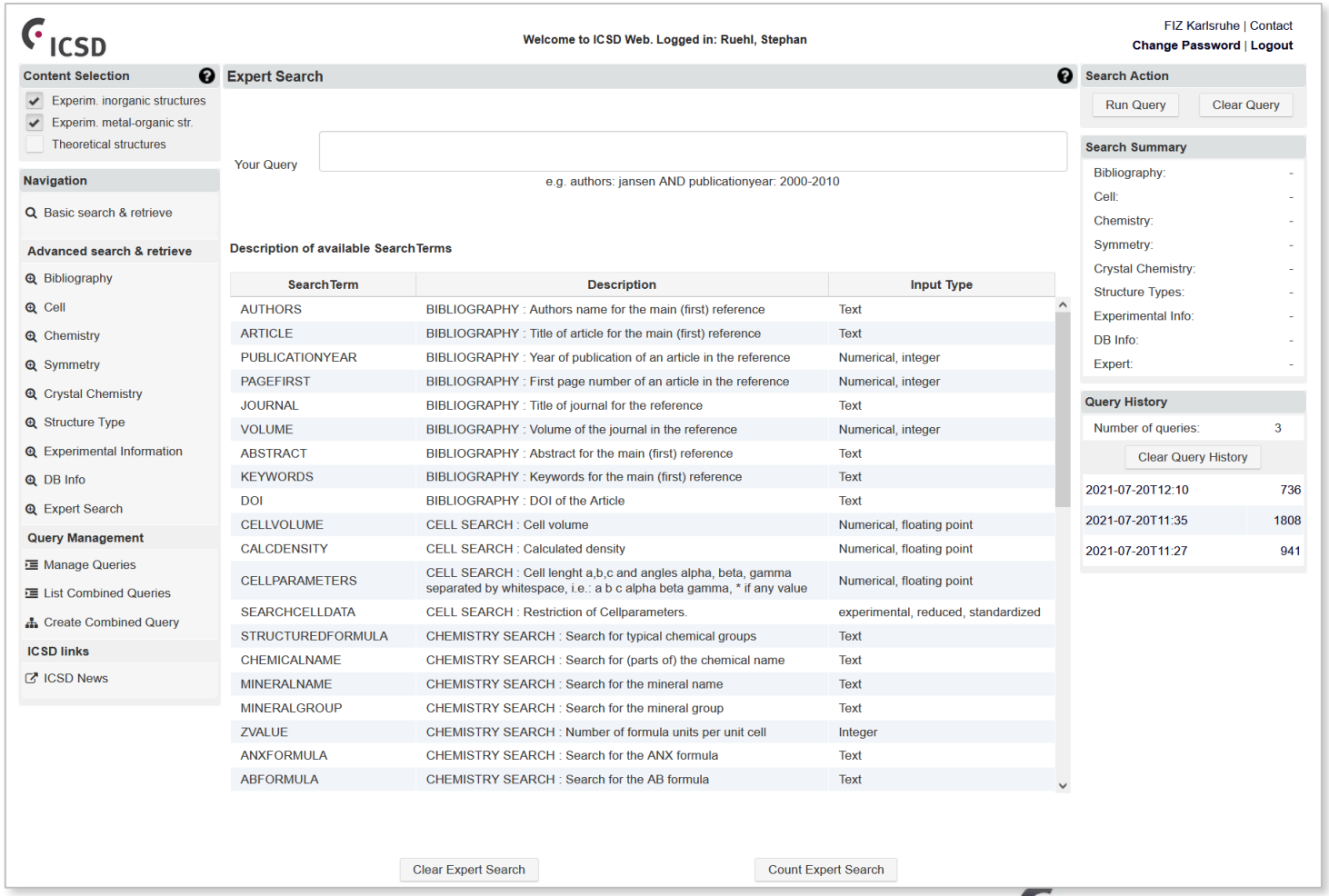
ICSD – Advanced search mask – Expert search

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



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

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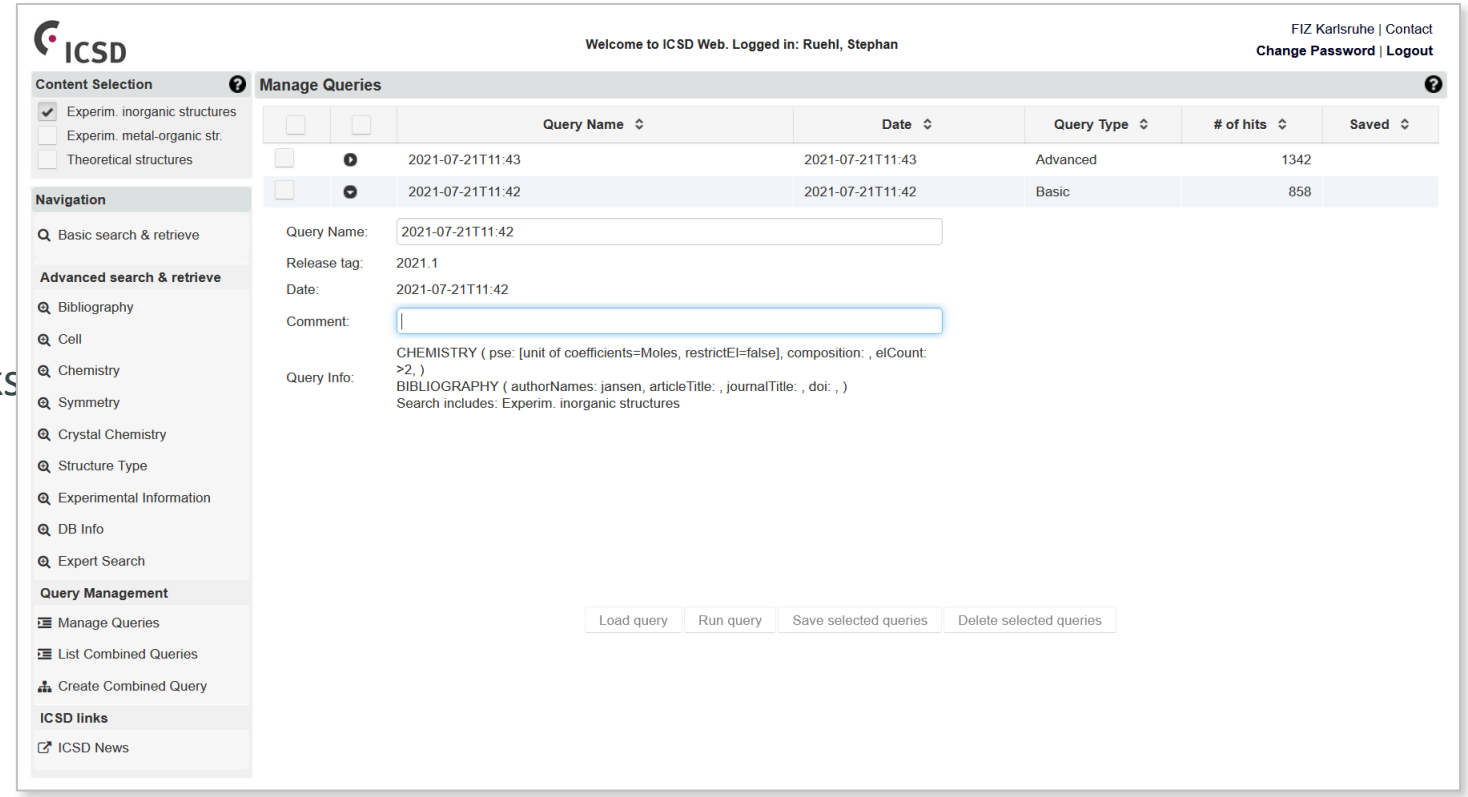
ICSD – Query Management – Manage Queries

- 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



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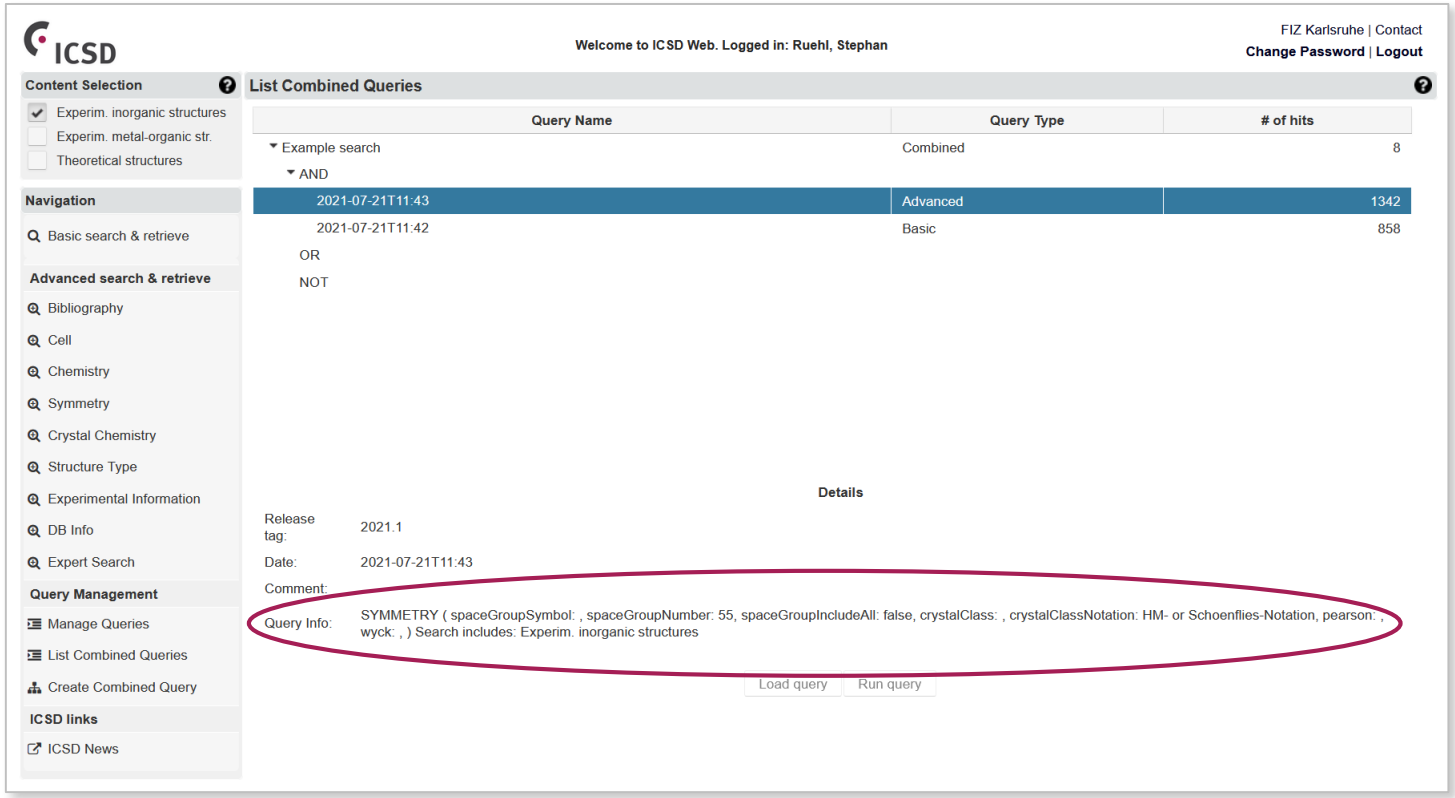
ICSD – Query Management – List Combined Queries

- 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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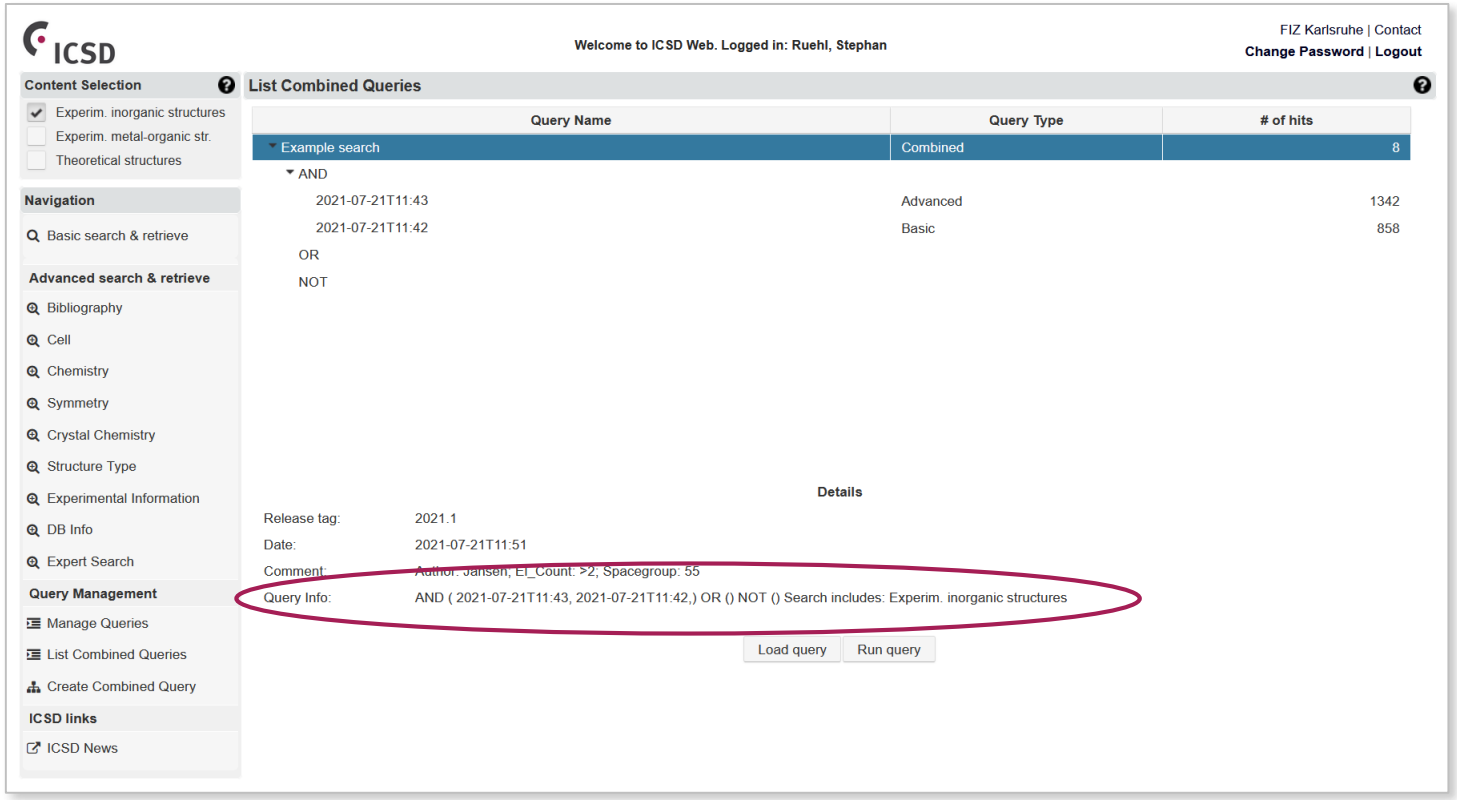

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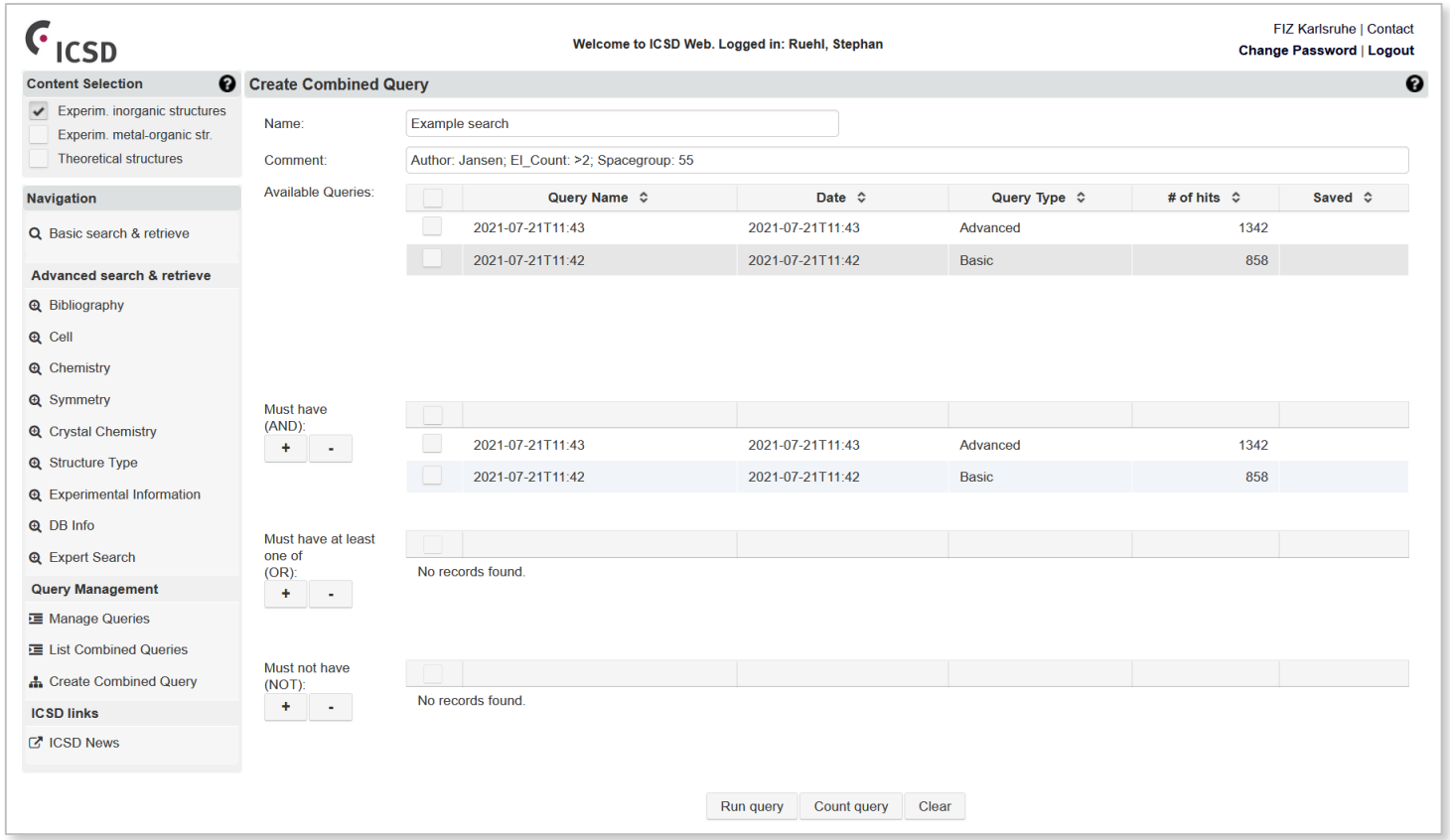
ICSD – Query Management – Create Combined Queries

- 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

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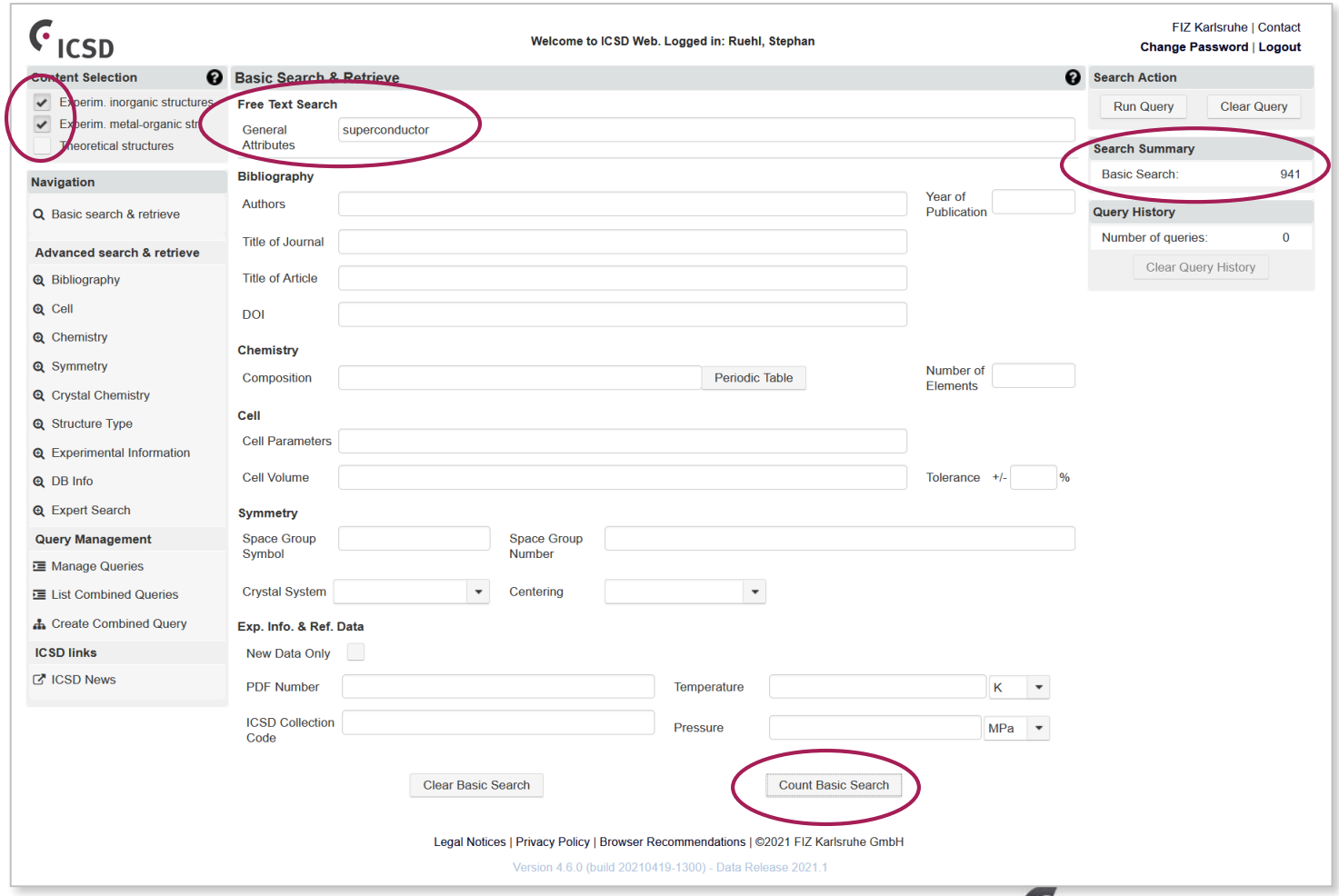
ICSD – Example: high temperature superconductors

Interest: high temperature superconducting ceramics

- First known: Ba2Cu3LaO7 (1986)
- Better Tc (~90k): YBa2Cu3O7−x > (1987)



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ICSD – Example: high temperature superconductors - Results

Result list

ICSD

Welcome to ICSD Web. Logged in: Ruehl, Stephan

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Change Password | **Logout**

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	Hg2.8 (As F6)0.94		A neutron diffraction	Schultz, A.J.; Willian	7.549(5) 7.549(5) 12	Inorganic Chemistry	1978	
9187	R -3 m H	Ce Ir3	NbBe3#ThCo3	$CeIr_3$: superconducti	Górnicka, Karolina; (	5.280(4) 5.280(4) 26	Superconductor Scie	2019	
11144	I m -3 m	Ba0.54 K0.46 Bi O3		Hydrothermal synthe	Saiduzzaman, Md; Y	8.5207(2) 8.5207(2)	Inorganic Chemistry	2019	
11418	R 3 2 H	Na3 Pt10 Si5		$Na_3Pt_{10}Si_5$. A non-c	Yamada, Takahiro; H	10.1305(5) 10.1305(	Inorganic Chemistry	2019	
11419	R 3 2 H	Na3 Pt10 Si5		$Na_3Pt_{10}Si_5$. A non-c	Yamada, Takahiro; H	10.1536(3) 10.1536(	Inorganic Chemistry	2019	
11420	R 3 2 H	Na3 Pt10 Si5		$Na_3Pt_{10}Si_5$. A non-c	Yamada, Takahiro; H	10.1345(5) 10.1345(	Inorganic Chemistry	2019	
11421	R 3 2 H	Na3 Pt10 Si5		$Na_3Pt_{10}Si_5$. A non-c	Yamada, Takahiro; H	10.1478(3) 10.1478(	Inorganic Chemistry	2019	
11422	R 3 2 H	Na3 Pt10 Si5		$Na_3Pt_{10}Si_5$. A non-c	Yamada, Takahiro; H	10.1421(4) 10.1421(	Inorganic Chemistry	2019	
11514	P 4/m m m	Fe Sr2 Y Cu2 O7.83	(Ba1.5La0.5)Cu3La(	Soft magnetic switch	López-Paz, Sara A.;	3.8145(3) 3.8145(3)	Inorganic Chemistry	2019	
11980	I 4/m	Mo4 Ga18.69 Sn1.8		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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Buildnumber 8bcae72c5d1a30b4303d5c9b05126084e32c4706

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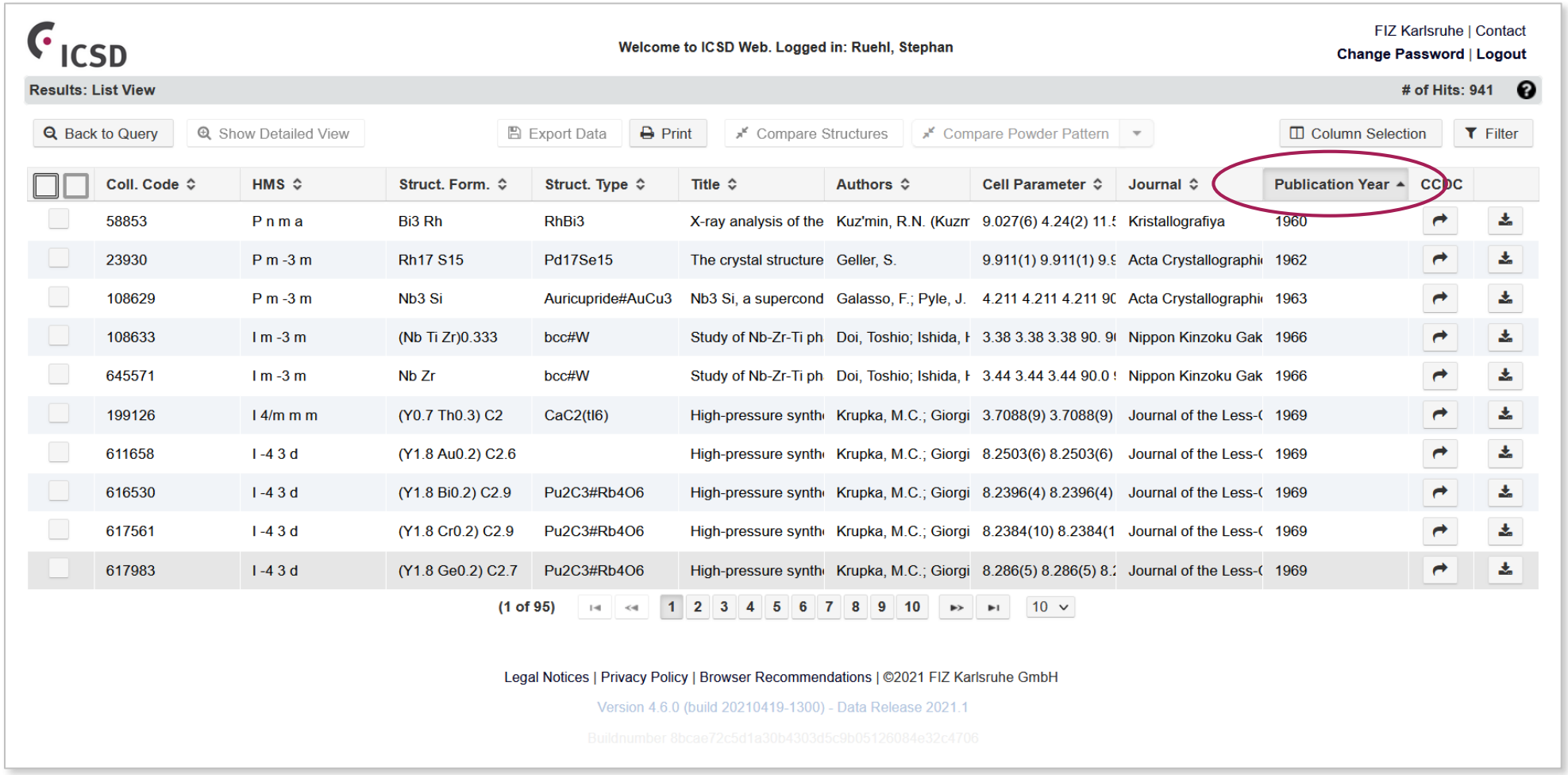
ICSD – Example: high temperature superconductors - Results

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. (Kuzm	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) 9.9	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, H	3.38 3.38 3.38 90. 90	Nippon Kinzoku Gak	1966	
645571	I m -3 m	Nb Zr	bcc#W	Study of Nb-Zr-Ti ph	Doi, Toshio; Ishida, H	3.44 3.44 3.44 90.0 9	Nippon Kinzoku Gak	1966	
199126	I 4/m m m	(Y0.7 Th0.3) C2	CaC2(tI6)	High-pressure synth	Krupka, M.C.; Giorgi	3.7088(9) 3.7088(9)	Journal of the Less-(	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-(	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-(	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-(	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) 8.2	Journal of the Less-(	1969	

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

Buildnumber 8bcae72c5d1a30b4303d5c9b05126084e32c4706

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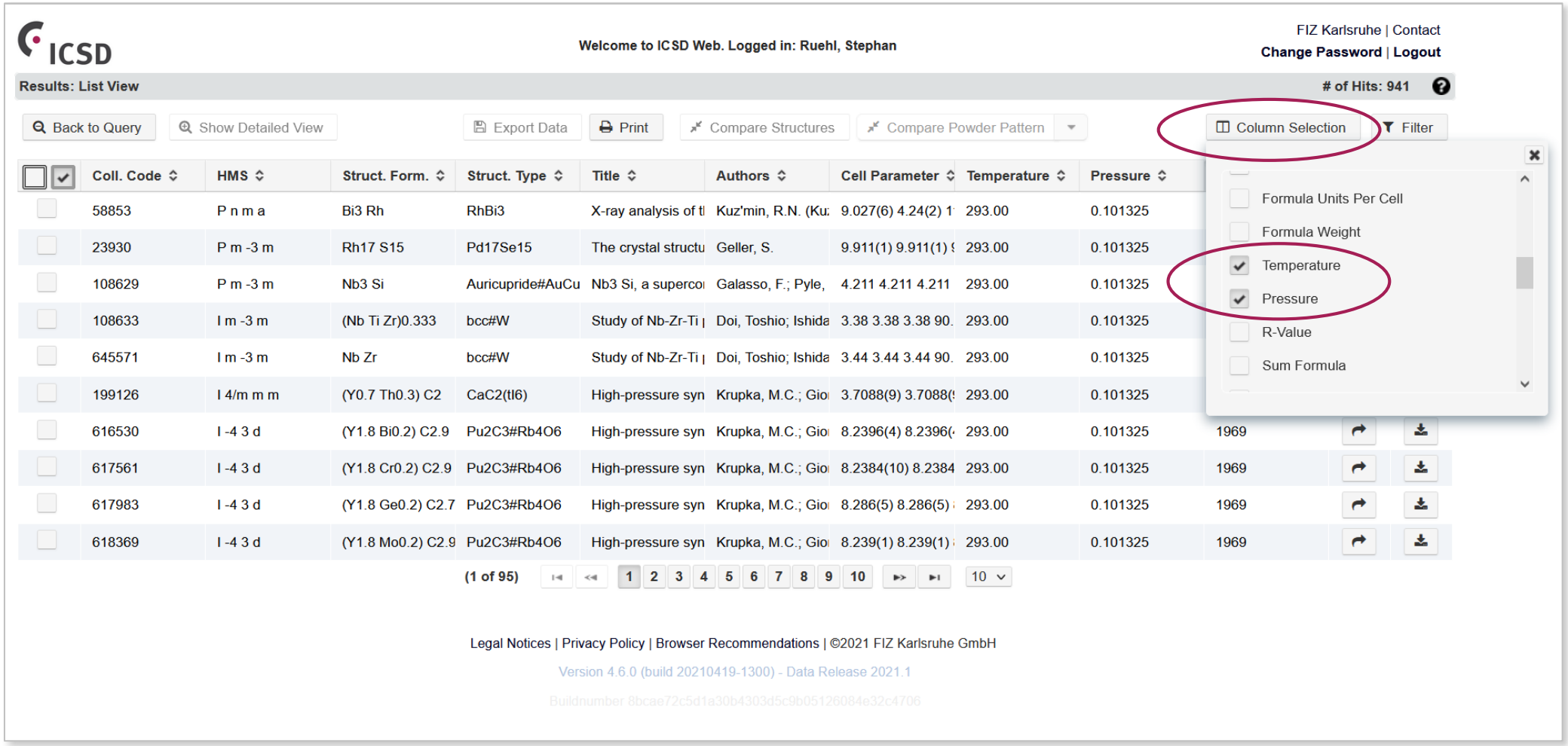
ICSD – Example: high temperature superconductors - Results

Result list:

Column selection



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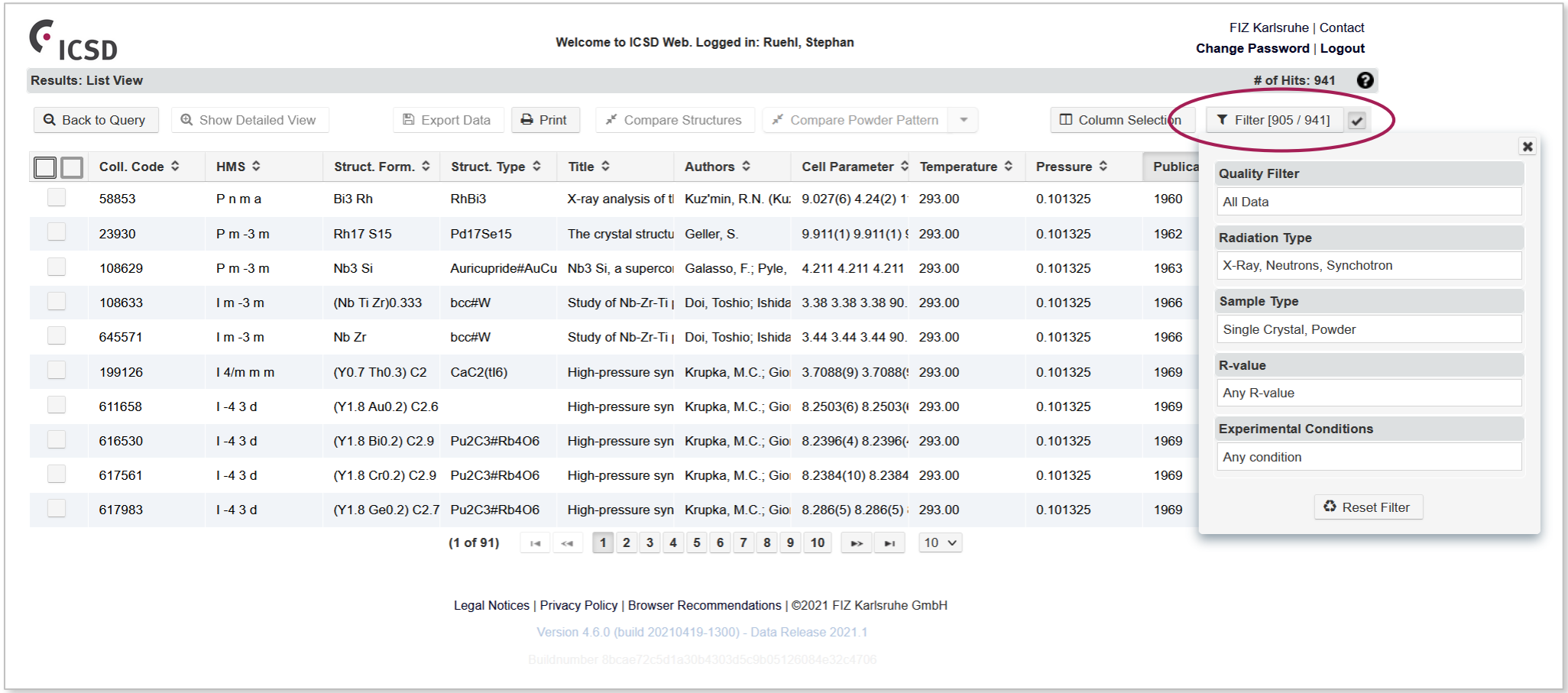
ICSD – Example: high temperature superconductors - Results

Result list:

Filter options



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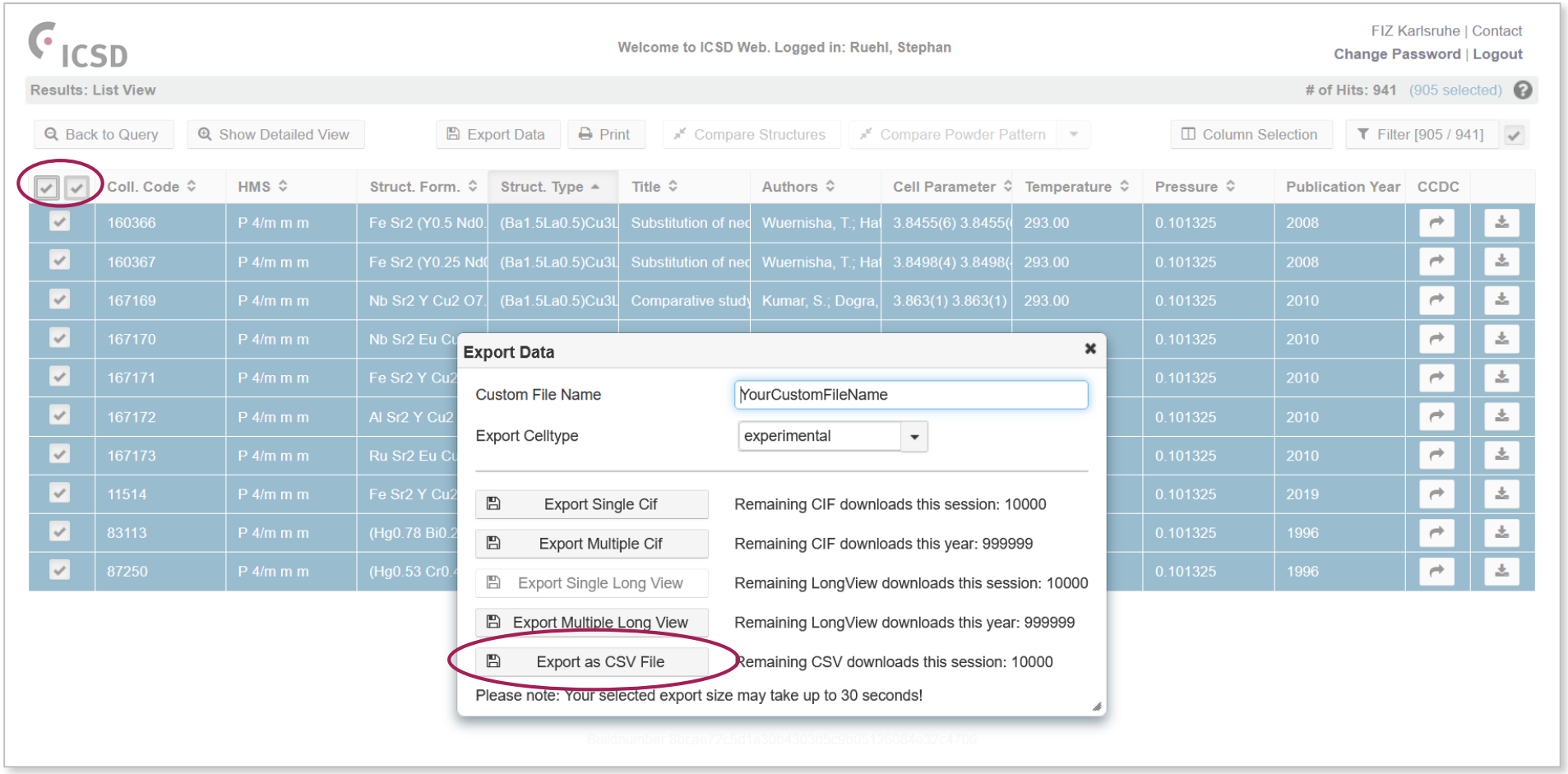
ICSD – Example: high temperature superconductors - Results

Result list:

Export data

-> CSV file



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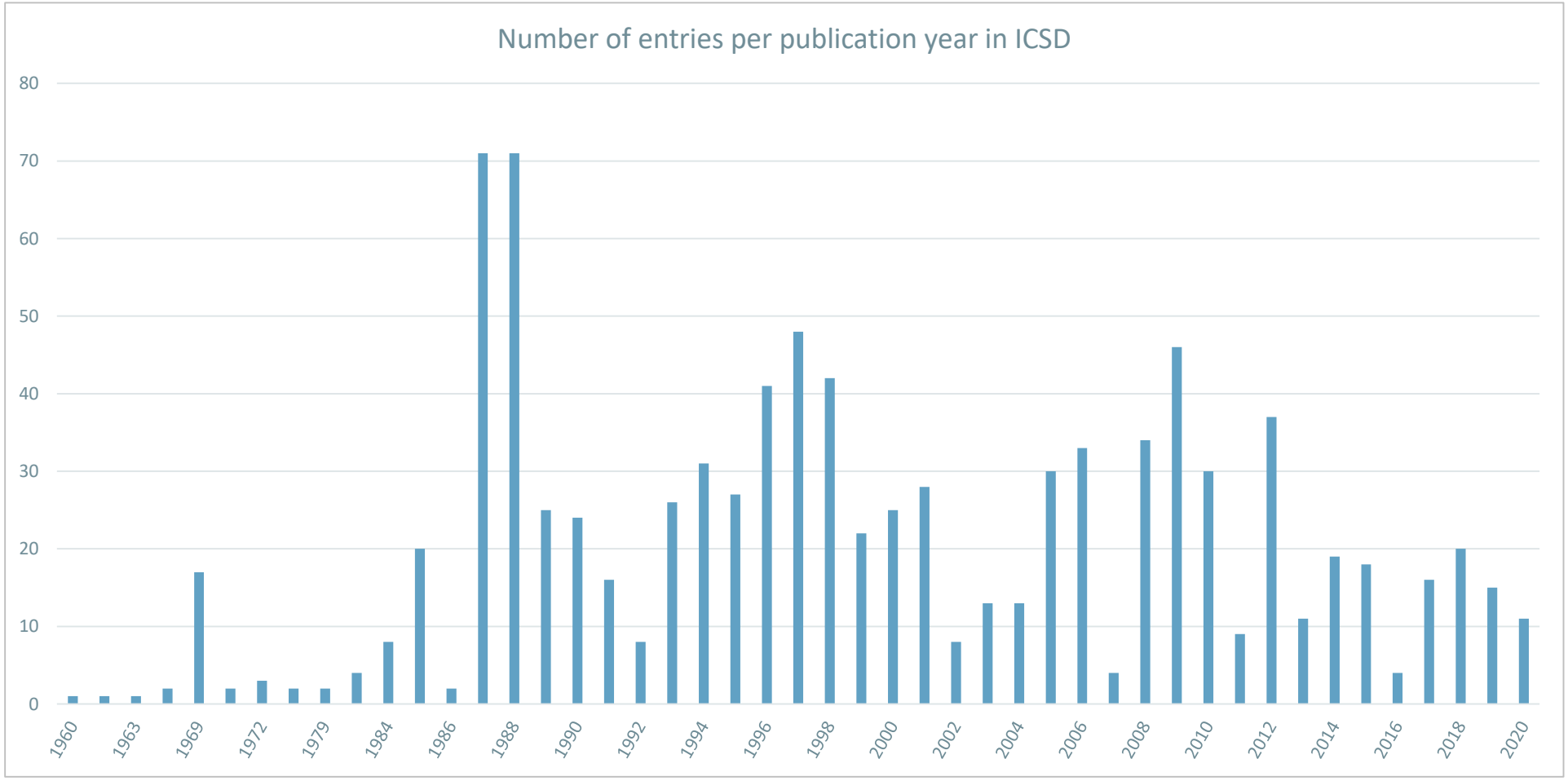
ICSD – Example: high temperature superconductors – External analysis

Information about super-conductors in ICSD



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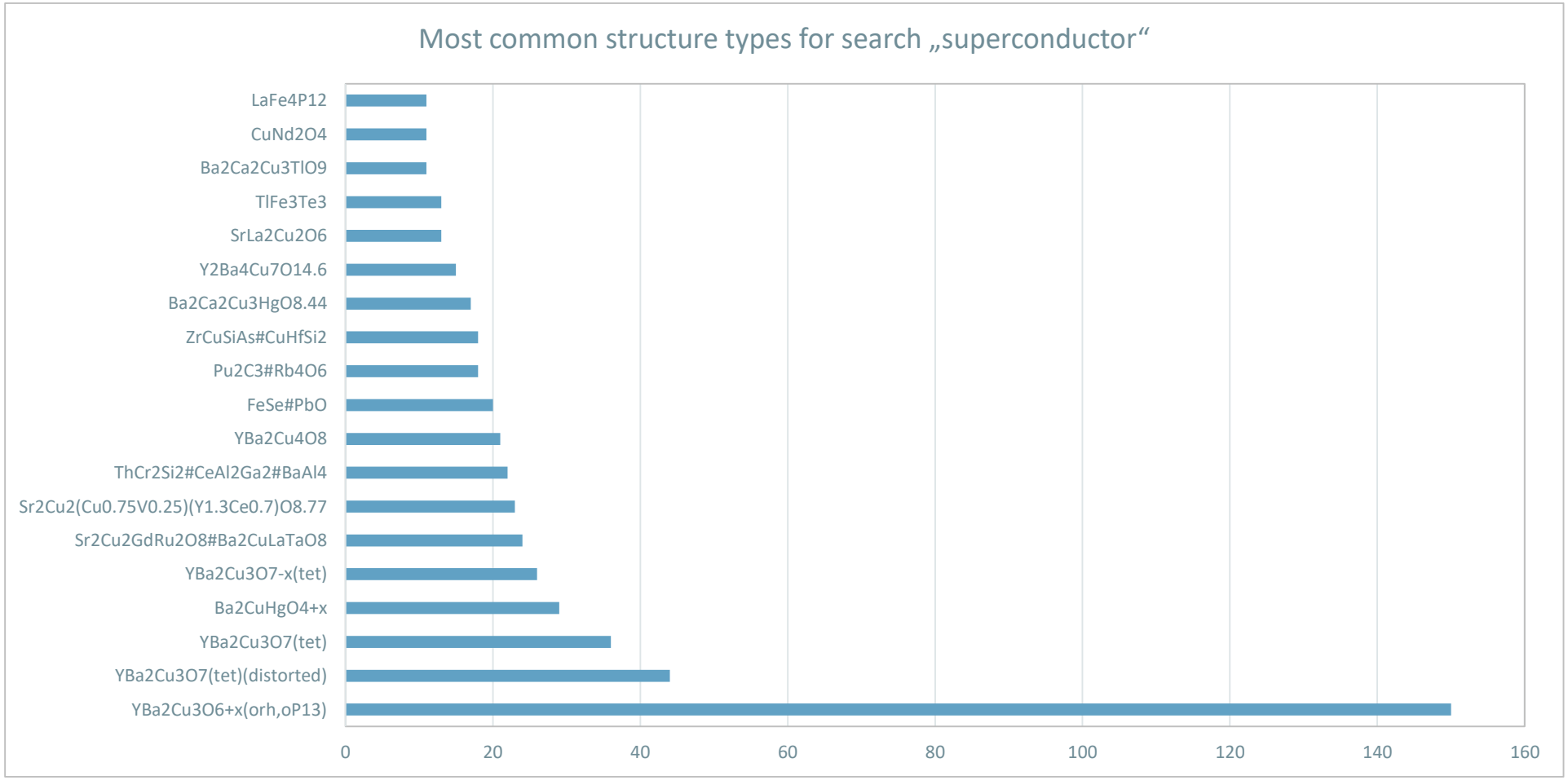
ICSD – Example: high temperature superconductors – External analysis

125 structure types with less than 10 entries left out



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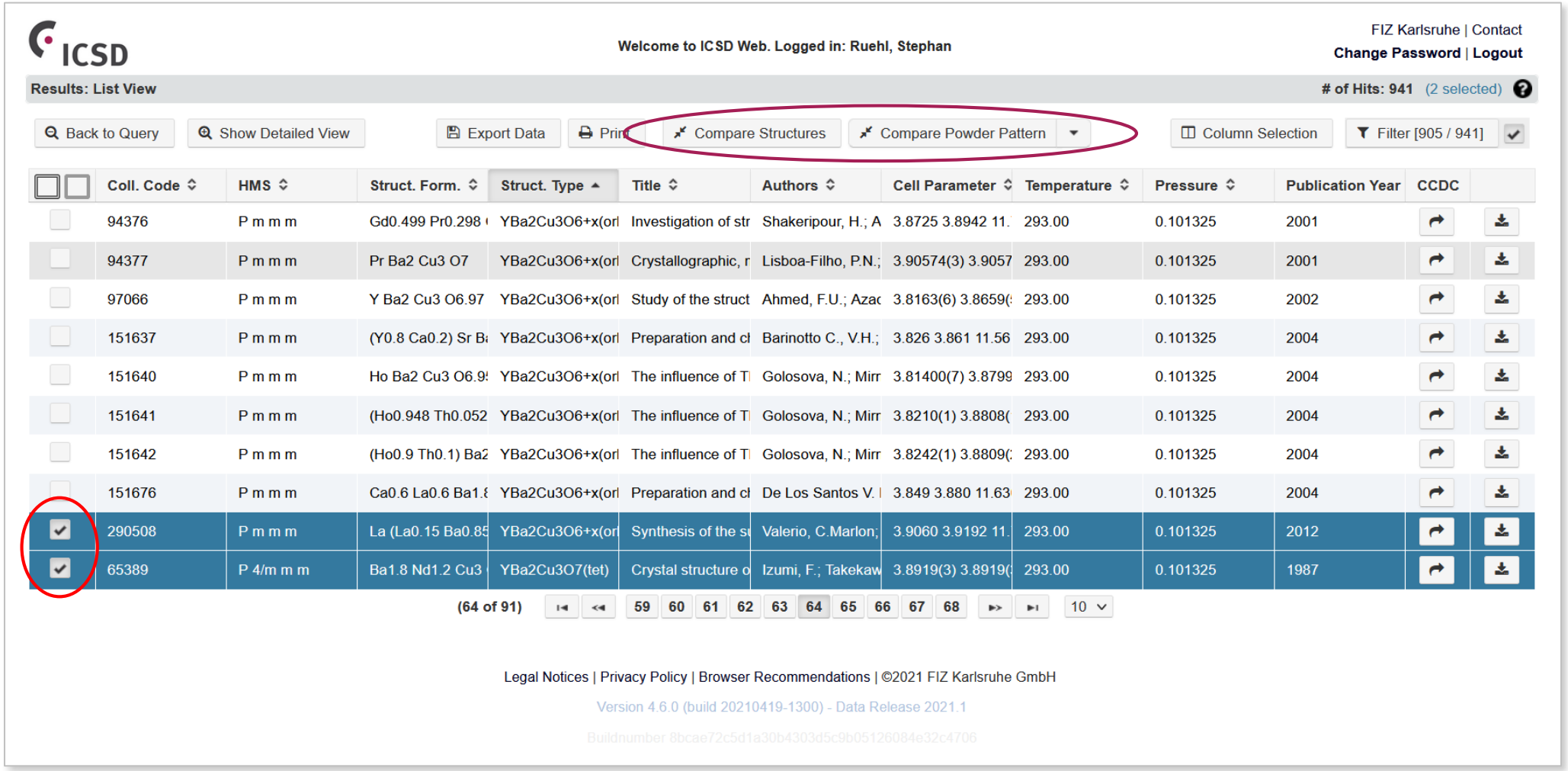
ICSD – Example: high temperature superconductors - Results

Result list:

Sorted by structure type



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(orl	Investigation of str	Shakeripour, H.; A	3.8725 3.8942 11.	293.00	0.101325	2001	
94377	P m m m	Pr Ba2 Cu3 O7	YBa2Cu3O6+x(orl	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(orl	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(orl	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(orl	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(orl	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(orl	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 Ba1.8	YBa2Cu3O6+x(orl	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(orl	Synthesis of the su	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(tet)	Crystal structure o	Izumi, F.; Takekaw	3.8919(3) 3.8919(	293.00	0.101325	1987	

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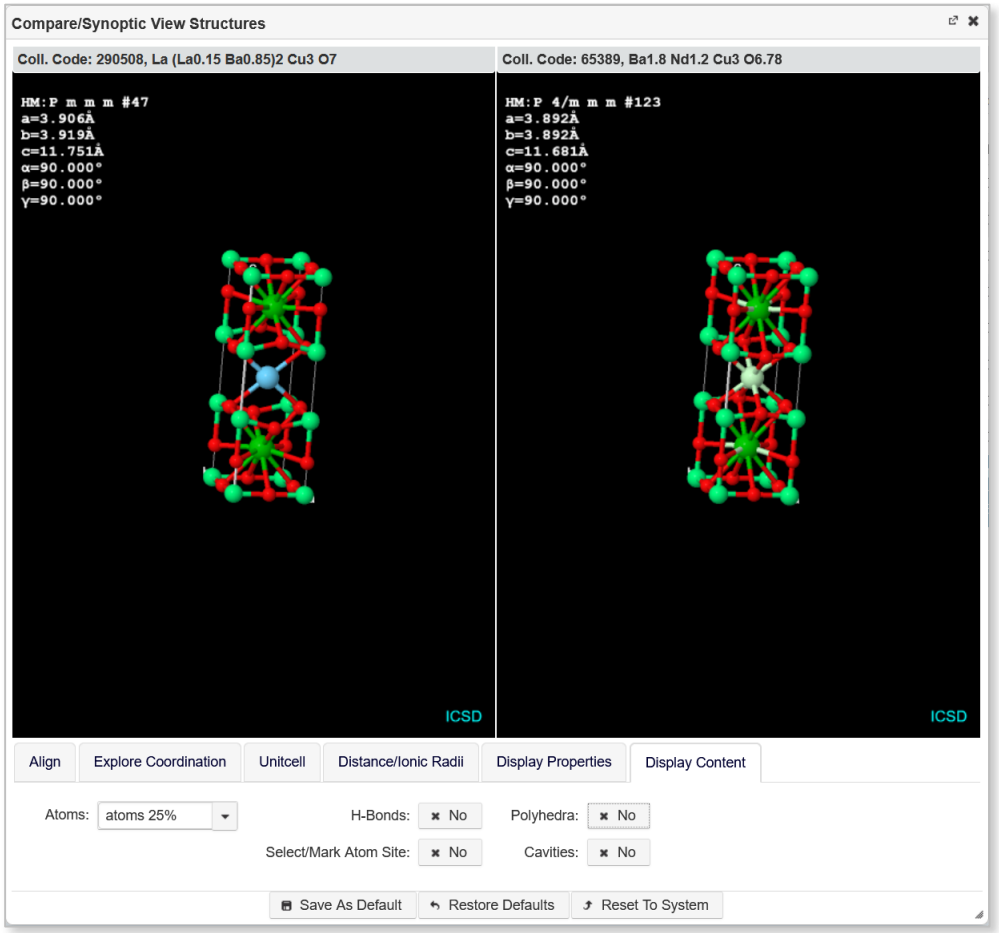
ICSD – Example: high temperature superconductors - Results

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



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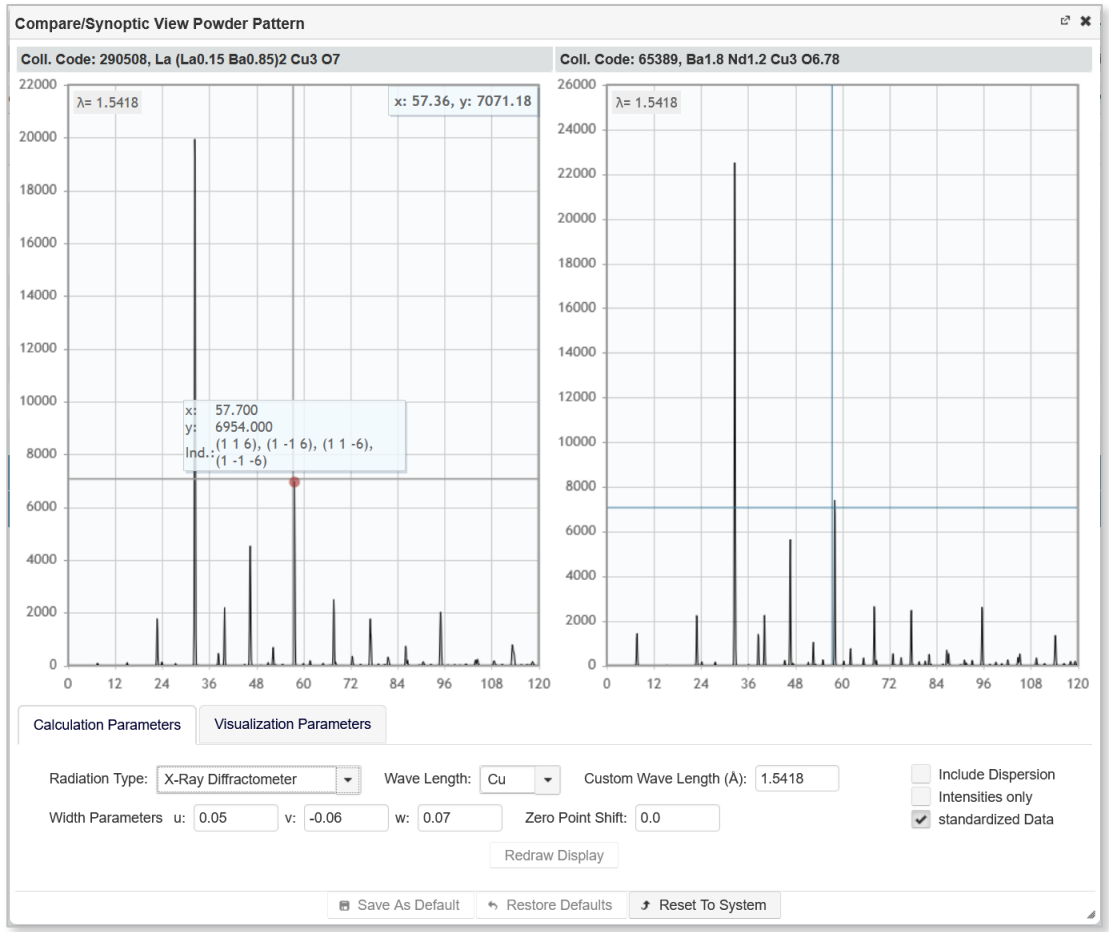
ICSD – Example: high temperature superconductors - Results

Comparison of the two simulated powder patterns for the structures

- side-by-side view



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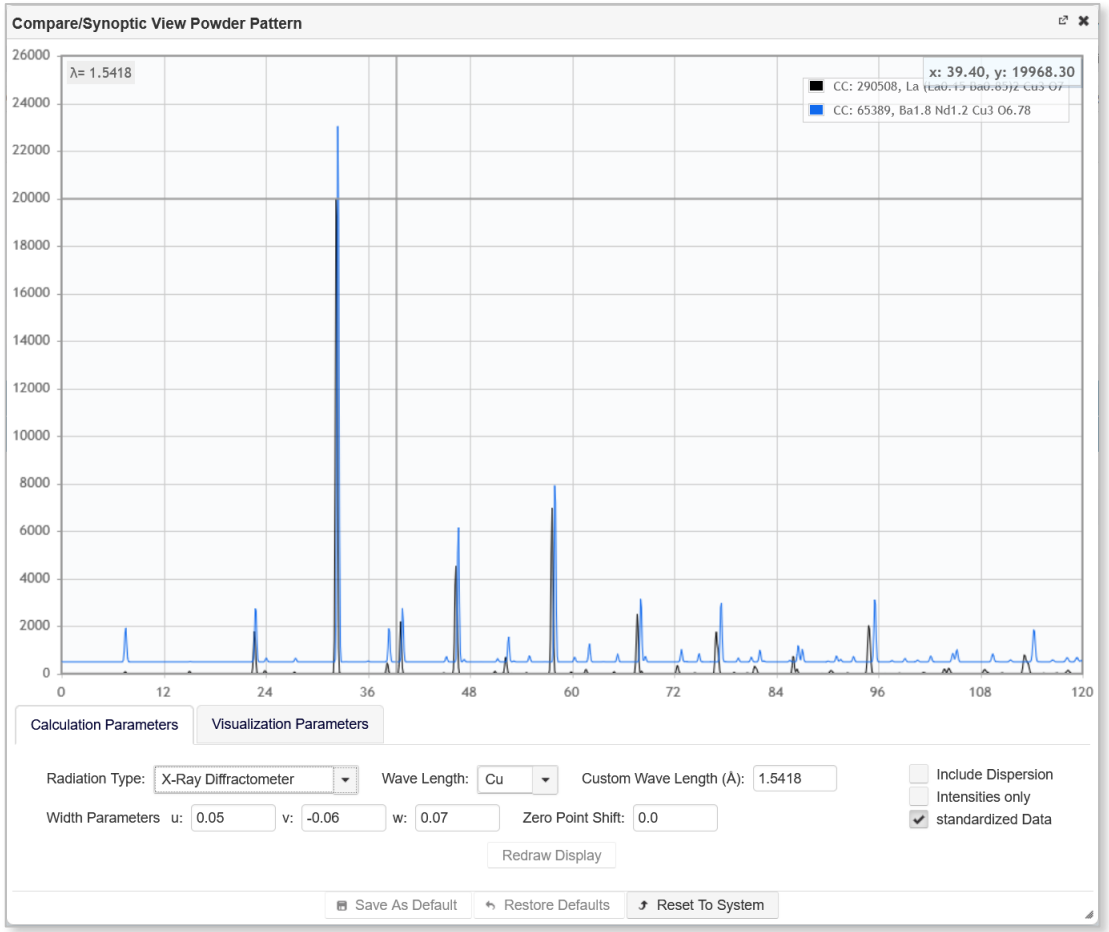
ICSD – Example: high temperature superconductors - Results

Comparison of the two simulated powder patterns for the structures

- staggered view



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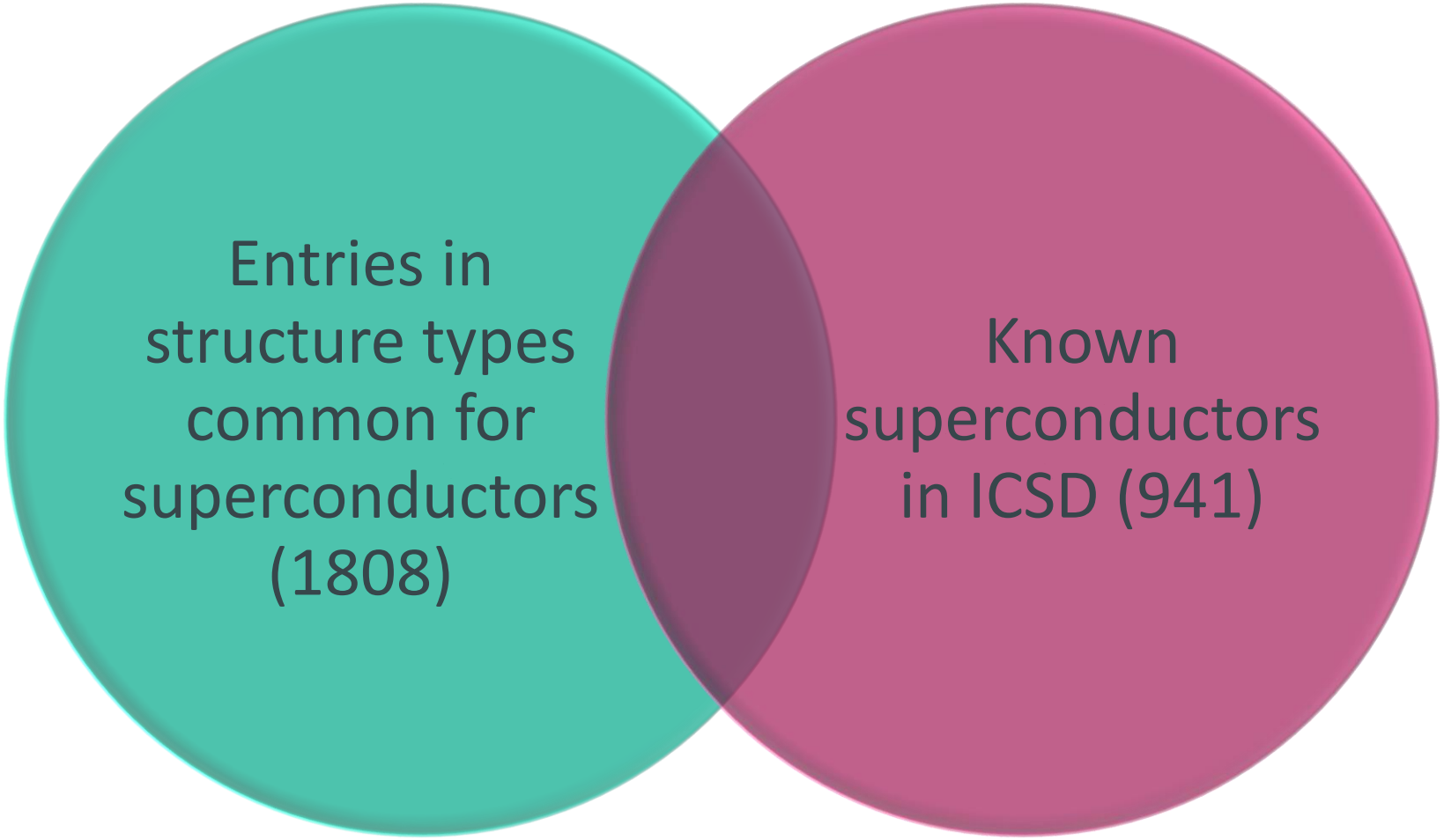
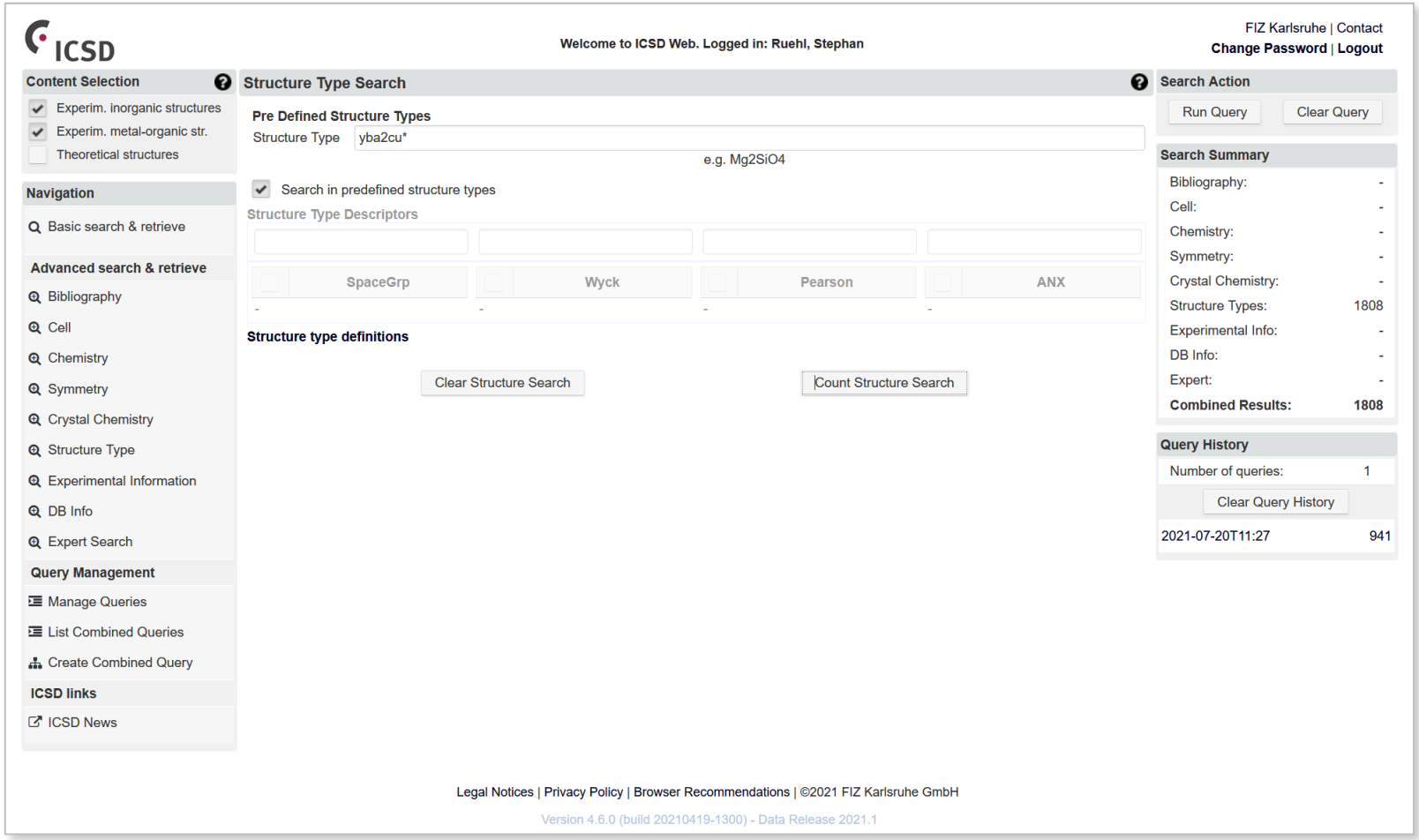
ICSD – Example: high temperature superconductors



ICSD – Example: high temperature superconductors – New search

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



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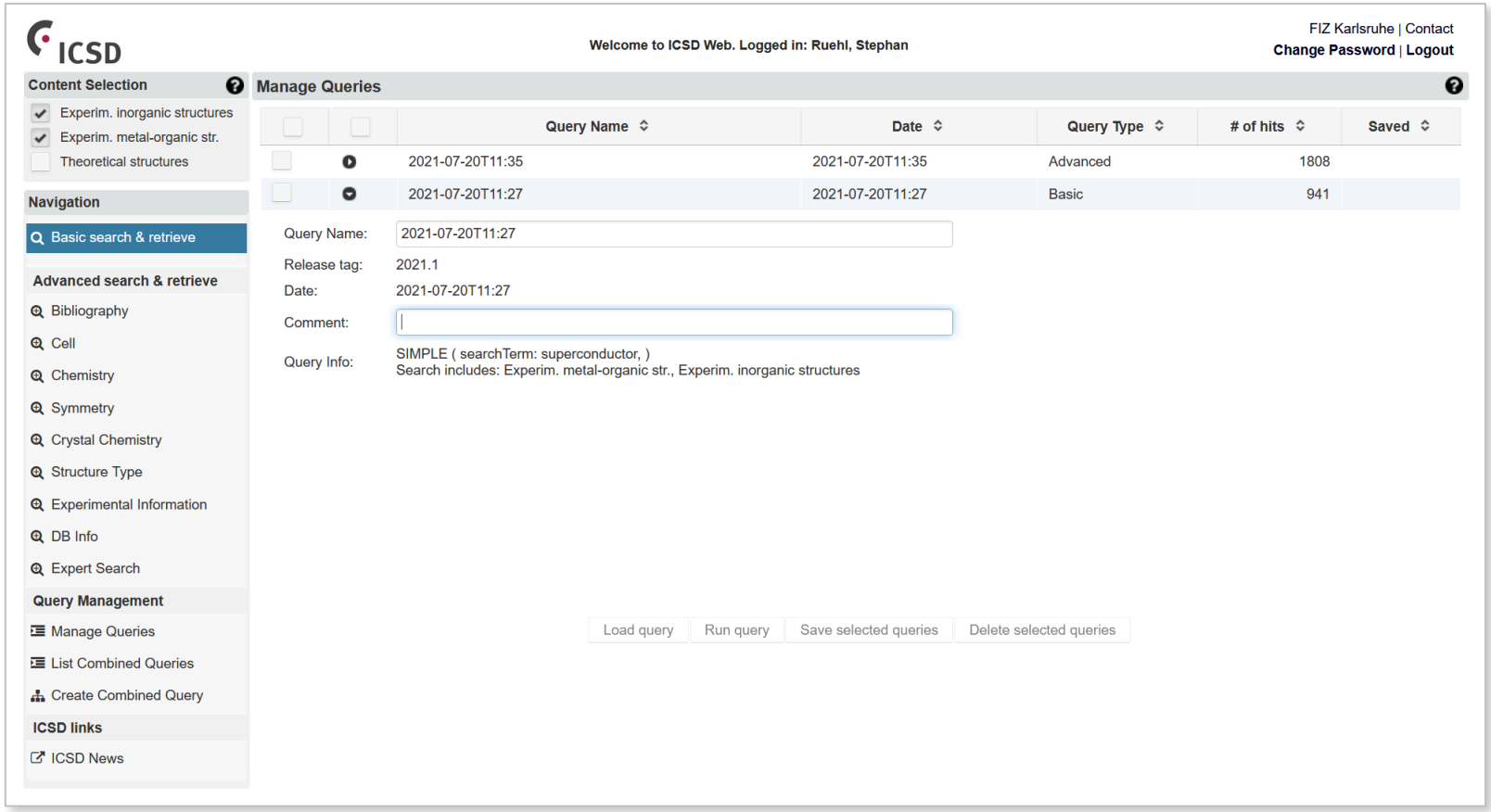
ICSD – Example: high temperature superconductors – Combine searches

Manage Queries shows the two queries from the Query History



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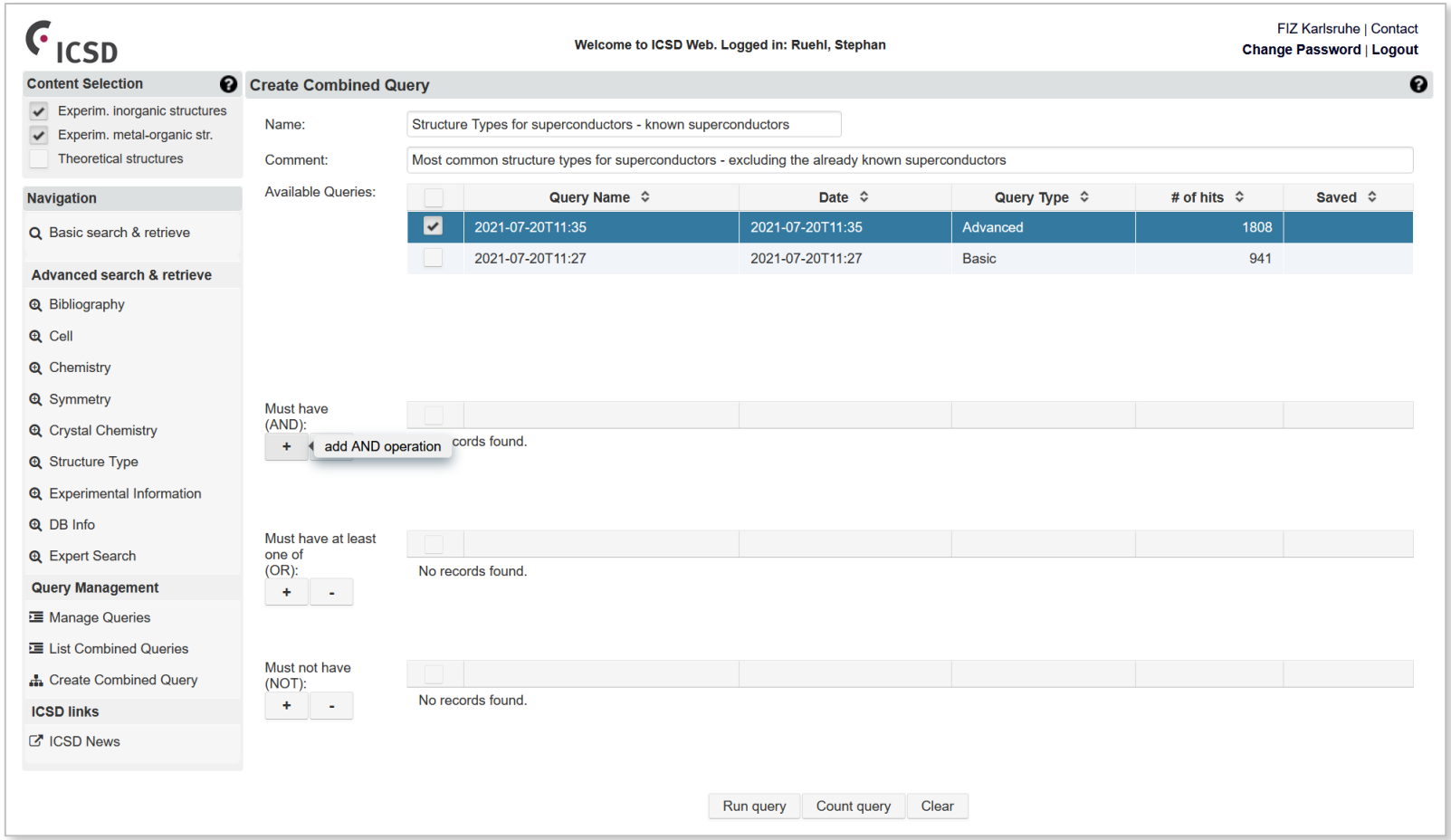
ICSD – Example: high temperature superconductors – Combine searches

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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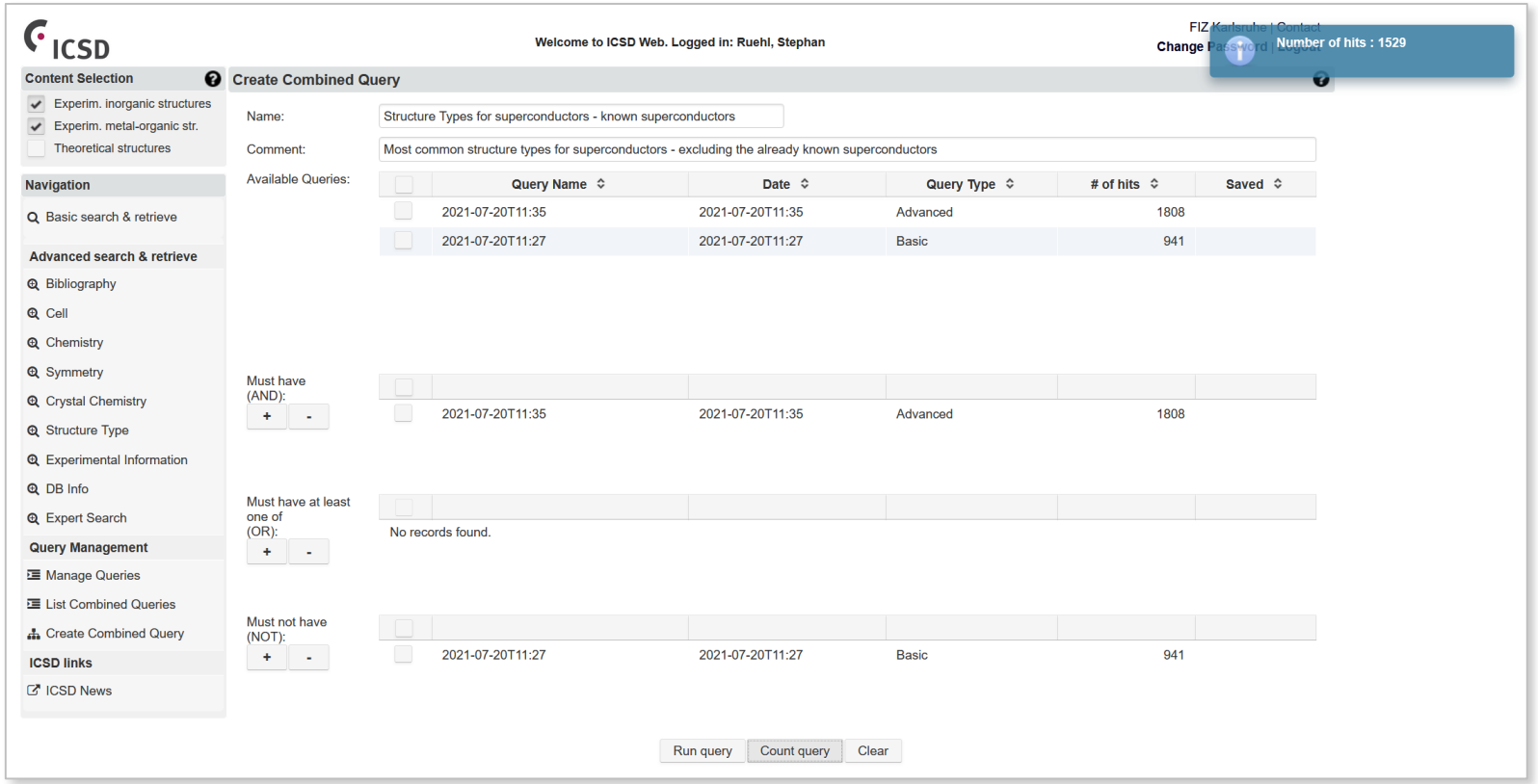
ICSD – Example: high temperature superconductors – Combine searches

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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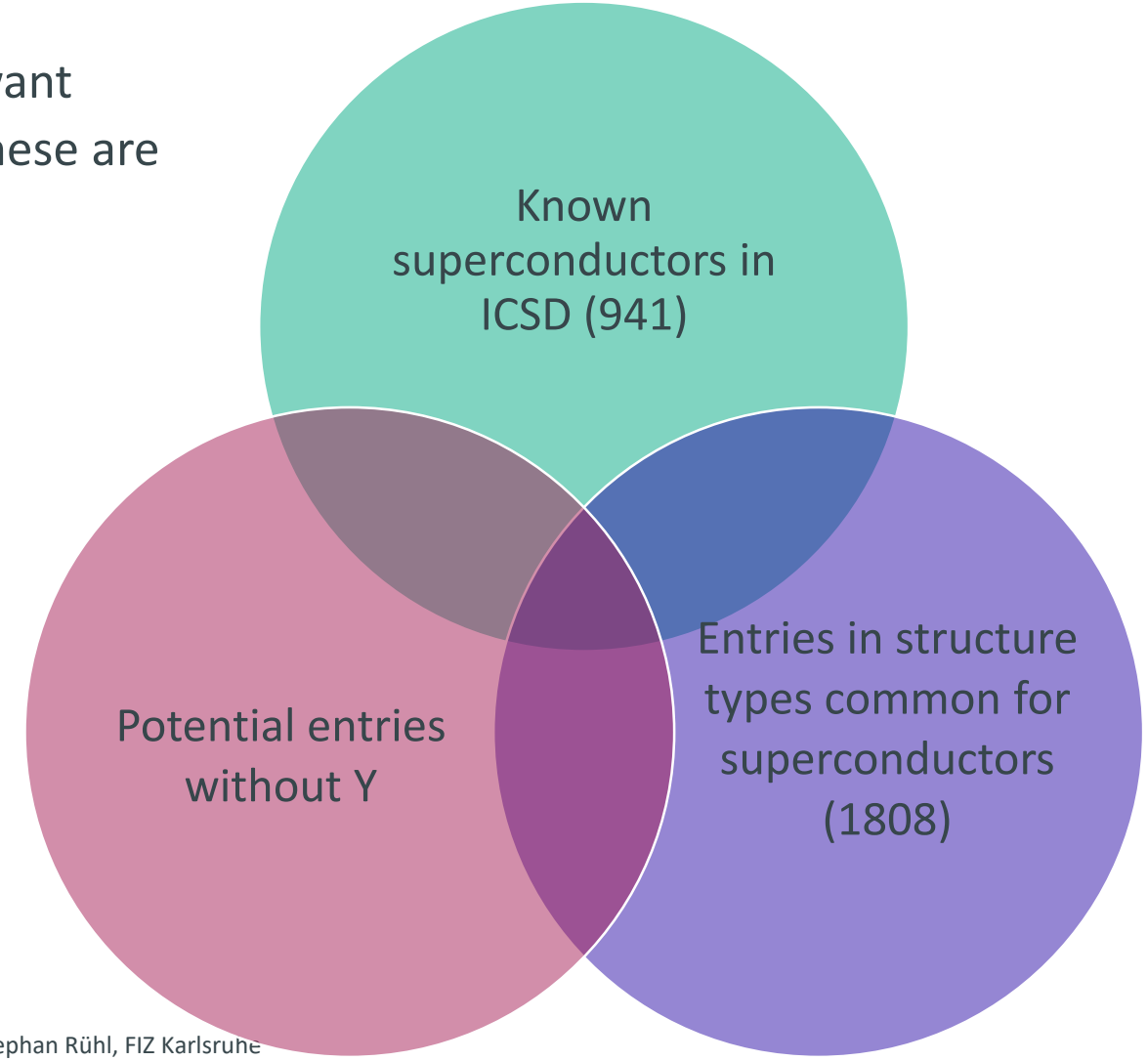
ICSD – Example: high temperature superconductors – Exclude Y

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



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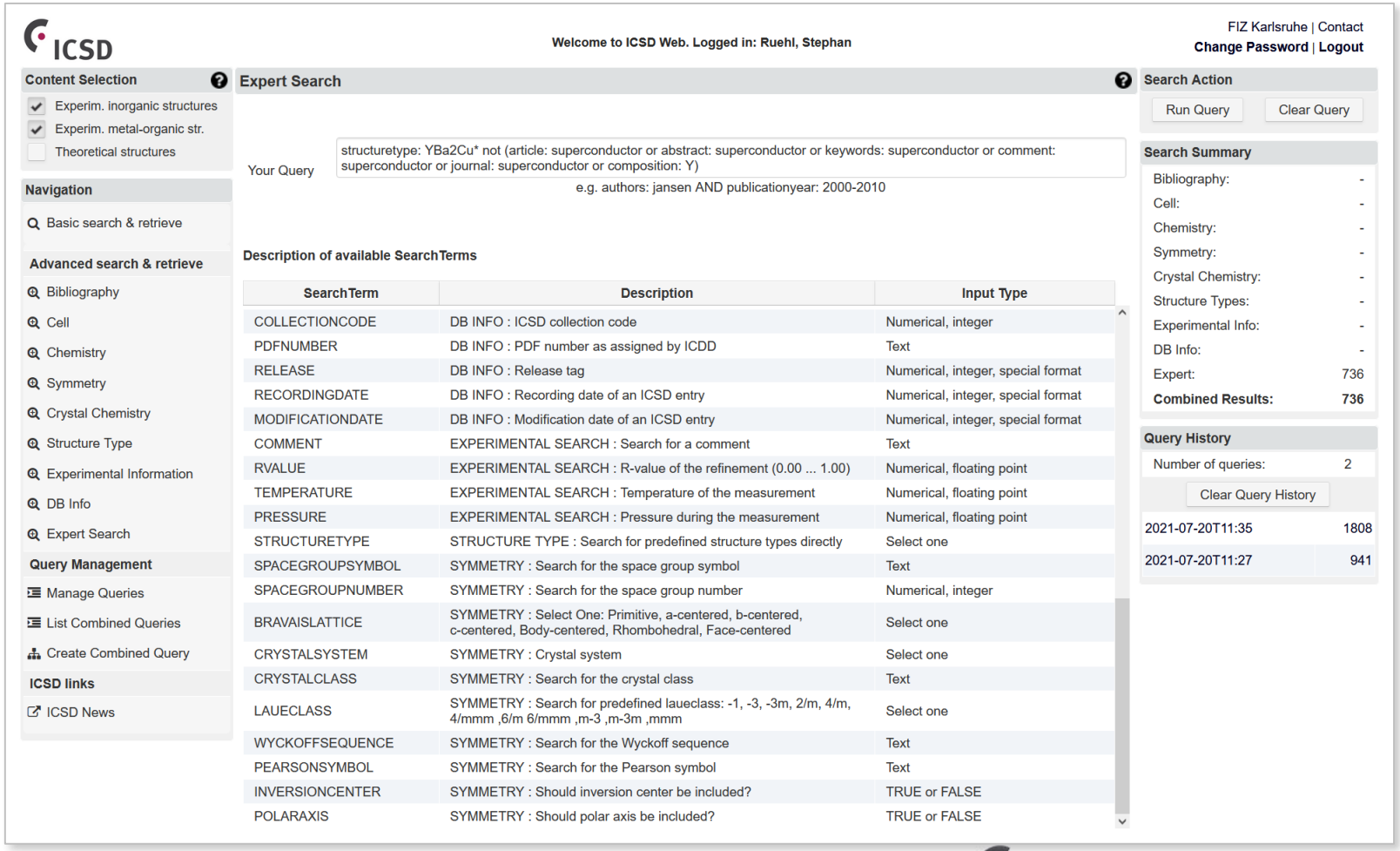
ICSD – Example: high temperature superconductors – Expert Search

Using the Expert Search Mask

Note: This search is also available for the ICSD API



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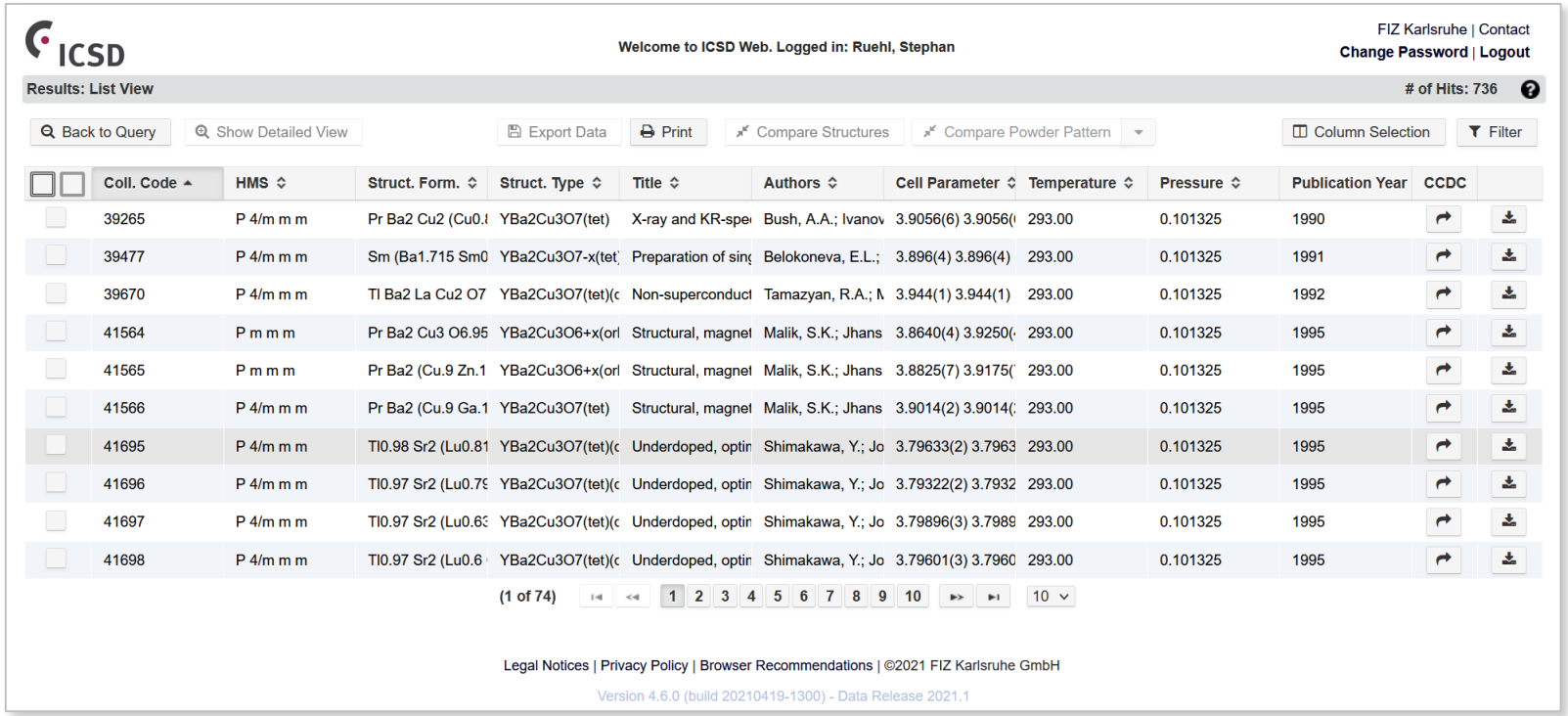
ICSD – Example: high temperature superconductors – Final result

Result list



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Results: List View

# of Hits: 736

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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 (Cu0.8	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 sing	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(orl	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(orl	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 (Lu0.79	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 (Lu0.63	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	

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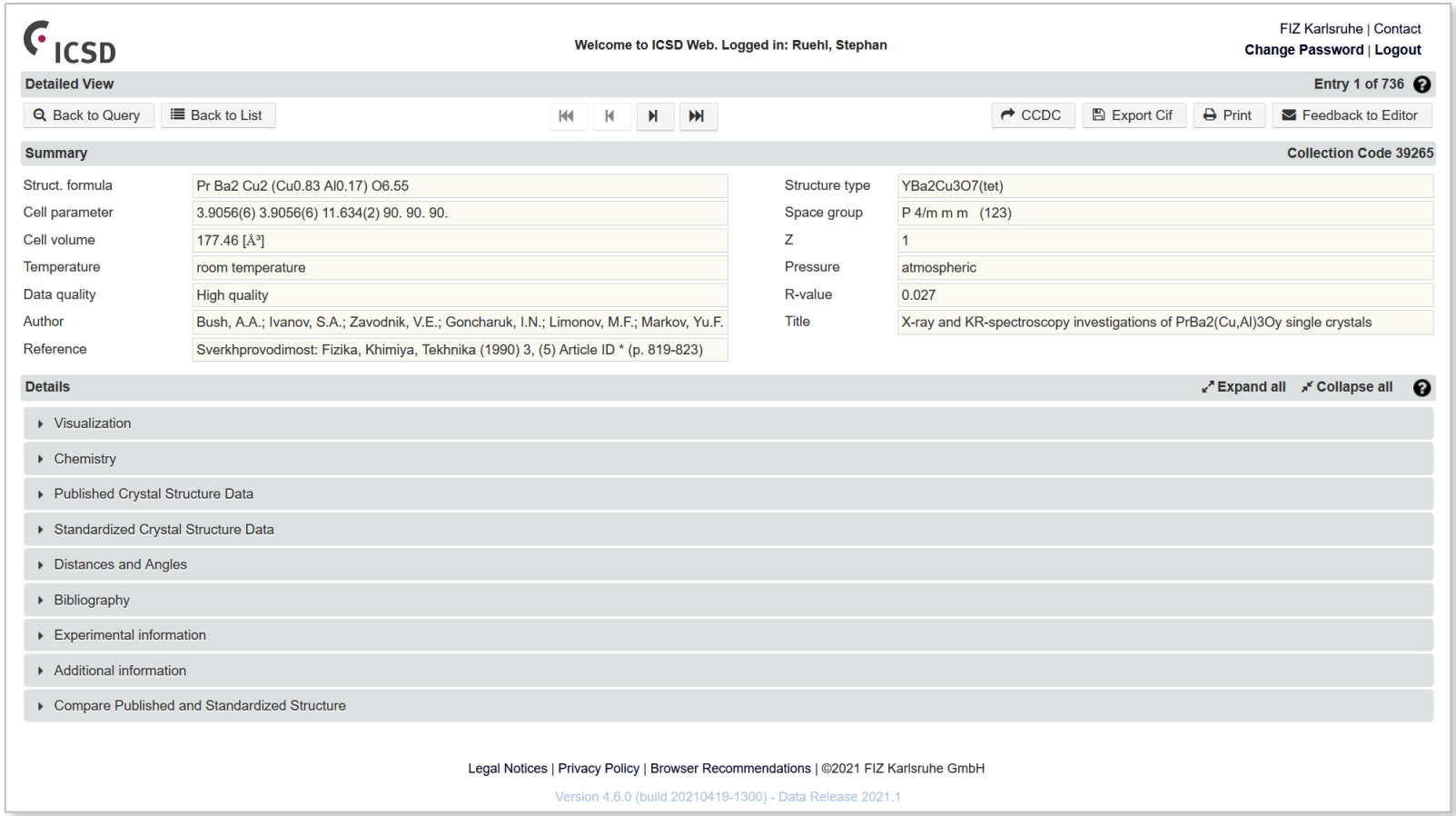
ICSD – Detailed View - Summary

Detailed Information for an entry:

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



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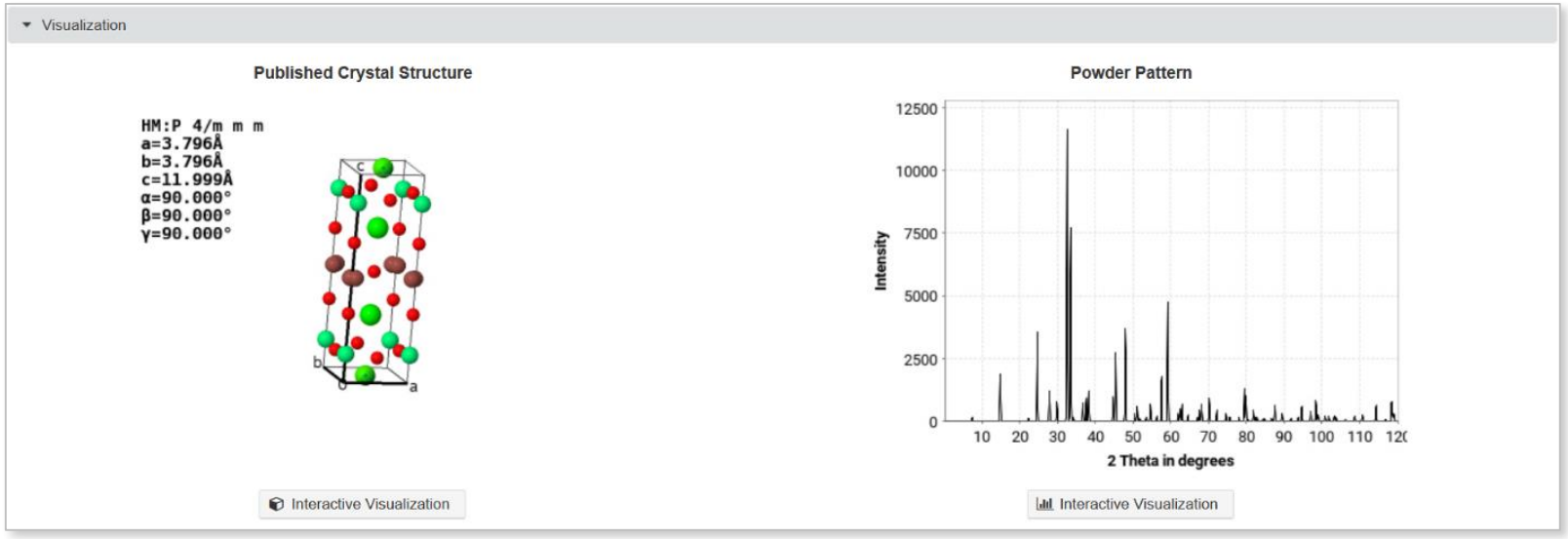
ICSD – Detailed View - Visualization

Pictures of:

- Crystal structure
- Simulated powder pattern

Interactive Visualization available with many options to customize it



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ICSD – Detailed View - Chemistry

Information on the Chemistry:

- Structured formula provides the formula split up into cations and anions

Chemistry

Sum. formula	Ca0.19 Cu2 Lu0.81 O6.96 Sr2 Tl0.98	Struct. formula	Tl0.98 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)		

- Mineral name/group infromation may be found here
- Chemical names are not necessarily IUPAC names - can be used to search for complex anions

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.
Cell volume	172.93 Å³
Crystal system	tetragonal
Laue class	4/mmm
Structure type	YBa2Cu3O7(tet)(distorted)
Pearson symbol	tP13
Wyckoff sequence	m i h g2 d c
Calc. density	7.33 [g/cm³]

Space group	P 4/m m m (123)		
Z	1		
Crystal class	4/mmm		
	a/b	b/c	c/a
Axis ratios	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 – Standardized structure

Crystallographic information for the standardized structure

Additional information:

- standardization

Standardized Crystal Structure Data

Cell parameter	3.7963 3.7963 11.9986 90.000 90.000 90.000	Space group	P 4/m m m (123)
Cell volume	172.92 Å³	Z	1
Crystal system	tetragonal	Crystal class	4/mmm
Laue class	4/mmm		
Structure type	YBa2Cu3O7(tet)(distorted)		
Pearson symbol	tP13		
Wyckoff sequence	n i h2 g b a	Axis ratios	a/b: 1.0000; b/c: 0.3164; c/a: 3.1606
Transformation info	TRANS Origin 1/2 1/2 1/2		

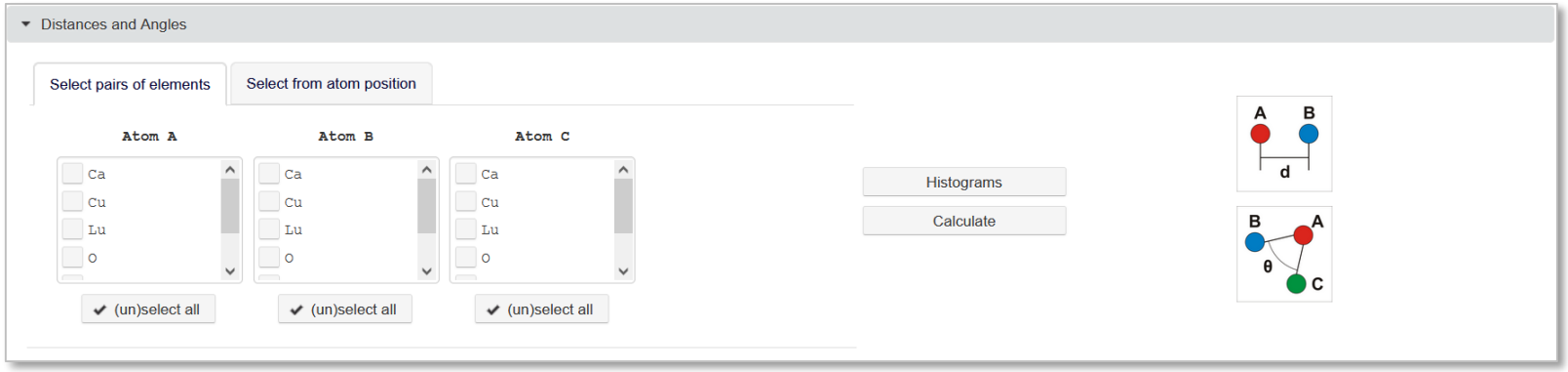
EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	B
Tl	1	+3.00	4 n	0.4357	0.5000	0.0000	0.245000	0.9100
Sr	1	+2.00	2 g	0.0000	0.0000	0.2102	1	0.7700
Lu	1	+3.00	1 b	0.0000	0.0000	0.5000	0.810000	0.3600
Ca	1	+2.00	1 b	0.0000	0.0000	0.5000	0.190000	0.3600
Cu	1	+2.08	2 h	0.5000	0.5000	0.3644	1	
O	1	-2.00	4 i	0.0000	0.5000	0.3797	1	
O	2	-2.00	2 h	0.5000	0.5000	0.1709	1	
O	3	-2.00	1 a	0.0000	0.0000	0.0000	0.960000	

EL	Lbl	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Cu	1	0.003200	0.003200	0.008700	0.000000	0.000000	0.000000
O	1	0.011200	0.004000	0.017900	0.000000	0.000000	0.000000
O	2	0.017200	0.017200	0.006000	0.000000	0.000000	0.000000
O	3	0.051000	0.051000	0.010000	0.000000	0.000000	0.000000

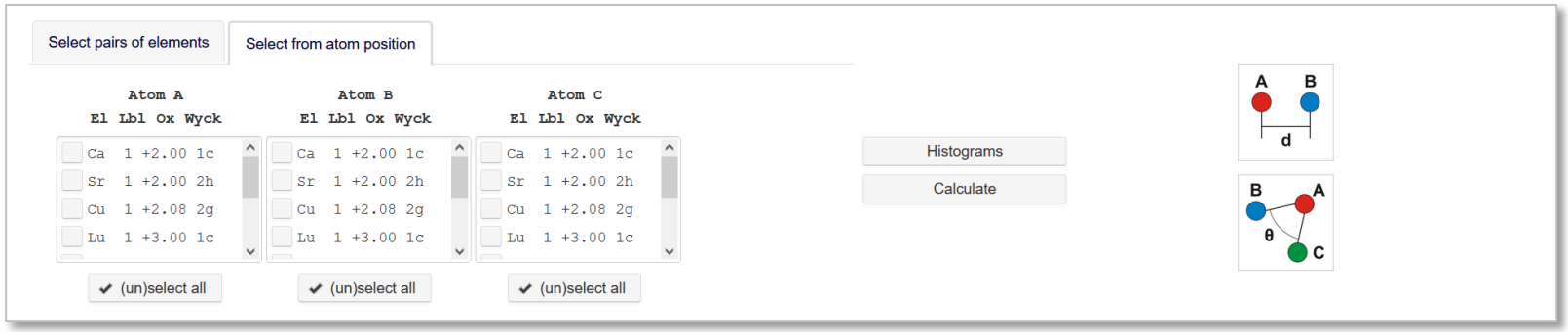
ICSD – Detailed View – Distances and Angles

Option to calculate distances and angles:

- Based on elements
- Based on atomic positions



Histograms for distances across e whole database



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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 Sr2 (R1-x Cax) Cu2 O7-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

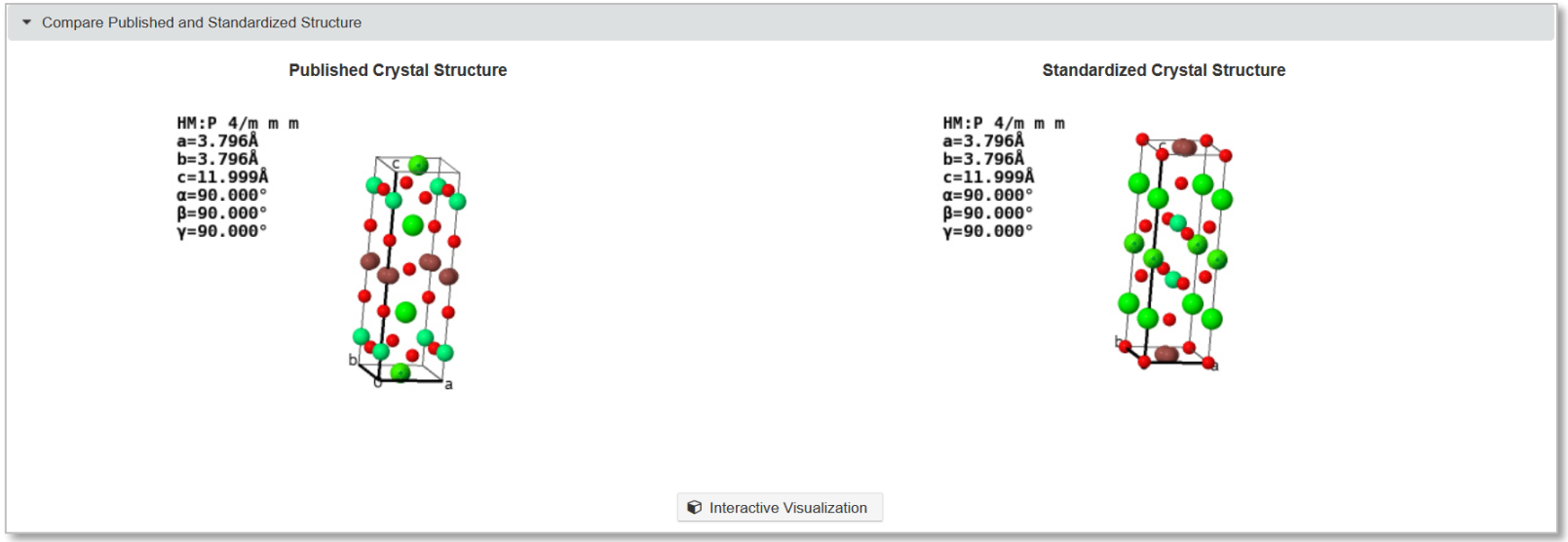
Additional information

Comments	Underdoped, Tc = 50 K

ICSD – Detailed View – Compare published/standardized structure

Pictures of the published and the standardized structure

Interactive view is also available



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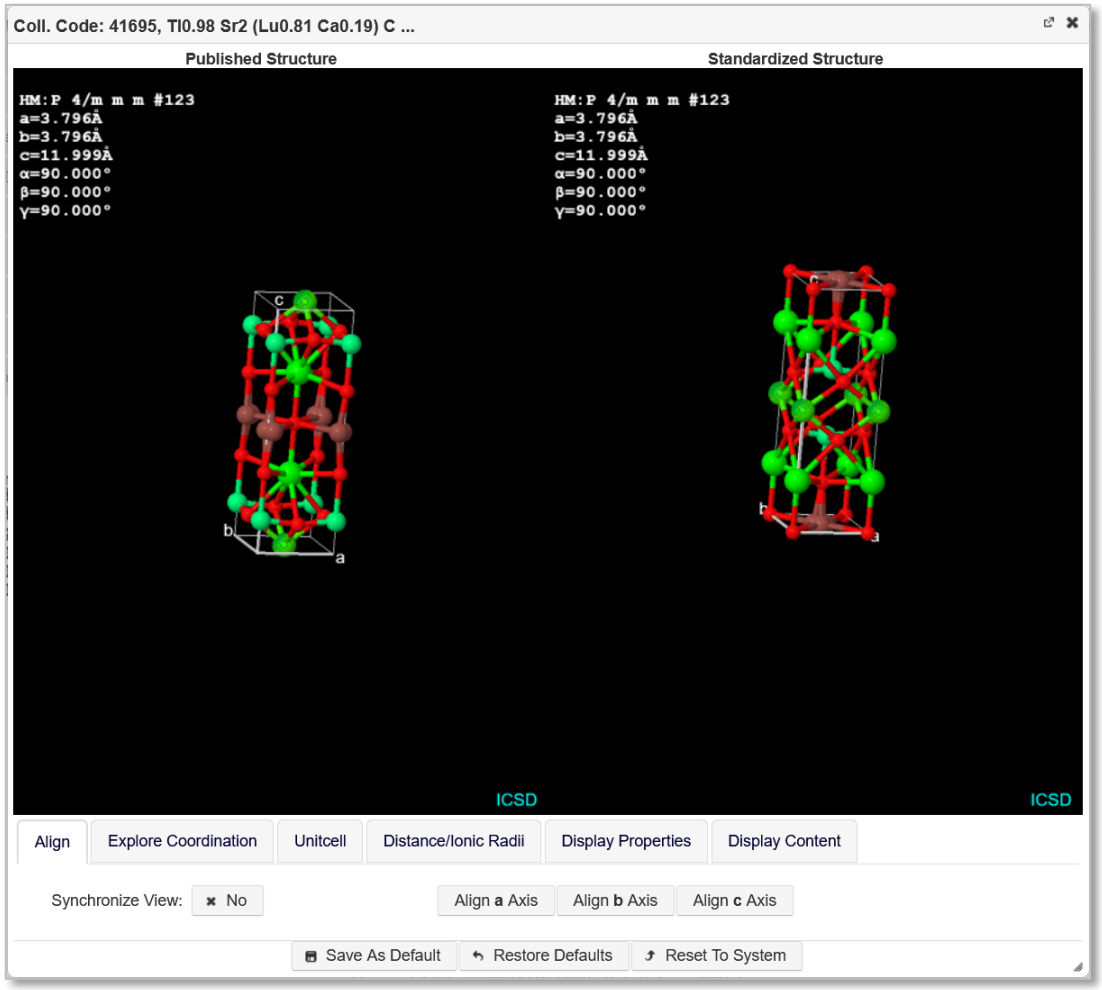
ICSD – Detailed View – Compare published/standardized structure

Interactive view of the published and standardized structure

Visualization can be adjusted as for single structures



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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/lrcfmd/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

ICSD

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 datbase

- 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. loginid
password string (formData)	The password of the ICSD account. If this parameter is not set, an IP-based authentication will be performed. your password

Execute

Responses Response content type text/plain

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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=your%20password"
```

Request URL

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

Server response

Code	Details
200	Response body

```
Already authenticated.
```

Download

Response headers

```
connection: keep-alive
content-length: 22
content-type: text/plain
date: Wed, 28 Jul 2021 09:32:05 GMT
icsd-auth-token: 69DC33FEB27BCDCEE8A7A5EA3390E0CD
keep-alive: timeout=20
strict-transport-security: max-age=31536000 ; includeSubDomains
```


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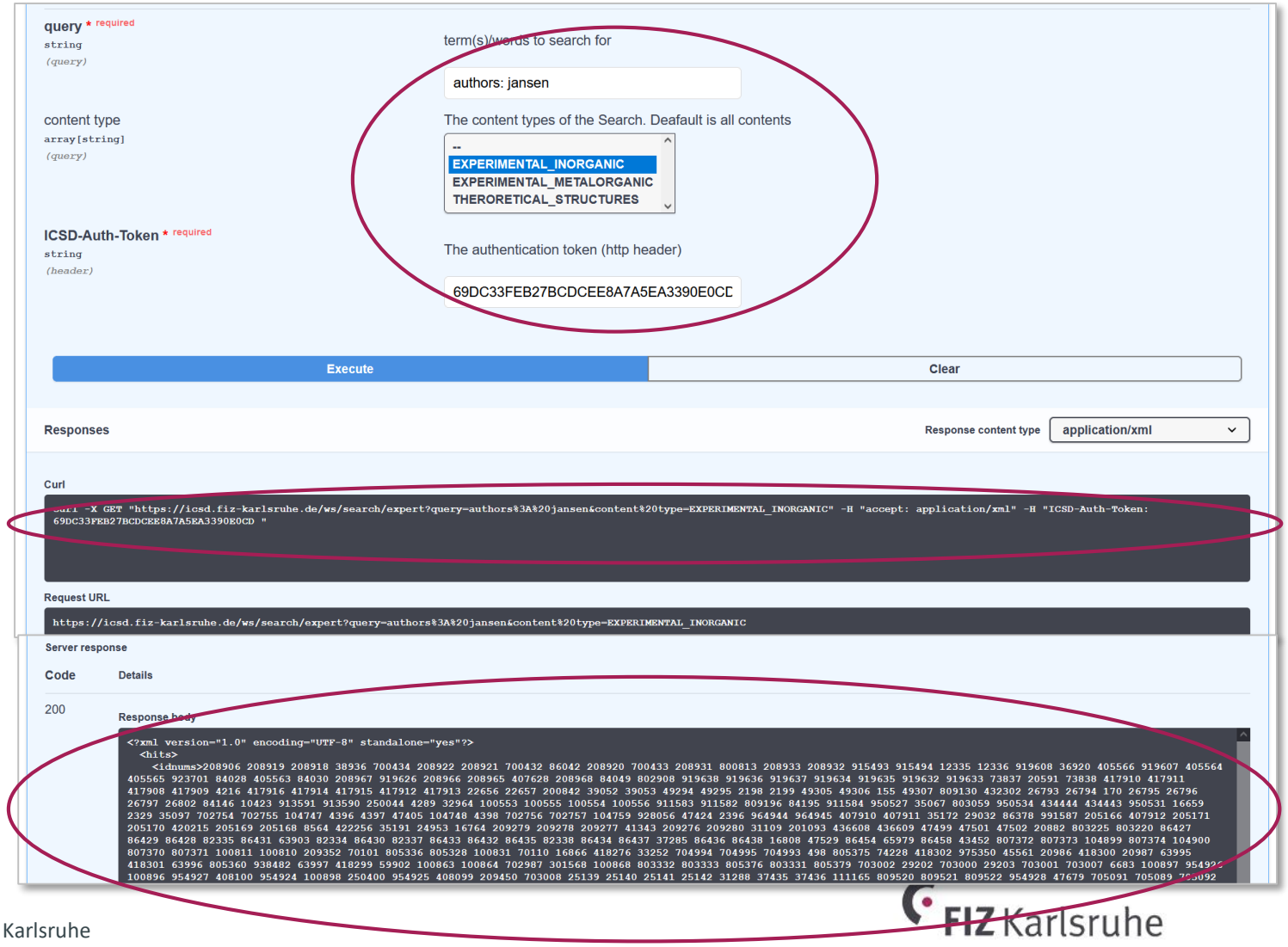
ICSD – API (Search)

Search uses the Expert Mask syntax

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



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Thank you for your attention

Contact

Stephan Rühl
Product Manager ICSD
FIZ Karlsruhe – Leibniz-Institute for Information Infrastructure
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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(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

Appl Cryst JAC Journal of Applied Crystallography

home archive editors for authors for readers submit subscribe open access

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

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

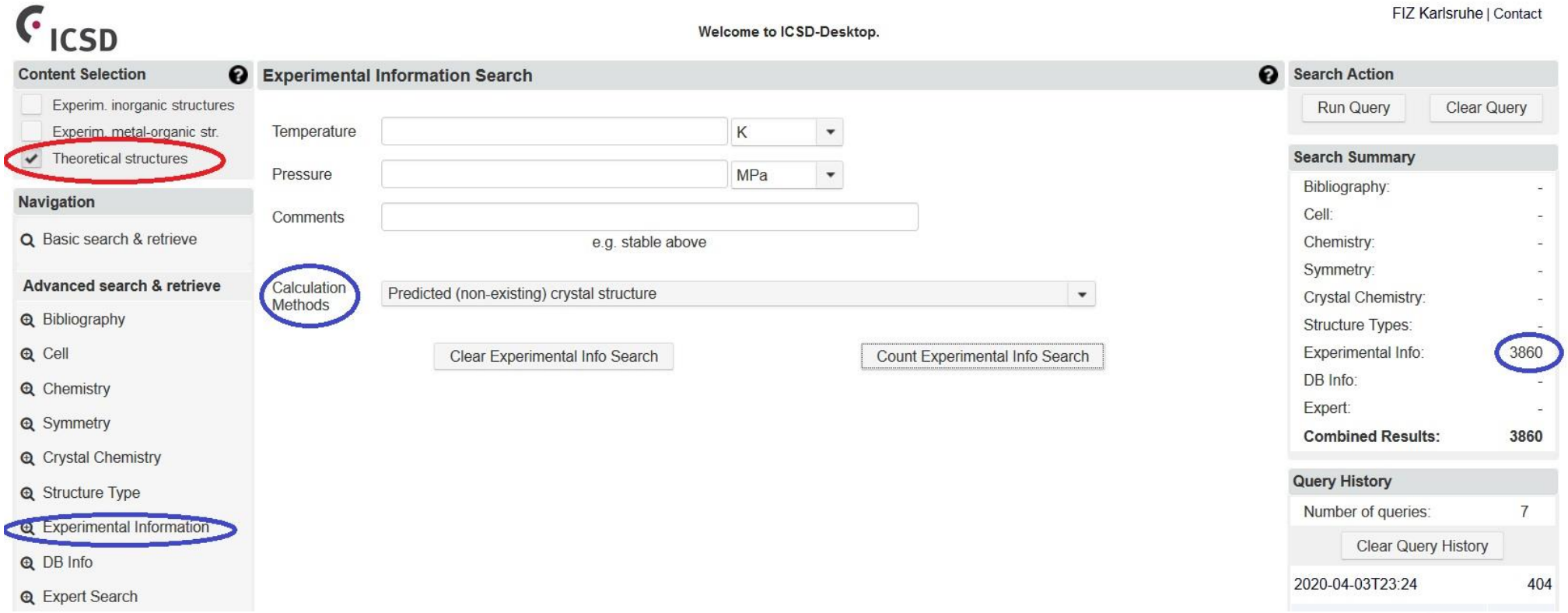
Upgrade of the theoretical CIF file

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.



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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

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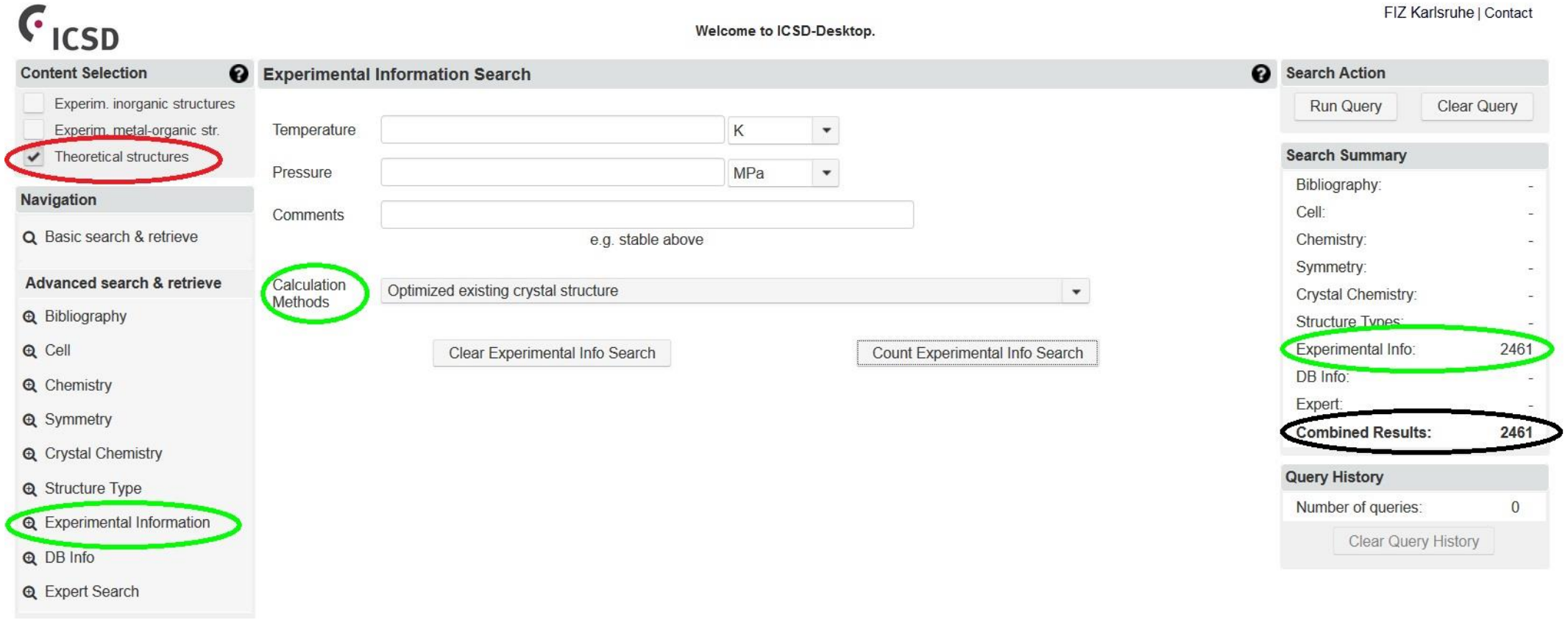
- Optimized (or existing) crystal structures are theoretically calculated structures of existing experimental crystal structures in the ICSD until the year of publication.
- In experimental materials science and related sciences, they can be used as an excellent tool for industrial and technological 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



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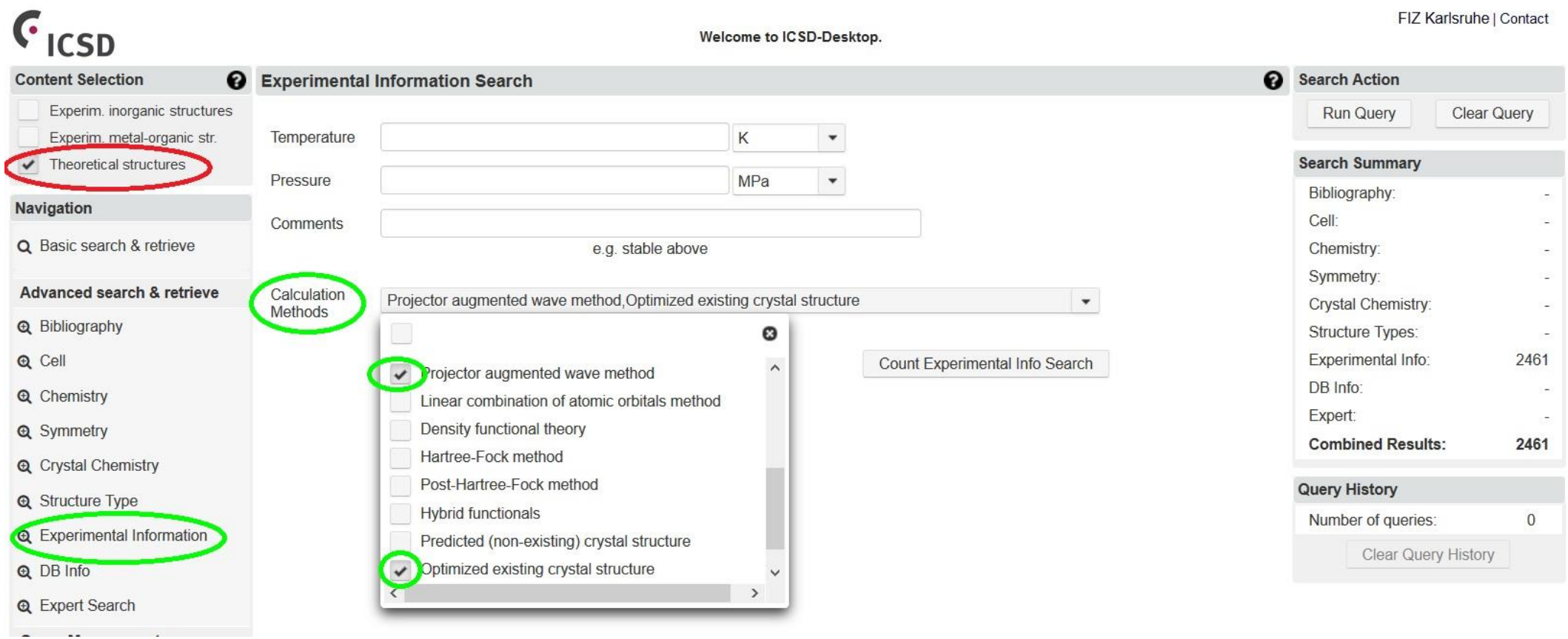
Search for parameters for method development and future calculations



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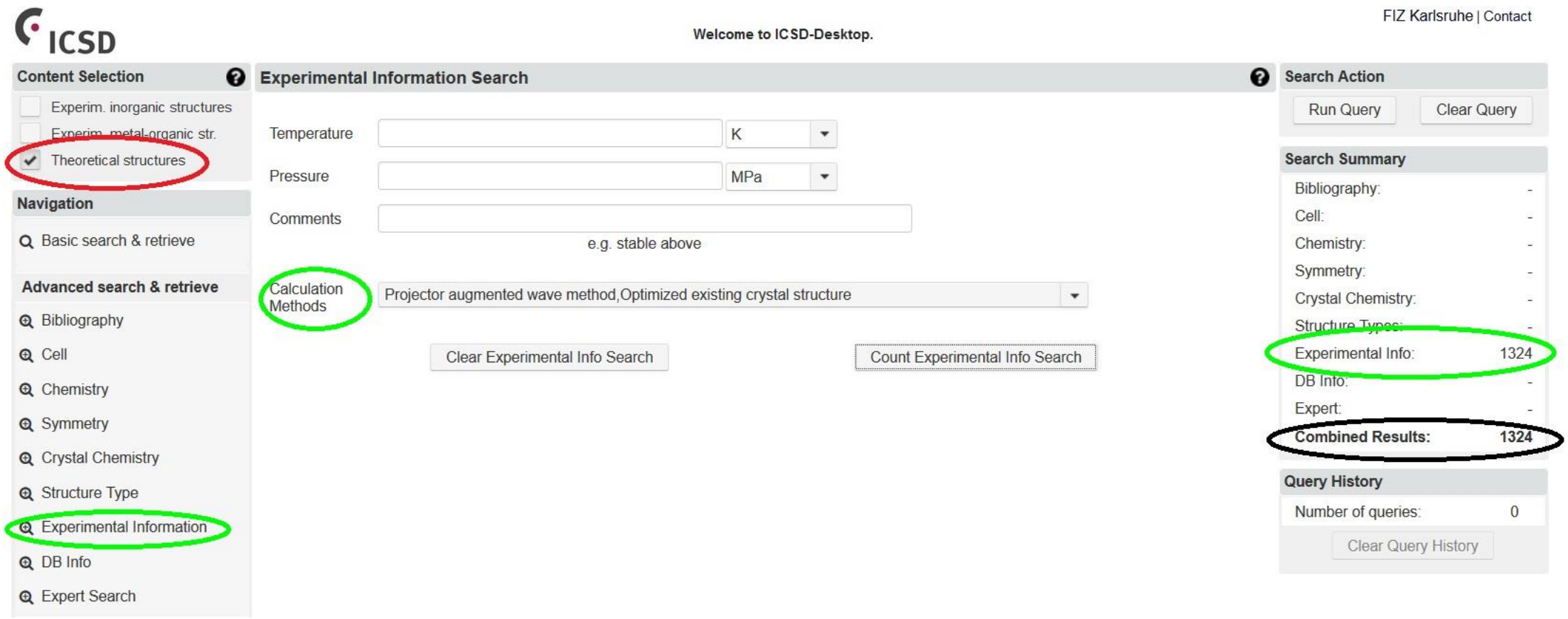
Search for parameters for method development and future calculations



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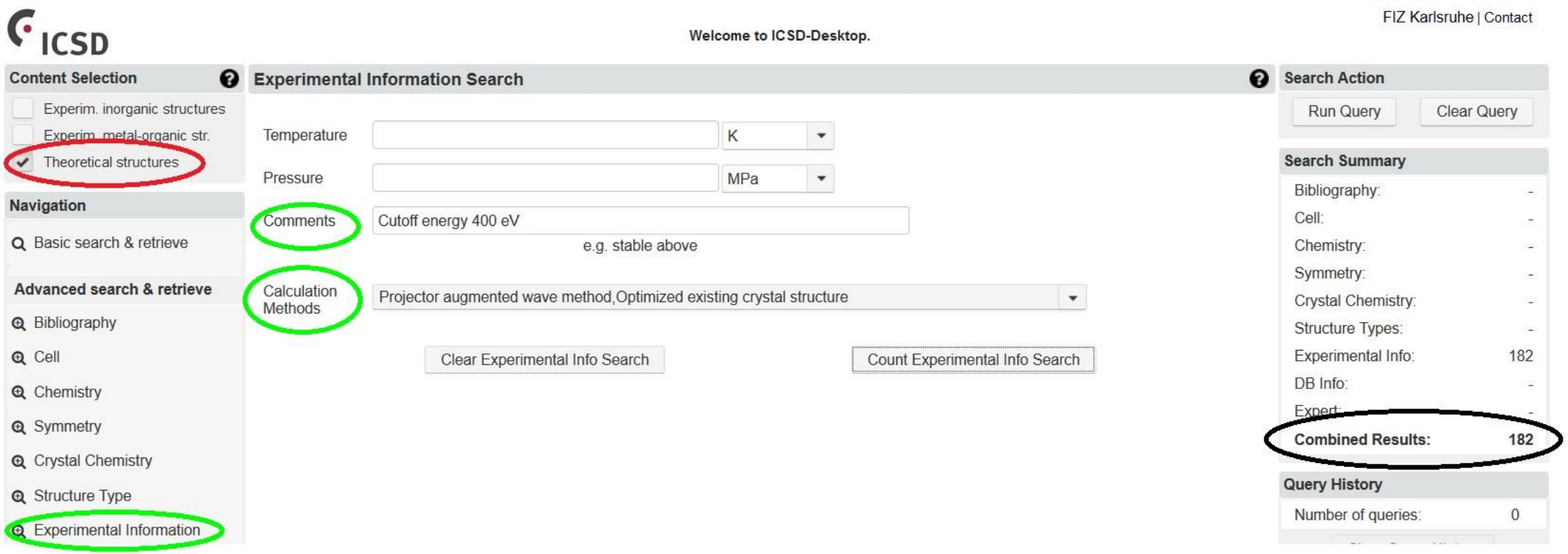
Search for parameters for method development and future calculations



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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

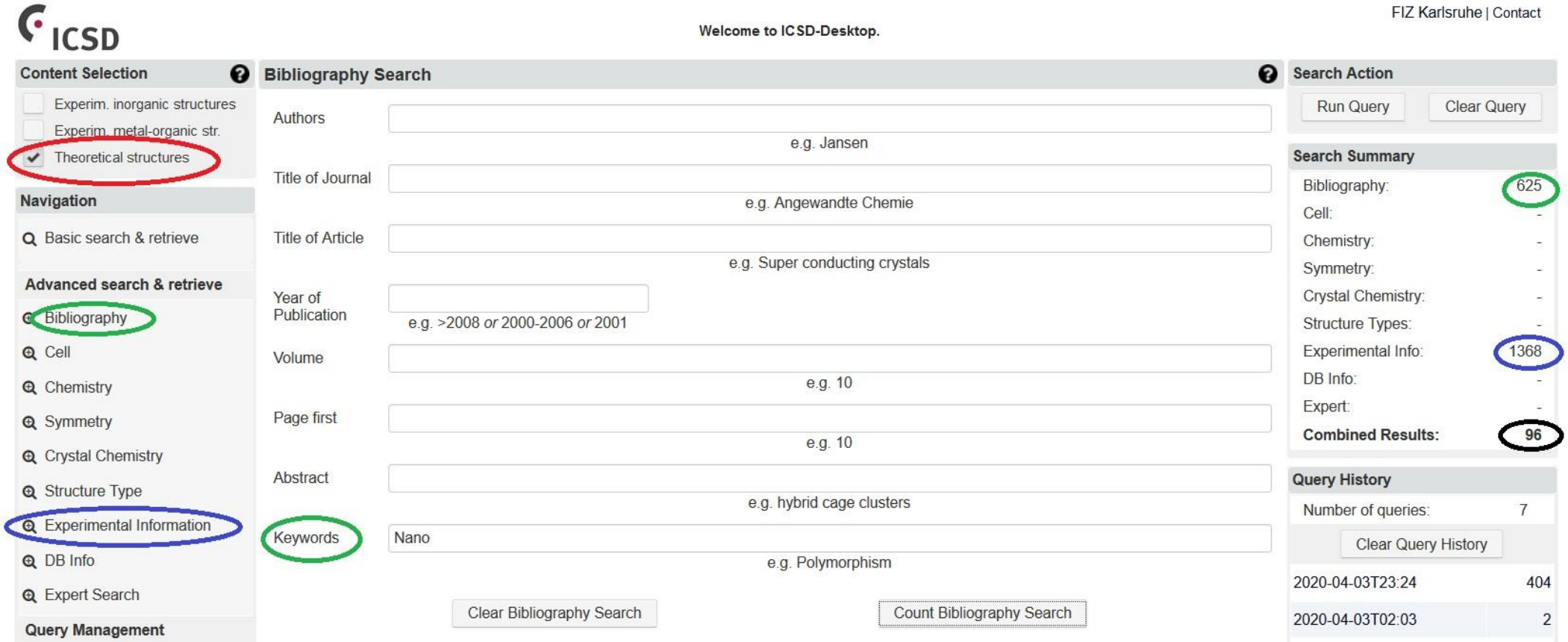

Figure 4a. Example on how to search the ICSD for theoretical nanostructures (ICSD Desktop 2019.2)

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

ICSD

Welcome to ICSD-Desktop.

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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 O2	Rutile-TiO2	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	Ni3 Sn	Heusler-AlCu2Mn	Modelling of phase diagrar	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemic
671335	F m -3 m	Ni	fcc(ccp)-Cu	Modelling of phase diagrar	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemic
671336	I 41/a m d Z	Ni		Modelling of phase diagrar	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemic
671337	P 63/m m c	Ni3 Sn2	Ni3SnP-Co1.75Ge	Modelling of phase diagrar	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemic
671338	F m -3 m	Sn	fcc(ccp)-Cu	Modelling of phase diagrar	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemic
671339	I 41/a m d Z	Sn		Modelling of phase diagrar	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemic

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

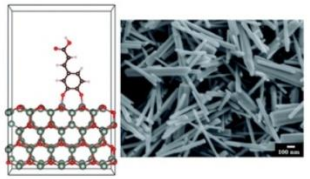
Density functional theory and experimental studies of caffeic acid adsorption on zinc oxide and titanium dioxide nanoparticles

Check for updates

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 TiO_2. 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 TiO_2. 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 electrosteric 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 TiO_2 nanorods and the EPD of TiO_2 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

ICSD

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Detailed View — Entry 1 of 1

Back to Query | Back to List | 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

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How to search ICSD using keywords

LOGIN TO ICSD

ICSD
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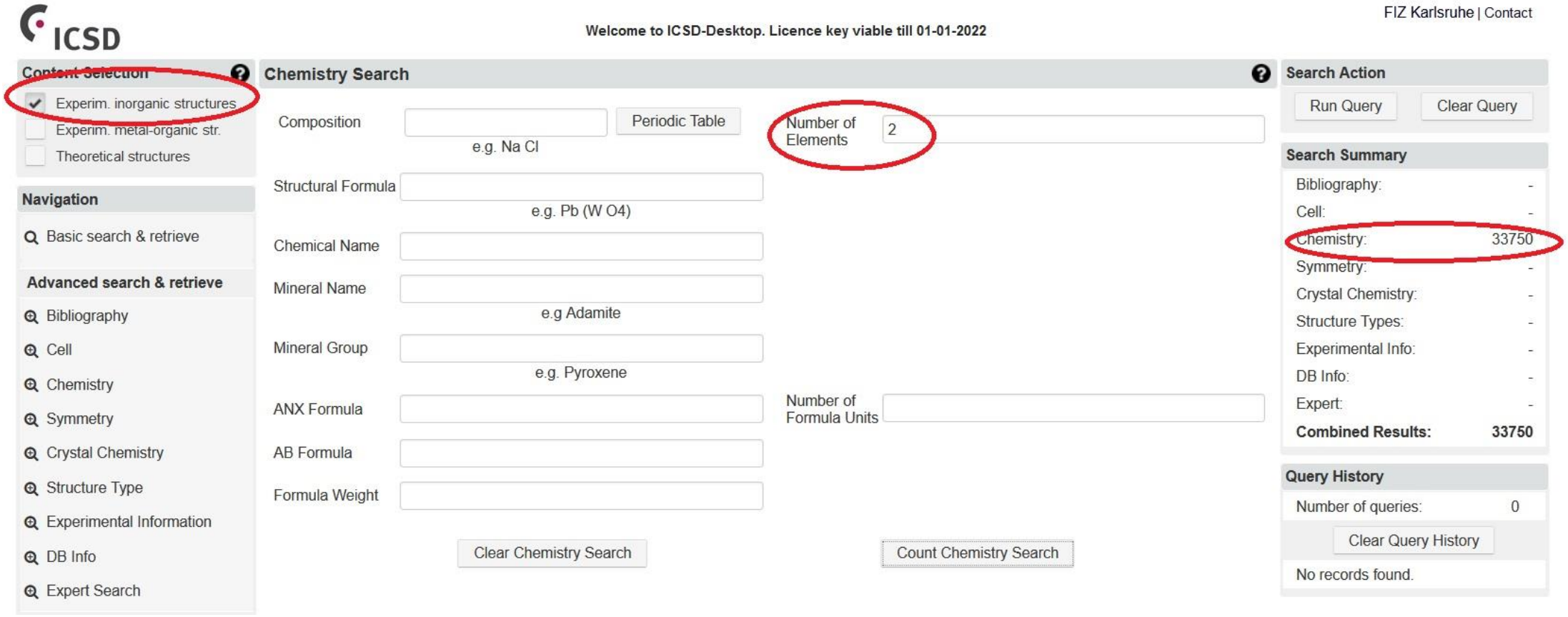
ABOUT ICSD PRODUCTS HOW TO USE SUPPORT CRYSTAL STRUCTURE DEPOT

Using keywords to perform very specific searches in ICSD

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



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

ICSD

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Content Selection

- [x] Experim. inorganic structures
- [ ] Experim. metal-organic str.
- [x] Theoretical structures

Navigation

- Basic search & retrieve

Advanced search & retrieve

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

Chemistry Search

Composition: e.g. Na Cl — Periodic Table

Number of Elements: 2

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

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

ICSD

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Content Selection

- [x] Experim. inorganic structures
- [ ] Experim. metal-organic str.
- [x] 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

Structure Type Search

Pre Defined Structure Types

Structure Type

e.g. Mg2SiO4

[ ] Search in predefined structure types

Structure Type Descriptors

ax

SpaceGrp	Wyck	Pearson	ANX
A112/m	a	aP16	AX
Aba2	a10	aP2	
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

Activate Windows

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

ICSD

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Content Selection

- [x] Experim. inorganic structures
- [ ] Experim. metal-organic str.
- [x] 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

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
- [x] Prototype Structure Type
- [ ] Structure Type

Clear Check Boxes

Clear Crystal Search

Count Crystal Search

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

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Results: List View

# of Hits: 140

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	Reference
59	P 63/m m c	Ga S	InSe(beta)#GaS	Refinement of the 2h (GaS	Kuhn, A.; Chevy, A.; Cheva	Acta Crystallographica, Se
109	P -1	Te I	TeI	Zur Kenntnis der Subhalog	Kniep, R.; Mootz, D.; Rabe	Zeitschrift fuer Anorganisch
1558	C 1 2/m 1	Bi I	BiI(mS32)	Wismutmonojodid Bi J, ein	von Schnering, H.G.; von E	Zeitschrift fuer Anorganisch
1559	C 1 2/m 1	Bi I	BiI(mS16)	Wismutmonojodid Bi J, ein	von Schnering, H.G.; von E	Zeitschrift fuer Anorganisch
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 tetrasul	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 Anorganisch
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

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

CrystEngComm

ROYAL SOCIETY OF CHEMISTRY

PAPER

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View Journal

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Cite this: DOI: 10.1039/c7ce01039g

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

J. Zagorac, *[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

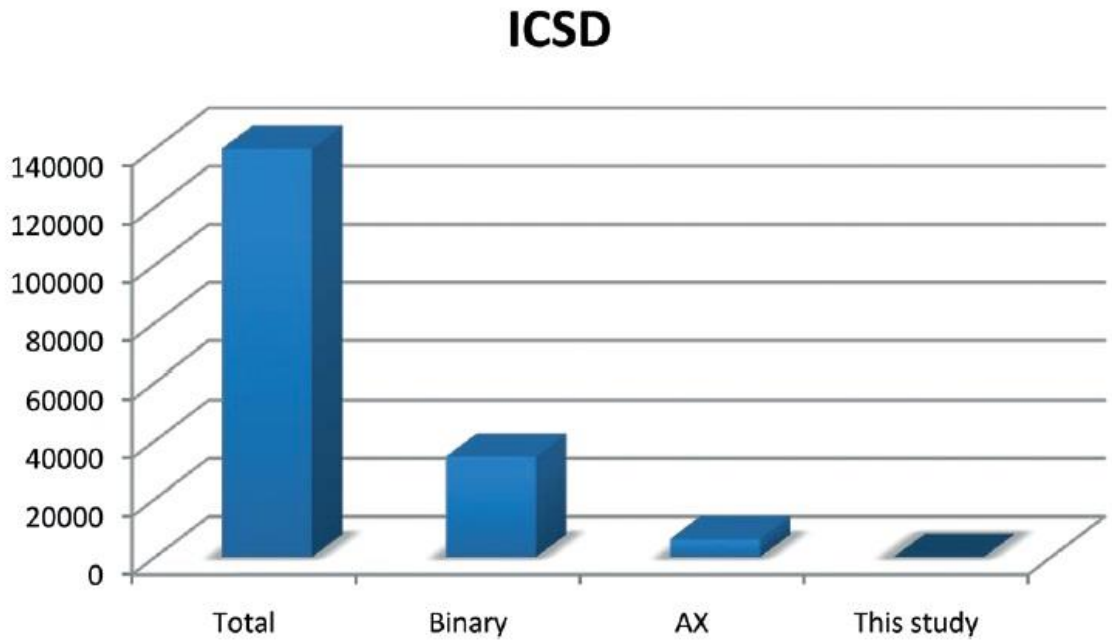

Fig. 2 Statistical analysis of the data mining *ab initio* approach. The figure depicts drastic reduction of possible structure candidates from this study to the total amount of structures listed in the ICSD database, saving time and computational cost.

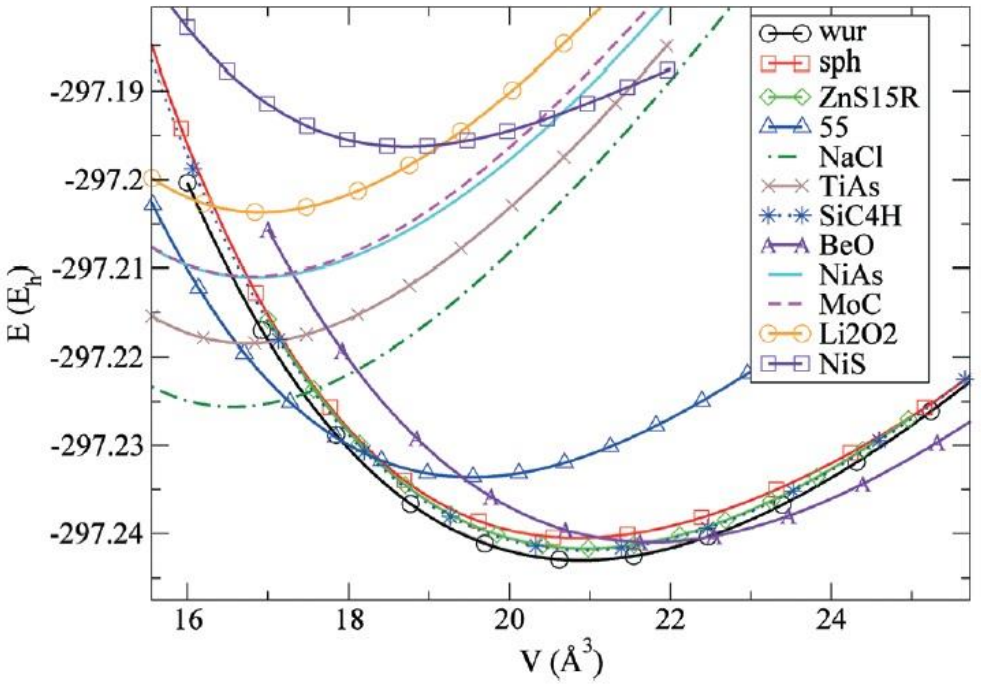

Fig. 3 Calculated $E(V)$ curves for the optimized AlN structure types obtained using the B3LYP functional. Energies per formula unit are given in hartrees (E_h).

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 B_6O

J Zagorac[1,2], D Jovanović[1,3], T Volkov-Husović[4], B Matović[1,2] and D Zagorac[1,2]

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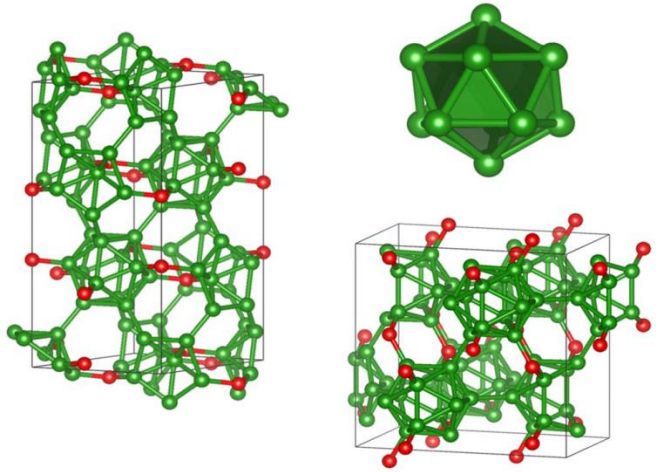
Modelling and Simulation in Materials Science and Engineering, Volume 28, Number 3

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

Springer Link

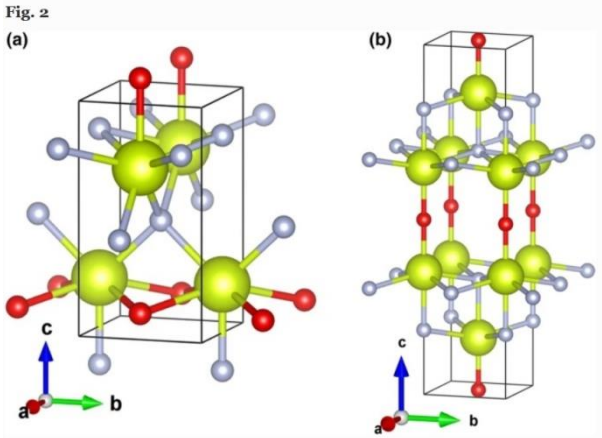


Open Access | Published: 06 July 2020

Predicting Feasible Modifications of Ce_2ON_2 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



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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: crysdata@fiz-karlsruhe.de

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