Content

ICSD Web Help

In order to get help to specific topics, please select one of the following points:

- General Information on searching in ICSD
- Basic Search and Retrieve
- Advanced Search and Retrieve
- Query Management
- Output Management
- Quality Filtering

Information about each input field will be displayed as a description together with some examples for the Basic Search and Advanced Search options. The help for Query Management explains the features used to handle previously performed queries and also offers a mask for more complex searches, i.e. combining queries using logical operators. The output management deals with viewing as well as exporting the results. And, finally, the quality filtering provides a post-query filtering system to refine the results by several criteria.

General information on searching in ICSD

Search fields in ICSD accept either numerical values or text. This is specified in the help for each search field. In addition to those two types there are also some dropdown boxes for specific definitions as well as some checkboxes to select certain properties.

In general, the different fields are combined by logical AND. Checkboxes are often grouped according to certain topics and all checkboxes within such a group are combined by logical OR. Groups are clearly marked by a frame.

More sophisticated queries can be easily created using the Create Combined Queries mask.

Numerical fields

Numerical fields usually accept single values (e.g. 42) or ranges (e.g. 2000-2009, ‹5, ‹=66, ›2.45, ›=1.33). Some fields (e.g. Tolerances) only accept a single value.

In numerical fields usually only one entry is allowed. The only exception is the field Cell Parameters in the Basic Search which accepts up to 6 values according to the 6 parameters describing the unit cell.

Values might either be integer or floating point numbers. It is possible to enter either type in any field and it will be converted (so the year 2012.5 will be handled as 2012) internally.

Text fields

Entries in text fields may contain wildcards. Wildcards are not used implicitly; they have to be placed by the user. The retrieval interface accepts the following two wildcards:

Wildcard	Function	Example	
*	Replace any number of characters	Sulf*	finds Sulfur, Sulfate, Sulfamic, …
#	Replace either 0 or 1 character	Sul##ur	finds Sulfur and Sulphur

There are some special text fields that do not accept wildcards. Those fields are currently: Composition, Atom A and Atom B in the Interatomic Distances and Minimum Search definition.

In text fields where several entries can be defined (e.g. Title of Article) the given texts are searched for in any order. If the search order matters, the entries can be put in quotes (e.g. “magnetic structure” will not find articles containing “… magnetic and electronic structure …”). Wildcards cannot be used within quotes.

The search interface

The ICSD interface is divided into 6 parts (Fig. 1):

(1) Header,
(2) Content Selection,
(3) Navigation,
(4) Main interface (search masks),
(5) Search Action field,
(6) Search Summary field and
(7) Query History field.

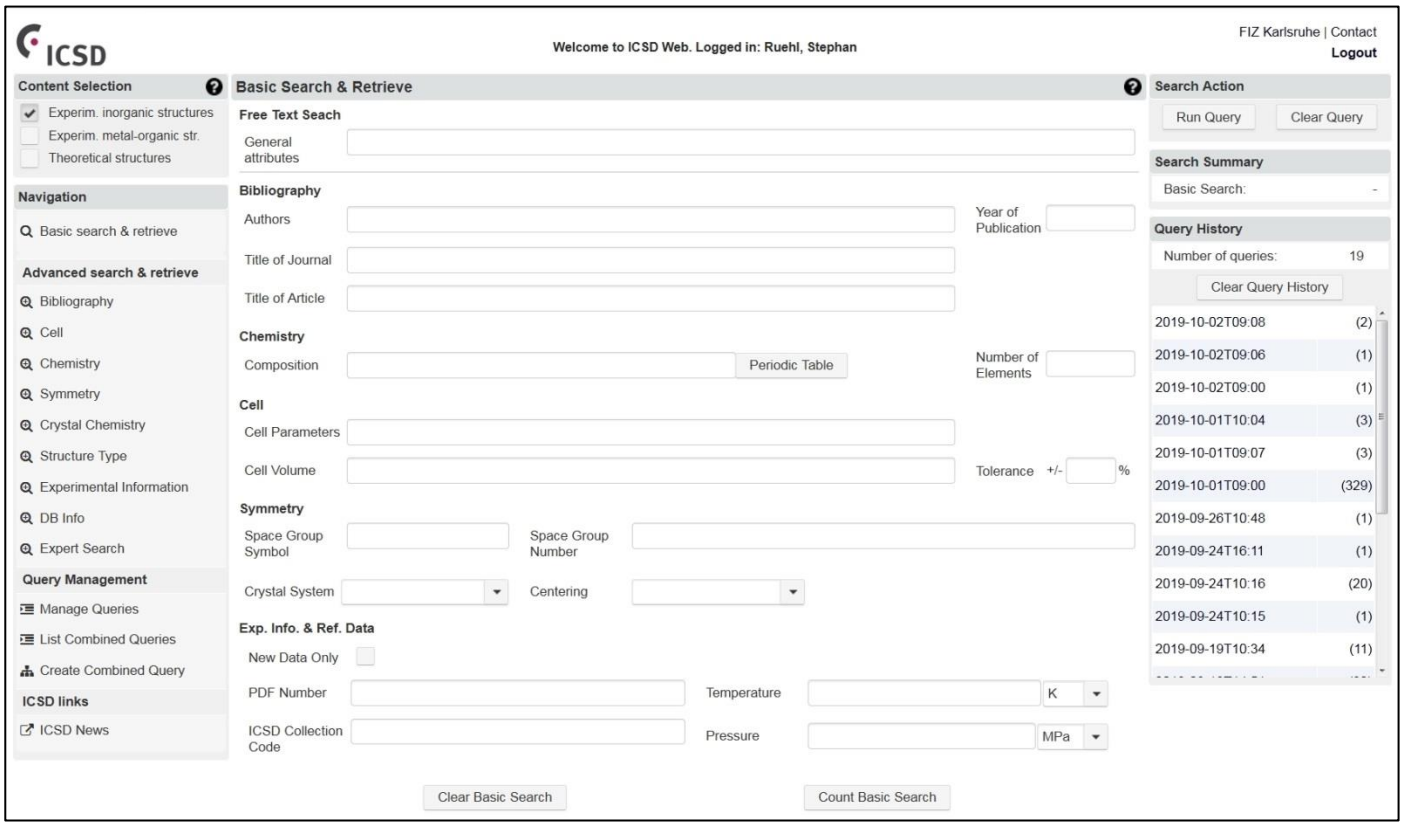


Figure 1: ICSD main screen.

The header shows a welcome message. On the right side you have the option to logout. This will close the current session. Please use this option instead of just closing the tab or the browser, because open sessions may prevent you from logging in again at a later time until the open session gets closed automatically by the server.

In the Content Selection you can define which kind of entries should be used in the queries. At the moment you can choose between:

- Experimental inorganic structures
- Experimental metal-organic structures
- Theoretical structures

The default setting is "Experimental inorganic structures". This setting incorporates only experimentally determined crystal structures.

The Navigation allows you to jump back to the "Basic Search" form, to access specialized pages for performing advanced searches, and to manage your queries.

The main interface is the central working place for the ICSD. Here you can enter and refine searches.

The Search Action field allows you to run and clear your current query.

In the Search Summary field preliminary numbers of results are shown when the Count button on the search masks is used.

The Query History field contains up to the last 30 performed searches and allows you to access them quickly and conveniently. Clicking on the descriptive text (per default the date and time the query was generated) will fill in the search masks with the stored information for this query. You can then modify the query before you run it. Clicking on the number on the right hand side will directly run the stored query and leads you to the results page (List View).

Performing searches

Searches are easily performed by entering specific criteria (details of search fields will be discussed in their context) into the corresponding search fields. In order to check if the set of results will have an easy to handle size, click the button "Count [...] Search". The Search Summary field will then be updated to show the number of results of the current search, without actually executing the search. This is a necessary procedure, because only result sets with no more than 10,000 hits will be displayed. By showing the number of potential candidates you will have the opportunity to narrow down your search. Figure 2 shows an example of a search resulting in more than 10,000 hits.

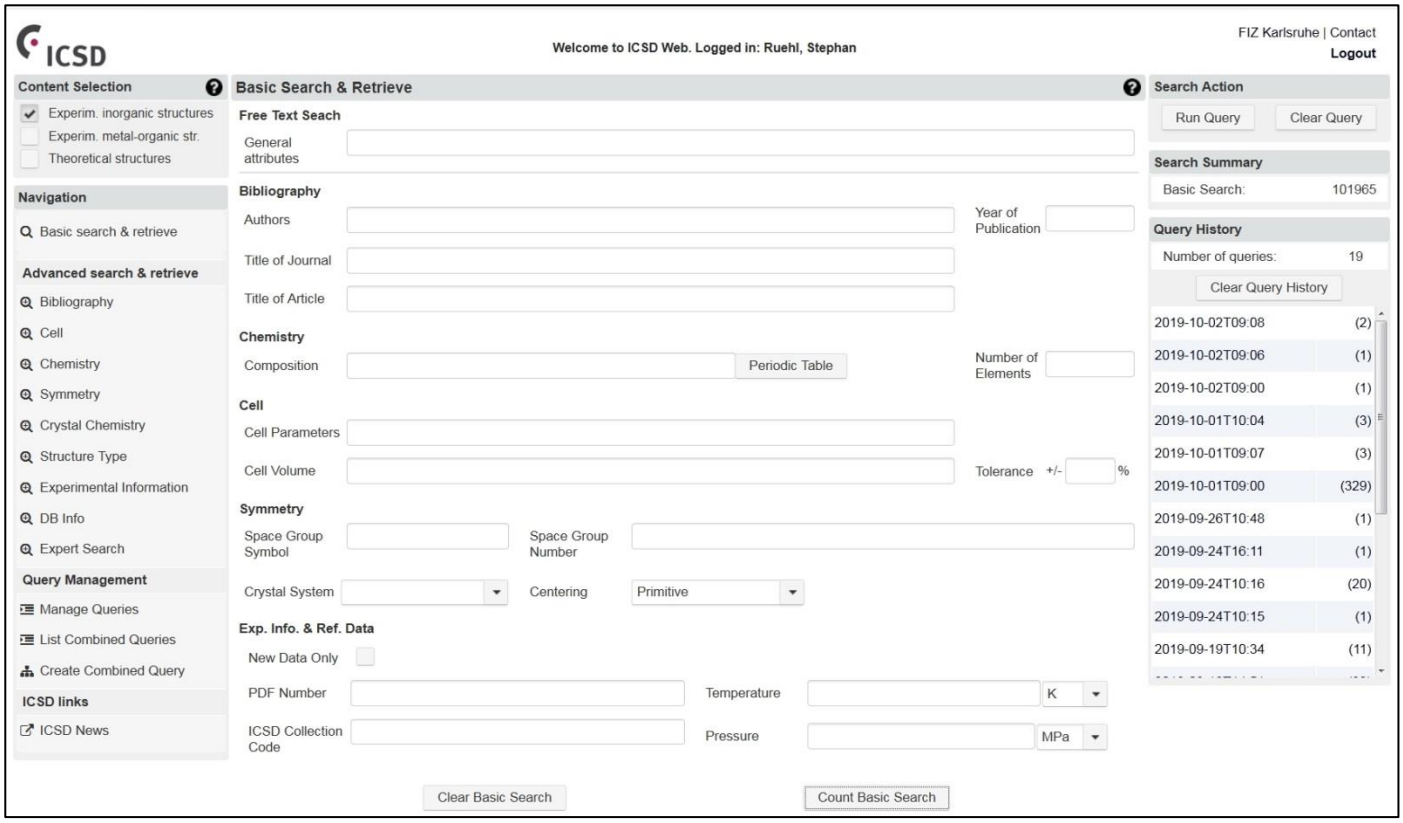


Figure 2: There are more than 10,000 records with P centering in ICSD.

Clicking “Run Query” will then produce a message explaining that there are more hits than can be processed (Fig. 3).

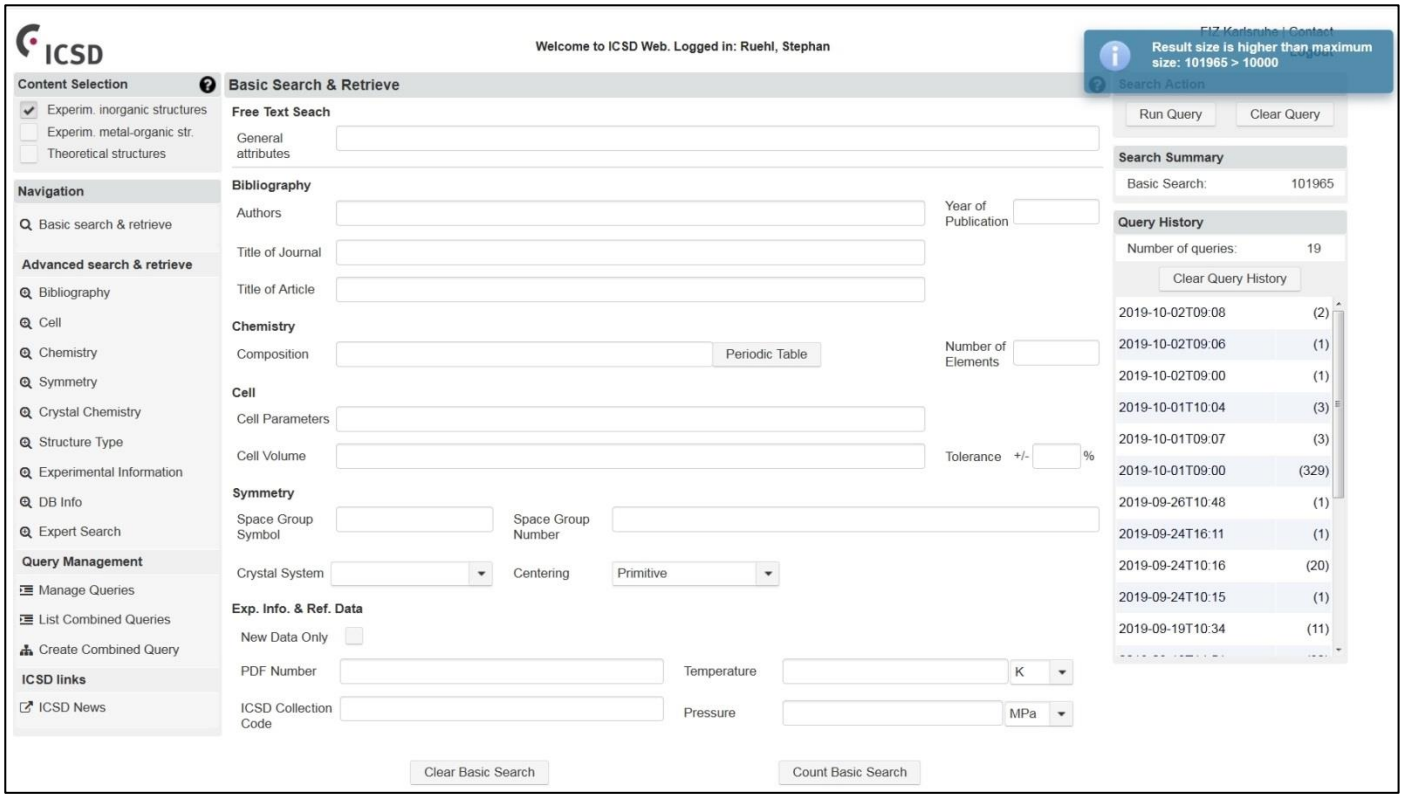


Figure 3: Message when the search results in too many hits.

Basic Search and Retrieve

The Basic Search mask highlights the most often used search fields from most of the Advanced Search masks. For most searches this will be the easiest way to get all relevant parameters defined on one single mask. The only search that is only found on this mask is the Free Text search.

Free text Search

The Free Text search offers a text search in all text fields in ICSD – the user then does not need to know in which field the information that interests the user can be found. For obvious cases like an author or a journal this may not be necessary, but in other cases it may not be known in advance where some specific information can be found – then this search field will be a good starting point.

Bibliography

Search Field	# of entries	Format	Type	Example
Authors	Unlimited	Single entry multiple entries #, * “ “	Text	Jansen Fink Bolte M##ller Ander*
Title of Journal	Unlimited	Single entry multiple entries #, * “ “	Text	Science Angewandte Chemie Crystallogr*
Title of Article	Unlimited	Single entry multiple entries #, * “ ”	Text	reactivity magnetic structure sul##ate
Year of Publication	1	Single value ‹, ‹=, ›, ›= -	Numeric	1913 ›2008 2000-2006

Chemistry

Search Field	# of entries	Format	Type	Example
Composition	unlimited	Single entry multiple entries no Wildcards	Text	Au Na Cl O
Number of Elements	1	Single value ‹, ‹=, ›, ›=, -	Numeric	3 4-5

Cell

Search Field	Units	# of entries	Format	Type	Example
Cell Parameters	angstrom, degree	6	Single value ‹, ‹=, ›, ›= - *	Numeric	5 5 5 90 90 90 3-4 3-4 * 90 * 90 15.5-16 * * 90 ›=90 90 10 * * * * *
Cell Volume	cubic angstrom	1	Single value ‹, ‹=, ›, ›= -	Numeric	2400 1000-1100 ‹=500
Tolerance[1]	%	1	Single value	Numeric	3

[1] Tolerances apply to Cell Parameters and Cell Volume

Symmetry

Search Field	# of entries	Format	Type	Example
Space Group Symbol	1	Single entry, #, * “ “	Text	P-1 P12#1 Fm*
Space Group Number	1	Single value ‹, ‹=, ›, ›= -	Numeric	14 ›225 83-145
Crystal System	1	-	Dropdown	-
Centering	1	-	Dropdown	-

Experimental Info and Reference Data

Search Field	Units	# of entries	Format	Type	Example
New Data Only	-	-	-	Checkbox	-
PDF Number	-	1	Single entry, #, *	Numeric	01-077-1145 47-1360
Collection Code	-	1	Single value ‹, ‹=, ›, ›= -	Numeric	22333 ‹=100000 600000-699999
Temperature	selectable	1	Single value ‹, ‹=, ›, ›= -	Numeric	100 ‹10 270-310
Pressure	selectable	1	Single value ‹, ‹=, ›, ›= -	Numeric	1.5 ›100000 0.01-

Advanced Search and Retrieve

Bibliographic Search

The Bibliographic Search allows you to look up crystal structure data by publication data (Fig. 1).

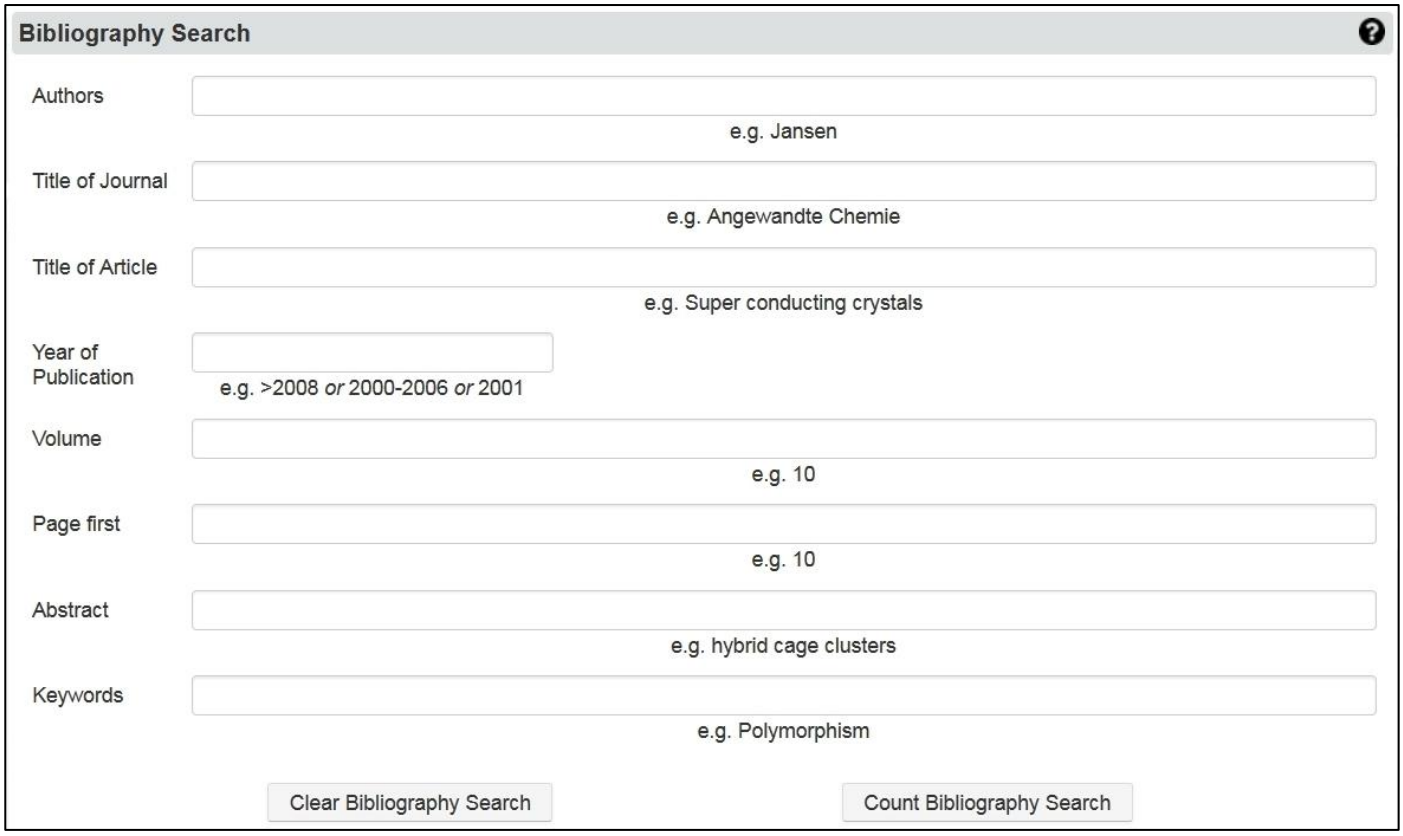


Figure 1: Bibliographic Search screen.

Authors

Search for Authors' names. Several Names or part of names can be given and they are combined by logical AND. Please note, that only the authors for the first reference are stored.

Description	Authors' name for the main (first) reference
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character " " exact term

Examples:

Search term	will find the following entries
jAnSEn	Jansen
“Jansen, M.”	M. Jansen
Jans*	Jans[arbitrary rest], such as Jansen, Janssen, Jansson etc.
Mu#ller	Muller AND Mueller

Title of Journal

Search for the title of a journal. You do not need to enter the complete title. Often a meaningful abbreviation is less error prone than a long journal title. Several parts of the journal can be given and they are combined by logical AND.

Description	Title of journal for the reference
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
nature	Finds all journals with the word “nature” in it, e.g.: Nature or Nature Chemistry
Acta Chim* Hung*	Acta Chimica Academiae Scientiarum Hungaricae
Z* f##r Anorg* Allg*	Zeitschrift fuer Anorganische und Allgemeine Chemie
“materials science“	Will find journals like “Journal of Materials Science” but not “Science and Technology of advanced materials”

Title of Article

Search for the title of an article. You do not have to enter the complete title; again, a meaningful abbreviation is less error prone than the whole title. Several parts of the title can be given and they are combined by logical AND. Titles are only stored for the main reference.

Description	Title of article for the main (first) reference
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
thio sulfate	thio AND sulfate, such as “X-ray study of two nickel(II)-thiosulfate compounds” and “X-ray diffraction study of copper(I)thiourea complexes formed in sulfate-containing acid solutions”
thiosul##ate	Thiosulfate or Thiosulphate, such as “Cadmium thiosulfate dihydrate” or “The crystal structure of anhydrous sodium thiosulphate”
“copper sulfate“	Finds exactly this phrase, such as “The crystal structure of spangolite, a complex copper sulfate sheet mineral”

Year of Publication

Search for the year of publication of an article. Either one year or a range of years can be specified.

Description	Year of publication of an article in the reference
Type	Numerical, integer
Format	Single value or range
# of entries	1
Wildcards	- range; year1 – year2 ‹ range; ‹year ‹= range; ‹=year › range; ›year ›= range; ›=year

Examples:

Search term	will find the following entries
1974	1974
1974-1976	1974 or 1975 or 1976
‹ 1915	1912 or 1913 (first structure published in 1912)
‹=1914	1912 or 1913
›2005	2006 or 2007 or 2008 or 2009 or 2010 …
›=2006	2006 or 2007 or 2008 or 2009 or 2010 …

Volume

Search for the volume of a journal. Either one volume or a range of volumes can be specified.

Description	Volume of the journal in the reference
Type	Numerical, integer
Format	Single value or range
# of entries	1
Wildcards	- range; volume1 – volume2 ‹ range; ‹volume ‹= range; ‹=volume › range; ›volume ›= range; ›=volume

Examples:

Search term	will find the following entries
22	22
10-12	10 or 11 or 12
‹4	1 or 2 or 3
›=67	66 or 67 or 68 or 69 or 70 ...

Page

Search for the first page number of an article. Either one page number or a range of page numbers can be specified.

Description	First page number of an article in the reference
Type	Numerical, integer
Format	Single value or range
# of entries	1
Wildcards	- range; page1 – page2 ‹ range; ‹page ‹= range; ‹=page › range; ›page ›= range; ›=page

Examples:

Search term	will find the following entries
197	197
197-199	197 or 198 or 199
‹65	64 or 63 or 62 or 61 or 60 ...
›=121	121 or 122 or 123 or 124 or 125 ...

Abstract

Search within the abstract (if available).

Description	Abstract of the article
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
Magnetic Proper*	magnetic [...] property (or properties, ...)
Supercond*	Superconductor, superconducting, ...

Keywords

Search for keywords. Please note that these keywords are not the ones given by the authors. We assign keywords mainly for materials properties or additional spectroscopic determinations that were mentioned for the crystal structure.

Description	Keywords for the crystal structure (magnetic properties or spectroscopic methods)
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
ferromanget*	Ferromagnetic, ferromagnetism
Raman	Raman spectroscopy was applied

Cell Search

The Cell Search mask (Fig. 1) allows the user to search for cell parameters and cell volumes in the experimental data and/or in the standardized data. It is also possible to search for reduced cells by either directly giving the cell parameters for the reduced cell or by converting the given cell parameter to the reduced cell. In each case the unit for the cell parameters a, b and c can be set to angstrom, nm or pm using a dropdown box. This unit in cubic form is also used for the cell volume.

In addition, it is possible to search for a calculated density.

Each search field can be given as a single value or a range. The Global Tolerance field allows to apply a percentage variation on top of this.

The search fields are combined by logical AND.

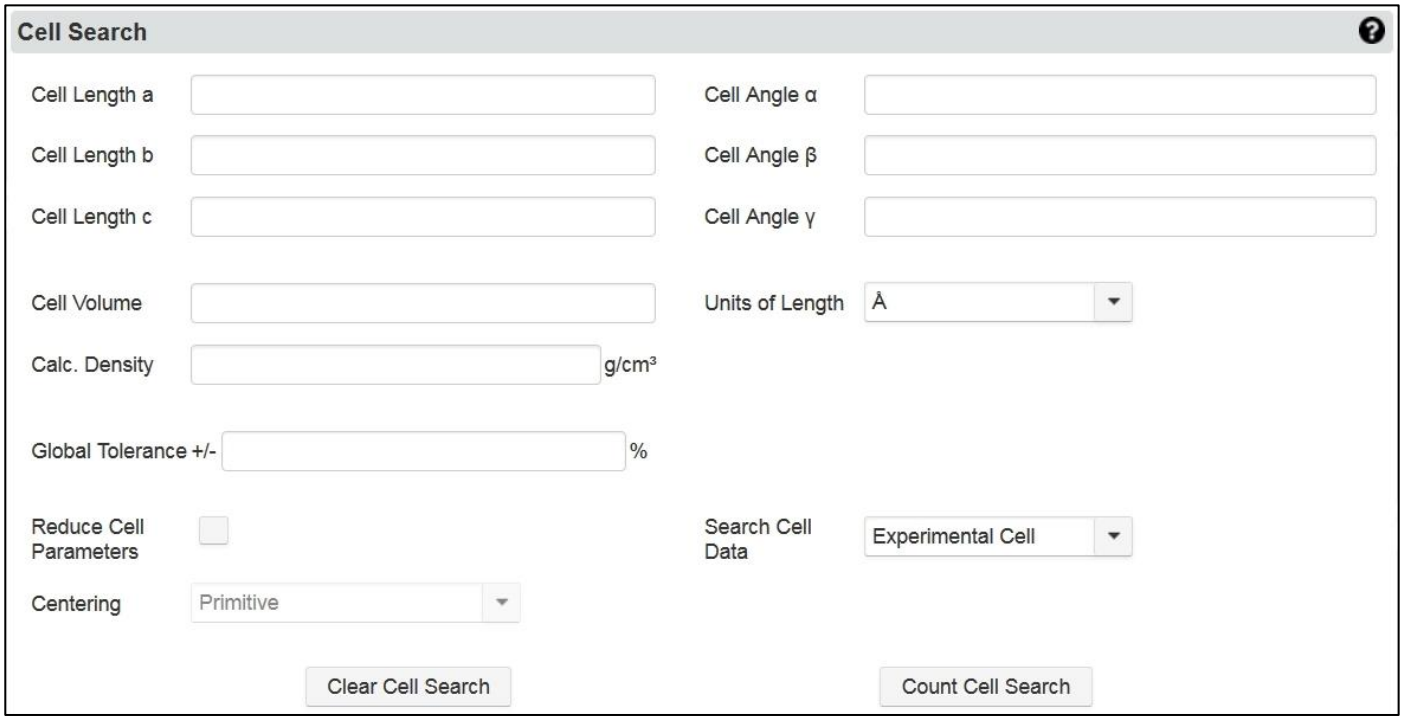


Figure 1: Cell search screen

You can search for reduced cell data in the following ways:

1. Enter the reduced cell parameters in the Cell Length and Cell Angles search fields and select "Reduced Cell" in the dropdown box Search Cell Data.

2. Enter the reduced cell parameters in the Cell Length and Cell Angles search fields and select "All Cell Data" in the dropdown box Search Cell Data. This will also find experimental and standardized cells corresponding to the given cell parameters.

3. Check the checkbox Reduce Cell Parameters. The dropdown box Search Cell Data will be changed to Reduced Cell and greyed out, so it cannot be changed directly anymore. Now you can select a centering by changing the dropdown box Centering. Note that any given entries in the cell length or

cell angle search fields will be reset if the centering is changed. Now you can define the cell parameters of the experimental cell. When you run this query or use the count button, the cell will be reduced on-the-fly and the reduced cell is used for the search. If you want to check the reduced cell before the search, you can take a look at the reduced cell calculated from the experimental cell by using the button Display Reduced Cell Parameter.

Cell Length a, b or c

Search for the cell parameters a, b and/or c. Each parameter can be specified as a single value or as a range. The percentage tolerance from the Global Tolerance field is added to the parameter value. You can define whether the cell length is to be searched in the experimental (published) cell, in the standardized cell, or in the reduced cell. The unit of the cell length is defined by the dropdown box Units of Length as angstrom, nm or pm.

Description	Cell length a or b or c
Type	Numerical, floating point
Format	Single value or range
# of entries	1
Wildcards	- range; cell_length; cell_length1 – cell_length2 ‹ range; ‹ cell_length ‹= range; ‹= cell_length › range; › cell_length ›= range; ›= cell_length

Examples:

Search term	will find the following entries
10	10.0000
11.0-11.5	11.0000 – 11.5000
‹10	0.0000 – 9.9999
›=100	100.0000 – 99999.9999 (currently the largest cell length in ICSD is more than 500 angstrom)

Cell Angle α, β or γ

Search for the cell parameters α, β and/or γ. Each parameter can be specified as a single value or as a range. The percentage tolerance from the Global Tolerance field is added to the parameter value. You can define whether the cell angle is to be searched in the experimental (published) cell, in the standardized cell, or in the reduced cell. Cell angles are given in degree.

Description	Cell angle α or β or γ
Type	Numerical, floating point
Format	Single value or range
# of entries	1
Wildcards	- range; cell_angle; cell_angle1 – cell_angle2 ‹ range; ‹ cell_angle ‹= range; ‹= cell_angle › range; › cell_angle ›= range; ›= cell_angle

Examples:

Search term	will find the following entries
90	90.0000
110.0-115.0	110.0000 – 115.0000
‹100	0.0000 – 99.9999
›=100	100.0000 – 179.9999

Cell Volume

Search for the cell volume. The cell volume can be specified as a single value or as a range. The percentage tolerance from the Global Tolerance field is added to the cell volume value. The unit of the cell volume is specified by the dropdown box Units of Length as the cubic form of the given unit.

Description	Cell volume
Type	Numerical, floating point
Format	Single value or range
# of entries	1
Wildcards	- range; cell volume; cell_volume1 – cell_volume2 ‹ range; ‹ cell_volume ‹= range; ‹= cell_volume › range; › cell_volume ›= range; ›= cell_volume

Examples:

Search term	will find the following entries
1000	1000.0000
2000.0-2500.0	2000.0000 – 2500.0000
‹100	0.0000 – 99.9999
›=100	100.0000 – 999999.9999 (largest cell volume in ICSD is over 350,000 $Å^3$)

Calculated Density

Search for the calculated density of the crystal structure. The percentage tolerance from the Global Tolerance field is added to the density value. The calculated density can be specified as a single value or as a range. The unit of the density is g/cm^3.

Description	Calculated density
Type	Numerical, floating point
Format	Single value or range
# of entries	1
Wildcards	- range; calculated density; density1 – density2 ‹ range; ‹ density ‹= range; ‹= density › range; › density ›= range; ›= density

Examples:

Search term	will find the following entries
1	1.0000
2.0-20.0	2.0000 – 20.0000
‹1.0	0.0000 – 0.9999
›=20	20.0000 – 99.9999

Global Tolerance

This does not define a searchable field. This field is used to extend the values specified for the cell parameters (Cell length a, b or c; Cell Angle α, β or γ) and for the Cell Volume and Calculated Density by the given percentage.

Description	This tolerance is applied to the cell parameters, volume and density
Type	Numerical, floating point
Format	Single value
# of entries	1
Wildcards	none

Units of Length

This dropdown box allows to select the unit for the search fields Cell length a, b and c. This unit also applies to the Cell Volume in the corresponding cubic forms.

Description	Units of Length
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Search Cell Data

This dropdown box allows to select which data are used for the cell parameter search. Selectable data sources are: Experimental Data; Standardized Data; Reduced Cell; All Cell Data.

Description	Specify the data used in the query
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Reduce Cell Parameters

This checkbox defines the cell parameters specified in the search fields cell lengths a, b and c and the cell angles α, β or γ as experimental cell parameters that should be transformed to the reduced cell. When selecting this checkbox, the dropdown box Search Cell Data is set to reduced cell and greyed out. In addition, another dropdown box is activated and can be used to define the centering of the cell.

Description	Transforms the specified cell parameters to the reduced cell
Type	Checkbox
Format	-
# of entries	-
Wildcards	-

Centering

This dropdown box allows to select the centering of the cell parameters. This is only used for the transformation of the experimental cell to the reduced cell. This dropdown box becomes accessible only when the Reduce Cell Parameters checkbox is checked.

Description	Centering of the cell
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Display Reduced Cell Parameter

This button transforms the experimental cell parameters specified in the search fields cell lengths a, b and c and cell angles α, β or γ to the reduced cell and displays it. This button becomes accessible only when the Reduce Cell Parameters checkbox is checked (Fig. 2).

Description	Units of Length
Type	Button
Format	-
# of entries	-
Wildcards	-

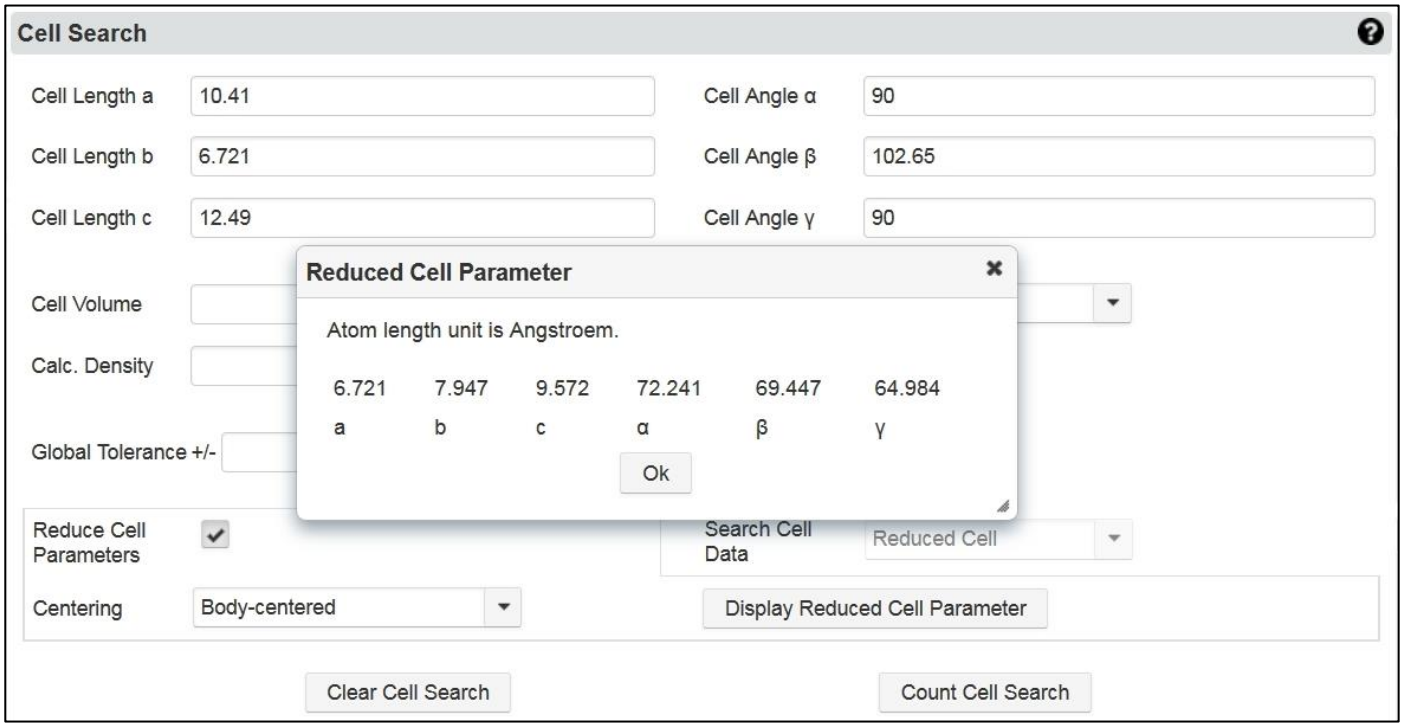


Figure 2: Display the Reduced Cell

Chemistry Search

With the Chemistry Search (Fig. 1) mask you can search for

- Composition
- Structural Formula
- Number of Elements
- Number of Formula Units
- Chemical Name
- Mineral Name
- Mineral Group
- ANX Formula
- AB Formula
- Formula weight

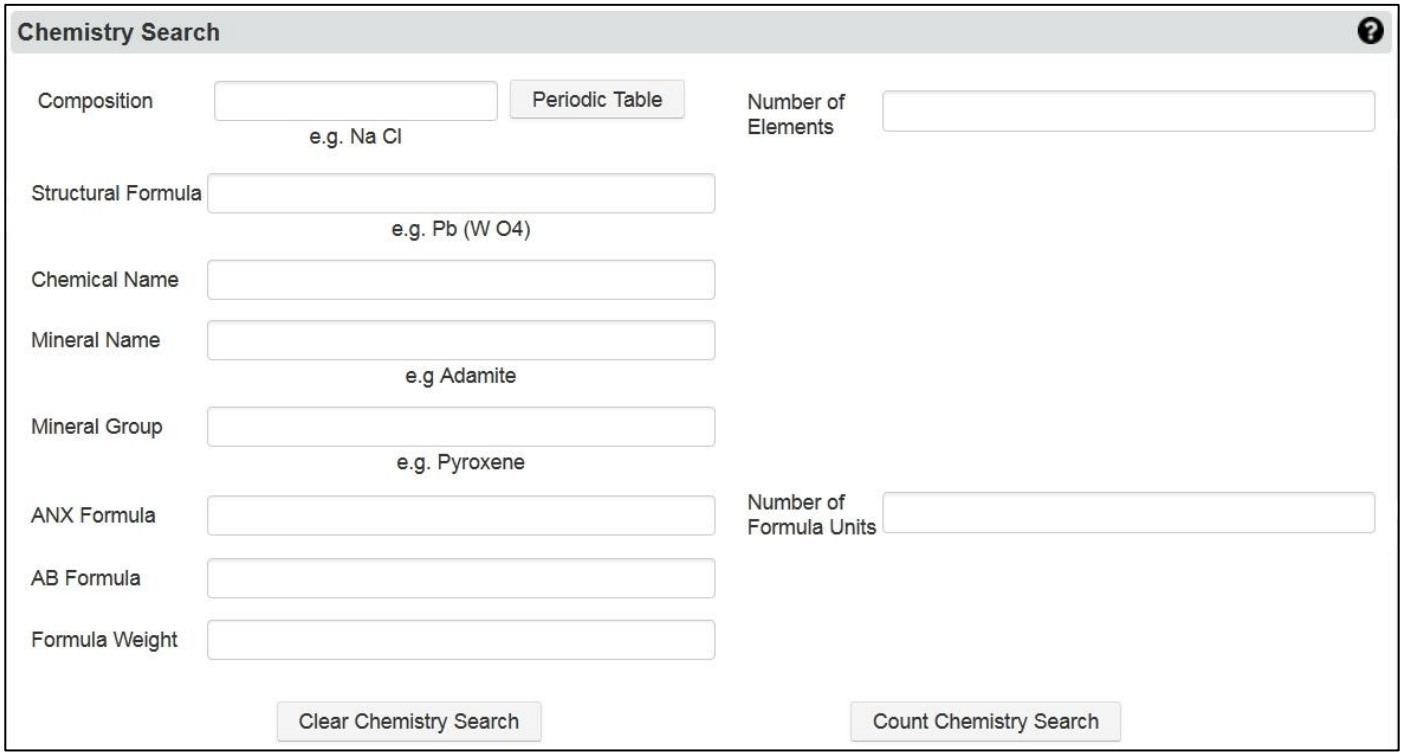


Figure 1: Chemistry Search mask.

Composition

The Composition search field is used to specify the chemical composition of the crystal structure. There are two ways to define the composition: Either enter the elements separated by blanks or select them from the periodic table (Fig. 2), which can be opened in a dialogue using the button “Periodic Table”.

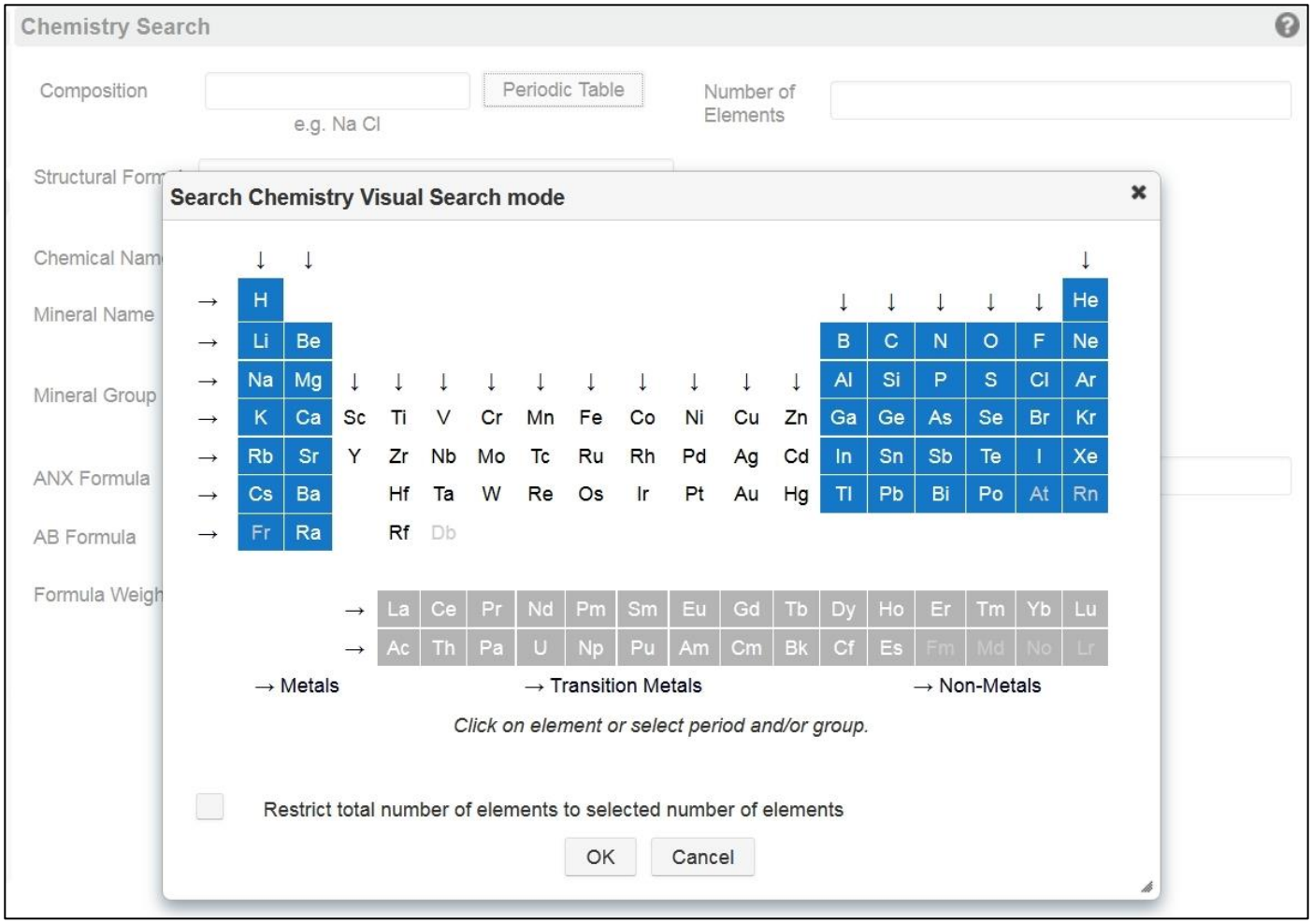


Figure 2: Select the composition directly using the periodic system

The following search terms are allowed:

- Chemical elements, **note**: D for Deuterium and T for Tritium is allowed,
- Groups (in the meaning of "Groups in the Periodic Table of Elements") of elements (see Tab. 1 for nomenclature),
- Periods of elements (see Tab. 2 for nomenclature) and
- Groups, such as metals, transition metals and non-metals (see Tab. 3 for nomenclature, Fig. 3 for information which elements belong to metals and non-metals).

Search terms are combined by logical AND; it is possible to use other boolean operators in the following ways to search for the composition:

- In order to combine certain elements/element groups by OR, put them in parentheses.
- In order to exclude certain elements/element groups (NOT), place a hyphen ("-") in front of the entry.

Additionally, searches can be refined even more by specifying the stoichiometric coefficients (Co. min/max) and/or the oxidation numbers (Ox. min/max) of elements (EL). The colon is used as a separator:

EL:Co.(min):Co.(max):Ox.(min):Ox.(max)

Note that the specified order has to be used. Trailing information can be omitted.

The periodic table dialogue (Fig. 2) allows easy entering of search terms: by clicking on an element symbol additional entry fields will be displayed, where the following modifications can be applied:

- the logical combination can be selected (AND/NOT),
- in the element symbol field more than one entry is possible (additional elements have to be added by hand); all entered symbols will be combined by logical OR,
- the range for stoichiometric coefficients (Co.(min)/Co.(max)) can be entered,
- the range for oxidation numbers (Ox.(min)/Ox.(max)) can be entered.

You can specify the maximum number of elements and the units of coefficients (moles, atom percent or mass percent) by selecting the appropriate entry from the dropdown box.

Checking the box "Restrict total number of elements to selected number of elements" will automatically limit the number of elements to the number of the selected ones.

Table 1: ICSD names for Periodic Table groups

Chemical Group	ICSD name	Conventional name(s)		
1	LIG	Alkali metals	group I A	1st main group
2	BEG	Alkaline earth metals	group II A	2nd main group
3	SCG	Scandium group	group III B	
4	TIG	Titanium group	group IV B	
5	VG	Vanadium group	group V B	
6	CRG	Chrome group	group VI B	
7	MNG	Manganese group	group VII B	
8	FEG	Iron group	group VIII B	
9	COG	Cobalt group	group VIII B	
10	NIG	Nickel group	group VIII B	
11	CUG	Copper group	group I B	
12	ZNG	Zinc group	group II B	
13	BG	Boron group	group III A	3rd main group
14	CG	Carbon group	group IV A	4th main group
15	NG	Nitrogen group	group V A	5th main group
16	OG	Oxygen group	group VI A	6th main group
17	FG	Fluorine group	group VII A	7th main group
18	HEG	Noble gases	group VIII A	8th main group

Table 2: ICSD names for Periods

Chemical Period	ICSD name	
1	1PE	H, D, T, He
2	2PE	Li, Be, B, C, N, O, F, Ne
3	3PE	Na, Mg, Al, Si, P, S, Cl, Ar
4	4PE	K, Ca, Sc, Ti, V, Cr, Mn, Fr, Co, Ni, Cu, Zn, Ga, ..., Br, Kr
5	5PE	Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, ..., I, Xe
6	6PE	Cs, Ba, La, Ce, ..., Yb, Lu, Hf, Ta, ..., At, Rn
7	7PE	Fr, Ra, Ac, Th, ... No, Lr, Rf

Table 3: ICSD names for other chemical groups of elements

Group	ICSD name	
Metals	MET	
Transition metals	TME	not including f-block elements
Non-metals	NME	
Lanthanoids	LAN	including La
Actinoids	ACT	including Ac

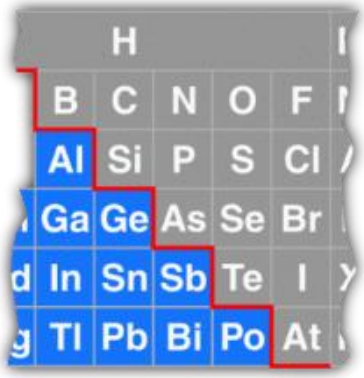


Figure 3: Border (red line) between metals ("MET", blue fields) and non-metals ("NME", grey fields) in ICSD

Description	Composition (including stoichiometric coefficients / oxidation numbers)
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	- excludes the following element/group (NOT) ( ) includes at least one of the elements/groups specified (OR)

Examples:

Composition	# of Elements	Result
Na Cl	2	NaCl
Na Cl	3	e.g. $NaClO_3$, $NaClO_2$, $NaMnCl_3$, $NaAlCl_4$, Na_2ZnCl_4
Na Cl O	3	$NaClO_3$, $NaClO_2$
Cl O	3	e.g. $NaClO_3$, $KClO_3$, $RbClO_3$, $Pb(ClO_3)_2$, $Hg_2(ClO_3)_2$
TME Cl O	3	$Hg_2(ClO_3)_2$, **but not** e.g. $NaClO_3$, $Pb(ClO_3)_2$ etc.
BEG Cl O	3	$Ba(ClO_3)_2$, $Sr(ClO_3)_2$, **but not** e.g. $NaClO_3$, $Pb(ClO_3)_2$, $Hg_2(ClO_3)_2$ etc.
LIG FG O	3	e.g. $RbIO_3$, $NaBrO_3$, $NaClO_4$, Rb_3IO_5, $Cs_2I_4O_{11}$
(Na K) Br	2	NaBr or KBr
-Na -K Br	2	all binary bromides except NaBr and KBr
-Na -K LIG:1:1 FG:1:1	2	all alkali metal halogenides except NaX and KX; will not include e.g. $CsBr_3$ and Cs_2I_8
Cr:::4:4	2	all compounds with an oxidation number of +4 for Cr, such as CrO_2 or Cr_3B_4
Cr:1:1:4:4	2	all compounds with an oxidation number of +4 for Cr and exactly one Chromium, such as CrO_2, but not Cr_3B_4

Number of Elements

Search for the number of different elements in the composition. Either one number or a range of numbers can be specified.

Description	Number of different elements in the composition
Type	Numerical, integer
Format	Single value or range
# of entries	1
Wildcards	- range; #ofelements1 – #ofelements2 ‹ range; ‹#ofelements ‹= range; ‹=#ofelements › range; ›#ofelements ›= range; ›=#ofelements

Examples:

Search term	will find the following entries
2	binary compounds
2-3	binary or ternary compounds
‹3	elements or binary compounds
›=5	compounds with at least 5 different elements in the composition

Structural Formula

This search field offers a more structured formula compared to the pure element listing in the composition field. You can search for typical functional groups like sulfates (S O4) or perchlorates (Cl O4). The charge is not given, only the elements in the correct ratio are specified. Several functional groups are combined by logical AND.

Description	Search for typical chemical groups
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term ( ) exact term

Examples:

Search term	will find the following entries
(S O4)	Sulfates, hydrogen sulfate, … (S is uniquely defined, As is not possible)
S O4	Sulfate, hydrogen sulfate and also arsenate as well as other structures with a S and O4 group somewhere in the formula
S2 O4	e.g. Cd8 (Be Si O4)6 S2

Chemical Name

Search for a compound’s common chemical name or parts of it. Several parts of the chemical name can be given and they are combined by logical AND. Please note that chemical names are not meant to be IUPAC conform. The chemical names are only intended to give a hint on the functional groups and elements found in the crystal structure.

Description	Search for (parts of) the chemical name
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
sul##ate	e.g. Na2SO4, Na2SO4·10H2O, NaHSO4, Na2S2O3, NaMg2Fe5(SO4)7(OH)6(H2O)33
ammonium osmate	e.g. ((CH3)4N)2(Os(NO)FI4), (((C4H9)4N)3(Se8(Re5OsCl6)))((C2H5)2O)2

Mineral Name

Search for the mineral name. Entries are combined by logical AND.

Description	Search for the mineral name
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
Adamite	“Adamite” and “Adamite, cuproan”
Whitlock*	“Whitlockite”, “Whitlockite (heated)”, “Whitlockite, magnesian” and “Whitlockite, manganoan”

Mineral Group

Search for the mineral group. Entries are combined by logical AND.

Description	Search for the mineral group
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
Feldspar	Feldspar
per*	Perovskite and Periclase

ANX Formula

Search for the ANX formula. This formula is invaluable for identifying structural analogues. The ANX formula is generated according to the following rules:

- H is not taken into account, even if coordinates are available.
- The coordinates for all sites of all other atoms must be determined.

- Different atom types on the same position are treated as one single atom type. The relevant atom type is the one with the highest site occupation factor. If the SOFs are equal, the first atom type is the relevant atom type.

  Exception to this rule: if anions and cations occupy the same site they will not be treated as one atom type.

- All sites occupied by the same atom type are combined unless the oxidation state is different:
  $Fe^{2+}(Fe^{3+})_2O_4$ → AB2X4
  $(Fe^{2.6667+})_3O_4$ → A3X4
- 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 the rounded sum is equal to zero all sums are being multiplied by a common factor so that the smallest sum is equal to 1.0, so no element will be omitted.
- 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 and the characters are assigned according to ascending indices: AB2X4, not A2BX4.
- All ANX formulae with more than 4 cation symbols, 3 neutral symbols or 3 anion symbols are deleted. This measure limits the number of different ANX formulae.

Chemical formula	ANX formula
$Mg_3Al_2(SiO_4)_3$	A2B3C3X12
$Ca_3(Al_{1.3325}Fe_{0.6675})Si_3O_{12}$	A2B3C3X12
$(Mg_{2.7}Fe_{0.3})(Al_{1.7}Cr_{0.3})Si_3O_{12}$	A2B3C3X12

Description	Search for the ANX formula	
Type	Text	
Format	Single entry	
# of entries	1	
Wildcards	*	any number of characters
	#	0 or 1 character
	“ “	exact term

Examples:

Search term	will find the following entries
N#	N, NO, NX
A*YZ	A2XYZ, AB2XYZ, ABXYZ and AXYZ
A*C*	all formulae that have at least AnnBnnCnn in it. AX or ABX are not included.

AB Formula

Search for the AB formula. In general, for generating the AB formula the same rules as those for generating the ANX formula apply. In contrast to the ANX formula, H is taken into account and there are no predefined letters for cations, anions or neutral atom types.

Chemical formula	AB formula
Li_2SO_4	AB2C4
H_2O	AB2
$K_2(O_2(SO_3)_2)$	ABC4
$K_2(S_2O_7)$	A2B2C7
$Na_6O(SO_4)_2$	A2B6C9

Description	Search for the AB formula	
Type	Text	
Format	Single entry	
# of entries	1	
Wildcards	*	any number of characters
	#	0 or 1 character
	" "	exact term

Examples:

Search term	will find the following entries
ABC	ABC, but not e.g. ABC2
A#	A, AB
A*D	A0.33BCD, A0.47BCD

Number of Formula Units

Search for the number of formula units per unit cell. Either one number or a range of numbers can be specified.

Description	Number of formula units per unit cell	
Type	Numerical, integer	
Format	Single value or range	
# of entries	1	
Wildcards	-	range; #offormulaunits1 – #offormulaunits2
	‹	range; ‹#offormulaunits
	‹=	range; ‹=#offormulaunits
	›	range; ›#offormulaunits
	›=	range; ›=#offormulaunits

Examples:

Search term	will find the following entries
2-3	Compounds with two or three formula unit per cell
‹2	only compounds with exactly one formula unit per cell
›=1	all records in the database

Formula Weight

Search for the formula weight of the asymmetric unit. Either one number or a range of numbers can be specified.

Description	Formula Weight of the asymmetric unit
Type	Numerical, integer
Format	Single value or range
# of entries	1
Wildcards	- range; weight1 – weight ‹ range; ‹ weight ‹= range; ‹= weight › range; ›weight ›= range; ›=weight

Examples:

Search term	will find the following entries
100-101	Compounds with a formula weight between 100 and 101
›=1.0	All records in ICSD

Symmetry Search

The Symmetry Search (Fig. 1) enables you to look up the following information:

- Space Group
- Wyckoff Sequence
- Centering
- Crystal Class
- Pearson Symbol
- Crystal System
- Laue Class
- Special symmetry (polar axis, inversion center)

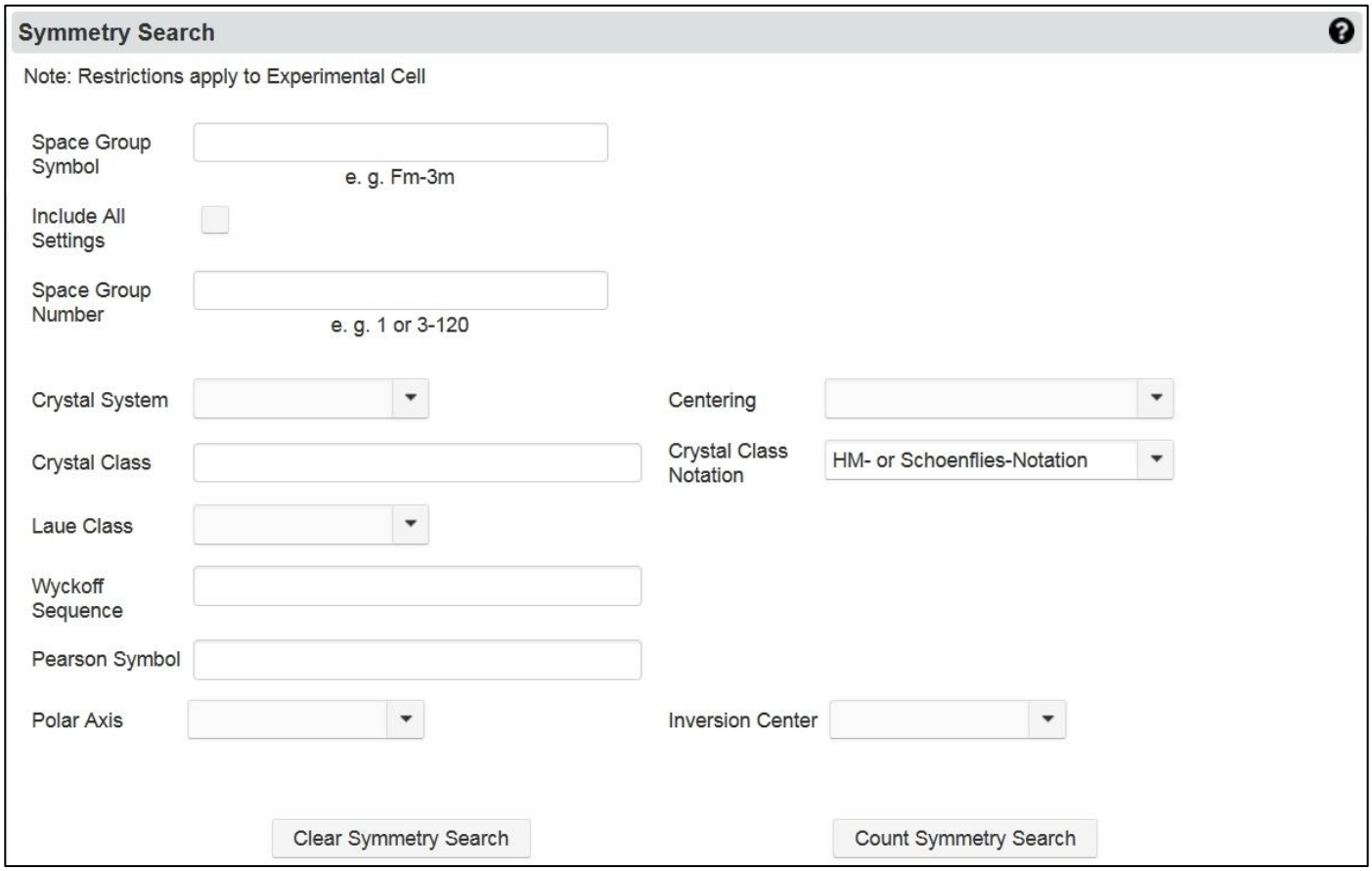


Figure 1: Symmetry Search mask

Please note that all restrictions made on this search mask apply to experimental cells only.

Space Group Symbol

Space group symbols are entered in Hermann–Mauguin (H–M) notation. The symbol for inversion ("bar") must be given as a minus sign ("-") in front of the corresponding axis. Blanks in the notation are ignored. Please note that only the given setting is searched for. If all possible settings for a given space group should be included, the checkbox "Include All Settings" must be checked.

Description	Search for the space group symbol
Type	Text
Format	Single entry
# of entries	1
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
p-1	Space group number 2
„P – 1“	Space group number 2
fm-*	Space groups: Fm-3, Fm-3c, Fm-3m
p 1 2 # 1	Space groups: P121 and P1211

Include All Settings

This checkbox mainly affects the search field “Space Group Symbol”. When checked, not only the specified space group symbol is searched for but all settings of the corresponding space group. In addition, a new field will be visible showing all space group settings as well as the space group number. In combination with a space group number, this checkbox displays the alternative settings of the given space group number.

Description	Includes all alternative settings for the specified space group
Type	Checkbox
Format	-
# of entries	-
Wildcards	-

Space Group Number

Space group numbers can be searched for in this field. Searching for a space group number automatically includes all possible settings for the space group. This means that, the checkbox “Include All Settings” does not have any effect with this search field apart from displaying all different settings in the database for the given space group number.

Description	Search for the space group number
Type	Numerical, integer
Format	Single value or range
# of entries	1
Wildcards	- range; spacegroupnumber1 – spacegroupnumber 2 ‹ range; ‹spacegroupnumber ‹= range; ‹=spacegroupnumber › range; ›spacegroupnumber ›= range; ›=spacegroupnumber

Examples:

Search term	will find the following entries
3	Space groups: P121 and P112
1-2	Space groups: B1, C1, F1, I1, P1 and A-1, B-1, C-1, F-1, I-1, P-1
›=229	Space groups: Im-3m and Ia-3d

Crystal System

With this drop-down-box the crystal system can be defined. The box allows the selection of any of the 7 crystal systems and an undefined (empty) selection.

Description	Crystal system
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Centering

With this drop-down-box the centering can be defined. The box allows the selection of any of the 7 centerings and an undefined (empty) selection.

Description	Centering
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Crystal Class

This search field allows searching for the crystal class. Depending on the setting of the dropdown box “Crystal Class Notation” the specified search term can follow either the Hermann–Mauguin, Schönflies notation, or both notations.

Description	Search for the crystal class
Type	Text
Format	Single entry
# of entries	1
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
Td	Td (-43m in H-M notation)
4##	4, -4, 4/m, 422, 432, 4mm (H-M notation)
“m-3m”	m-3m in H-M notation or Oh in Schoenflies notation

Crystal Class Notation

With this drop-down-box the notation used for the crystal class can be defined. The box allows the selection of either Herman-Mauguin (H-M) notation, Schoenflies (Schoen) notation or both. Per default, both notations are possible.

Description	Notation for the crystal class
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Laue Class

With this drop-down-box the Laue class can be defined. The box allows the selection of any of the 11 Laue class and an undefined (empty) selection.

Description	Search for the Laue class
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Wyckoff Sequence

The Wyckoff Sequence is a descending sequence of Wyckoff symbols (usually lower letters). The Wyckoff symbols are separated by blanks. The sequence can be specified in any order, because each Wyckoff symbol is treated individually. Apart from Pmmm all space groups need less than 26 Wyckoff letters, so the International Tables use for the 27th Wyckoff position an "α", which cannot be used due to technical reasons. Thus, the ICSD uses an "A" (capital letter) instead.

Description	Search for Wyckoff sequence	
Type	Text	
Format	Single entry or multiple entries	
# of entries	Unlimited	
Wildcards	*	any number of characters
	#	0 or 1 character
	“ “	exact term

Examples:

Search term	will find the following entries
a	all sequences with Wyckoff symbol a, but not with e.g. a2 or a3 e.g.: “c12 b8 a”, “d12 c a” or “A2 z y t s r o k j2 f a”
c# d*	all sequences with Wyckoff symbols c or c1 – c9 and any d, but not e.g. c12 e.g.: “d c a3”, “d25 c b a5” or “o9 n8 m8 l f e d c”
"f2 e d b"	all sequences with exactly this phrase as part of the Wyckoff sequence e.g.: “f2 e d b”, “f2 e d b a” or “g3 f2 e d b a”

Pearson Symbol

The Pearson Symbol consists of a single letter for the crystal class, followed by the Bravais lattice type symbol, followed by the number of atoms in the unit cell.

Table 1: Crystal class letters and Bravais lattice types

Crystal class	Abbreviation	Bravais lattice	Abbreviation
triclinic (anorthic)	a	primitive	P
monoclinic	m	side-centered (A, B, or C)	S
orthorhombic	o	face-centered	F
tetragonal	t	body-centered	I
cubic	c	rhombohedral	R
hexagonal	h		

Description	Search for the Pearson symbol
Type	Text
Format	Single entry
# of entries	1
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
oF100	all orthorhombic, face-centered structures with 100 atoms in the unit cell
mS*	all monoclinic, side-centered structures with any number of atoms in the unit cell
cP##	all cubic, primitive structures with up to 99 atoms in the unit cell

Inversion Center

With this drop-down-box you can define whether the space group contains an inversion center or not. The default setting is undefined.

Description	Inclusion/Exclusion of an inversion center
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Polar Axis

With this drop-down-box you can define whether the space group contains a polar axis or not. The default setting is undefined.

Description	Inclusion/Exclusion of an inversion center
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Crystal Chemistry Search

With the Crystal Chemistry Search (Fig. 1) you can look up atomic distances.

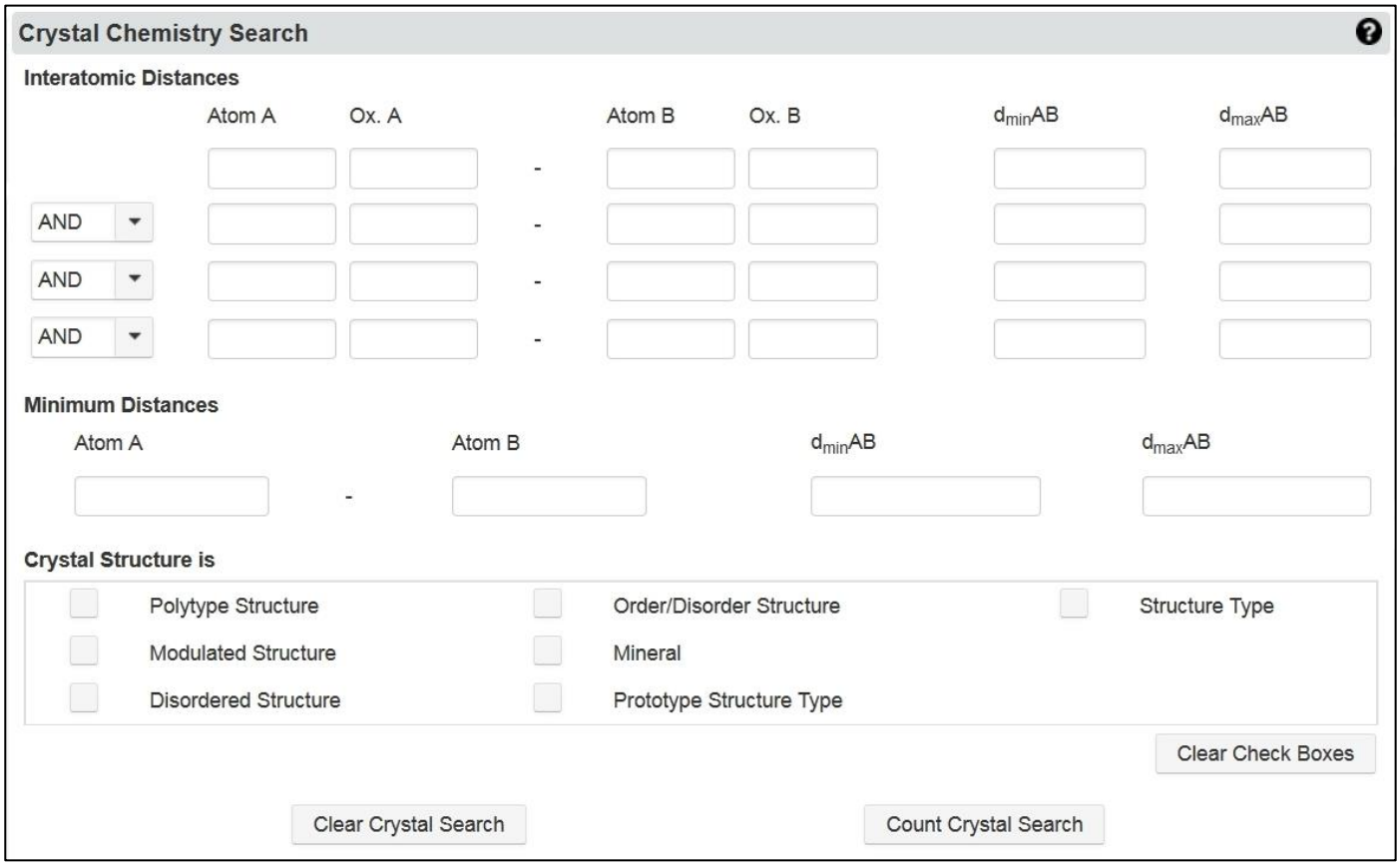


Figure 1: Crystal Chemistry Search

Interatomic distances

These search fields allow searching for distances between two atoms in the unit cell. At least the following data are required:

- Atom A,
- Atom B,
- d_{min}AB,
- d_{max}AB.

For further refinement of the search oxidation states can be entered.

Please note that oxidation states are internally handled with a tolerance of 0.1. This means that giving an oxidation state of say 2.66 in the respective field is internally seen as a range of 2.56-2.76. The reason for this tolerance is the ambiguity in determining oxidation states especially for not fully occupied positions.

Up to four distances can be specified at once. For the additional three interatomic distances a logical operator (AND / OR) can be set.

Atom A / Atom B

These two search fields set the atoms. Atoms must be chemical elements. Wildcards are not allowed.

Description	Defines the atoms for the interatomic distances
Type	Text
Format	Single entry
# of entries	1
Wildcards	-

Ox. A / Ox. B

In these fields the oxidation number can be specified for atoms A and/or B. Neither of these fields are mandatory for an interatomic distance search.

Description	Defines the oxidation number of the atoms
Type	Numerical, floating point
Format	Single entry
# of entries	1
Wildcards	-

d_{min} AB/ d_{max} AB

These two search fields set the minimum and maximum distance for the interatomic distance search. The maximum distance cannot exceed 5 angstrom.

Description	Defines the minimum/maximum distance
Type	Numerical, floating point
Format	Single entry
# of entries	1
Wildcards	-

Minimum distances

These search fields allow searching for structures that have the shortest distance between the two specified atoms within the given range. At least the following data are required:

- Atom A,
- Atom B,
- d_{min}AB,
- d_{max}AB.

Atom A / Atom B

These two search fields set the atoms. Atoms must be chemical elements. Wildcards are not allowed.

Description	Defines the atoms for the minimum distances
Type	Text
Format	Single entry
# of entries	1
Wildcards	-

d_{min} AB/ d_{max} AB

These two search fields set the minimum and maximum distance for the minimum distance search. The maximum distance cannot exceed 5 angstrom.

Description	Defines the minimum/maximum distances in the minimum distance search
Type	Numerical, floating point
Format	Single entry
# of entries	1
Wildcards	-

You can also limit your structure search by checking for one or more of the following flags (flags are combined by logical operator OR):

- Polytype Structure,
- Order/Disorder Structure,
- Structure Type,
- Modulated Structure,
- Mineral,
- Disordered Structure,
- Prototype Structure Type.

Structure Type Search

The Structure Type Search (Fig. 1) enables you to search within the comprehensive collection of structure types, compiled and assigned by R. Allmann, and integrated into ICSD by R. Hinek ("The introduction of structure types into the Inorganic Crystal Structure Database ICSD").

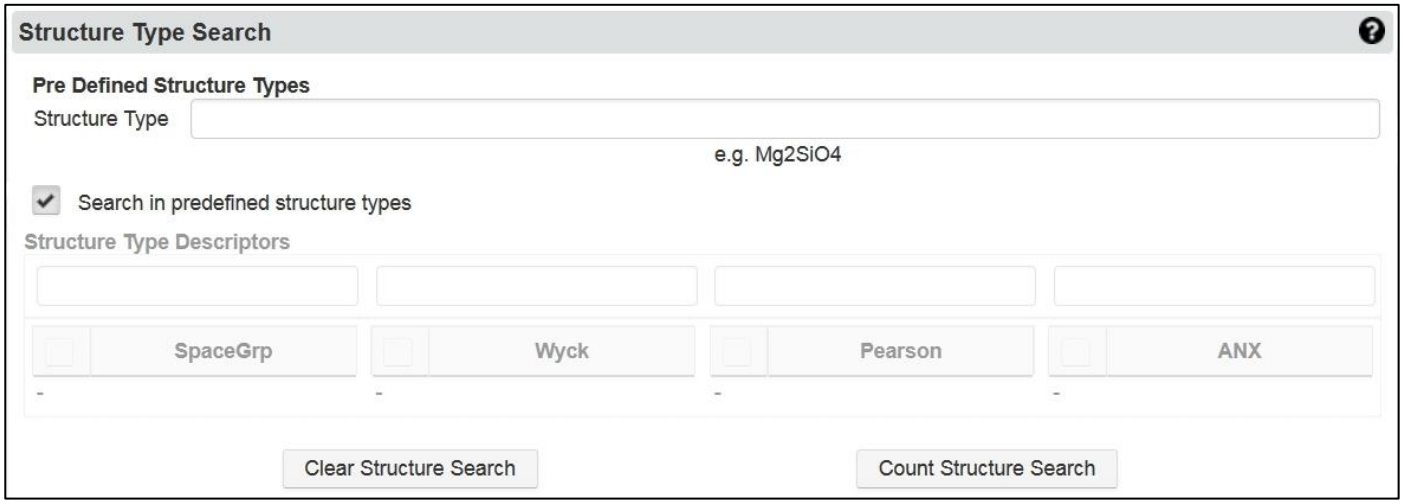


Figure 1: Structure Type Search using the predefined structure types

Structure types can be searched directly or using the most relevant descriptors for the structure types (space group, Wyckoff sequence, Pearson symbol and ANX formula).

Search in predefined structure types

This checkbox switches between the search using the predefined structure types (checked) and the search using the structure type descriptors (unchecked). In each case the other search option is greyed out and not accessible.

Description	Search for predefined structure types directly
Type	Checkbox
Format	-
# of entries	-
Wildcards	-

Structure Type

With this search field structure types can be searched directly by typing in the names or part of the names using wildcards. In ICSD there are currently more than 9000 structure types defined.

Description	Search for structure types
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
Zeolite	all records with this exact term, e.g. Zeolite-A-frame, Zeolite-ABW-frame, …
Pe*	structure types containing a part starting with “pe”, e.g. pectolite, perrierite
"Quartz,low"	Structure type with this exact phrase

Structure Descriptors

Alternatively to the direct search of structure types, you can also search via the defining structure type descriptors (Fig. 2):

- Space Group Symbol
- Wyckoff Sequence
- Pearson Symbol
- ANX Formula

For each of these descriptors the rules for input apply according to the respective fields as found on the other search masks.

The checkbox next to the column name allows for selecting/deselecting all entries shown for this descriptor. If there are several pages of entries, only the entries for the current page are selected.

Space group symbol

Description	Search for the space group symbol
Type	Text
Format	Single entry
# of entries	1
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
p-1	Space group number 2
„P – 1“	Space group number 2
fm-*	Space groups: Fm-3, Fm-3c, Fm-3m
p 1 2 # 1	Space groups: P121 and P1211

Wyckoff Sequence

Description	Search for Wyckoff sequence	
Type	Text	
Format	Single entry or multiple entries	
# of entries	Unlimited	
Wildcards	*	any number of characters
	#	0 or 1 character
	“ “	exact term

Examples:

Search term	will find the following entries
a	all sequences with Wyckoff symbol a, but not with e.g. a2 or a3 e.g.: “c12 b8 a”, “d12 c a” or “A2 z y t s r o k j2 f a”
c# d*	all sequences with Wyckoff symbols c or c1 – c9 and any d, but not e.g. c12 e.g.: “d c a3”, “d25 c b a5” or “o9 n8 m8 l f e d c”
"f2 e d b"	all sequences with exactly this phrase as part of the Wyckoff sequence e.g.: “f2 e d b”, “f2 e d b a” or “g3 f2 e d b a”

Pearson Symbol

Description	Search for the Pearson symbol	
Type	Text	
Format	Single entry	
# of entries	1	
Wildcards	*	any number of characters
	#	0 or 1 character
	“ “	exact term

Examples:

Search term	will find the following entries
oF100	all orthorhombic, face-centered structures with 100 atoms in the unit cell
mS*	all monoclinic, side-centered structures with any number of atoms in the unit cell
cP##	all cubic, primitive structures with up to 99 atoms in the unit cell

ANX formula

Description	Search for the ANX formula
Type	Text
Format	Single entry
# of entries	1
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
N#	N, NO, NX
A*YZ	A2XYZ, AB2XYZ, ABXYZ and AXYZ
A*C*	all formulae that have at least AnnBnnCnn in it. AX or ABX are not included.

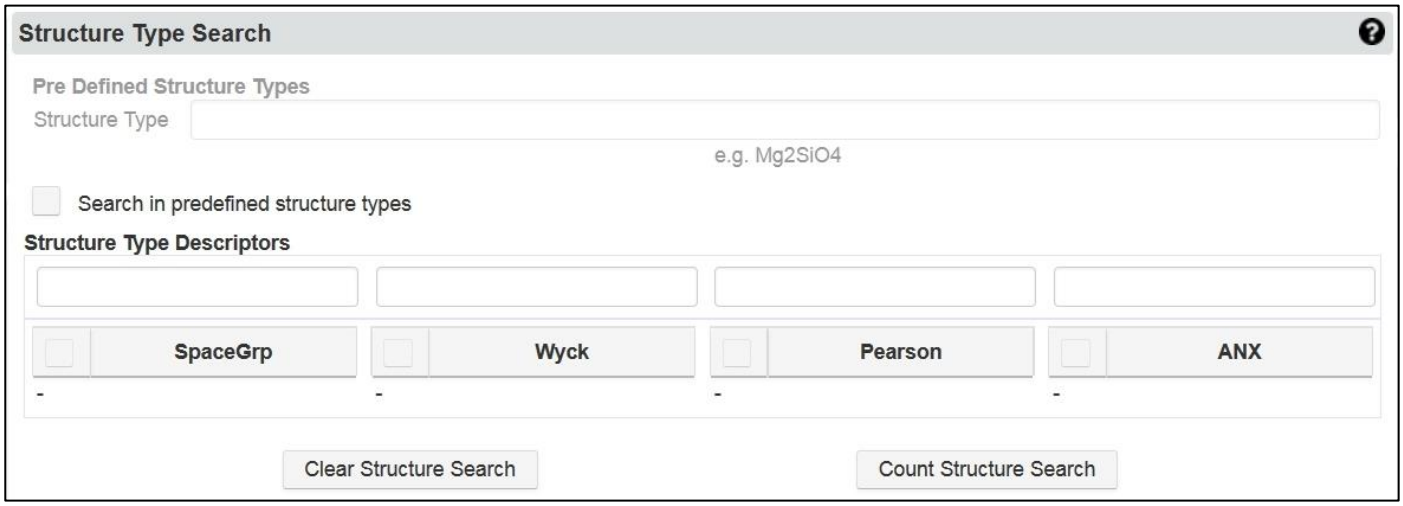


Figure 2: Structure Type Search using the descriptors (space group, Wyckoff sequence, Pearson symbol and ANX formula)

As soon as one of the structure type descriptors has been defined (Fig. 3) all possible values for the other descriptors are shown in the columns. If the first descriptor was defined using a wildcard this descriptor column will also show all possible entries according to the definition given. The descriptor defined in the search field does not have to be selected to be included in the search. This is done automatically.

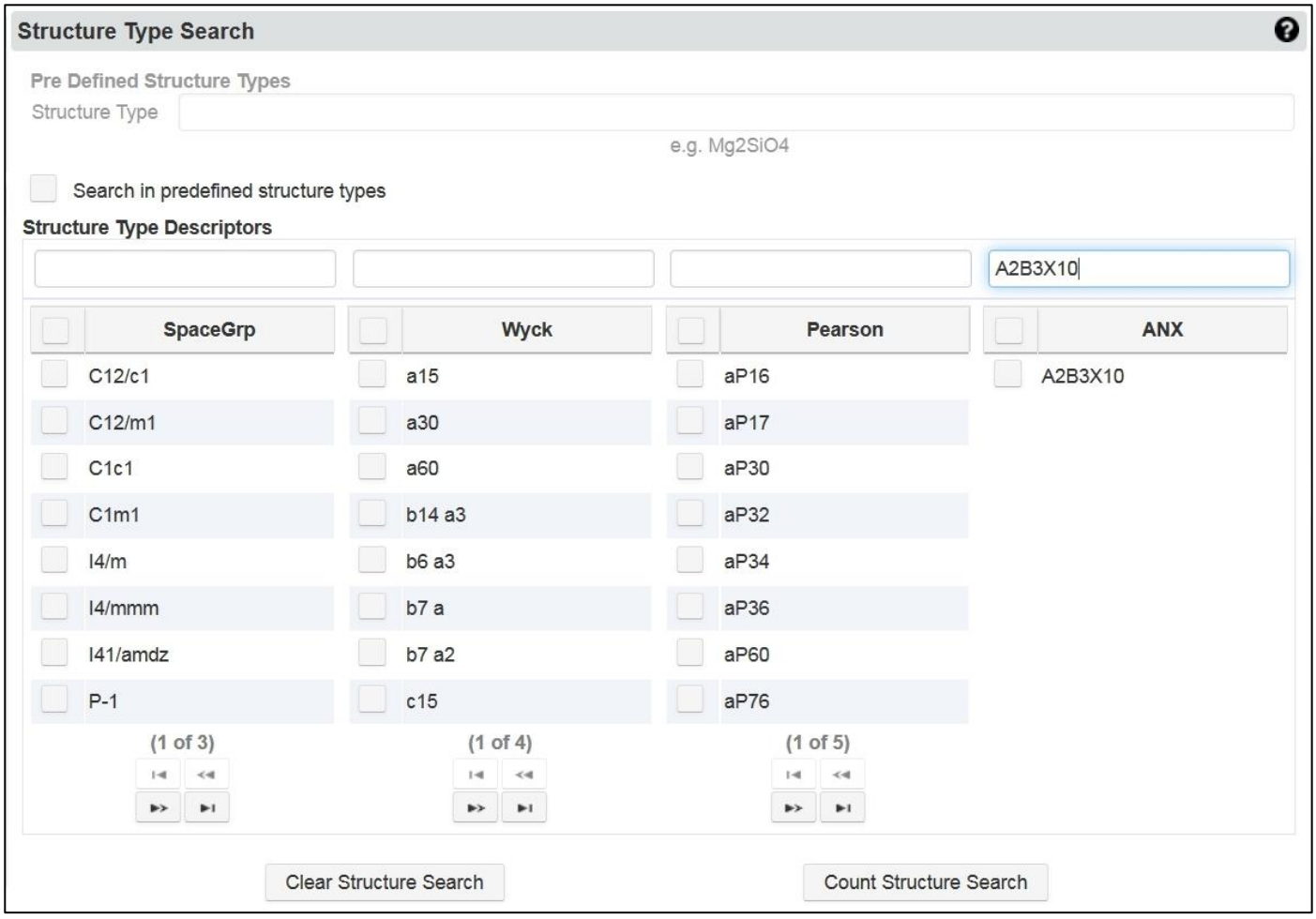


Figure 3: Initial definition of an ANX formula

All further selections will change the shown entries (Fig. 4). Selections within one column are combined by OR, while selections in different columns are combined by AND.

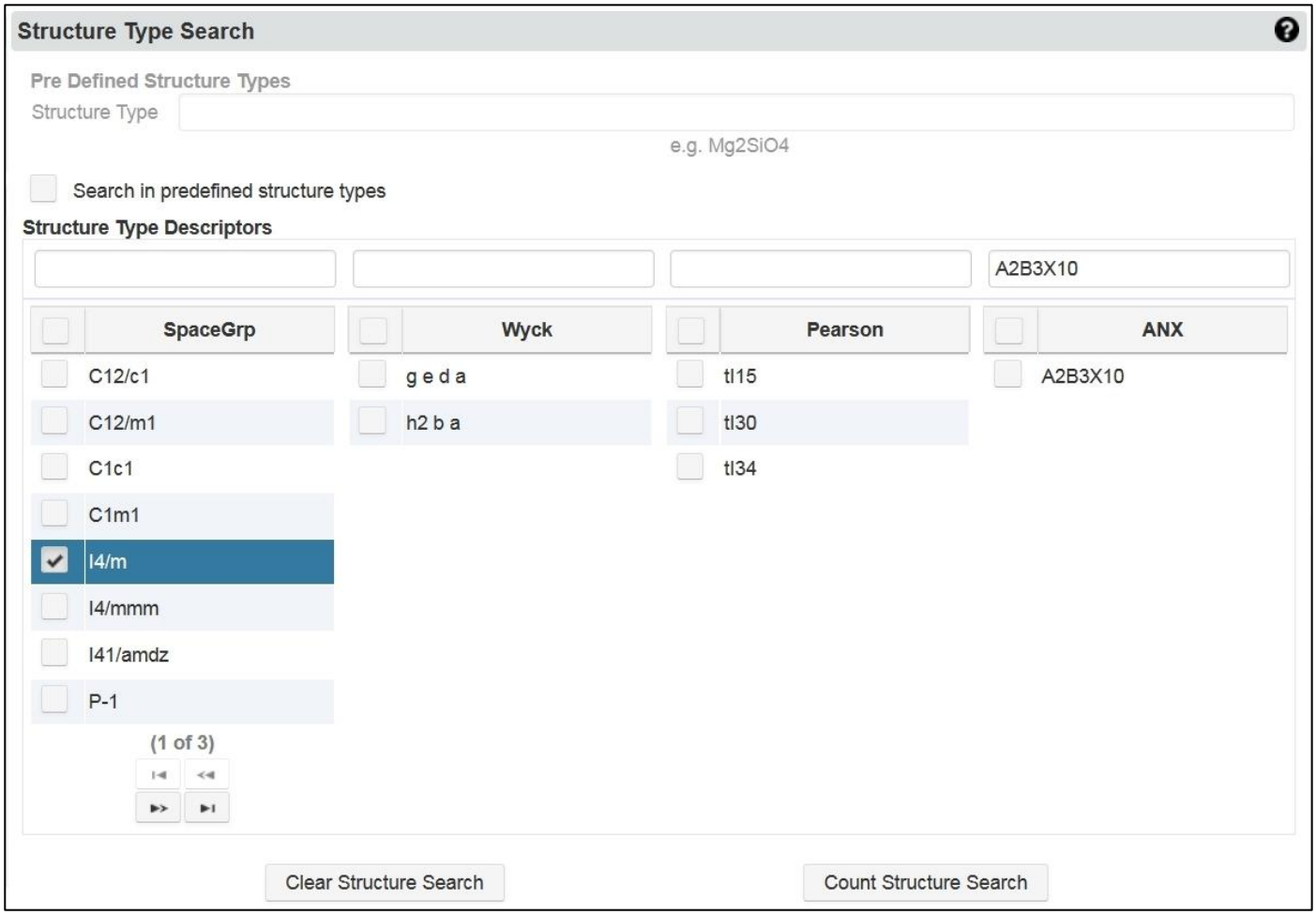


Figure 4: Additionally selecting a space group changes the possible entries

Please note that selecting several entries in one column and then selecting an entry in another column will often remove selections from the previous table, if those selections are not all true for the AND combination of the two tables (Fig. 5).

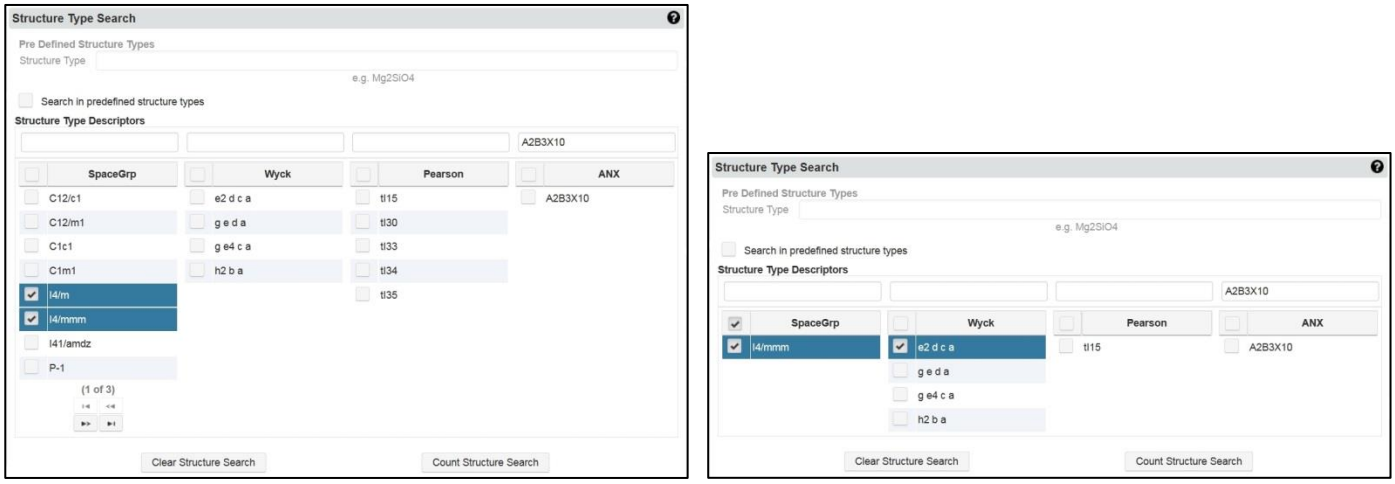


Figure 5: left) Selection of 2 entries in one column (Wyckoff sequence). right) Selection of one entry in another column (Wyckoff sequence) is often not compatible with the AND combination of those

columns for all selected entries resulting in some selections (space group I4/m) being automatically removed.

It is also possible to define all descriptors directly using the search fields (Fig. 6). In the example below the search will include one space group, two Wyckoff sequences, two Pearson symbols and two ANX formula.

Figure 6: All structure type descriptors can be specified

Experimental Information Search

The Experimental Information Search enables you to search explicitly for records with certain ambient conditions, experimental setups and additional properties, such as structures from a Rietveld refinement etc.

Please note that this search mask depends on the selection made in the Content Selection area. The "Calculation method" search field is only available if "Theoretical structures" is selected and the groups "Radiation Type", "Sample Type", "Additional Properties", and the R-value search field are only shown if at least one of the two experimental structures options ("Experimental inorganic structures" or "Experimental metal-organic structures") is selected (Figure 1)

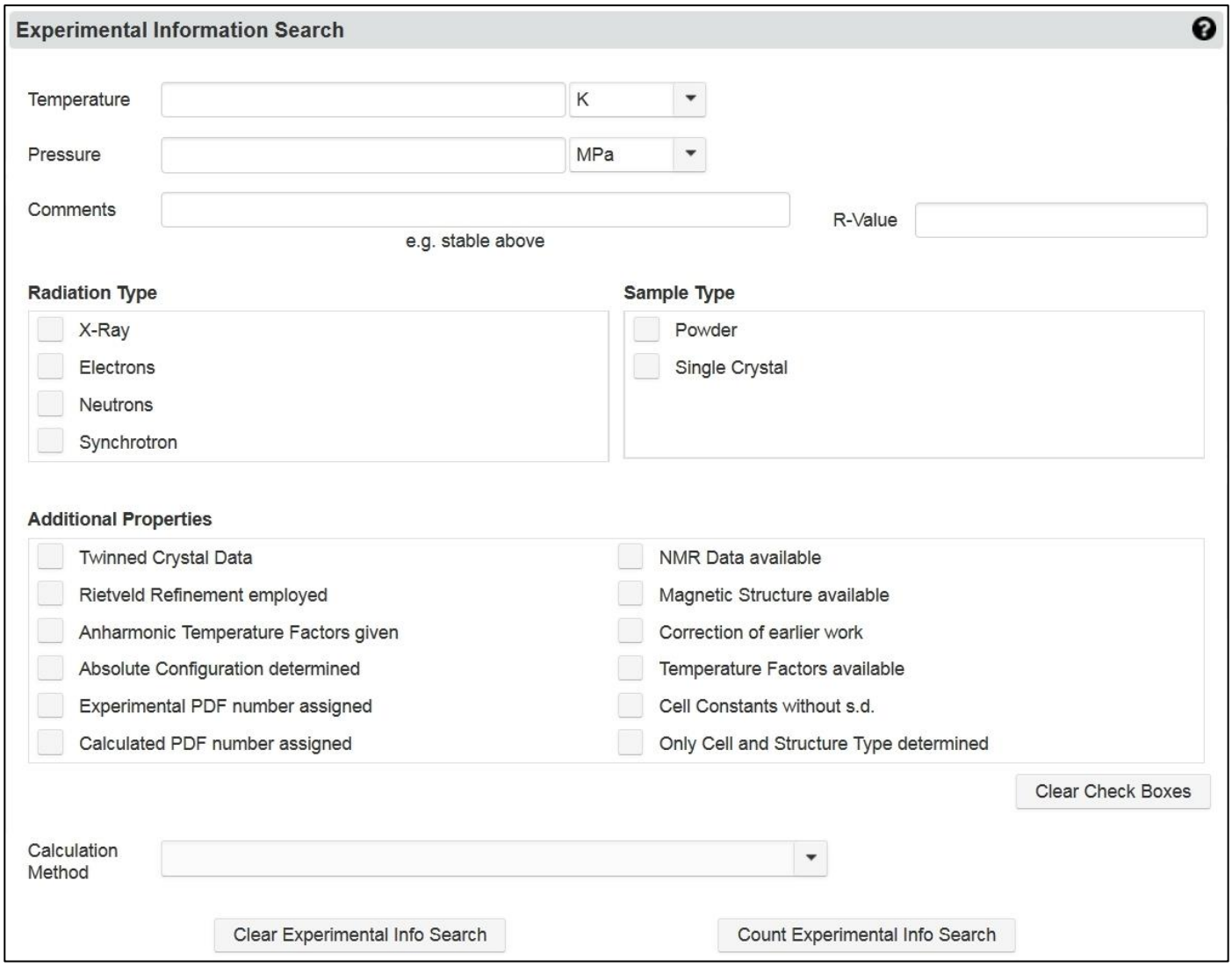


Figure 1: Experimental Information Search mask with all possible search fields. This is available if at least one of "Experimental inorganic structures" or "Experimental metal-organic structures" together with "Theoretical structures" is selected

Temperature

This search field allows to specify the temperature at which the crystal structure has been determined. Possible units can be defined using the dropdown box next to it.

Note: If no temperature was given by the author, a default temperature of 293K is assumed by the system!

Description	Temperature of the measurement
Type	Numerical, floating point
Format	Single value or range
# of entries	1
Wildcards	- range; temperature1 – temperature2 ‹ range; ‹ temperature ‹= range; ‹= temperature › range; › temperature ›= range; ›= temperature

Examples:

Search term	will find the following entries (assuming K as unit)
2-3	crystal structures measured between 2.0 K and 3.0 K
‹1.0	crystal structures measured at a lower temperature than 1.0 K
›=350	Crystal structures measured at temperatures above 350 K

Unit of Temperature

With this drop-down-box the unit for the temperature search can be defined. Possible units are Kelvin (default) and Celsius.

Description	Unit of temperature
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Pressure

This search field allows to specify the pressure at which the crystal structure has been determined. Possible units can be defined using the dropdown box next to it.

Note: If no pressure was given by the author, a default pressure of 0.101325 MPa is assumed by the system!

Description	Pressure during the measurement
Type	Numerical, floating point
Format	Single value or range
# of entries	1
Wildcards	- range; pressure1 – pressure 2 ‹ range; ‹ pressure ‹= range; ‹= pressure › range; › pressure ›= range; ›= pressure

Examples:

Search term	will find the following entries (assuming MPa as unit)
1000	crystal structures measured at exactly 1000.0 MPa (1.0 GPa)
‹1.0	crystal structures measured at a lower pressure than 1.0 MPa
›100000	Crystal structures measured at pressures higher than 100.0 GPa

Unit of Pressure

With this drop-down-box the unit for the pressure search can be defined. Possible units are MPa (default), bar, kPa, hPa, Pa and atm.

Description	Unit of pressure
Type	Dropdown box
Format	Single value, selectable, pre-defined
# of entries	1
Wildcards	-

Comments

This field allows to search for comments on a crystal structure.

Description	Search for a comment
Type	Text
Format	Single entry or multiple entries
# of entries	Unlimited
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
F-Atoms	records with the term in the comments, e.g. “F-atoms (AsF6) around As(4) were not determined.“ or “After 2nd ref. (Gagarinsky) H-atoms are 0.95(3) A away from the F-atoms in direction to the next F-Atom at F-F=2.49”
“F-Atoms (AsF6)”	records containing the exact phrase in the comments, e.g. “F-atoms (AsF6) around As(4) were not determined.“
cryst*	records containing the term starting with “cryst”, e.g. “Cell parameters from single crystal data.”

R-Value

This search field allows searching for goodness of fit values from employed structure refinements, e.g. Rietveld refinements. Usually the conventional R-value is stored in the database. For Rietveld refinements the R_p value is used if possible and in addition the R_{Bragg} can be stored in an additional remark field.

This search field is only visible if “Experimental inorganic structures” and/or “Experimental metal-organic structures” is selected in the “Content Selection”.

Only values between 0.00 and 1.00 are possible.

Description	R-value of the refinement
Type	Numerical, floating point
Format	Single value or range
# of entries	1
Wildcards	- range; r_value1 – r_value2 ‹ range; ‹ r_value ‹= range; ‹= r_value › range; › r_value ›= range; ›= r_value

Examples:

Search term	will find the following entries
0.015	structures with an R-value of exactly 0.015
0-1.0	all records with a stored R-value
‹0.05	all records with R-values smaller than 0.05

Radiation Type

This group of checkboxes allows to limit a query to certain radiation types used for the experiment:

- X-ray
- electrons
- neutrons
- synchrotron

All checked radiation types in this group will be combined by OR.

This search field is only visible if “Experimental inorganic structures” and/or “Experimental metal-organic structures” is selected in the “Content Selection”.

Sample Type

This group of checkboxes allows to limit the query to one of the two sample types used in the experiment:

- Powder
- Single crystal

All checked sample types in this group will be combined by OR.

This search field is only visible if “Experimental inorganic structures” and/or “Experimental metal-organic structures” is selected in the “Content Selection”.

Additional Properties

This last group of checkboxes allows to limit the query using one or more of the additional properties:

- 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 Standard Deviations
- Only Cell and Structure Type determined

All checked additional properties in this group will be combined by OR.

This search field is only visible if “Experimental inorganic structures” and/or “Experimental metal-organic structures” is selected in the “Content Selection”.

Calculation Method

This drop-down-box is only relevant for theoretically calculated structures. Here you can select the method used for the calculation. Please note that more than one method can be selected and the selected methods are combined by logical AND.

Description	Method used for the calculation of theoretical structures
Type	Dropdown box
Format	Multiple value, selectable, pre-defined
# of entries	1
Wildcards	-

This dropdown box is only visible if “Theoretical structures” is selected in the “Content Selection”.

DB Info Search

Using the Database Information Search (Fig. 1) you can search for records with certain database-related properties, such as the ICSD collection code or release date.

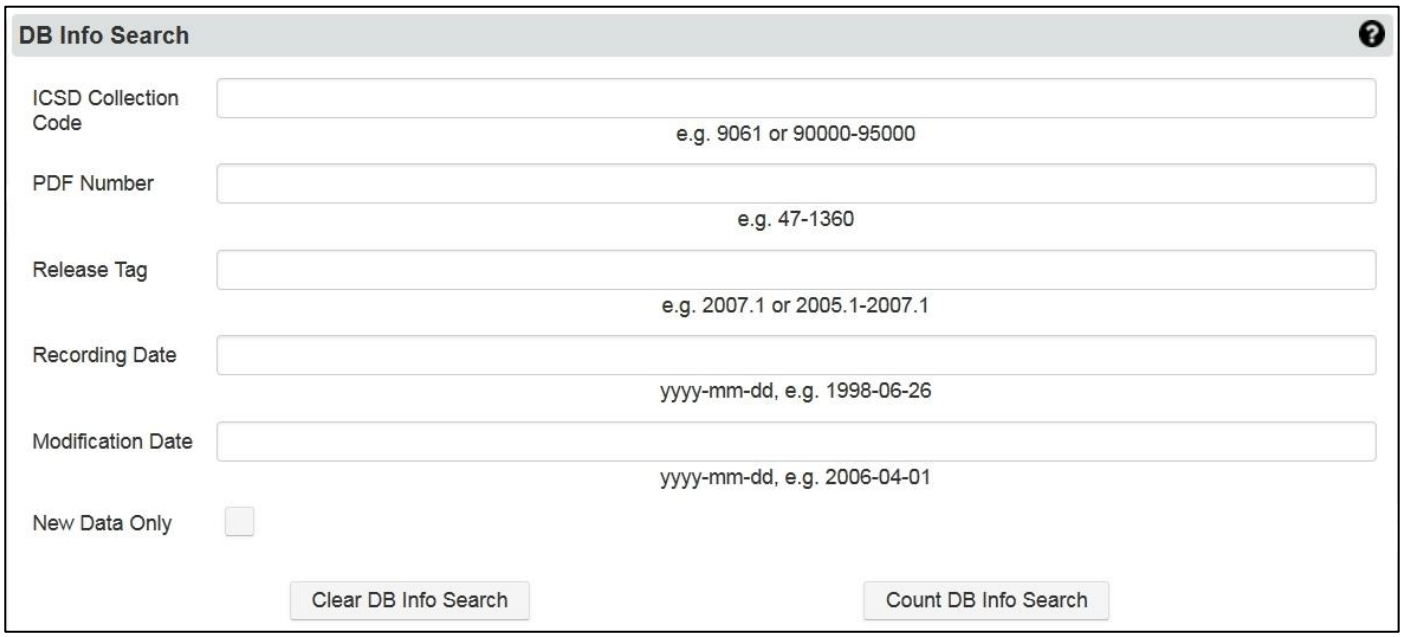


Figure 1: Database Information Search mask

ICSD Collection code

Allows to search for the Collection Code. Each record in ICSD is assigned a collection code, which serves as a reference for this record. Collection codes are not necessarily succeeding.

Description	ICSD collection code
Type	Numerical, integer
Format	Single value or range
# of entries	1
Wildcards	- range; collection_code1 – collection_code2 ‹ range; ‹ collection_code ‹= range; ‹= collection_code › range; › collection_code ›= range; ›= collection_code

Examples:

Search term	will find the following entries
10203	crystal structure with CC 10203
1-10	all records with CCs 1 – 10 (not necessarily 10 records!)
›=600000	all records with CC 600000 - 9999999

PDF number

PDF(Powder Diffraction File)-numbers are assigned by the ICDD. The pdf numbers follow a certain scheme n-n-n or n-n.

Description	PDF number as assigned by ICDD
Type	Text
Format	Single value or range
# of entries	1
Wildcards	* any number of characters # 0 or 1 character “ “ exact term

Examples:

Search term	will find the following entries
12-100	exact this PDF number 12-100
01-070-*	all PDF numbers in the range 01-070-0001 to 01-070-9999
01-07#-*	all PDF numbers in the range 01-070-0001 to 01-079-9999

Release Tag

Regular updates of ICSD are carried out twice per year. Those updates are then named according to the following pattern:

ReleaseYear.Release

E.g. the 2nd release in the year 2003 is named 2003.2. Each record in ICSD gets assigned a release tag when it is included in ICSD.

Description	Release tag
Type	Numerical, integer, special format
Format	Single value or range
# of entries	1
Wildcards	- range; release_tag1 – release_tag2 ‹ range; ‹ release_tag ‹= range; ‹= release_tag › range; › release_tag ›= range; ›= release_tag

Examples:

Search term	will find the following entries
2013.2	all records that were newly included in release 2 in 2013
2012.1-2012.2	all records included in the 2012 releases (not necessarily structures published in 2012)
‹2000.1	all records included before 2000

Recording Date

Recording dates have the following format:

yyyy-mm-dd

where yyyy is the year, mm the month and dd the day when the structure was included in ICSD. Please note that for each release all structures are included in ICSD on one specific date, so most dates will not produce any results.

Description	Recording date of an ICSD entry
Type	Numerical, integer, special format
Format	Single value or range
# of entries	1
Wildcards	- range; recording_date1 – recording_date 2 ‹ range; ‹ recording_date ‹= range; ‹= recording_date › range; › recording_date ›= range; ›= recording_date

Examples:

Search term	will find the following entries
2012-02-1	all records that were newly included on February 01, 2012
2000-01-01 – 2000-12-31	all records included in 2000
‹2000-01-01	all records included before 2000

Modification Date

Recording/Modification dates have the following format:

yyyy-mm-dd

where yyyy is the year, mm the month and dd the day when the record has last been modified. Please note that for each release all structures are modified in ICSD on one specific date, so most dates will not produce any results.

Description	Modification date of an ICSD entry
Type	Numerical, integer, special format
Format	Single value or range
# of entries	1
Wildcards	- range; modification_date1 – modification_date2 ‹ range; ‹ modification_date ‹= range; ‹= modification_date › range; › modification_date ›= range; ›= modification_date

Examples:

Search term	will find the following entries
2012-08-01	all records that were modified on August 01, 2012
2010-01-01 – 2010-01-31	all records that were modified in January 2010
‹1990-01-01	all records modified before 1990

New Data Only

This checkbox restricts the search to those structures that were added or modified in the current release.

Description	Only entries added or modified in current release
Type	Checkbox
Format	-
# of entries	-
Wildcards	-

Expert Search

The Expert Search does not offer a new search field, rather this search represents a possibility to build very complex searches in ICSD. For this purpose, 42 search fields, which are also available in the regular interface, can be combined almost arbitrarily using Boolean operators and/or brackets. The possible search fields are listed in tabular form under the Expert Search input field, each with a brief description of the Advanced Search & Retrieve mask on which the corresponding search is to be found and the type of search (text, numeric, logical) (Fig. 1). An exact description of the search fields can then be found on the specified search mask.

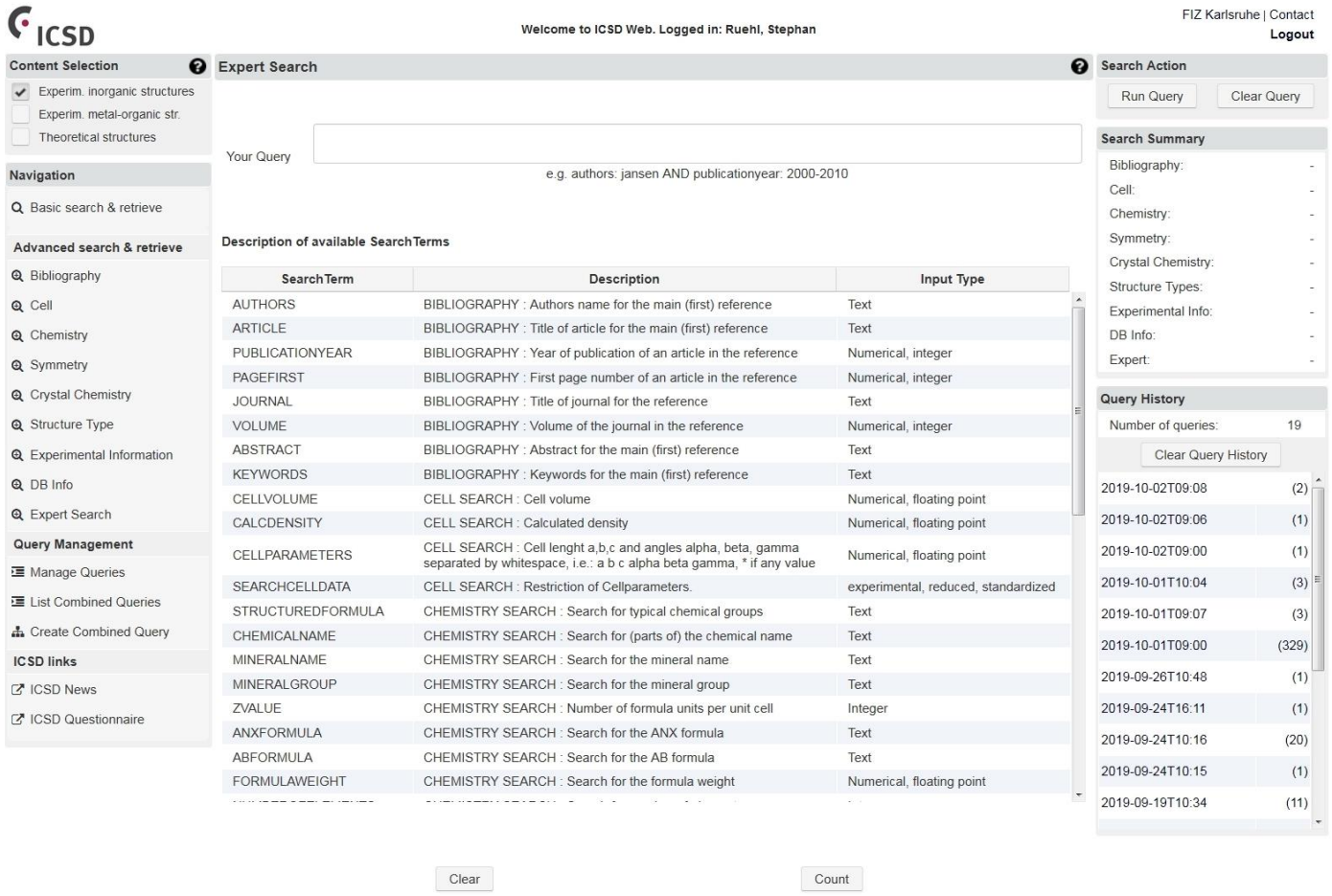


Figure 1: Expert Search: The search is defined in the input field. The table below lists the possible search fields that can be used in the Expert Search.

The search always consists of the search field followed by a colon, followed by the search term. The search term can also contain wildcards for text searches and the usual options such as “<”, “<=”, “>”, “>=” or a range for numeric searches. A search can consist of several search fields combined with Boolean operators (AND, OR, NOT). In addition, brackets "(" and ")" can be used to further restrain the search.

Below are some simple examples of how to use the Expert Search:

(1) searchcelldata: reduced AND cellparameters: 10-11 11-12 12-13 90 90 90 AND zvalue: >=8
(2) authors: jansen AND (journal: angewandt* OR journal: acta*) NOT publicationyear: 2000
(3) (crystalsystem: orthorhombic OR crystalsystem: tetragonal) AND inversioncenter: true and bravaislattice: face-centered

Query Management

The query management system for ICSD allows you to load, save, modify and delete queries. In addition, the Create Combined Queries mask can be used to create very complex searches by combining existing queries using logical operators (AND, OR, NOT).

Manage Queries

On the Manage Queries mask you can save, load, delete and modify queries from the Query History (the last 30 queries) or already saved queries (Fig. 1).

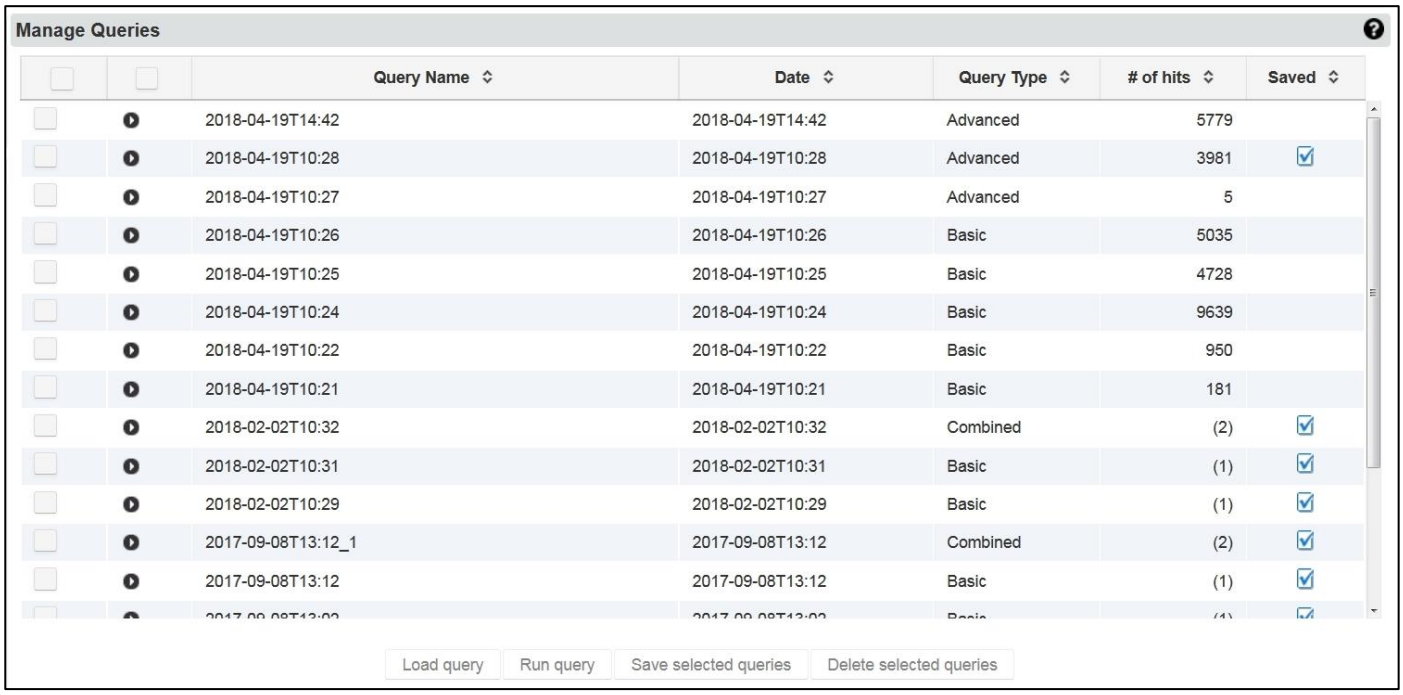


Figure 1: Manage Queries mask

The mask is basically a large table with one row per query. For each query the following information is given in a separate column:

- Query name: This shows the name of the query. Please note that queries from the Query History have automatically generated names in the format yyyy-mm-ddThh:nn with yyyy being the year, mm the month, dd the day, hh the hour and nn the minutes. When hovering over the Query name, a tool tip will be displayed with information on the search fields used for this query. The tool tip is identical to the information given in the details for the Query Info.
- Date: This gives the date in which the query was performed in the format yyyy-mm-ddThh:nn with yyyy being the year, mm the month, dd the day, hh the hour and nn the minutes.
- Query Type: The query type is Basic (if only the Basic Search mask was used in the query), Advanced (if the Advanced Search mask(s) were used in the query) or Combined. Combined queries can include any query type including Combined.
- # of hits: This shows the hits for this query using the current release. If the number is given in brackets, the number of hits correspond to a previous release and may be different for the current release. If this query is performed again, the number is updated.

- Saved: A small icon (a checked box) marks saved queries. All other queries are not saved and may be removed automatically. (Note: Queries from the Query History are only temporarily in this list. As soon as a new query enters the list of 30 queries, the oldest entry is removed).

The first two columns allow to select the entry or to show more details by clicking on the little triangle icon. The details given for a query are as follows (Fig. 2):

- Query name: As before, but here it can be changed.
- Release tag: This shows the release tag that corresponds to the shown # of hits. If the release tag is not the current one, the # of hits display is put in brackets.
- Date: The date on which the query was performed.
- Comment: Shows a user definable comment for this query.
- Query Info: Shows details of the fields used for this query.

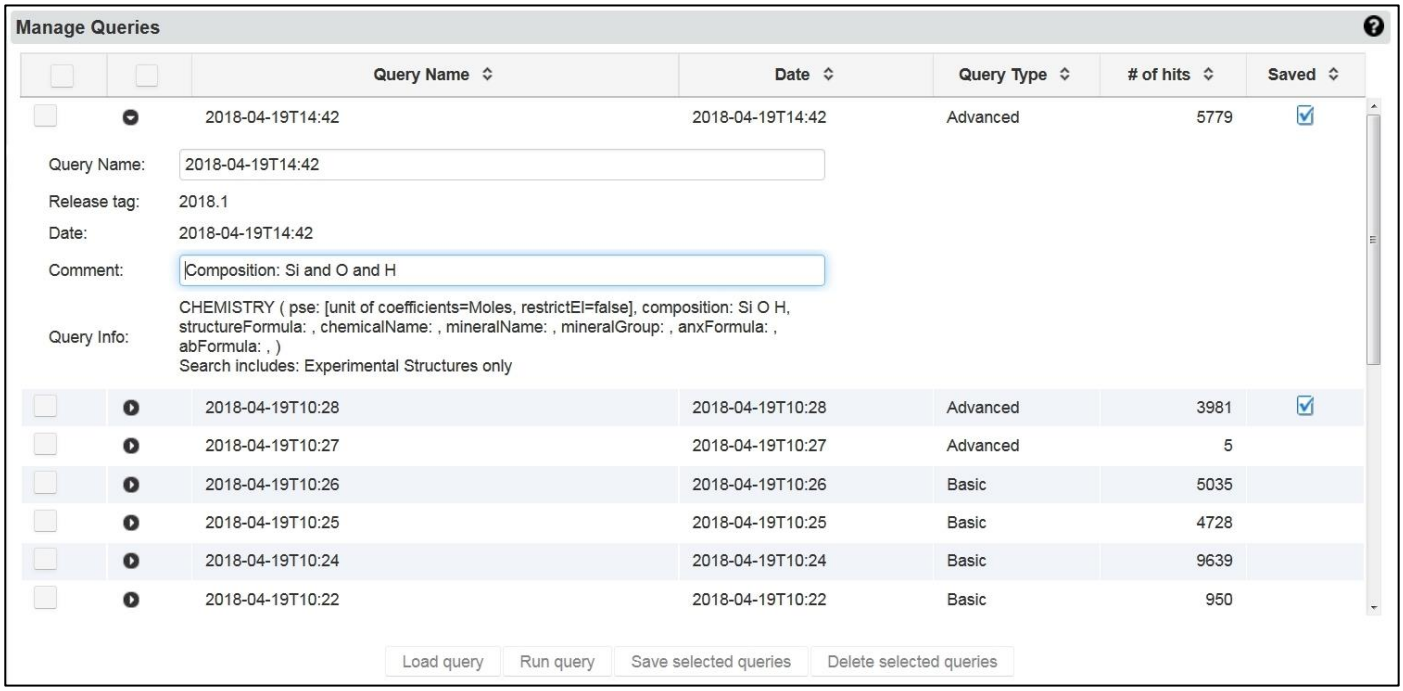


Figure 2: Show the details of the query by clicking on the little triangle in the second column. In this example a comment was included.

In the example in Figure 2 a comment was added. In order to save this comment, select the query and then save it (Fig. 3). A little icon indicates that comment was saved.

Figure 3: First the entry is selected (left), then the Save selected queries button is used to store the query for later use (right).

Figure 3 shows also that selecting one entry activates all buttons (Load query, Run query, Save selected queries, Delete selected queries). If more than one entry is selected only the last two buttons are activated (Fig. 4), because it is not possible to Load or Run more than one entry at a time.

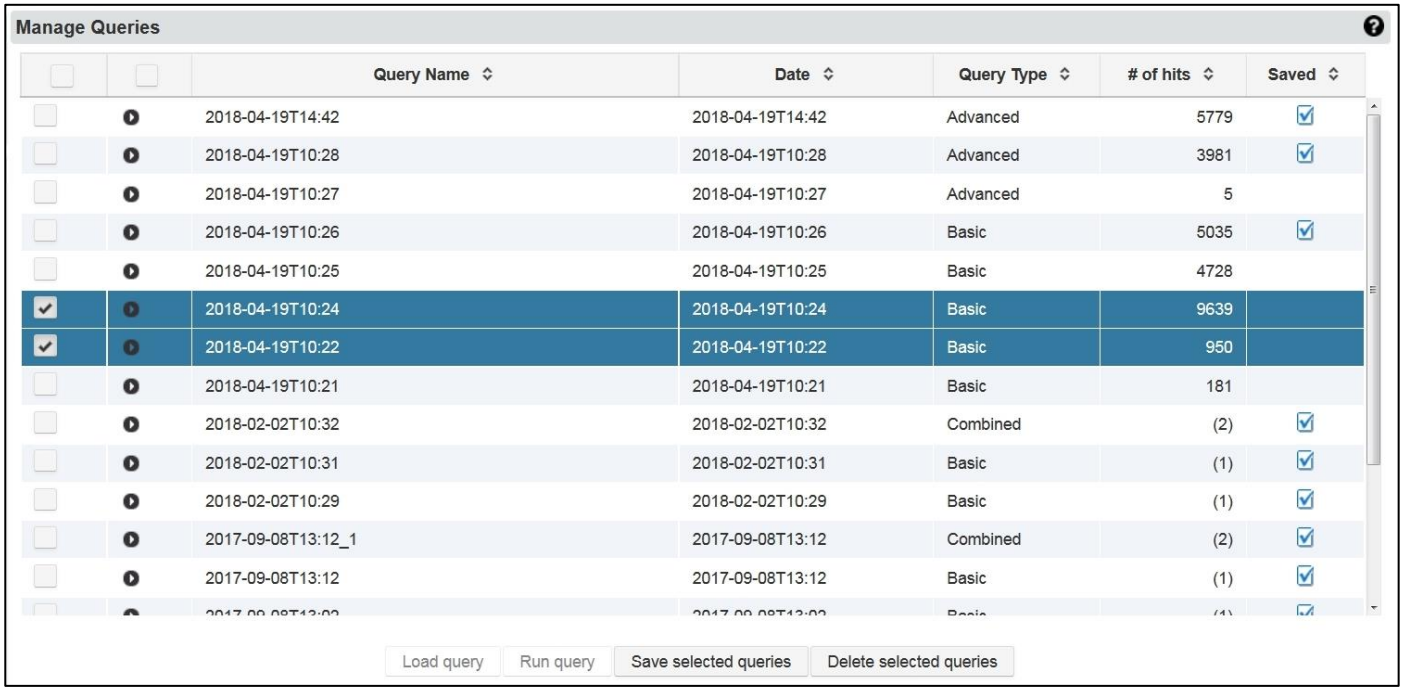


Figure 4: For two or more selected entries only the Save selected queries and Delete selected queries options are available.

The Load query button will restore the search fields of the query and open the respective mask for Advanced or Basic searches and the Create Combined Query mask for combined queries. The query can then be modified.

The Run query button will restore the search fields as well but it directly performs the search and the results will be shown in the List View.

The entries in the Manage Queries mask are listed by date as a default. You can change the order of entries by clicking on the little icon next to the column name. Each click on this icon will change the order from ascending and to descending (Fig. 5) and vice versa.

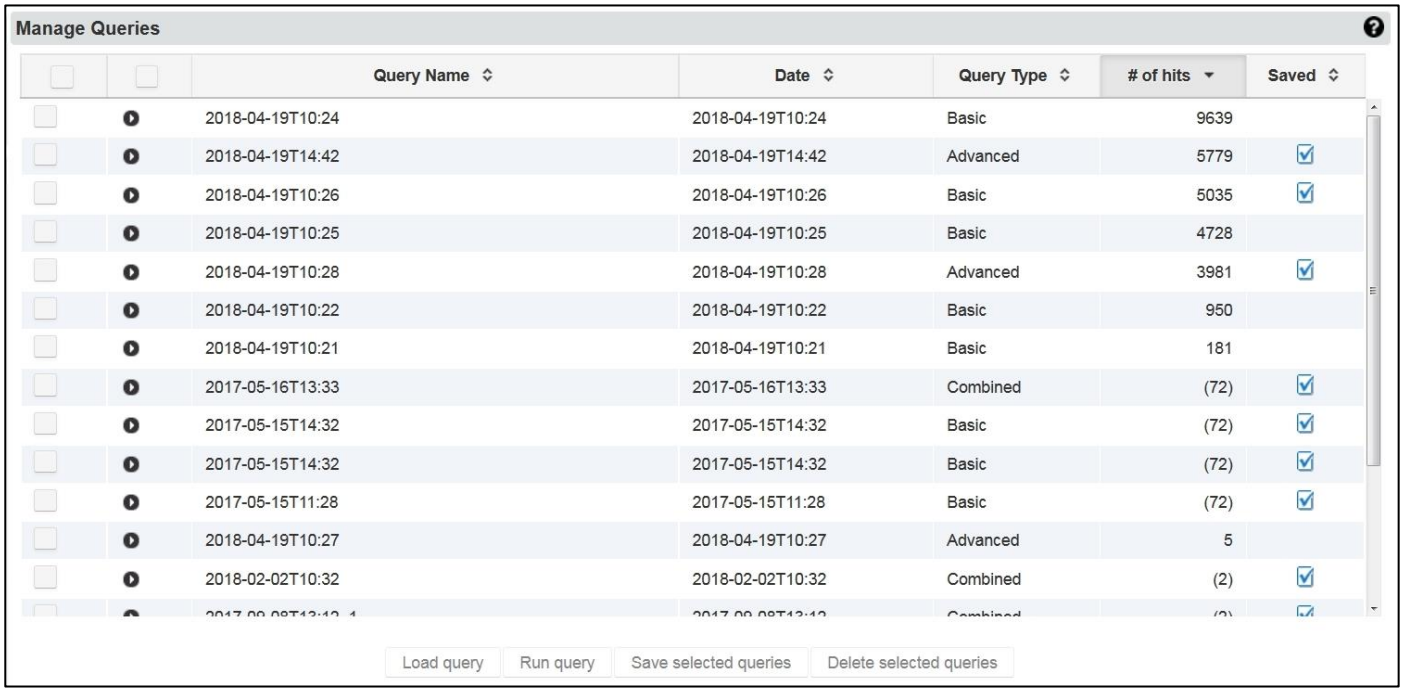


Figure 5: Change the order to ascending or descending by clicking on the little icon next to the column name. Here the column # of hits has been listed in descending order.

The two checkboxes in the title row offer a shortcut to select/deselect all entries (first checkbox (Fig. 6)) and to show/hide details for all entries (second checkbox).

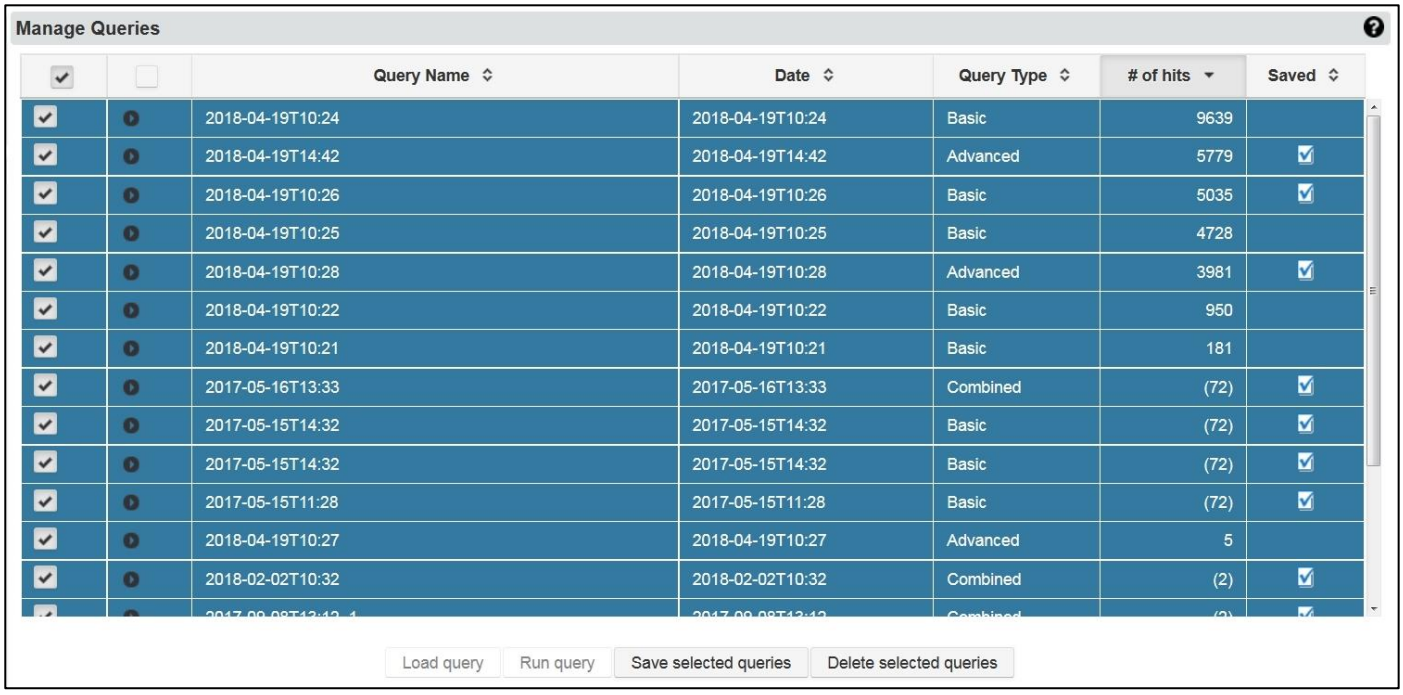


Figure 6: Select/Deselect all entries by using the checkbox in the title row.

List Combined Queries

This mask is specifically for combined queries (Fig. 1) and lists for each combined query all incorporated queries with their logical operators.

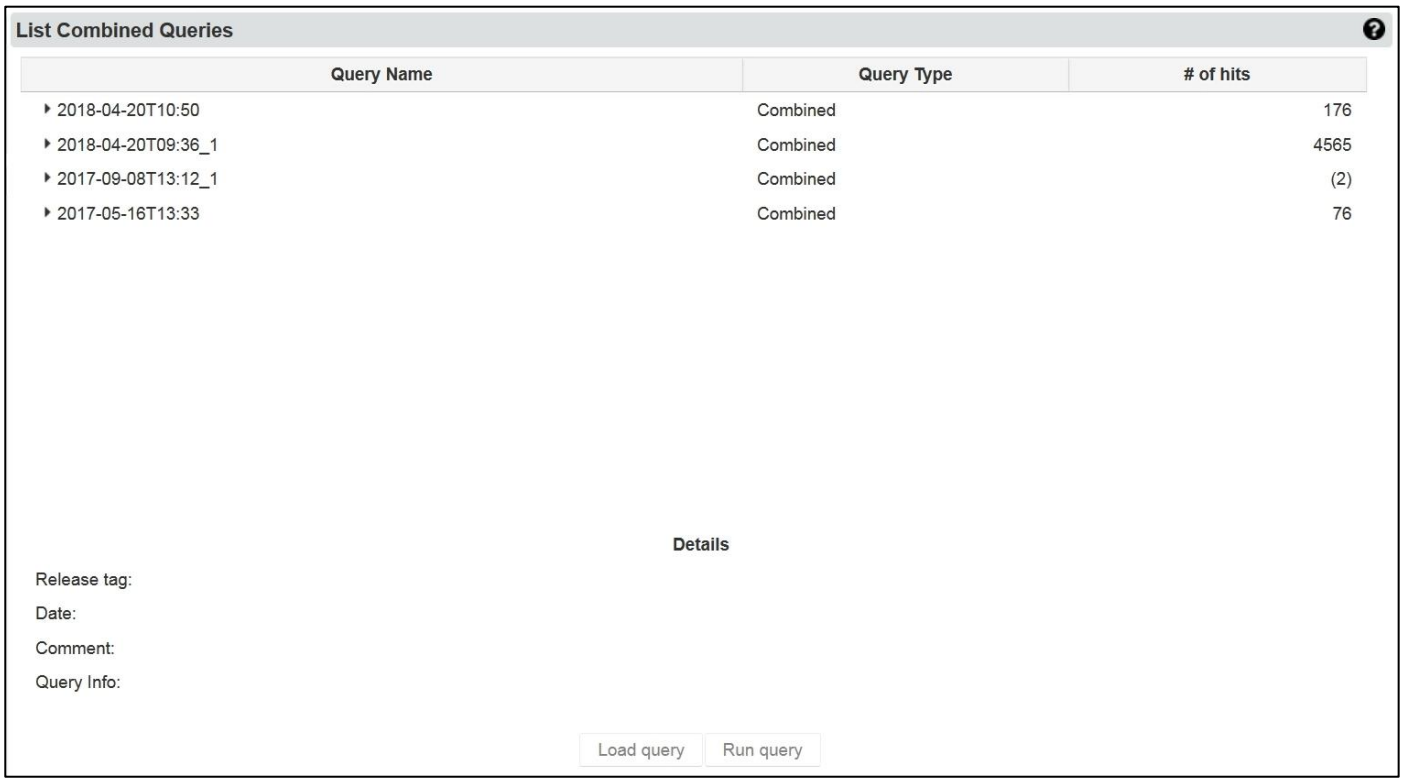


Figure 1: List Combined Queries mask

This mask makes it easier to check combined queries compared to the Manage Queries mask, because it is directly possible to view the Query Info of the logically connected queries for the query types Advanced and Basic (Fig. 2).

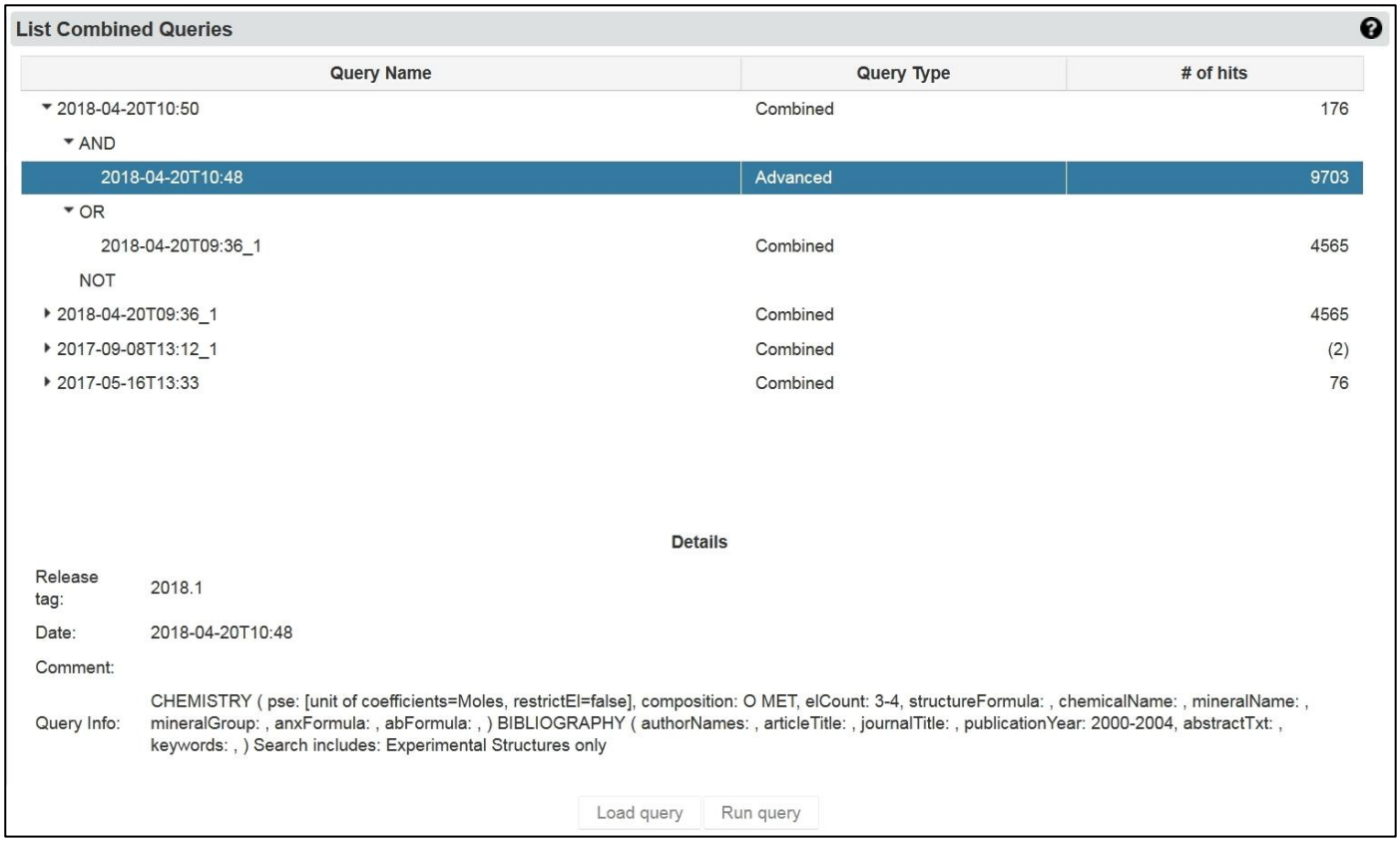


Figure 2: Details for the connected queries can be displayed (only for Query Type: Advanced and Basic)

In case a combined query is incorporated, the Query Info is not shown directly (Fig. 3), but the combined query in question can easily be selected to check on the definitions of this query.

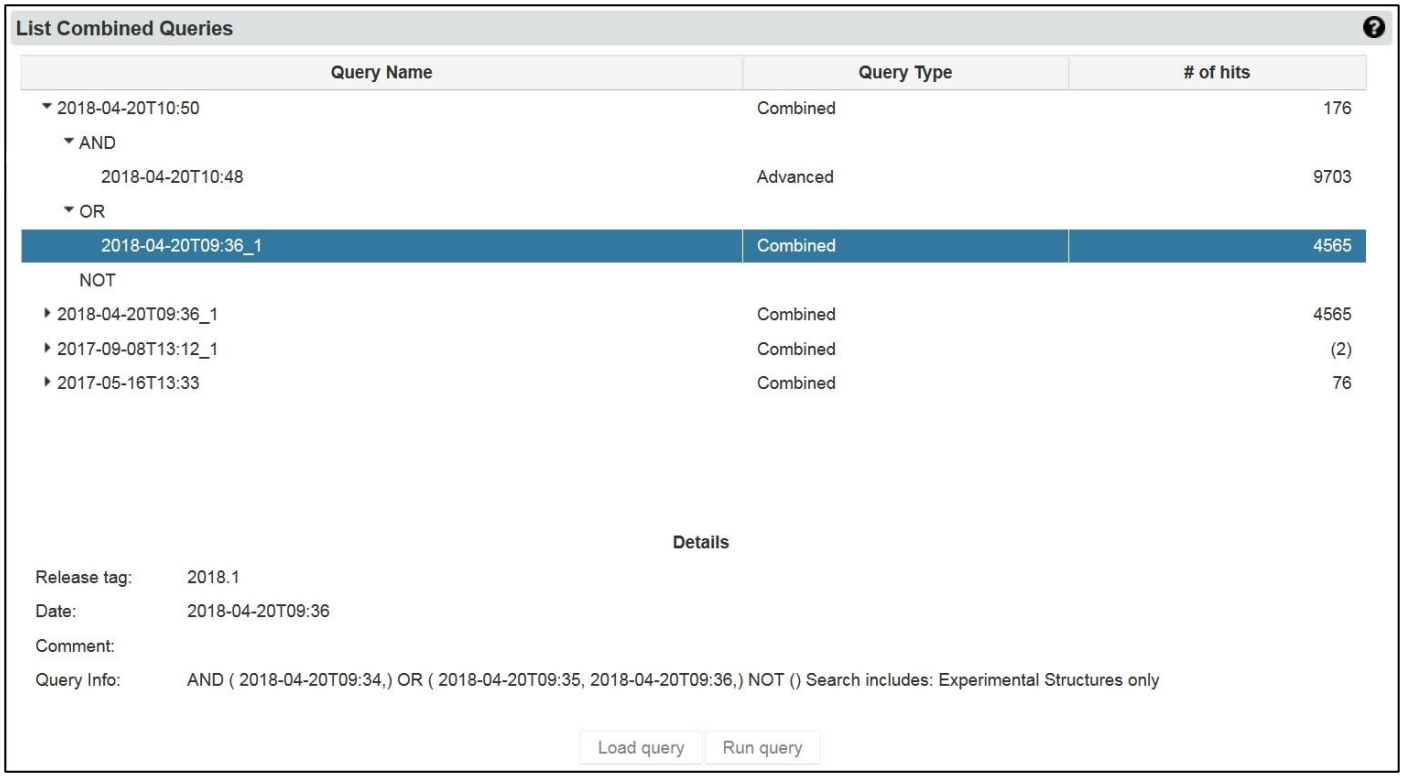


Figure 3: Details for a logically connected combined query are not shown directly. This information is accessible by selecting the main entry for this combined query.

The List Combined Queries mask can also be used to either load a query into the Create Combined Query mask for further modifications or to run the query directly. To perform any of these actions, the combined query needs to be selected (Fig. 4). Then the two buttons on the bottom are activated and can be used. Please note that the buttons only work for the combined queries and not for those incorporated in either of the logical operators.

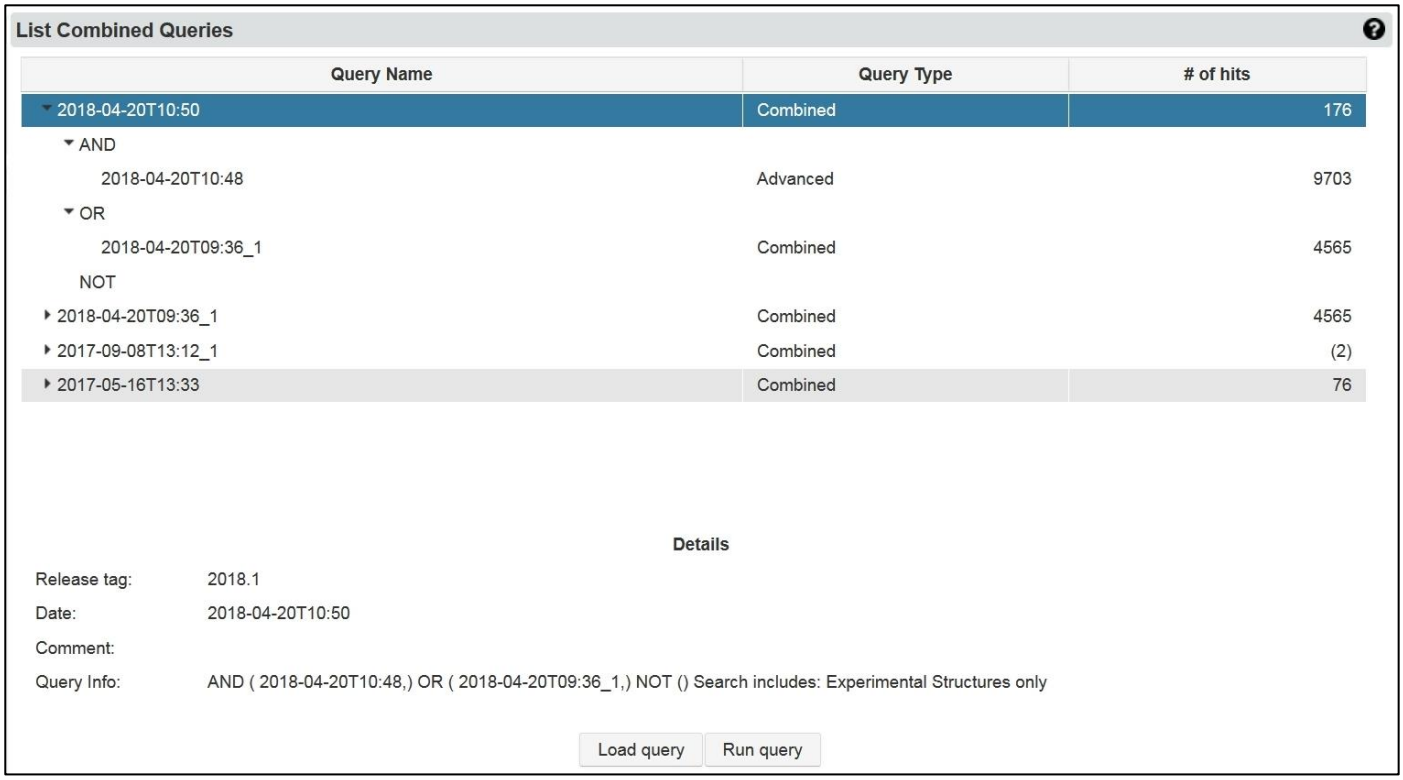


Figure 4: The two buttons at the bottom are activated once a combined query has been selected.

Create Combined Queries

This mask allows to create very complex queries by combining existing queries using the logical operators AND, OR and/or NOT (Fig. 1). In addition, it is also possible to edit existing combined queries using this mask, but this feature can only be reached via the Manage Queries mask using the "Edit Queries"-button on a combined query.

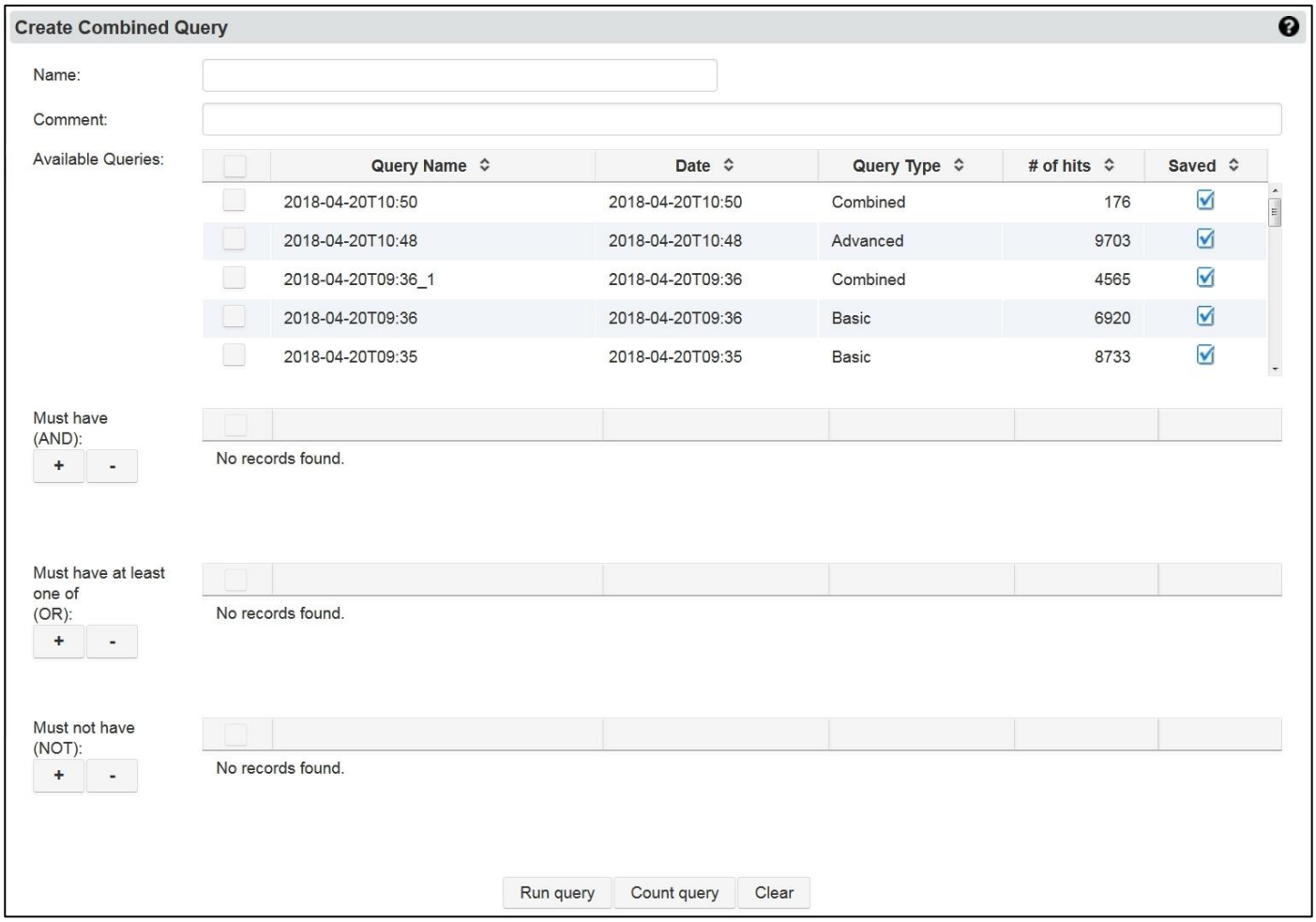


Figure 1: Create Combined Queries mask

In order to create a new query, enter a name for this query in the field Name. If no name is given a name will be generated automatically when the query is performed. In addition, a comment on this combined query can be made in the Comment field.

Next there is a table of the Available Queries. Those include up to 30 queries from the query history as well as any queries saved either manually in the Manage Queries mask or automatically by creating a combined query. For each query in this table the following information is given:

- Query name: This shows the name of the query. Please note that queries from the Query History have automatically generated names in the format yyyy-mm-ddThh:nn with yyyy being the year, mm the month, dd the day, hh the hour and nn the minutes. When hovering over the Query name, a tool tip will be displayed with information on the search fields used for this query. The tool tip is identical to the information given in the details for the Query Info.

- Date: This gives the date on which the query has been run in the format yyyy-mm-ddThh:nn with yyyy being the year, mm the month, dd the day, hh the hour and nn the minutes.
- Query Type: The query type is Basic (if only the Basic Search mask was used in the query), Advanced (if the Advanced Search mask(s) were used in the query) or Combined. Combined queries can include any query type including Combined.
- # of hits: This shows the hits for this query using the current release. If the number is given in brackets, the number of hits corresponds to a previous release and may be different for the current release. If this query is run, the number is updated.
- Saved: A small icon (a checked box) marks saved queries. All other queries are not saved and may be removed automatically. (Note: Queries from the Query History are only temporarily in this list. As soon as a new query enters the list of 30 queries, the oldest entry is removed).

The table of available queries can be sorted by any of these fields.

In order to include any of these queries to the combined query check the checkbox in front of the query/queries (Fig. 2).

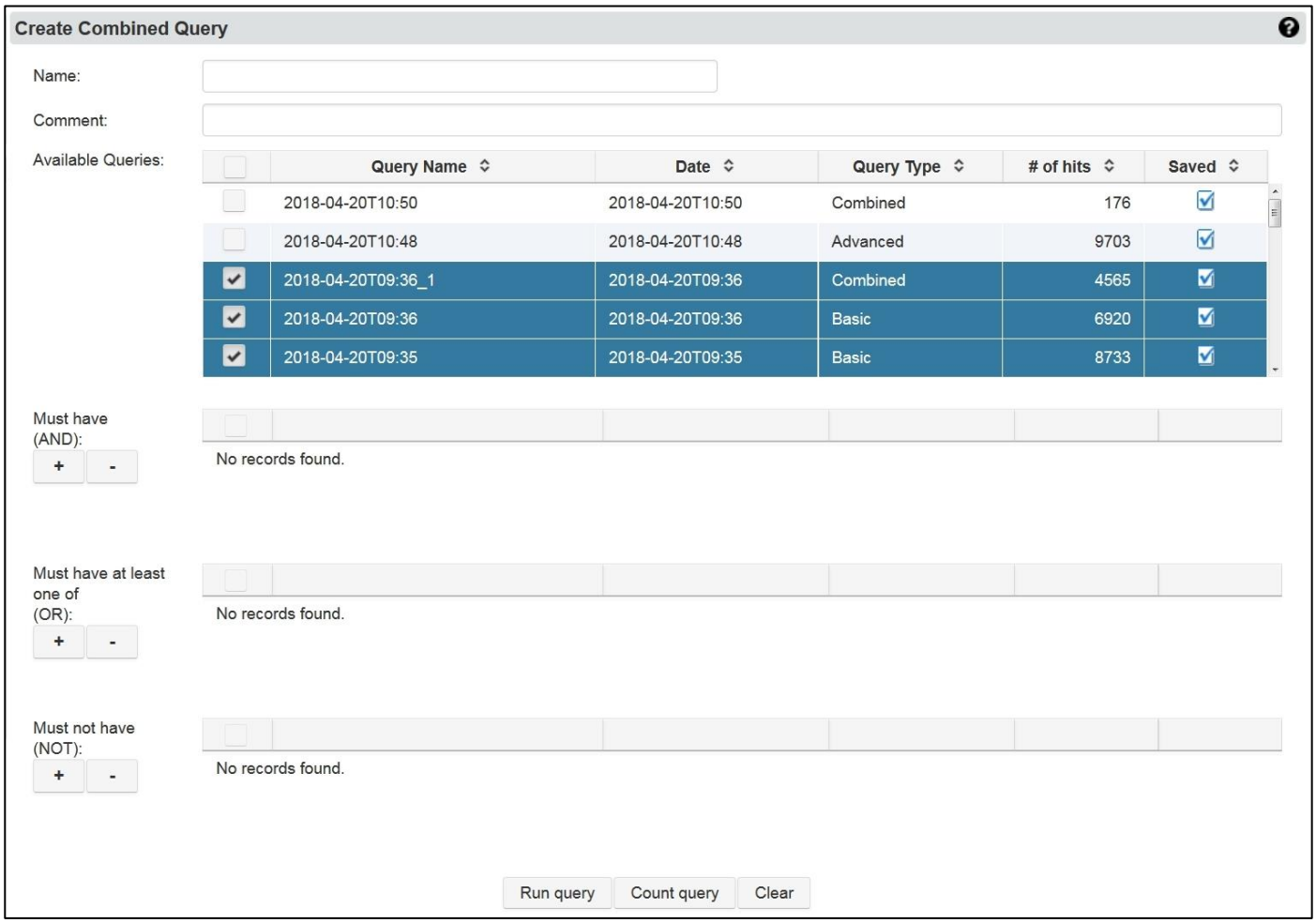


Figure 2: Select desired queries

The query/queries can now be added to the combined query using one of the following buttons (Fig. 3):

- AND: This adds the query/queries to the combined query using the logical operator AND.
- OR: This adds the query/queries to the combined query using the logical operator OR.
- NOT: This adds the query/queries to the combined query using the logical operator NOT (since NOT is a unary connective and therefore does not connect two queries this is internally handled as an “AND (NOT query)”).

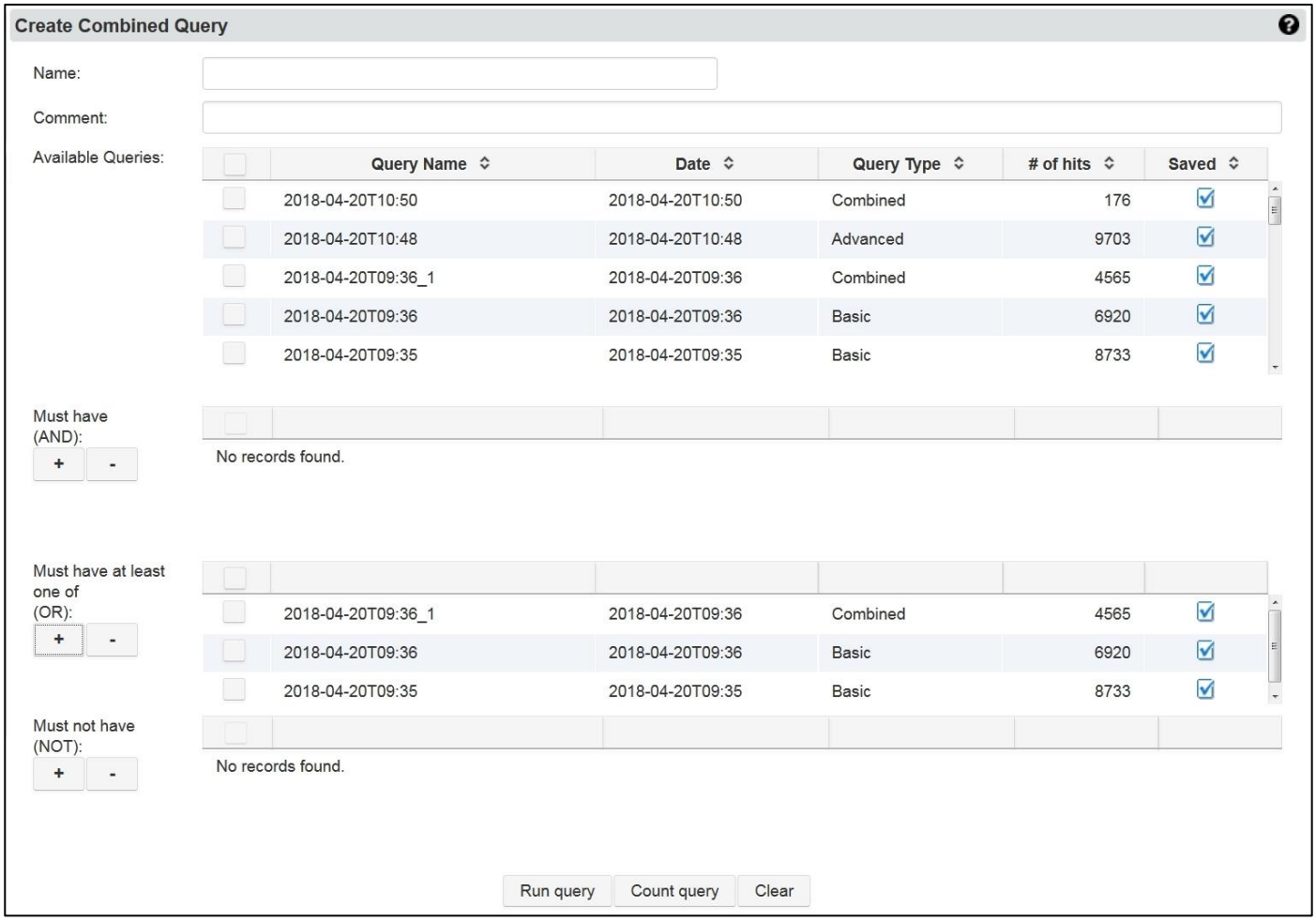


Figure 3: Add queries via any of the three logical operators

The queries will then be visible in one of the tables for the three different logical operators. Each table shows the same information as the Available Queries table.

A query can be removed from the table by checking the checkbox and clicking the corresponding “-“-button (Fig. 4).

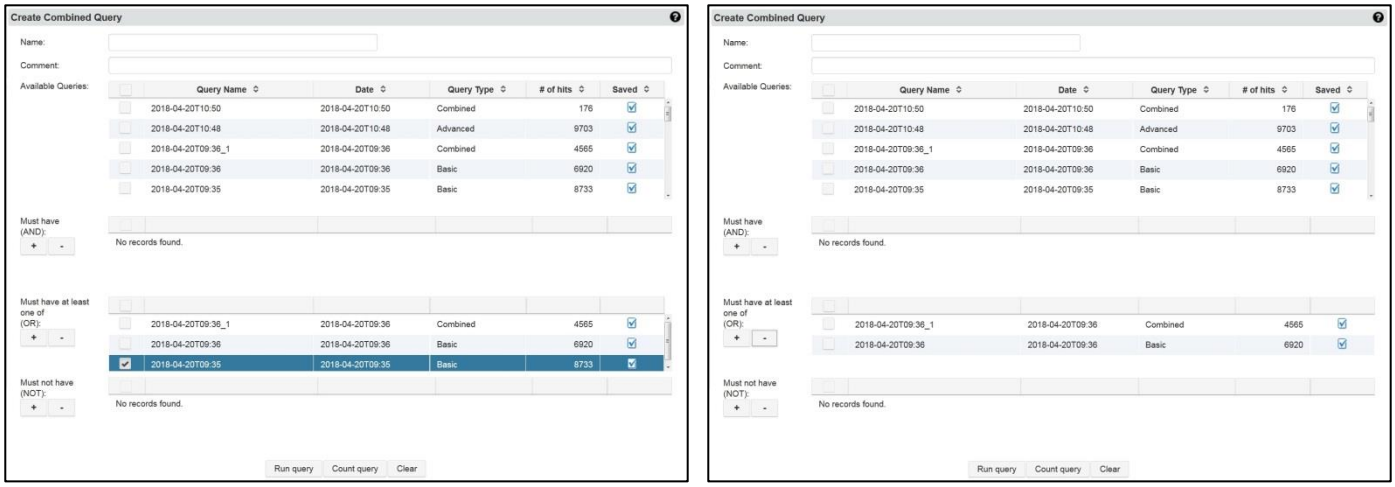


Figure 4: Remove a query from the combined query by first selecting the entry (left) and then click on the corresponding "-"-button.

The three buttons at the bottom of the mask perform (Run Query), check (Count Query) or clear (Clear Query) the query. The functionality is identical to the buttons for the other search masks. Additionally, the Run Query-button saves the combined query as well as all queries used to create it.

Output Management

In order to get help to specific topics, please select one of the following items in the left column:

- List View
- Detailed View
- Export Data
- Print
- Visualize/Compare Structures
- Visualize/Compare Powder Patterns
- Column Selection
- Filter

Information on each input field will be displayed together with some examples.

List View

The List View displays selected properties of the database records contained in the result set (Fig. 1). These properties are displayed on a one-row-per-record basis. Each property is described in one column. Up to 50 hits can be displayed on one page.

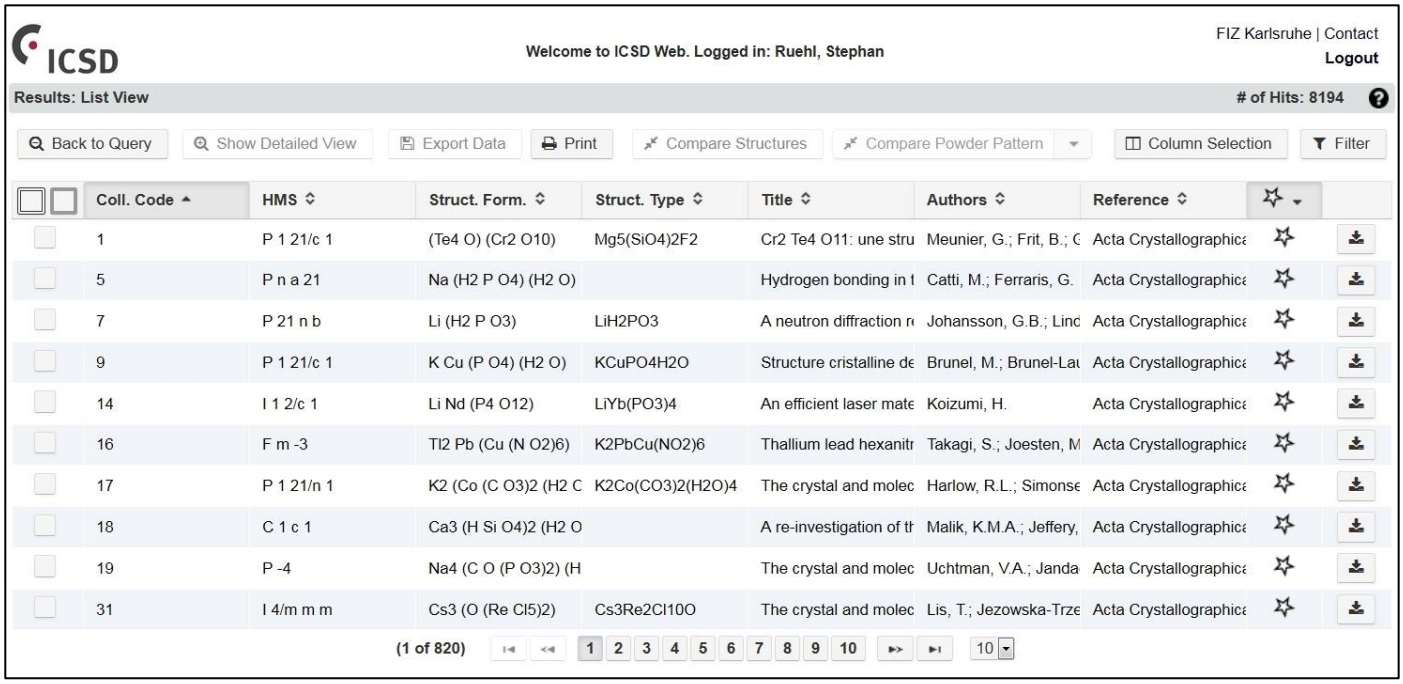


Figure 1: Result set

The columns to be displayed can be selected using the button “Column Selection”. At the moment there are about 30 properties or bibliographic information you can chose for display.

The number of hits to be displayed can be further refined using the Filter settings. If some filters apply a restriction on the displayed hits, the number of hits for the current filter settings and the number of total hits are given in brackets.

The two checkboxes in the first column allow you to select/deselect all entries (left checkbox) or all entries on this page (right checkbox).

Once at least one entry has been selected the options Show Detailed View, Visualize Structure, Visualize Powder Pattern, and Report become available. Once two to six records have been selected the buttons Visualize Structure and Visualize Powder Pattern change to Compare Structures and Compare Powder Patterns, respectively.

The Print button is a convenient shortcut to the regular print option of the browser.

While hovering with the mouse over either the Space group column or the structured formula column, a picture of the structure is displayed as a tooltip. Hovering over all other columns will provide a tooltip with the full information from this field – this is often helpful for fields with much text or many numbers.

Sorting

The data may be sorted by any column in ascending or descending order. Just click on the caption of the column you want to have sorted; a small arrow head will appear, indicating whether records are sorted in ascending (Fig. 2 (left)) or descending (Fig. 2 (right)) order.

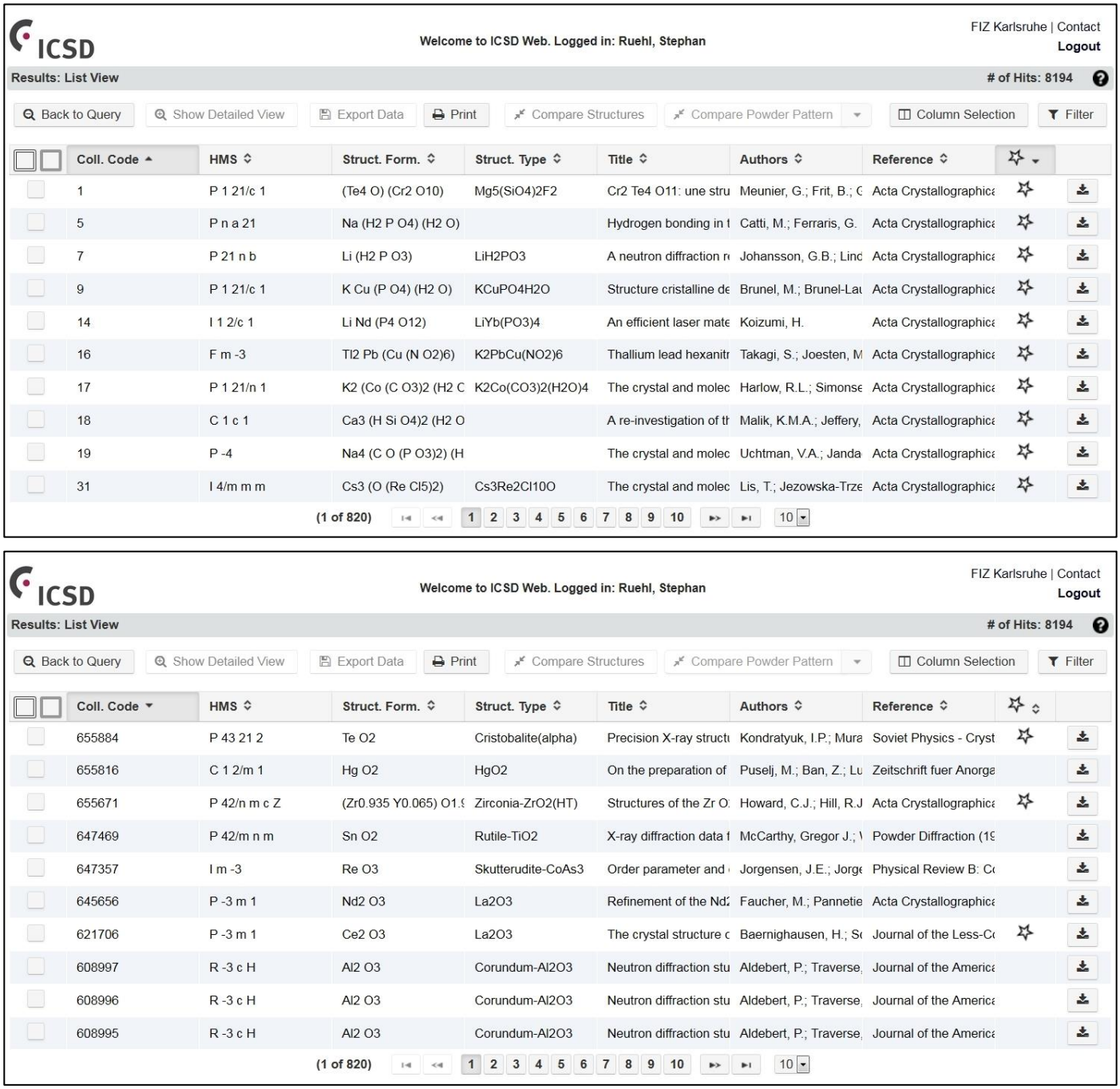


Figure 2: Sorting by ICSD Collection Code. Ascending (top), descending (bottom), indicated by the arrow head to the right of the column caption

To move columns, click on the column caption and keep the left mouse button pressed. Drag and drop the column to the desired position (Fig. 3). In the example the “Authors” column is now at its new position (Fig. 4).

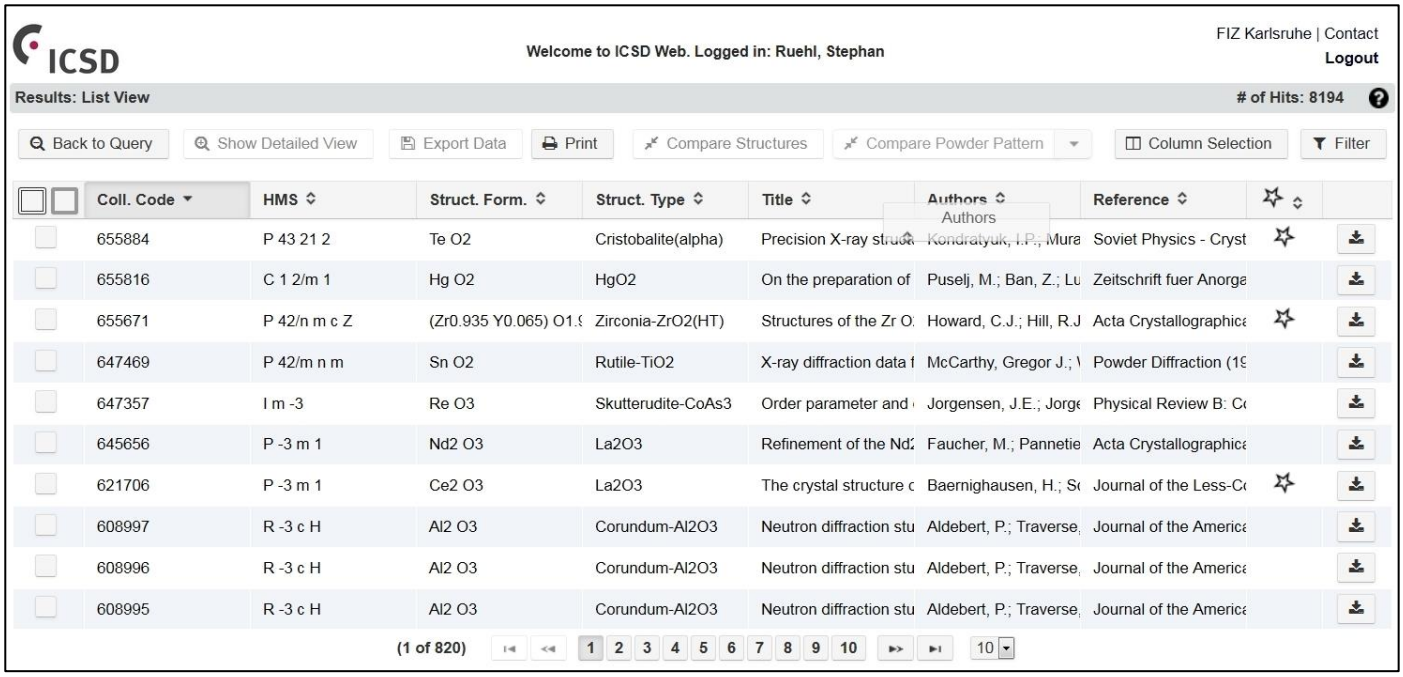


Figure 3: Moving columns

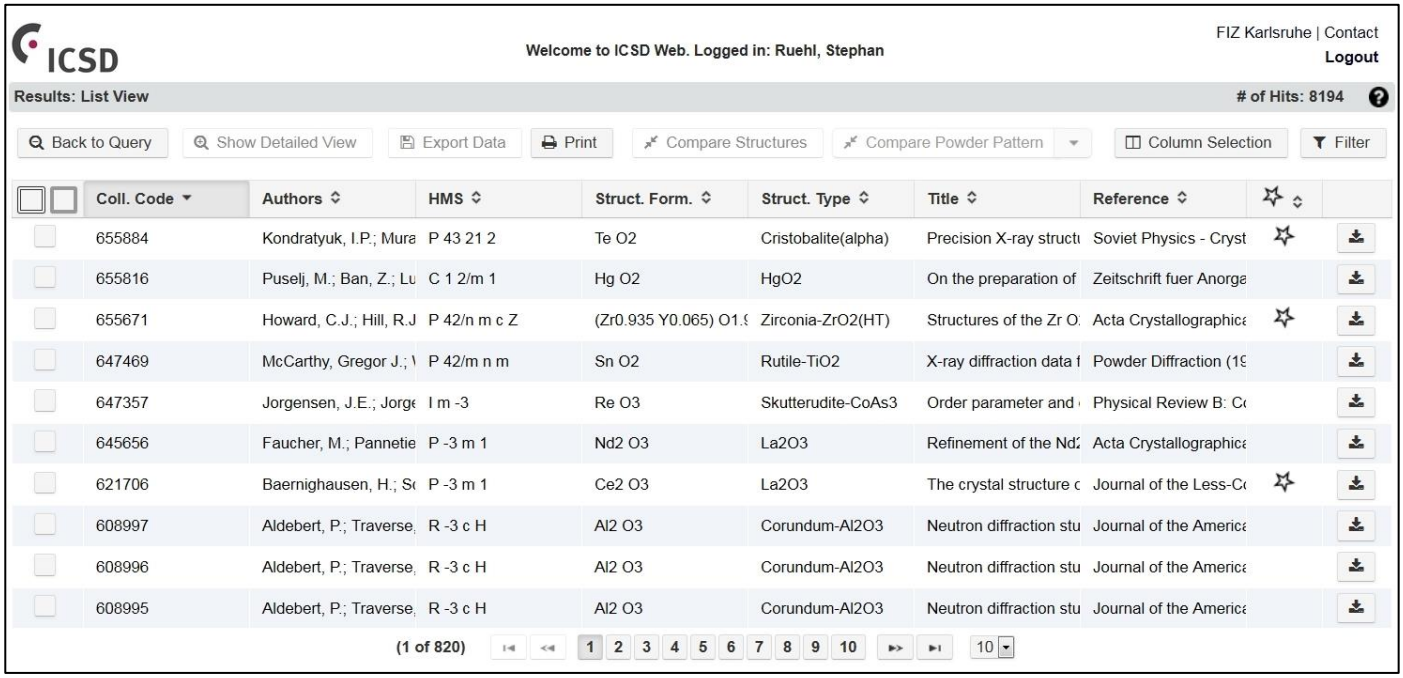


Figure 4: New position of the “Authors” column

To change the width of columns, move the mouse pointer between the columns until it changes its shape to the “Resize mouse pointer”. Click and keep the mouse button pressed. Moving the mouse will change the column width.

Detailed View

The detailed view provides a comprehensive summary of the most important features of an entry. Select the data set(s) you wish to examine: Use the checkboxes of specific records or click on the checkbox in the title of the selection column to select/deselect all records of the current page. The button "Show Detailed View" will be activated when at least one record is selected (Fig. 1).

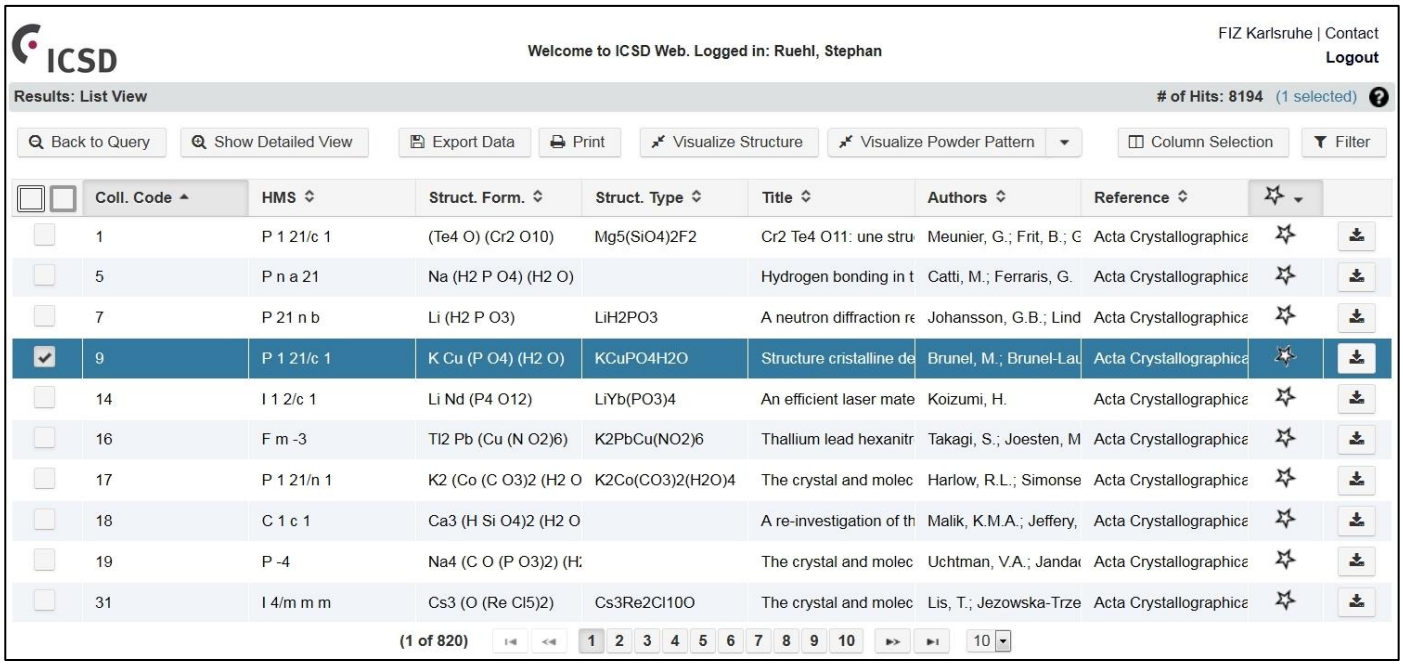


Figure 1: Result set

"Show Detailed View" shows the selected data sets in detailed view mode (Fig. 2). The window consists of three main parts:

1. The navigation shows which record is currently displayed, in this case "Entry 1 of 1".

   The button "Back to Query" deletes the current query and jumps back to the search mask or the Create Combined Query mask depending on where the query was started. The button "Back to List View" shows the result list without deleting the current query. The arrow buttons allow you to jump to the first selected record, to turn to the previous record, to the next record and to the last record, respectively. The "Print"-button provides a shortcut to the regular print function of the browser. And the "Feedback to Editor"-button provides an easy way to send us a feedback on the current record.

2. The summary briefly describes the main features of the current record, such as ICSD Collection Code, unit cell data, reference etc. The fields are also shown in the "Details" section, and will be described there.

3. The Detailed View gives a complete and comprehensive listing of all important record data. It is possible to expand individual sections by clicking on the desired caption, to expand ("Expand all") or to close all sections ("Collapse all"). The individual detail fields will be described below.

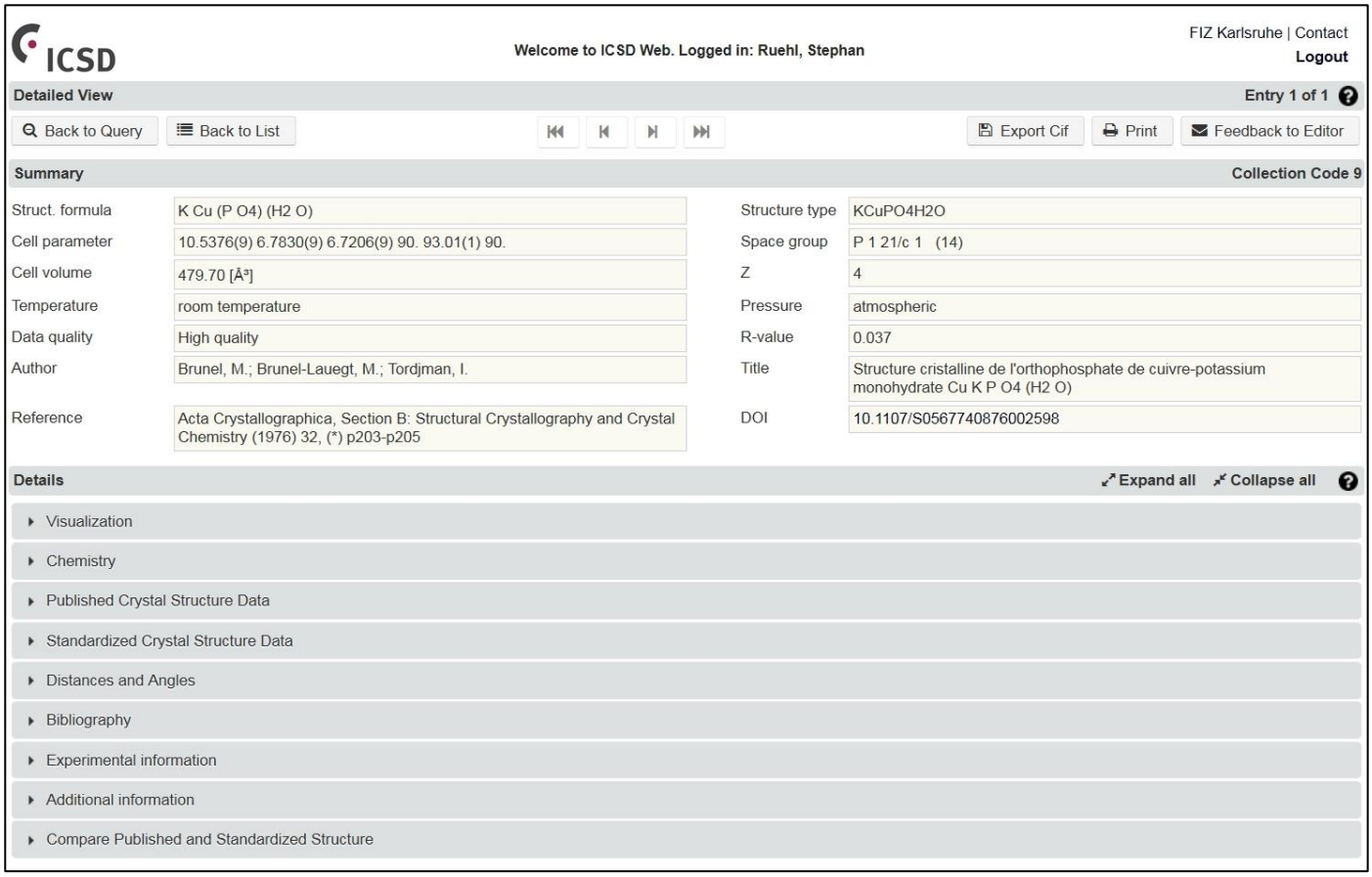


Figure 2: Main parts of the detailed view with the navigation bar, Summary, and Details for several aspects of the selected crystal structure

Description of fields in section “Details”

Visualization

The Visualization field consists of a crystal structure display (Fig. 3, left) and a powder pattern display (Fig. 3, right) part.

The crystal structure display starts with of a picture of the structure. In addition, an interactive crystal structure display can be started in a new window by clicking on the “Interactive Visualization” button (Fig. 4). This makes use of the JSmol [1] applet, showing the most important data within the display box: Space group and lattice constants as published by the author(s), and a 3D picture of the unit cell. The sum formula and the collection code are displayed in the title bar of the JSmol window.

Right-clicking into the structure display box (JSMol applet) opens a pop-up menu, from where you can change the display properties and perform geometric analyses of the displayed structure.

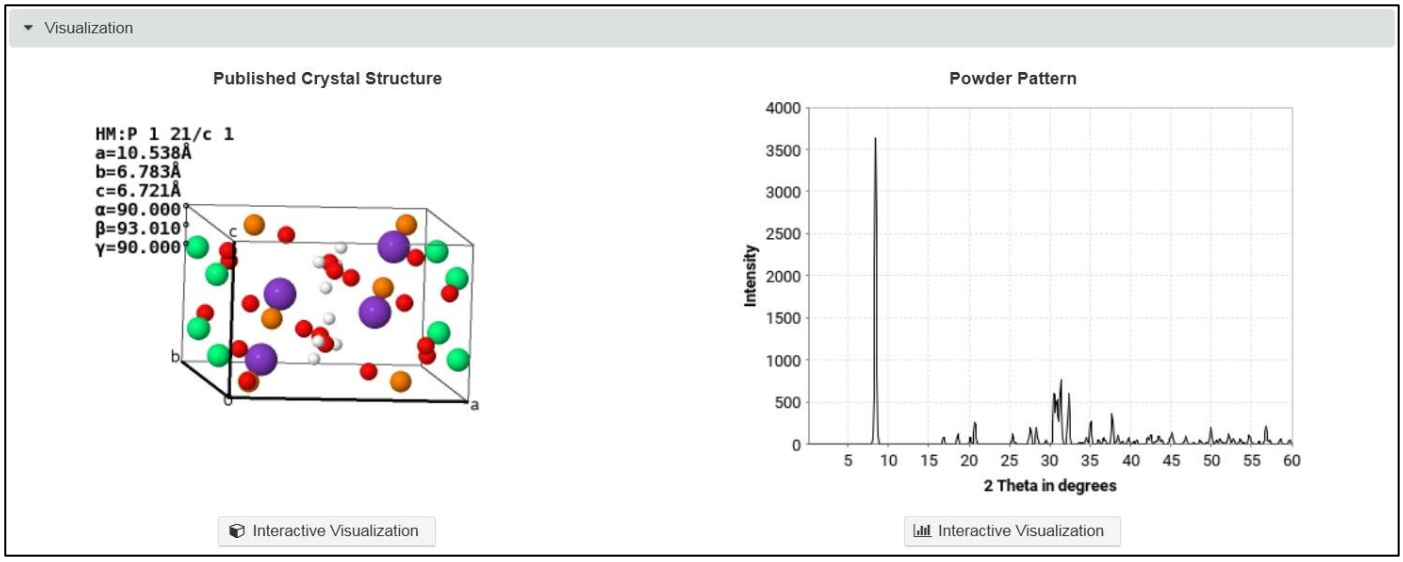


Figure 3: Picture of the crystal structure (left) and powder pattern display (right)

Some options to manipulate the interactive display for the current crystal structure are given in tabs below the display:

- Align: Here you can align the view along the a, b or c axis. The option “Synchronize View” is greyed out as this option is only accessible if several structures are displayed simultaneously. This kind of visualization can be started in the ListView.

- Explore Coordination: This allows to interactively visualize the environment of a selected atom. To start one has to activate the by setting the “Show Coordination” to “Yes”. Then two new options are displayed. First one has to select the central atom by clicking in the field to the right of the Central Atom description. The display now shows all atoms in the unit cell. Once one of these atoms is selected, only the central atom (selected) and the atoms in a certain radius around it are shown. The radius can be increased or decreased using the Distance field.

  On the right there are two additional buttons which offer quick ways to measure distances and angles in the crystal structure display. Clicking on one of the two buttons will display a short description of what is needed to display distances or angles.

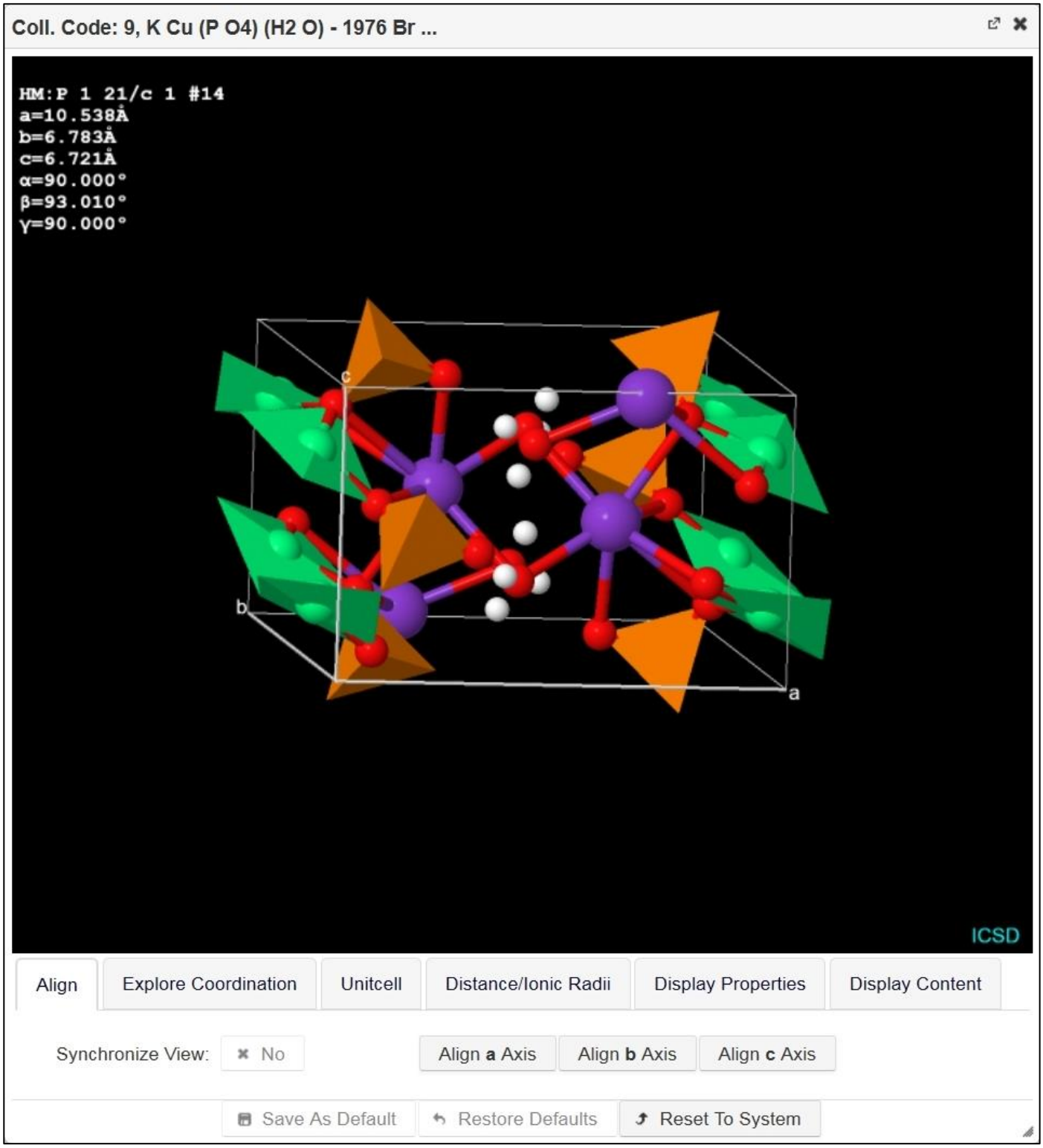


Figure 4: Visualization of the crystal structure in interactive mode in a separate window.

- Unit Cells: Enter the number of unit cells for each lattice direction you want to have displayed. Note: Although it is possible to enter decimal fractions, the fractions will be cut off. The values for a, b, and c are limited to 1.0 - 4.0.

  It is necessary to click on “Apply Unitcell” after making changes in the number of unit cells displayed along each lattice direction.

- Distance/Ionic Radii: The generation and display of bonds can be limited either by defining minimum and maximum distances or by providing minimum and maximum percentages of the sum of the ionic radii of the involved atoms/ions.

- Display Properties: Allows changing certain aspects of displaying the crystal structure, such as

    - background (on/off)
    - perspective drawing (on/off)
    - stereo (red/green) display
    - "Spin" will let the currently displayed structure rotate around the vertical axis
    - "Display Labels" will put the atom labels beside the appropriate atom.

- Display Content: A dropdown box allows for atom display customization. Hydrogen bonds, polyhedral and/or cavities can be shown/hidden by switching the appropriate box on/off. The Select/Mark Atom Site switch lets you highlight the equivalent atoms in the display by clicking on one atom.

- Three additional buttons allow for customization.
    - You can save preferred structure display settings with Jmol by pressing the "Save As Default"-button.
    - Clicking the "Restore Default"-button changes the display properties to the previously saved defaults or to the system defaults if no saved defaults have been created.
    - The "Reset to System"-button will always restore the properties to the original defaults.

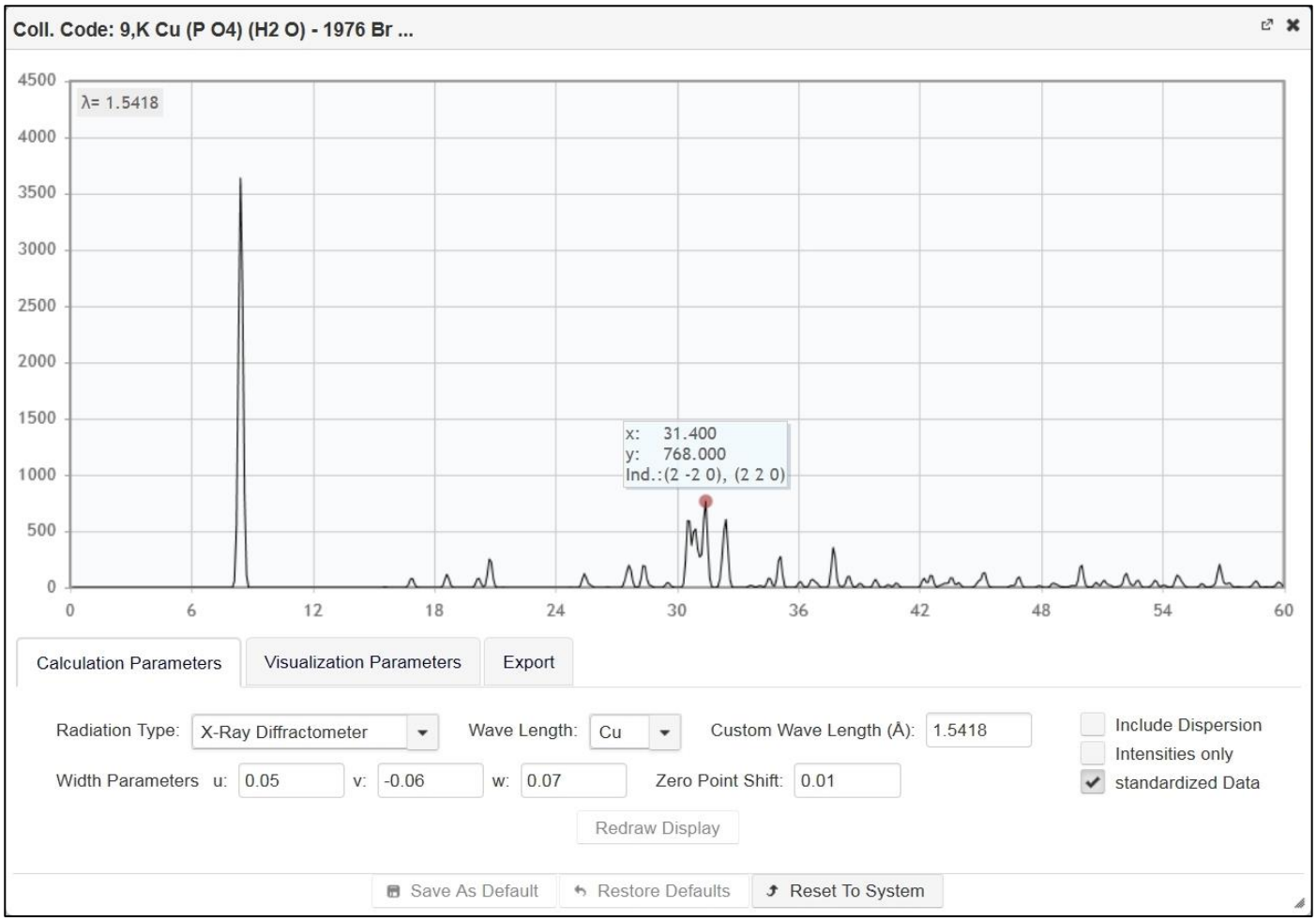


Figure 5: Simulated powder pattern in interactive mode in a separate window.

The right part of the Visualization window shows a picture of a simulated powder pattern of the currently displayed crystal structure. Again, an interactive simulated powder pattern display can be started in a new window by clicking on the "Interactive Visualization" button (Fig. 5) below the powder pattern. In the interactive display one can check the indices of reflections by hovering the mouse over the peak position in the diagram.

Similar to the interactive visualization display, the powder pattern display shows some basic information in the title bar (collection code, sum formula, publication year and authors).

There are also some options to manipulate the interactive calculation of the simulated powder pattern which are given in tabs below the display:

- Calculation Parameters: With the dropdown box "Radiation Type" one can select either X-Ray Diffraction or Neutron Diffraction. The appropriate wavelength can either be selected from a dropdown box (possible sources are Cu, Cr, Fe, Mo, and Ag) or one can enter a custom wavelength (Angstrom units).

  The reflex profile parameters *U*, *V* and *W* can be changed. In addition one can set a zero shift parameter.

  Toggling between line diagrams (checkbox "Intensities only") and standard powder patterns (Gauß envelope) is possible, too. One can also include or exclude dispersion. The default setting is to use the standardized data for the powder pattern generation, but one can also switch this off and then the published data are used. Of course, this does not change the powder pattern, but the indices may be different.

  It is necessary to click on "Redraw Display" after making any changes.

- Visualization Parameters: Here one can choose between 2 plot types: 2theta and d. 2theta plots in the range 0.1-60° in 0.1° steps are shown per default. x_{min}, x_{max}, and x_{step} describe the starting, the ending and the step value according to the chosen plot type, respectively.

  Additionally, it is possible to display the corresponding indices for each reflection and to colour the powder pattern in red.

  It is necessary to click on "Redraw Display" after making any changes.

- Export: You can export the simulated powder pattern as a two-column x-y data file or export it as a PDF file. In addition, a table can be created with hkl, 2 theta, d, multiplicity and intensity for each reflection in a txt-file.

Chemistry

Figure 6 highlights some chemical information on the structure. The sum formula is shown with all stoichiometric coefficients, where the elements are sorted in the order C, H (D), (the rest of the elements in alphabetic order). In the field "Struct. Formula" (Structured Formula – not Structural Formula!) certain building blocks of a chemical compound are grouped, e.g. Ca (C O3) (H2 O)6, where the sum formula just lists all elements with their coefficients, e.g. C1 H12 Ca1 O9.

The "Molecular weight" is calculated based on the sum formula.

The number of formula units (Z) shows how many times the unit cell contains the atoms in the field "Sum Form".

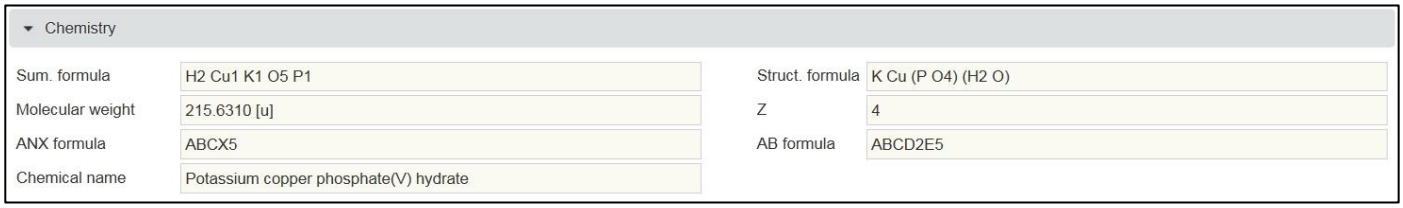


Figure 6: Chemistry details

The ANX formula is generated according to the following rules (see Tab. 1 for examples):

- H^+ is not taken into account, even if coordinates are available.
- The coordinates for all sites of all other atoms must be determined.
- Different atom types on the same position are being treated as one single atom type. The relevant atom type is the one with the highest site occupation factor (SOF). If the SOFs are equal, the first atom type is the relevant atom type.
  Exception to this rule: if anions and cations occupy the same site they will not be treated as one atom type.
- All sites occupied by the same atom type are combined unless the oxidation state is different.

  $Fe^{2+}(Fe^{3+})_2O_4 \rightarrow AB2X4$
  $(Fe^{2.6667+})_3O_4 \rightarrow A3X4$

- 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 the rounded sum is equal to zero all sums are multiplied by a common factor so that the smallest sum is equal to 1.0, so no element will be omitted.
- 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 and the characters are assigned according to ascending indices: AB2X4, not A2BX4.
- All ANX formulae with more than 4 cation symbols, 3 neutral symbols or 3 anion symbols are deleted. This measure limits the number of different ANX formulae.

Table 1: Examples for ANX formulae

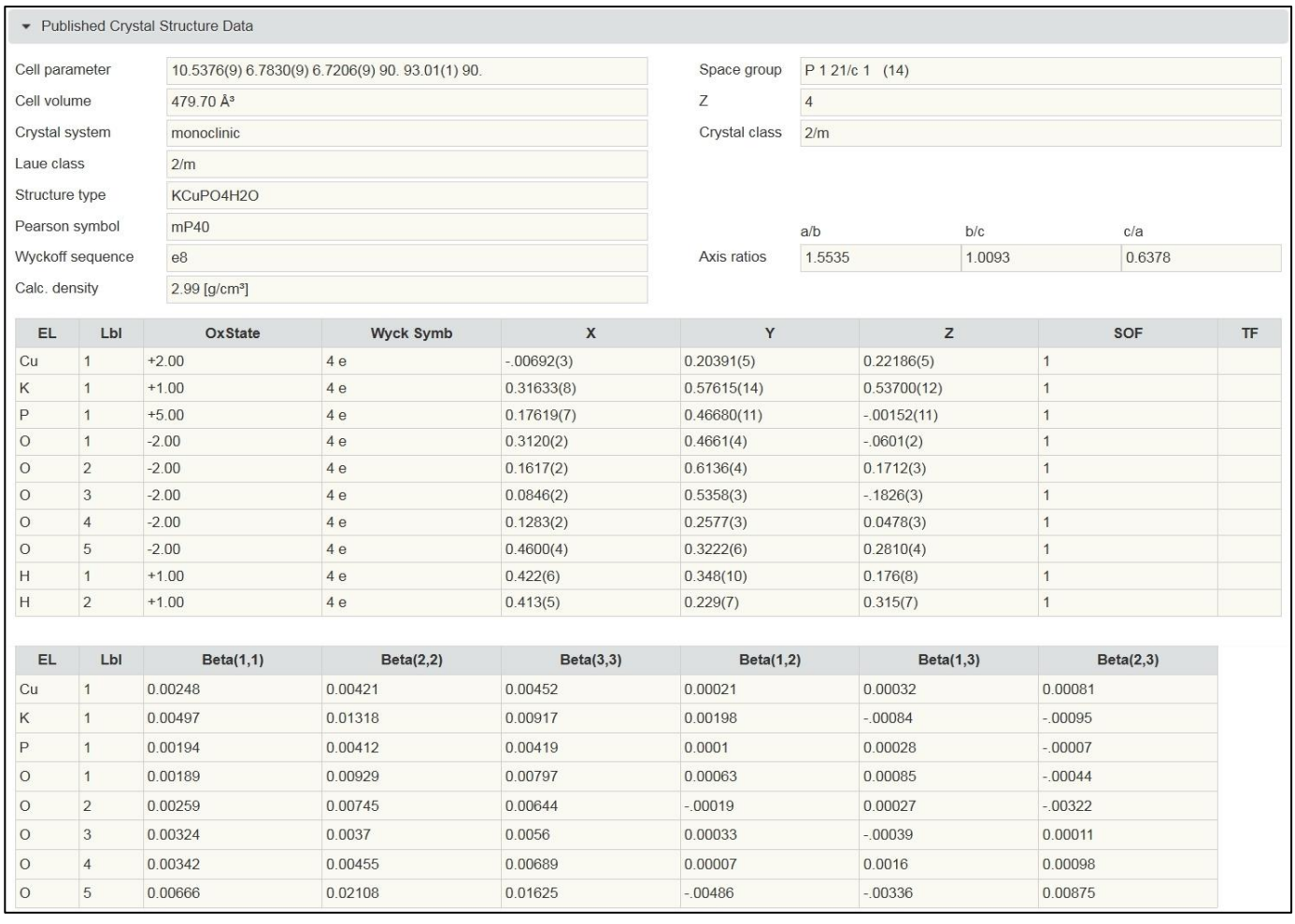
Chemical formula	ANX formula
$Mg_3Al_2(SiO_4)_3$	A2B3C3X12
$Ca_3(Al_{1.3325}Fe_{0.6675})Si_3O_{12}$	A2B3C3X12
$(Mg_{2.7}Fe_{0.3})(Al_{1.7}Cr_{0.3})Si_3O_{12}$	A2B3C3X12

The chemical name, the mineral name and the mineral group are listed accordingly. The place where the mineral is found may be given in the field "Mineral origin".

Published Crystal Structure Data

The field "Published Crystal Structure Data" (Fig. 7) shows the crystallographic information as given by the author(s) or derived from the symmetry. Among the cell parameters, space group, crystal system, crystal class, and Laue class you will find the cell volume, number of formula units (Z) and structure type information. In addition there is some information about the most important descriptors for the structure types: Pearson symbol, Wyckoff sequence, and Axis ratios. Finally, the calculated density and, if given in the publication, the measured density are also listed.

The list of atomic coordinates and, if available, the anisotropic displacement parameters are also contained. If the atomic coordinates were derived based on another structure with the same structure type, there will be a Remarks field mentioning that only "Derived coordinates" are shown.



Published Crystal Structure Data

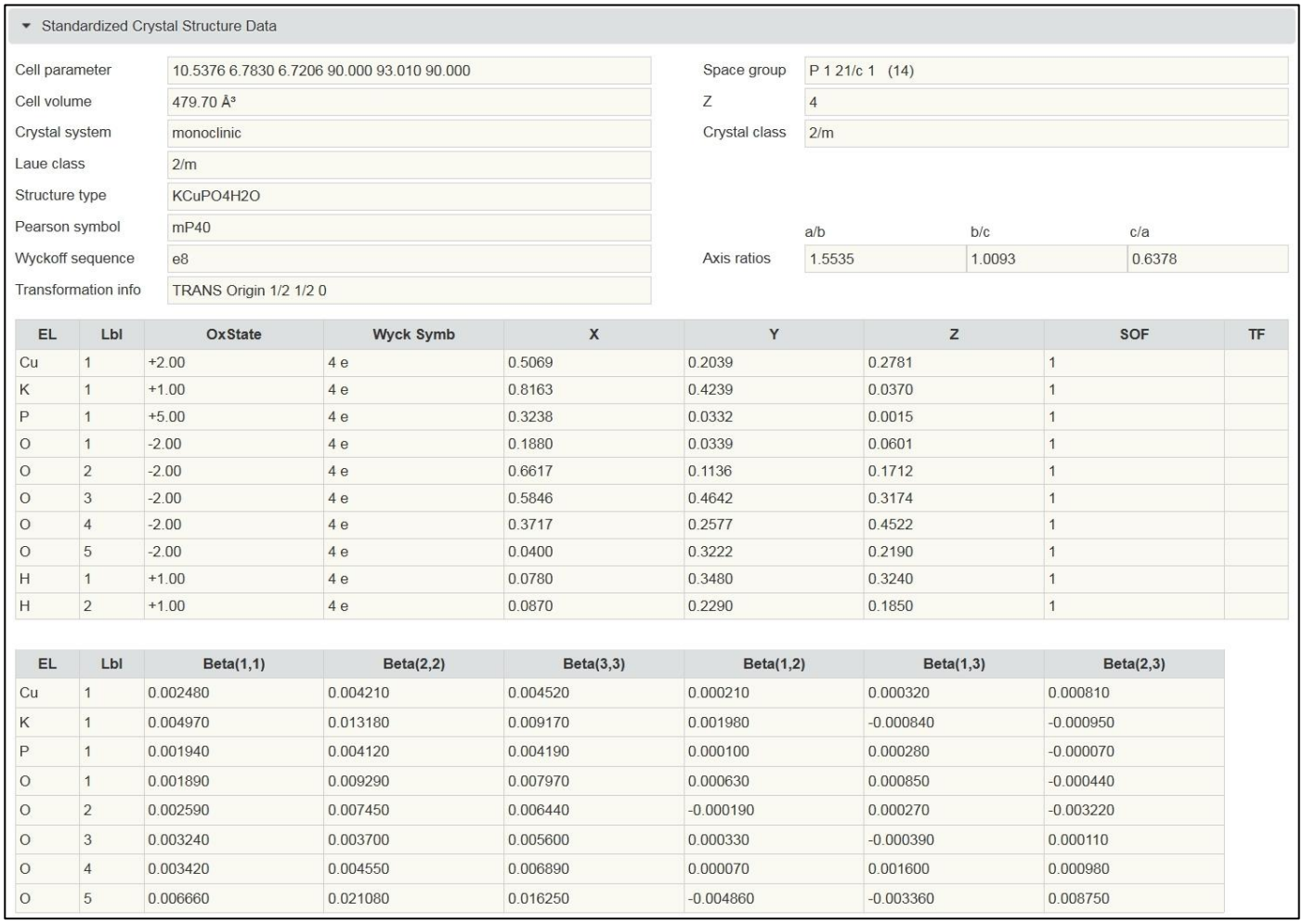
Cell parameter	10.5376(9) 6.7830(9) 6.7206(9) 90. 93.01(1) 90.	Space group	P 1 21/c 1 (14)
Cell volume	479.70 Å³	Z	4
Crystal system	monoclinic	Crystal class	2/m
Laue class	2/m		
Structure type	KCuPO4H2O		
Pearson symbol	mP40		
Wyckoff sequence	e8	Axis ratios	a/b 1.5535, b/c 1.0093, c/a 0.6378
Calc. density	2.99 [g/cm³]		

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	TF
Cu	1	+2.00	4 e	-.00692(3)	0.20391(5)	0.22186(5)	1	
K	1	+1.00	4 e	0.31633(8)	0.57615(14)	0.53700(12)	1	
P	1	+5.00	4 e	0.17619(7)	0.46680(11)	-.00152(11)	1	
O	1	-2.00	4 e	0.3120(2)	0.4661(4)	-.0601(2)	1	
O	2	-2.00	4 e	0.1617(2)	0.6136(4)	0.1712(3)	1	
O	3	-2.00	4 e	0.0846(2)	0.5358(3)	-.1826(3)	1	
O	4	-2.00	4 e	0.1283(2)	0.2577(3)	0.0478(3)	1	
O	5	-2.00	4 e	0.4600(4)	0.3222(6)	0.2810(4)	1	
H	1	+1.00	4 e	0.422(6)	0.348(10)	0.176(8)	1	
H	2	+1.00	4 e	0.413(5)	0.229(7)	0.315(7)	1	

EL	Lbl	Beta(1,1)	Beta(2,2)	Beta(3,3)	Beta(1,2)	Beta(1,3)	Beta(2,3)
Cu	1	0.00248	0.00421	0.00452	0.00021	0.00032	0.00081
K	1	0.00497	0.01318	0.00917	0.00198	-.00084	-.00095
P	1	0.00194	0.00412	0.00419	0.0001	0.00028	-.00007
O	1	0.00189	0.00929	0.00797	0.00063	0.00085	-.00044
O	2	0.00259	0.00745	0.00644	-.00019	0.00027	-.00322
O	3	0.00324	0.0037	0.0056	0.00033	-.00039	0.00011
O	4	0.00342	0.00455	0.00689	0.00007	0.0016	0.00098
O	5	0.00666	0.02108	0.01625	-.00486	-.00336	0.00875

Figure 7: Published Crystal Structure data

The “Standardized Crystal Structure Data” (Fig. 8) is derived from the published data and gives information on most of the fields as for the published data. Some more information about the standardization is given in the field “Transformation info”. The standardization is done following the rules given by L. M. Gelato and E. Parthé in J. Appl. Cryst. (1987) 20, 139-143.



Standardized Crystal Structure Data

Cell parameter	10.5376 6.7830 6.7206 90.000 93.010 90.000	Space group	P 1 21/c 1 (14)
Cell volume	479.70 Å³	Z	4
Crystal system	monoclinic	Crystal class	2/m
Laue class	2/m		
Structure type	KCuPO4H2O		
Pearson symbol	mP40		a/b b/c c/a
Wyckoff sequence	e8	Axis ratios	1.5535 1.0093 0.6378
Transformation info	TRANS Origin 1/2 1/2 0		

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	TF
Cu	1	+2.00	4 e	0.5069	0.2039	0.2781	1	
K	1	+1.00	4 e	0.8163	0.4239	0.0370	1	
P	1	+5.00	4 e	0.3238	0.0332	0.0015	1	
O	1	-2.00	4 e	0.1880	0.0339	0.0601	1	
O	2	-2.00	4 e	0.6617	0.1136	0.1712	1	
O	3	-2.00	4 e	0.5846	0.4642	0.3174	1	
O	4	-2.00	4 e	0.3717	0.2577	0.4522	1	
O	5	-2.00	4 e	0.0400	0.3222	0.2190	1	
H	1	+1.00	4 e	0.0780	0.3480	0.3240	1	
H	2	+1.00	4 e	0.0870	0.2290	0.1850	1	

EL	Lbl	Beta(1,1)	Beta(2,2)	Beta(3,3)	Beta(1,2)	Beta(1,3)	Beta(2,3)
Cu	1	0.002480	0.004210	0.004520	0.000210	0.000320	0.000810
K	1	0.004970	0.013180	0.009170	0.001980	-0.000840	-0.000950
P	1	0.001940	0.004120	0.004190	0.000100	0.000280	-0.000070
O	1	0.001890	0.009290	0.007970	0.000630	0.000850	-0.000440
O	2	0.002590	0.007450	0.006440	-0.000190	0.000270	-0.003220
O	3	0.003240	0.003700	0.005600	0.000330	-0.000390	0.000110
O	4	0.003420	0.004550	0.006890	0.000070	0.001600	0.000980
O	5	0.006660	0.021080	0.016250	-0.004860	-0.003360	0.008750

Figure 8: Standardized Crystal Structure data

Distances and Angles

The distances and angles dialogue enables you to perform statistical analyses of interatomic distances and angles. You can either choose from the element type lists (Fig. 9) or from the atom position lists (Fig. 10).

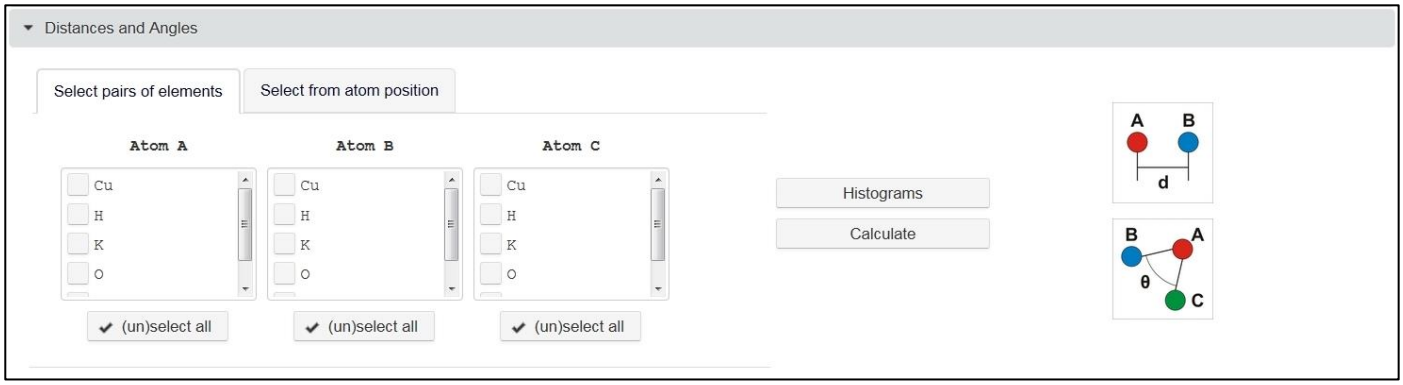


Figure 9: Distances and Angles screen: selection by elements

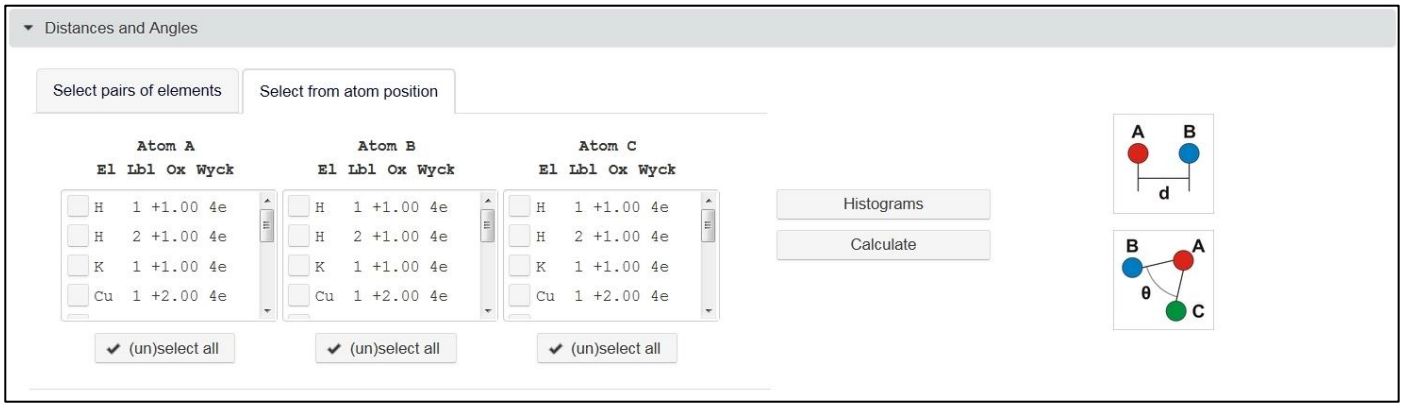
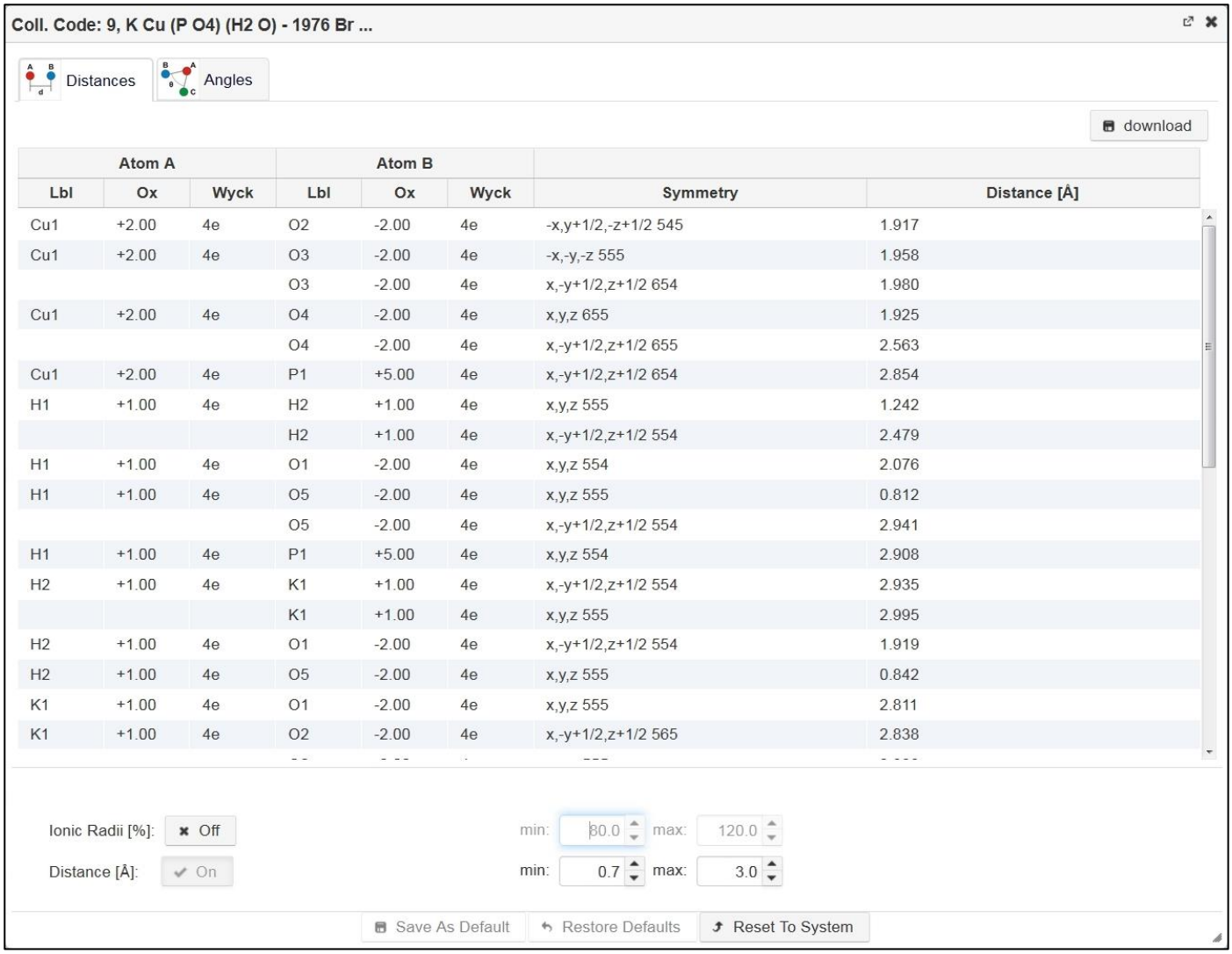


Figure 10: Distances and Angles screen: selection by atom positions

When at least one element/atom position each in Atom A and Atom B is selected, you may click the "Histograms" or the "Calculate" button.

"Calculate" will generate a list of bond length if only Atom A and Atom B contain selected element/atom positions. Bond angles are calculated if in addition at least one element/atom position is selected in the Atom C field. The maximum search range (Rmax) is 5 Angstrom for distances and 200% for the sum of ionic radii (again 5 Angstrom is the internal upper limit). This can be changed in the newly opened window. The result can be exported as a csv file by using the download button on the top right.

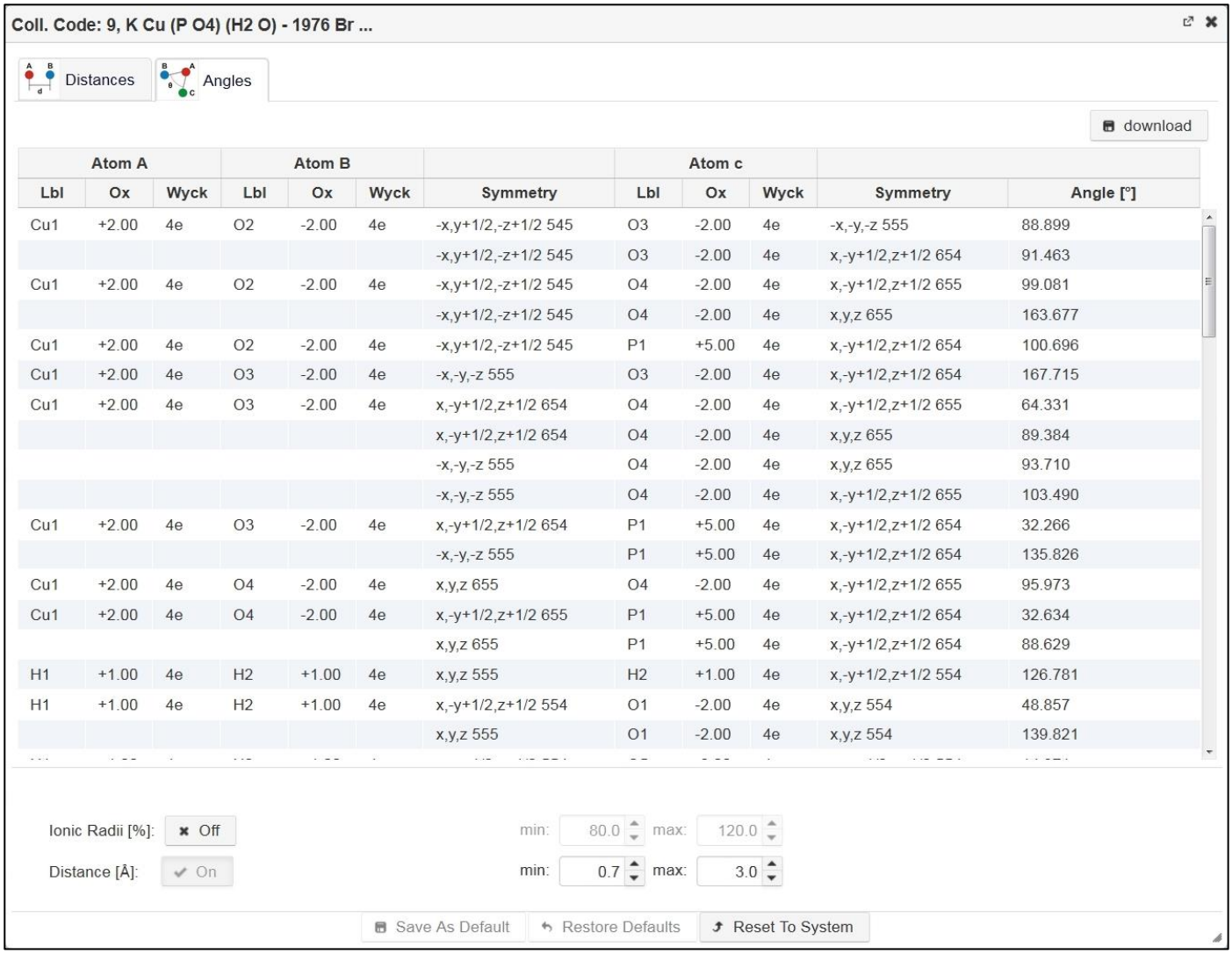


Atom A			Atom B				
Lbl	Ox	Wyck	Lbl	Ox	Wyck	Symmetry	Distance [Å]
Cu1	+2.00	4e	O2	-2.00	4e	-x,y+1/2,-z+1/2 545	1.917
Cu1	+2.00	4e	O3	-2.00	4e	-x,-y,-z 555	1.958
			O3	-2.00	4e	x,-y+1/2,z+1/2 654	1.980
Cu1	+2.00	4e	O4	-2.00	4e	x,y,z 655	1.925
			O4	-2.00	4e	x,-y+1/2,z+1/2 655	2.563
Cu1	+2.00	4e	P1	+5.00	4e	x,-y+1/2,z+1/2 654	2.854
H1	+1.00	4e	H2	+1.00	4e	x,y,z 555	1.242
			H2	+1.00	4e	x,-y+1/2,z+1/2 554	2.479
H1	+1.00	4e	O1	-2.00	4e	x,y,z 554	2.076
H1	+1.00	4e	O5	-2.00	4e	x,y,z 555	0.812
			O5	-2.00	4e	x,-y+1/2,z+1/2 554	2.941
H1	+1.00	4e	P1	+5.00	4e	x,y,z 554	2.908
H2	+1.00	4e	K1	+1.00	4e	x,-y+1/2,z+1/2 554	2.935
			K1	+1.00	4e	x,y,z 555	2.995
H2	+1.00	4e	O1	-2.00	4e	x,-y+1/2,z+1/2 554	1.919
H2	+1.00	4e	O5	-2.00	4e	x,y,z 555	0.842
K1	+1.00	4e	O1	-2.00	4e	x,y,z 555	2.811
K1	+1.00	4e	O2	-2.00	4e	x,-y+1/2,z+1/2 565	2.838

Figure 11: A text-only list of interatomic distances

The bond length dialogue consists of a text-only list of interatomic distances within the defined range, including oxidation states, Wyckoff symbols and the symmetry operation necessary to create Atom B (Fig. 11). Please note, that the translational part is encoded. 555 is the current unit cell. If 1.0 is added to the y-coordinate, 555 becomes 565. A number 456 means that 1.0 is substracted from the x-coordinate and 1.0 is added to the z-coordinate.

The dialogue for bonds and angles shows a text-only list of interatomic distances as above as well as a list of bond angles in a different tab. The angles list consists of the atom, oxidation state and Wyckoff symbol as well as for all atoms the symmetry operation necessary to generate Atoms B and C (Fig. 12).



Atom A			Atom B				Atom c				
Lbl	Ox	Wyck	Lbl	Ox	Wyck	Symmetry	Lbl	Ox	Wyck	Symmetry	Angle [°]
Cu1	+2.00	4e	O2	-2.00	4e	-x,y+1/2,-z+1/2 545	O3	-2.00	4e	-x,-y,-z 555	88.899
						-x,y+1/2,-z+1/2 545	O3	-2.00	4e	x,-y+1/2,z+1/2 654	91.463
Cu1	+2.00	4e	O2	-2.00	4e	-x,y+1/2,-z+1/2 545	O4	-2.00	4e	x,-y+1/2,z+1/2 655	99.081
						-x,y+1/2,-z+1/2 545	O4	-2.00	4e	x,y,z 655	163.677
Cu1	+2.00	4e	O2	-2.00	4e	-x,y+1/2,-z+1/2 545	P1	+5.00	4e	x,-y+1/2,z+1/2 654	100.696
Cu1	+2.00	4e	O3	-2.00	4e	-x,-y,-z 555	O3	-2.00	4e	x,-y+1/2,z+1/2 654	167.715
Cu1	+2.00	4e	O3	-2.00	4e	x,-y+1/2,z+1/2 654	O4	-2.00	4e	x,-y+1/2,z+1/2 655	64.331
						x,-y+1/2,z+1/2 654	O4	-2.00	4e	x,y,z 655	89.384
						-x,-y,-z 555	O4	-2.00	4e	x,y,z 655	93.710
						-x,-y,-z 555	O4	-2.00	4e	x,-y+1/2,z+1/2 655	103.490
Cu1	+2.00	4e	O3	-2.00	4e	x,-y+1/2,z+1/2 654	P1	+5.00	4e	x,-y+1/2,z+1/2 654	32.266
						-x,-y,-z 555	P1	+5.00	4e	x,-y+1/2,z+1/2 654	135.826
Cu1	+2.00	4e	O4	-2.00	4e	x,y,z 655	O4	-2.00	4e	x,-y+1/2,z+1/2 655	95.973
Cu1	+2.00	4e	O4	-2.00	4e	x,-y+1/2,z+1/2 655	P1	+5.00	4e	x,-y+1/2,z+1/2 654	32.634
						x,y,z 655	P1	+5.00	4e	x,-y+1/2,z+1/2 654	88.629
H1	+1.00	4e	H2	+1.00	4e	x,y,z 555	H2	+1.00	4e	x,-y+1/2,z+1/2 554	126.781
H1	+1.00	4e	H2	+1.00	4e	x,-y+1/2,z+1/2 554	O1	-2.00	4e	x,y,z 554	48.857
						x,y,z 555	O1	-2.00	4e	x,y,z 554	139.821

Figure 12: A text-only list of angles

Switching to the “Histograms” view (Fig. 13) opens a new window which shows two graphs. The upper one shows the number of occurrences of interatomic distances of the selected pair(s) of atoms in the whole database. The interatomic distance(s) found in the current record are marked blue; they are explicitly shown in the lower graph. While the x-axis shows distances in Angstrom units, the y-axis shows the number of occurrences.

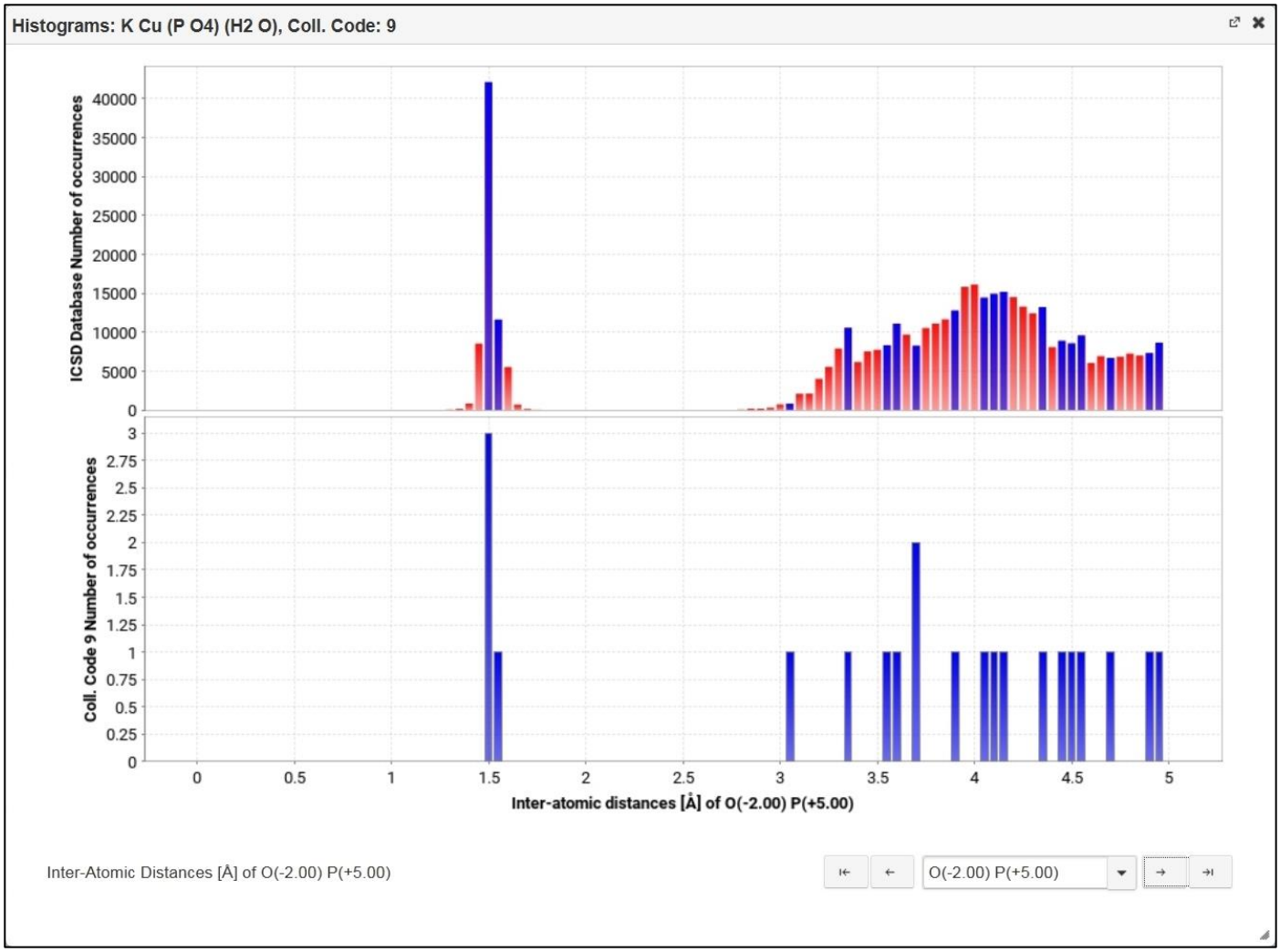


Figure 13: Histograms of interatomic distances

Bibliography

Fig. 14 shows the bibliographic information of the current record: authors, title of the article, reference and DOI. If an abstract is available for this record it is also shown. The “Get full text” link provides a connection to the publication for the current record.

If your institution has a SFX link resolver installed you can provide us with the necessary information (URL of the server and URL of a small logo). In this case your logo and an optional descriptive text is displayed and requests for original articles are redirected to your SFX link resolver.

This implementation of OpenURL is compatible with link resolvers like SFX or with document delivery services like FIZ Autodoc.

If no link resolver information is stored the default is linking to Google Scholar to search for the article.

Figure 14: Bibliography

If an abstract is available for this record it is displayed after the keywords.

Experimental Information/Theoretical information

The information displayed for this section depends on the kind of structure selected (Fig. 15). The section is called Experimental Information for each experimental structure and Theoretical Information for calculated structures. In any case some details about the experiment/calculation are provided.

For experimentally determined structures information about the temperature and the pressure of the measurement is given as published by the authors. If no pressure or temperature has been published, default values of 0.101325 MPa and 293 K are assumed and added. The corresponding fields then show “atmospheric” for the pressure and “room temperature” in the temperature field.

The “Radiation type” used for the measurement is given as one of: X-ray, electrons, neutrons, or synchrotron. Possible “Sample types” are either polycrystalline powder or single crystal. The “R-value” of a subsequent refinement is also given if available.

Some further information can be given as “Remarks”.

Theoretically calculated structures also provide some information about the temperature and pressure assumed for the calculation. Further technical details on the applied methods can be found in the field “Calculation method”. There may also be more information in the field “Remarks”.

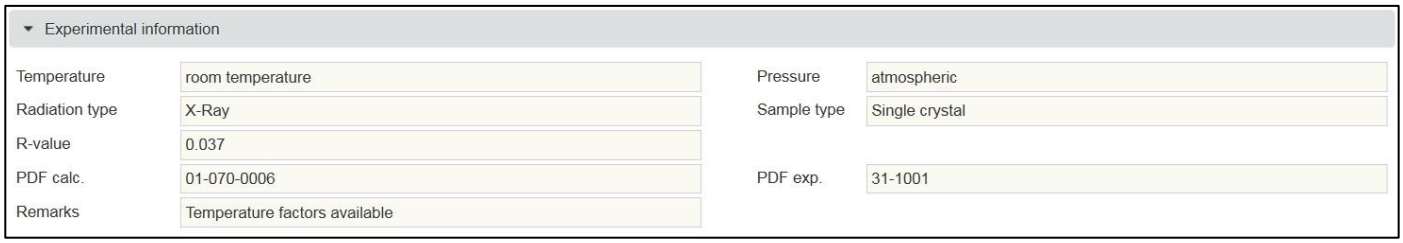


Figure 15: Experimental Information

Additional Information

Here you will find more information about known properties, or technical applications of the structure provided as keywords (Fig. 16). In the comments there may be some more details about the structure (for experimental structures) or about the technical details of the calculation (for theoretical structures).

Figure 16: Additional information

Compare Published and Standardized Structure

Figure 17 shows pictures of the published and the standardized structure side-by-side for easy comparison. Again, you can open the two structures side-by-side in a new window by clicking the "Interactive Visualization"-button (Fig. 18).

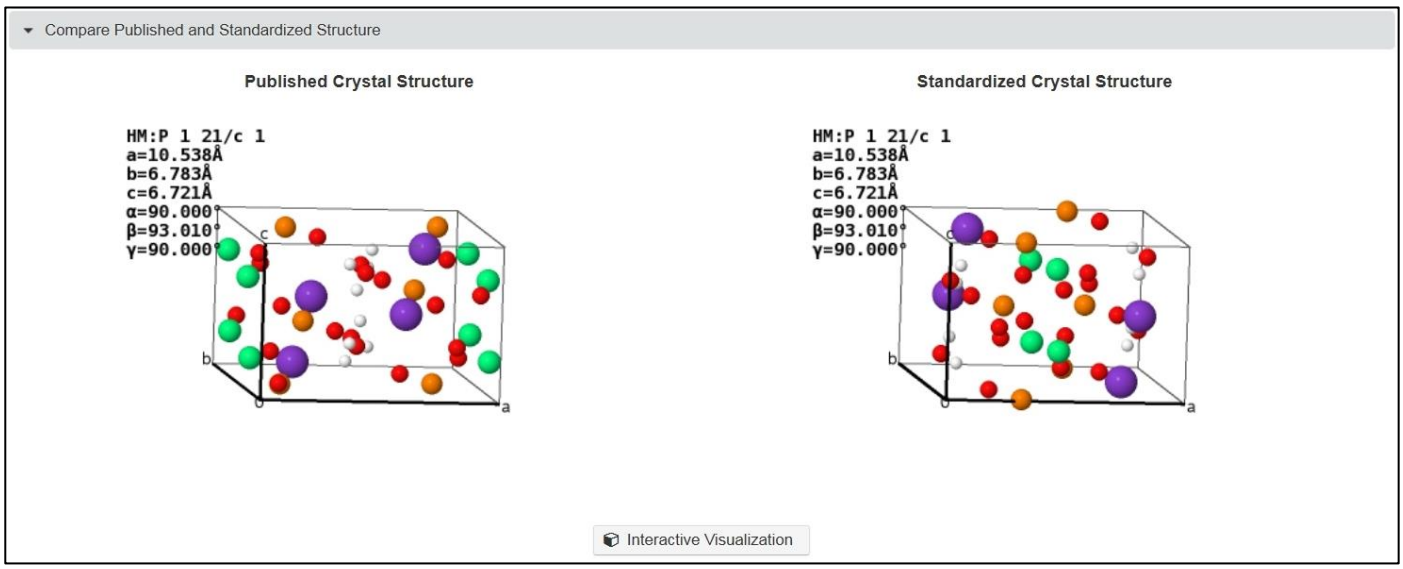


Figure 17: Comparison of published and standardized structures

Right-clicking into the structure display box (only in the JSMol applet not in the simple picture shown at the beginning) opens a pop-up menu, from where you can change the display properties and perform geometric analyses of the displayed structure.

Some options to manipulate the interactive display for the current crystal structure are given in tabs below the display:

- Align: Here you can align the view along the a, b or c axis. The option "Synchronize View" is greyed out as this option is only accessible if several structures are displayed simultaneously. This kind of visualization can be started in the ListView.

- Explore Coordination: This allows to interactively visualize the environment of a selected atom. To start one has to activate the by setting the "Show Coordination" to "Yes". Then two new options are displayed. First one has to select the central atom by clicking in the field to the right of the Central Atom description. The display now shows all atoms in the unit cell. Once one of

these atoms is selected, only the central atom (selected) and the atoms in a certain radius around it are shown. The radius can be increased or decreased using the Distance field.

On the right there are two additional buttons which offer quick ways to measure distances and angles in the crystal structure display. Clicking on one of the two buttons will display a short description of what is needed to display distances or angles.

- Unit Cells: Enter the number of unit cells for each lattice direction you want to have displayed. Note: Although it is possible to enter decimal fractions, the fractions will be cut off. The values for a, b, and c are limited to 1.0 - 4.0.

  It is necessary to click on “Apply Unitcell” after making changes in the number of unit cells displayed along each lattice direction.

- Distance/Ionic Radii: The generation and display of bonds can be limited either by defining minimum and maximum distances or by providing minimum and maximum percentages of the sum of the ionic radii of the involved atoms/ions.

- Display Properties: Allows changing certain aspects of displaying the crystal structure, such as

  - background (on/off)
  - perspective drawing (on/off)
  - stereo (red/green) display
  - “Spin” will let the currently displayed structure rotate around the vertical axis
  - “Display Labels” will put the atom labels beside the appropriate atom.

- Display Content: A dropdown box allows for atom display customization. Hydrogen bonds, polyhedral and/or cavities can be shown/hidden by switching the appropriate box on/off. The Select/Mark Atom Site switch lets you highlight the equivalent atoms in the display by clicking on one atom.

- Three additional buttons allow for customization.
  - You can save preferred structure display settings with Jmol by pressing the "Save As Default"-button.
  - Clicking the "Restore Default"-button changes the display properties to the previously saved defaults or to the system defaults if no saved defaults have been created.
  - The "Reset to System"-button will always restore the properties to the original defaults.

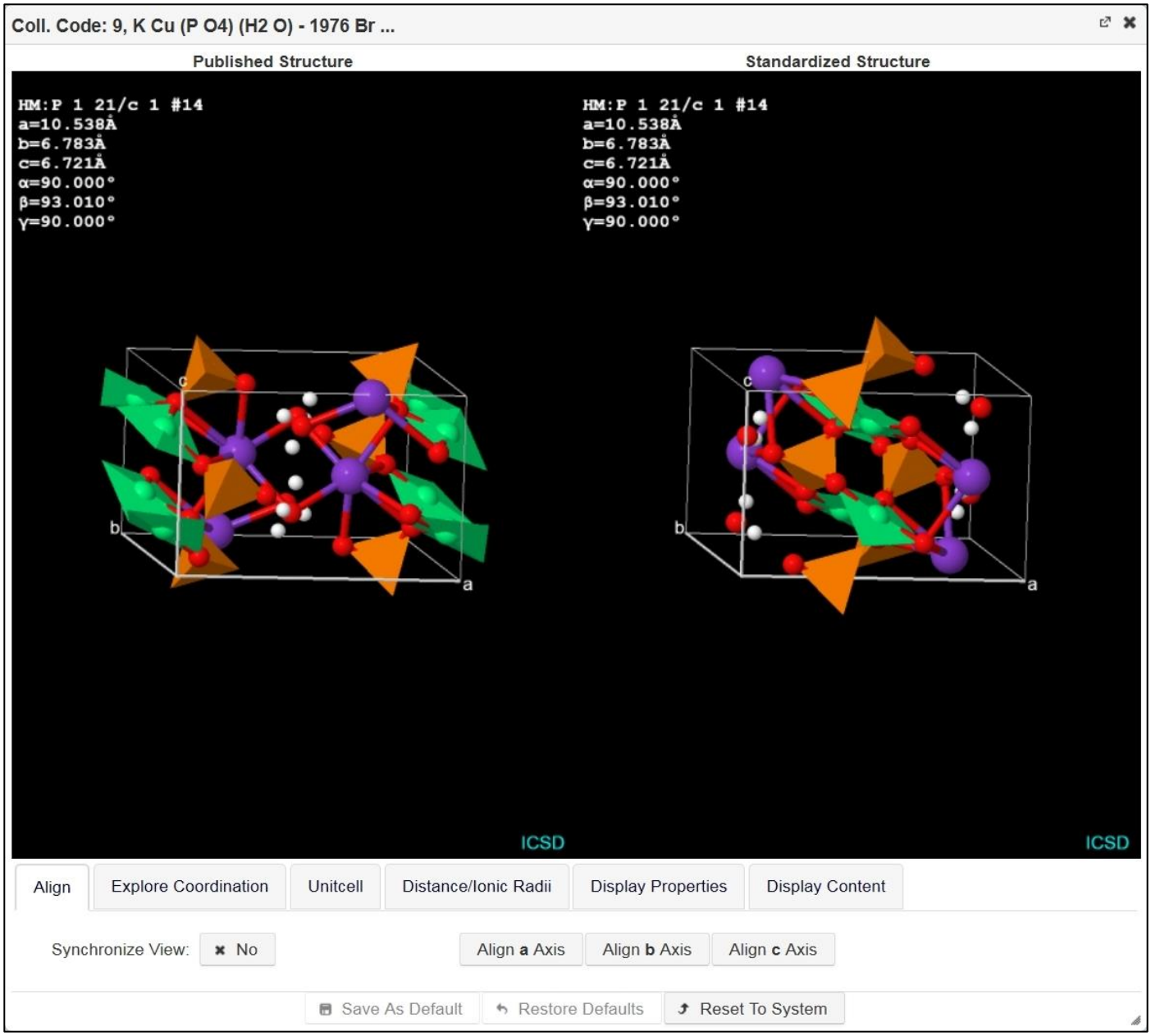


Figure 18: Interactive comparison of published and standardized structures

[1] JSmol: an open-source HTML5 viewer for chemical structures in 3D. http://wiki.jmol.org/index.php/JSmol

Export Data

Currently, data sets can be exported in CIF (Crystallographic Information File), TXT (text file), or csv (comma-separated values file) format.

Select the data set(s) you wish to export from the result list: Use the checkboxes of specific records or click on the checkbox in the title of the selection column to select/deselect all records of the current page. The button "Export Data" will be activated (Fig. 1) as soon as at least one record is selected. You may also export a record directly as a CIF file by clicking on the download symbol in the right column.

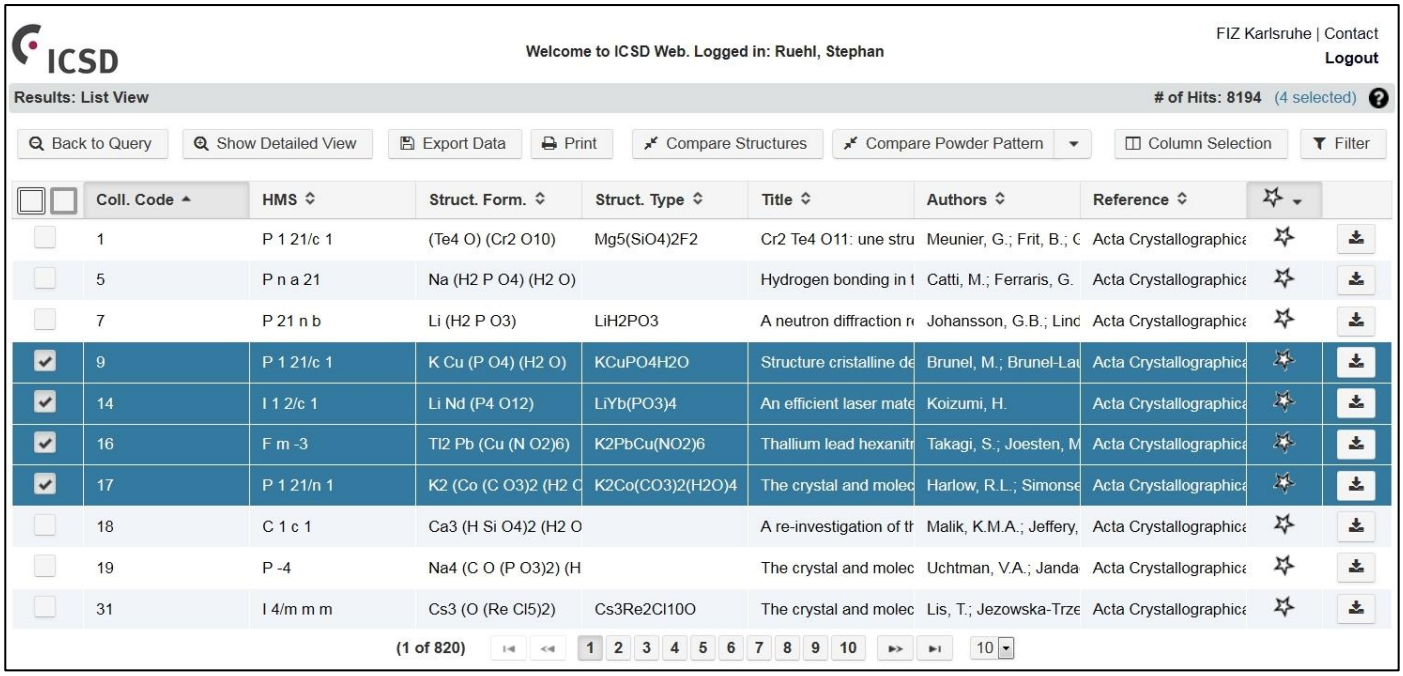


Figure 1: Result set

Clicking on the button "Export Data" will show a dialogue as shown in Figure 2. Enter the base file name for the records you want to export.

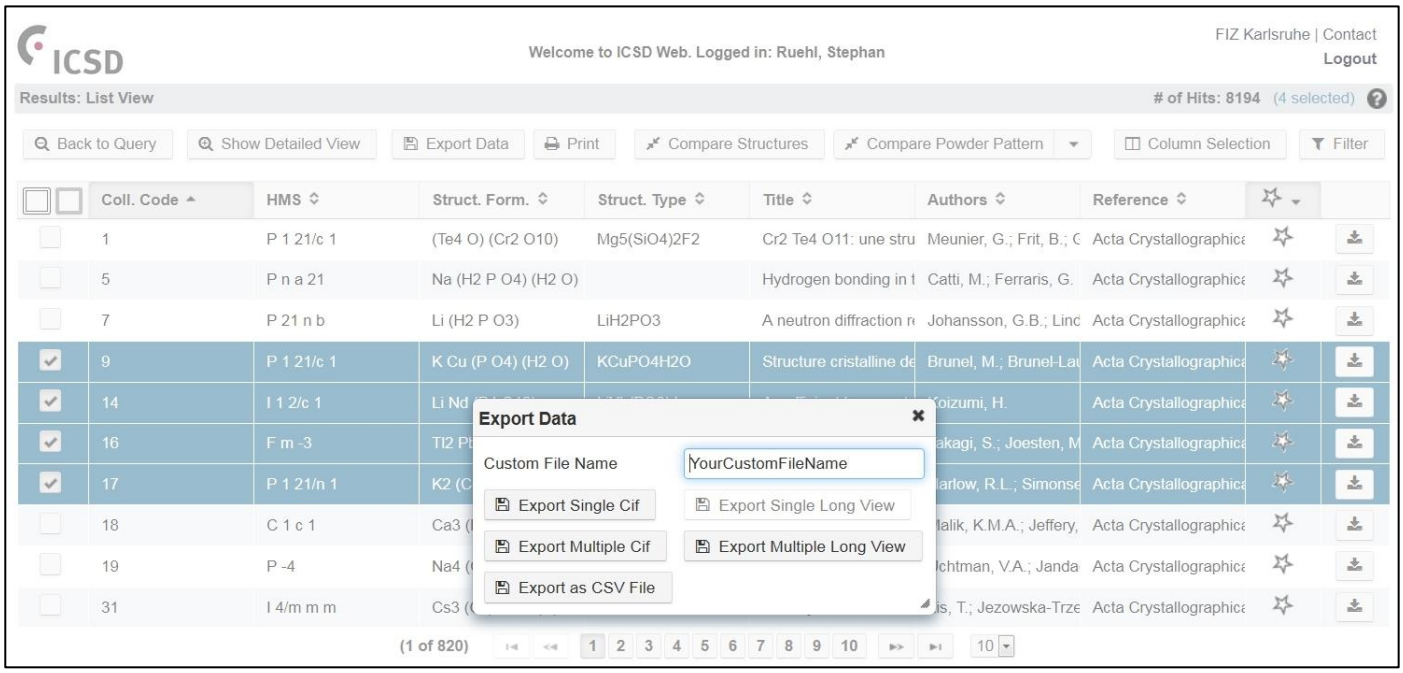


Figure 2: Export data dialogue

Exporting as a single CIF will lead to one file, in which the exported records are sequentially listed. Multiple CIFs will result in individual files for each record packed into a zip archive; filenames always contain the Collection Code.

Exporting TXT files is similar to the CIF export options. You can either export all files into one zip file or you can export single txt files. Please note that the Single Long View option does not list the TXT files sequentially as the similar function for CIF files does.

The csv option lets you export the current page of the List View with the customized settings as a csv-file.

Clicking on the download symbol in the column on the right allows you to either open the CIF file directly in a program associated with the extension .cif or to save the file. The predefined filename contains the ICSD Collection Code of the exported record. You may, of course, also change the suggested file name.

Print

The Print button provides a convenient shortcut to the regular print function of the browser. The customized list will be printed in a concise format.

Visualize Structure/Compare Structures

You can display up to six structures simultaneously in a separate window. Once you have selected one record the button "Visualize Structure" becomes accessible, and it changes to the "Compare Structures" button as soon as a second record is selected (Fig. 1). Please note that either of the two buttons is only accessible when up to six records are selected.

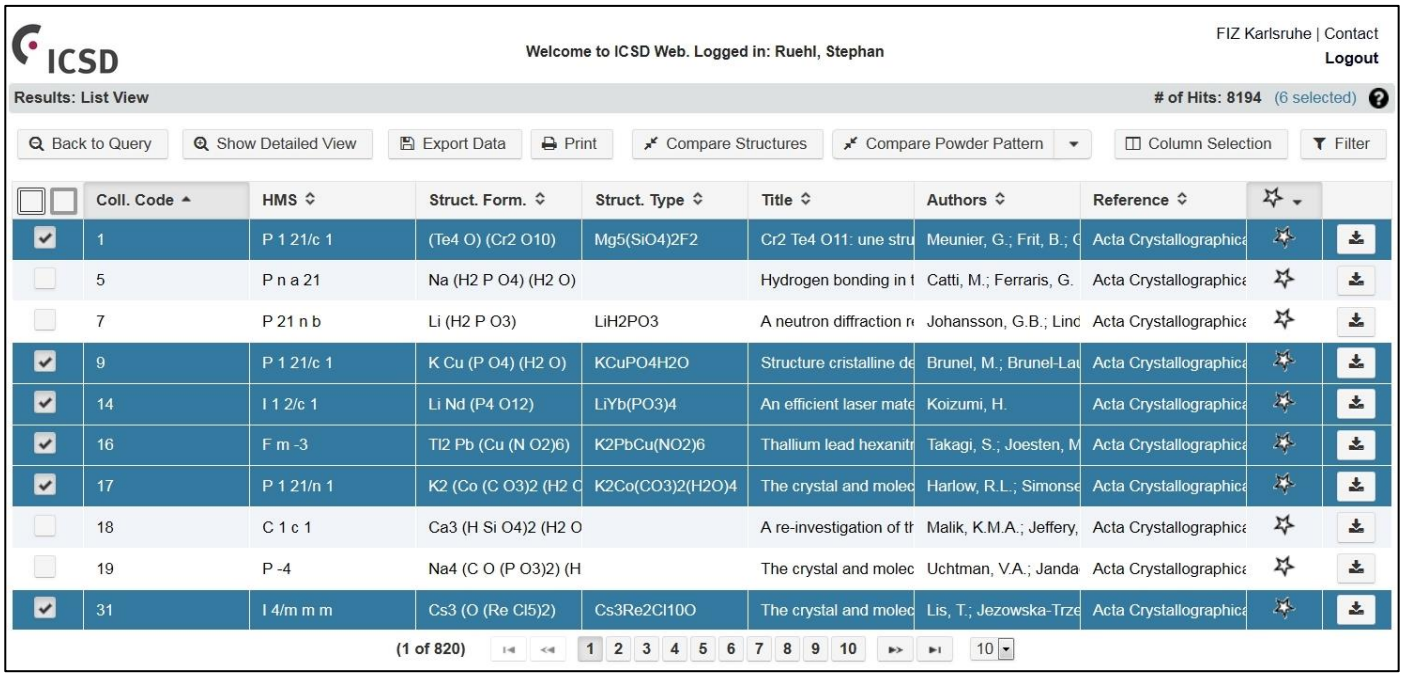


Figure 1: Result set

For each structure the collection and the structured formula is given in the title bar. The space group, the space group number and the lattice parameter are displayed next to the structure (Fig. 2). You can change the arrangement of the displayed structures by using drag-and-drop techniques.

Right-clicking into the structure display box (only in the JSMol applet not in the simple picture shown at the beginning) opens a pop-up menu, from where you can change the display properties and perform geometric analyses of the displayed structure.

Some options to manipulate the interactive display for the current crystal structure(s) are given in tabs below the display:

- Align: Here you can align the view along the a, b or c axis. The option "Synchronize View" allows to manipulate all currently displayed structure in the same way; e.g. turning one structure around results in all structures being turn simultaneously.

- Explore Coordination: This allows to interactively visualize the environment of a selected atom. To start one has to activate the by setting the "Show Coordination" to "Yes". Then two new options are displayed. First one has to select the central atom by clicking in the field to the right of the Central Atom description. The display now shows all atoms in the unit cell. Once one of these atoms is selected, only the central atom (selected) and the atoms in a certain radius around it are shown. The radius can be increased or decreased using the Distance field.

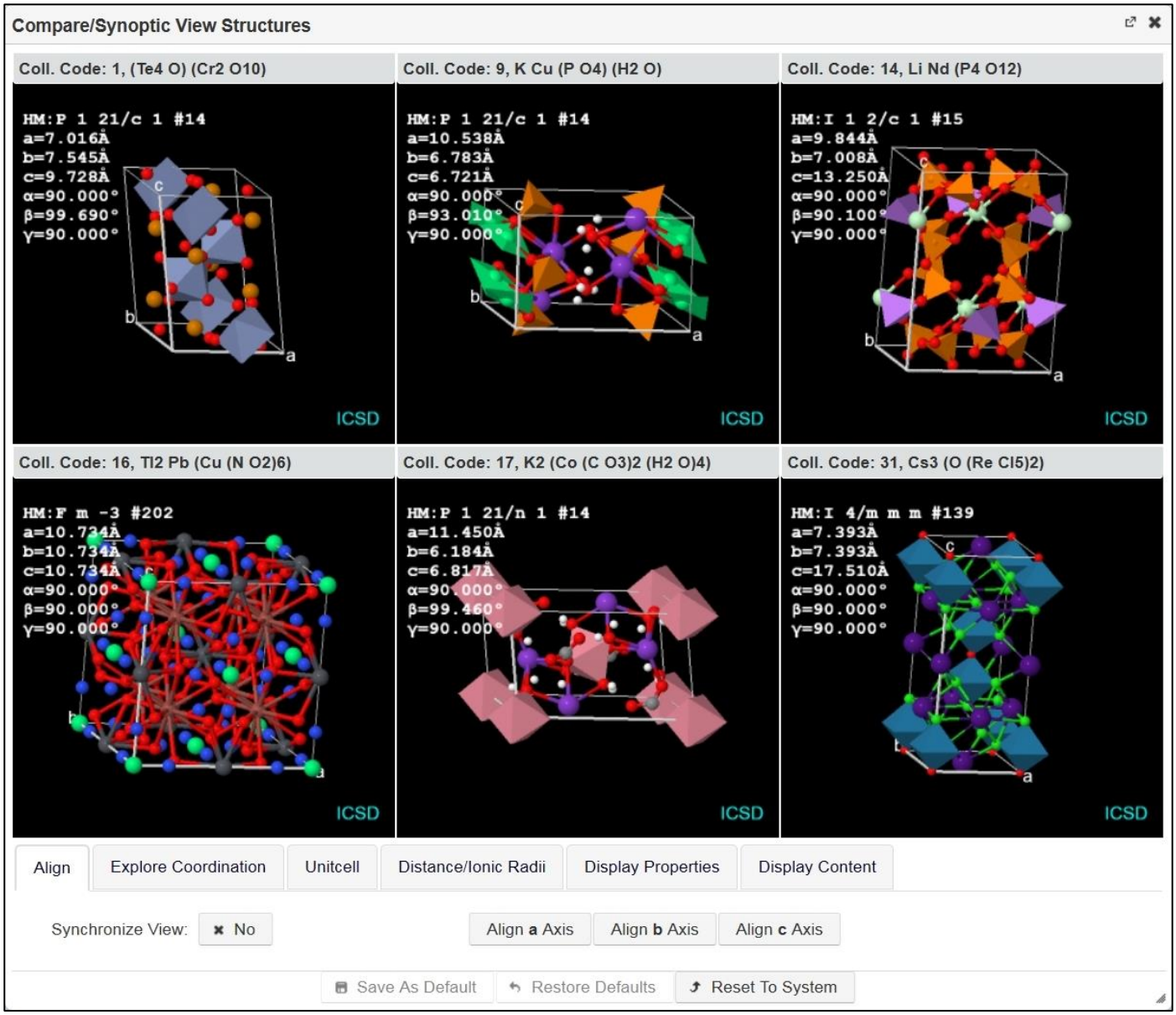


Figure 2: Compare Structures: Multiple plots of crystal structures

On the right there are two additional buttons which offer quick ways to measure distances and angles in the crystal structure display. Clicking on one of the two buttons will display a short description of what is needed to display distances or angles.

- Unit Cells: Enter the number of unit cells for each lattice direction you want to have displayed. Note: Although it is possible to enter decimal fractions, the fractions will be cut off. The values for a, b, and c are limited to 1.0 - 4.0.

  It is necessary to click on “Apply Unitcell” after making changes in the number of unit cells displayed along each lattice direction.

- Distance/Ionic Radii: The generation and display of bonds can be limited either by defining minimum and maximum distances or by providing minimum and maximum percentages of the sum of the ionic radii of the involved atoms/ions.

- Display Properties: Allows changing certain aspects of displaying the crystal structure, such as

    - background (on/off)
    - perspective drawing (on/off)
    - stereo (red/green) display
    - “Spin” will let the currently displayed structure rotate around the vertical axis
    - “Display Labels” will put the atom labels beside the appropriate atom.

- Display Content: A dropdown box allows for atom display customization. Hydrogen bonds, polyhedral and/or cavities can be shown/hidden by switching the appropriate box on/off. The Select/Mark Atom Site switch lets you highlight the equivalent atoms in the display by clicking on one atom.

- Three additional buttons allow for customization.
    - You can save preferred structure display settings with Jmol by pressing the "Save As Default"-button.
    - Clicking the "Restore Default"-button changes the display properties to the previously saved defaults or to the system defaults if no saved defaults have been created.
    - The "Reset to System"-button will always restore the properties to the original defaults.

Visualize Powder Pattern/Compare Powder Pattern

You can display up to six simulated powder patterns simultaneously in a separate window. Once you have selected one record the button "Visualize Powder Pattern" becomes accessible, and it changes to the "Compare Powder Pattern" button as soon as a second record is selected. Please note that either of the two buttons is only accessible when up to six records are selected.

For each simulated powder pattern the collection and the structured formula is given in the title bar (Fig. 1). You can change the arrangement of the displayed powder patterns by using drag-and-drop techniques.

There are two other options for displaying up to six powder patterns: You can display them as overlapped patterns (Fig. 2) or staggered patterns (Fig. 3). These two options can be accessed using the dropdown-box icon on the right of the "Compare Powder Pattern" button.

There are also some options to manipulate the interactive calculation of the simulated powder pattern which are given in tabs below the display:

- Calculation Parameters: With the dropdown box "Radiation Type" one can select either X-Ray Diffraction or Neutron Diffraction. The appropriate wavelength can either be selected from a dropdown box (possible sources are Cu, Cr, Fe, Mo, and Ag) or one can enter a custom wavelength (Angstrom units).

  The reflex profile parameters *U*, *V* and *W* can be changed. In addition one can set a zero shift parameter.

  Toggling between line diagrams (checkbox "Intensities only") and standard powder patterns (Gauß envelope) is possible, too. One can also include or exclude dispersion. The default setting is to use the standardized data for the powder pattern generation, but one can also switch this off and then the published data are used. Of course, this does not change the powder pattern, but the indices may be different.

  It is necessary to click on "Redraw Display" after making any changes.

- Visualization Parameters: Here one can choose between 2 plot types: 2theta and d. 2theta plots in the range 0.1-60° in 0.1° steps are shown per default. x_{min}, x_{max}, and x_{step} describe the starting, the ending and the step value according to the chosen plot type, respectively.

  Additionally, it is possible to display the corresponding indices for each reflection and to colour the powder pattern in red.

  It is necessary to click on "Redraw Display" after making any changes.

- Export: You can export the simulated powder pattern as a two-column x-y data file or export it as a PDF file. In addition, a table can be created with hkl, 2 theta, d, multiplicity and intensity for each reflection in a txt-file.

Figure 1: Multiple plots of powder patterns

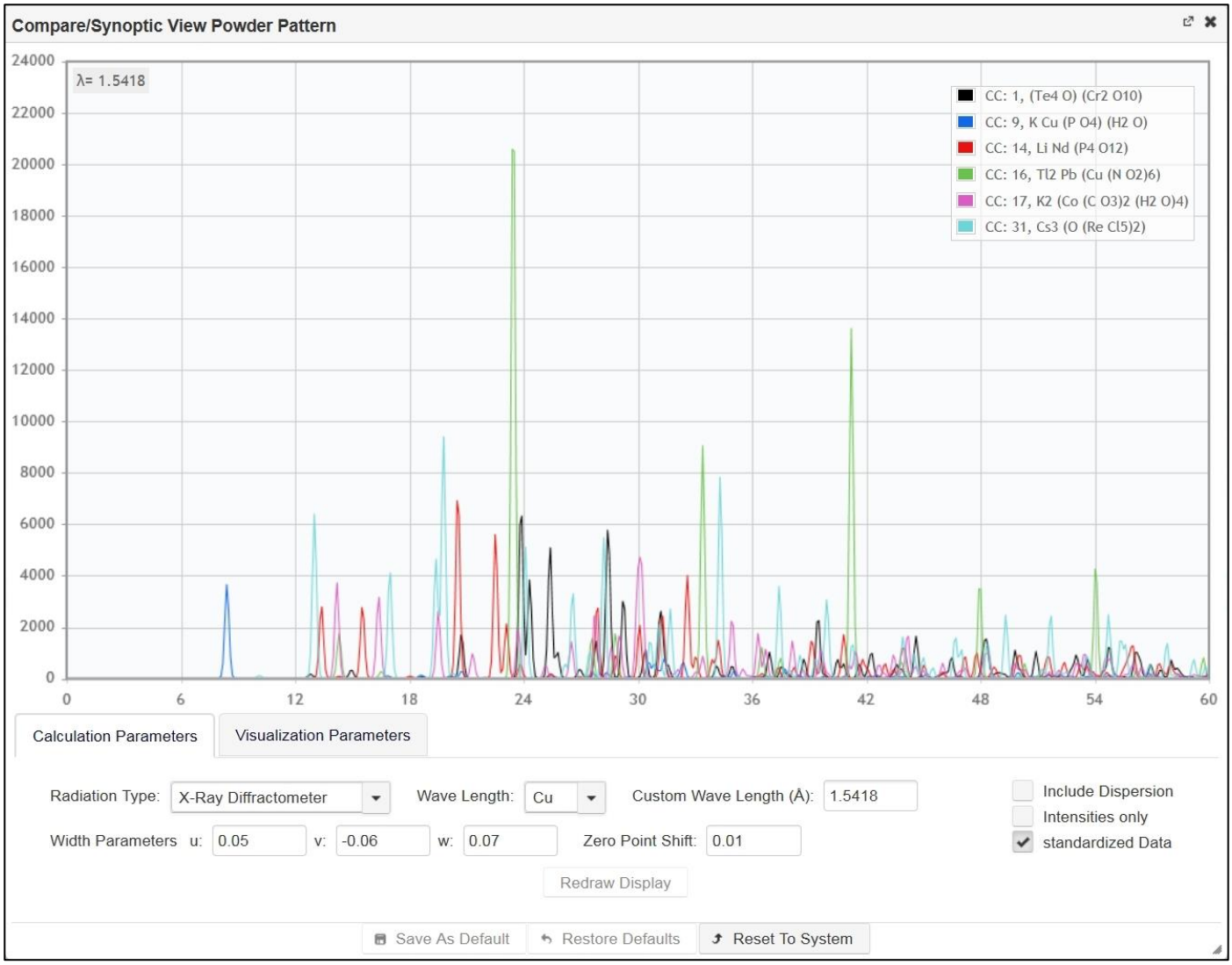


Figure 2: Overlayed plot of powder patterns

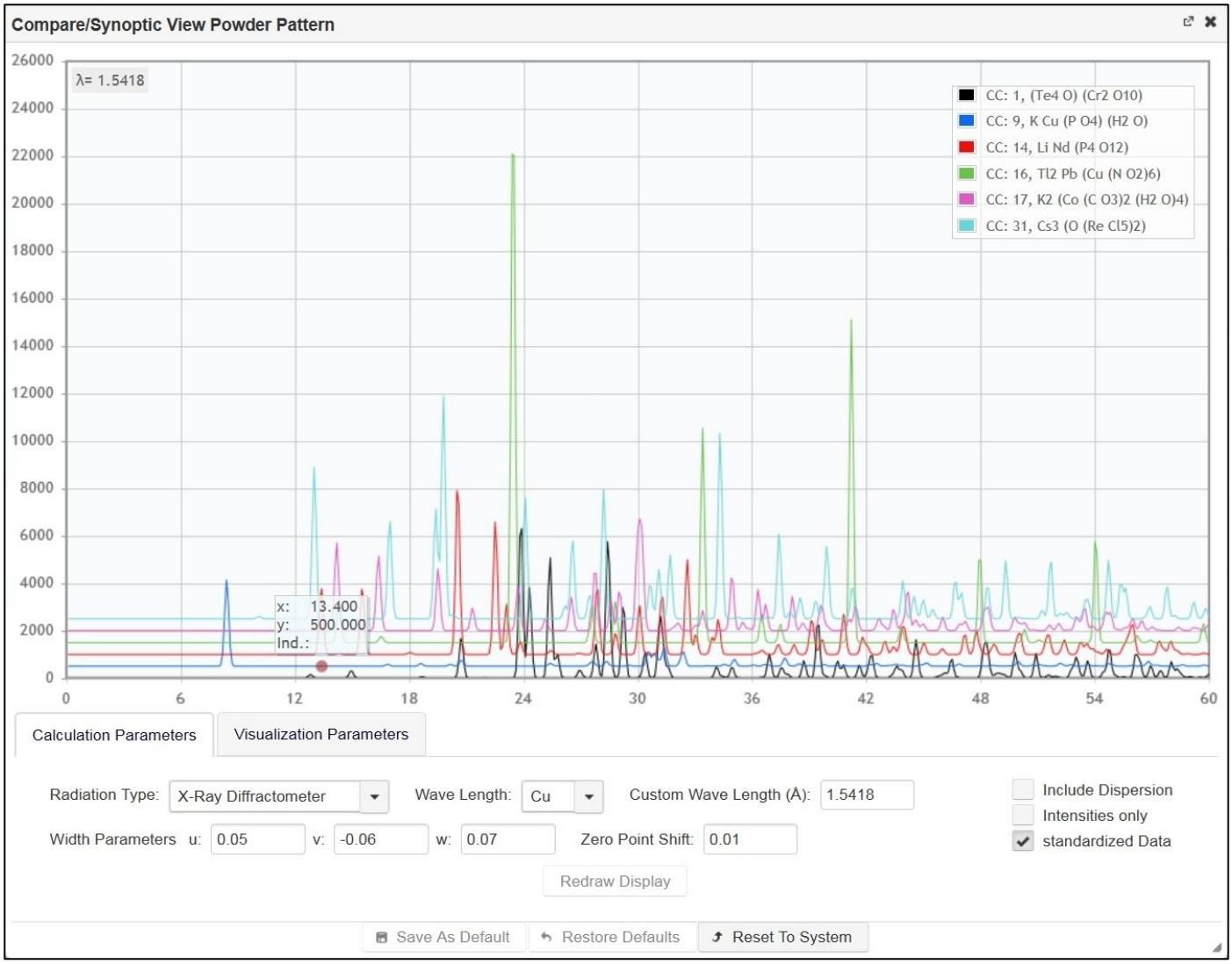


Figure 3: Staggered plot of powder patterns

Column Selection

The column selection allows you to choose the fields displayed in the List View. Just click on the button and a new window opens with all options. Just select the ones you want to display and deselect the ones you want to be removed from the List View (Fig. 1). These settings are stored server side, so they are retained after logout.

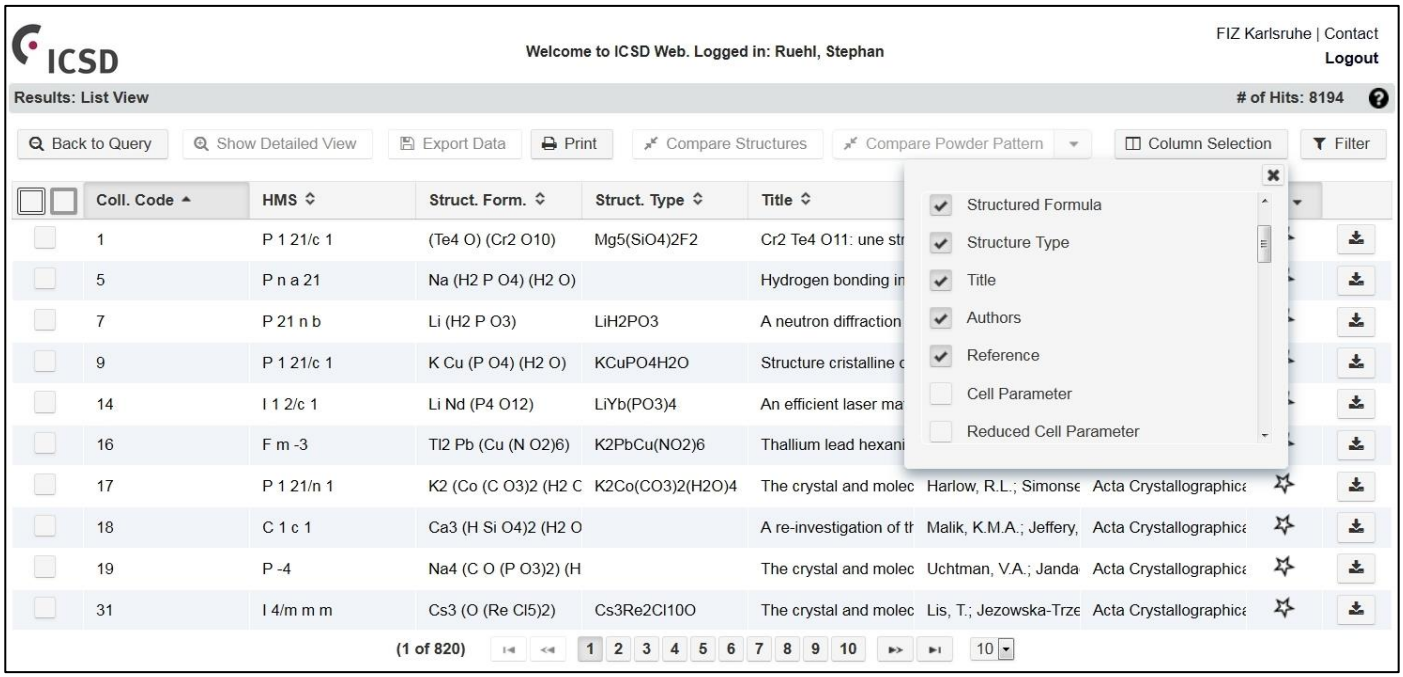


Figure 1: Column selection: Here you can choose the fields that are relevant to you.

The following options are available:

- Collection code
- HMS (space group)
- Structured Formula
- Structure Type
- Title
- Authors
- Reference (journal, volume, year, page)
- Cell parameter (a,b,c,alpha,beta,gamma)
- Reduced cell parameter (a,b,c,alpha,beta,gamma)
- Standardised cell parameter (a,b,c,alpha,beta,gamma)
- Cell volume
- Formula units per cell (Z)
- Formula weight
- Temperature
- Pressure
- R-value
- Sum formula
- ANX-formula
- AB-formula
- Chemical name
- Mineral name

- Mineral group
- Calculated density
- Measured density
- Pearson symbol
- Wyckoff sequence
- Journal
- Volume
- Publication year
- Page number
- Quality

Please note that the column to the right (download) and to the left (selection) cannot be removed.

Filter

A post-query filtering has been implemented that allows to further refine the number of hits of a query without having to re-execute the query. Using the "Filter" button on the top right opens a new window, which allows you to set and/or unset the filters.

The filters are divided into five groups: Quality Filter, Radiation Type, Sample Type, R-Value and Experimental Conditions (Fig. 1).

- Quality Filter: Here you can choose between displaying all structures (the default), only high quality structures or standard quality structures. High quality structures need to fulfill the following criteria:
    - structure determination including refinement (in case of powder data including Rietveld refinement)
    - temperature factors given
    - pressure in the range 0.09-0.11 MPa
    - temperature in the range 285-300 K
    - standard deviation given for cell parameters
    - an R-value must be specified
- Radiation Type: Here you can select the type of radiation used (X-Ray, electron, neutron or synchrotron radiation). Per default all options are selected.
- Sample Type: Here you can choose between structures determined from single crystals and from powders.
- R-value: Here you can confine the structures to be displayed by the R-Value. Options are: Any R-Value; R-value ‹=0.1 and R-value ‹=0.05.
- Experimental Conditions: This currently offers the options to use Any condition, Structures that were measured at low temperature (T‹=200k) and/or high-pressure structures (P›=1Mpa)

Once some filters are applied, the number of current hits and the number of total hits without the filters is displayed in the button in brackets. In addition, directly next to the button is now a selected checkbox (Fig. 2). This checkbox applies the selected filter criteria. Unselecting the box displays again all records from the current query.

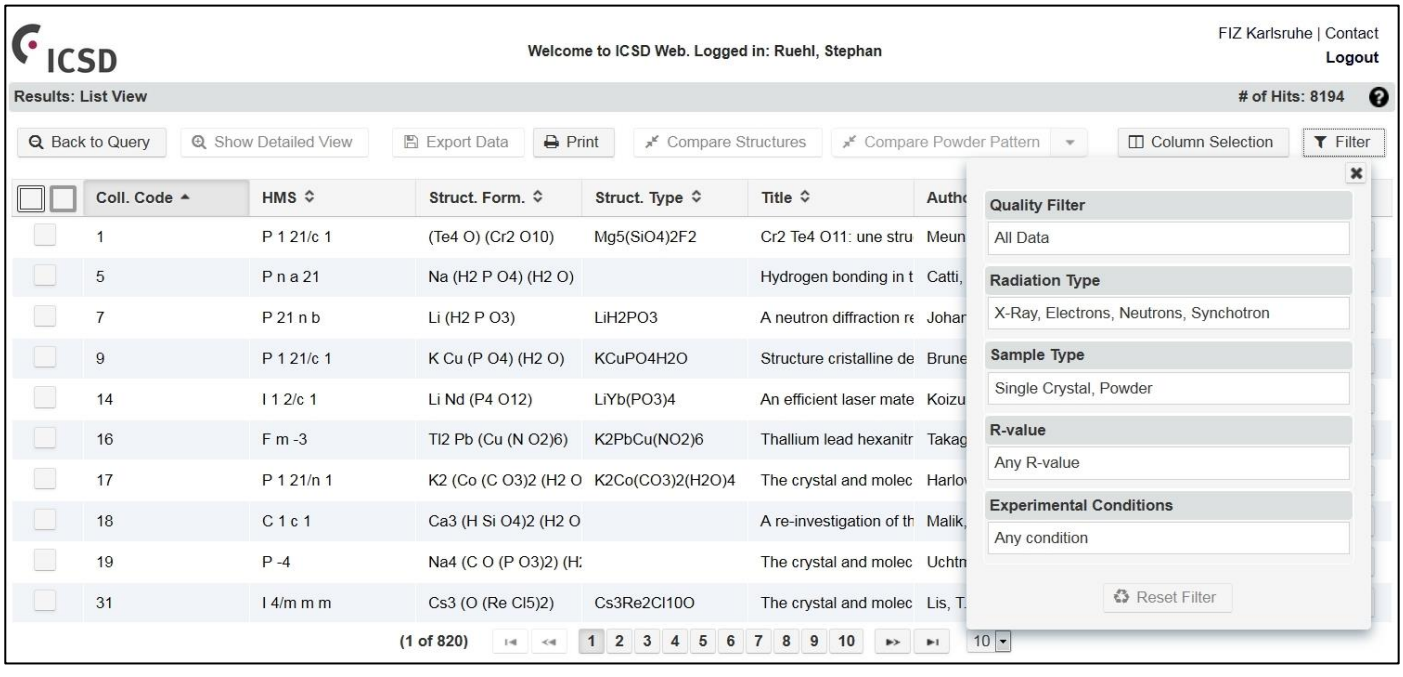


Figure 1: The post-query Filter window with its options.

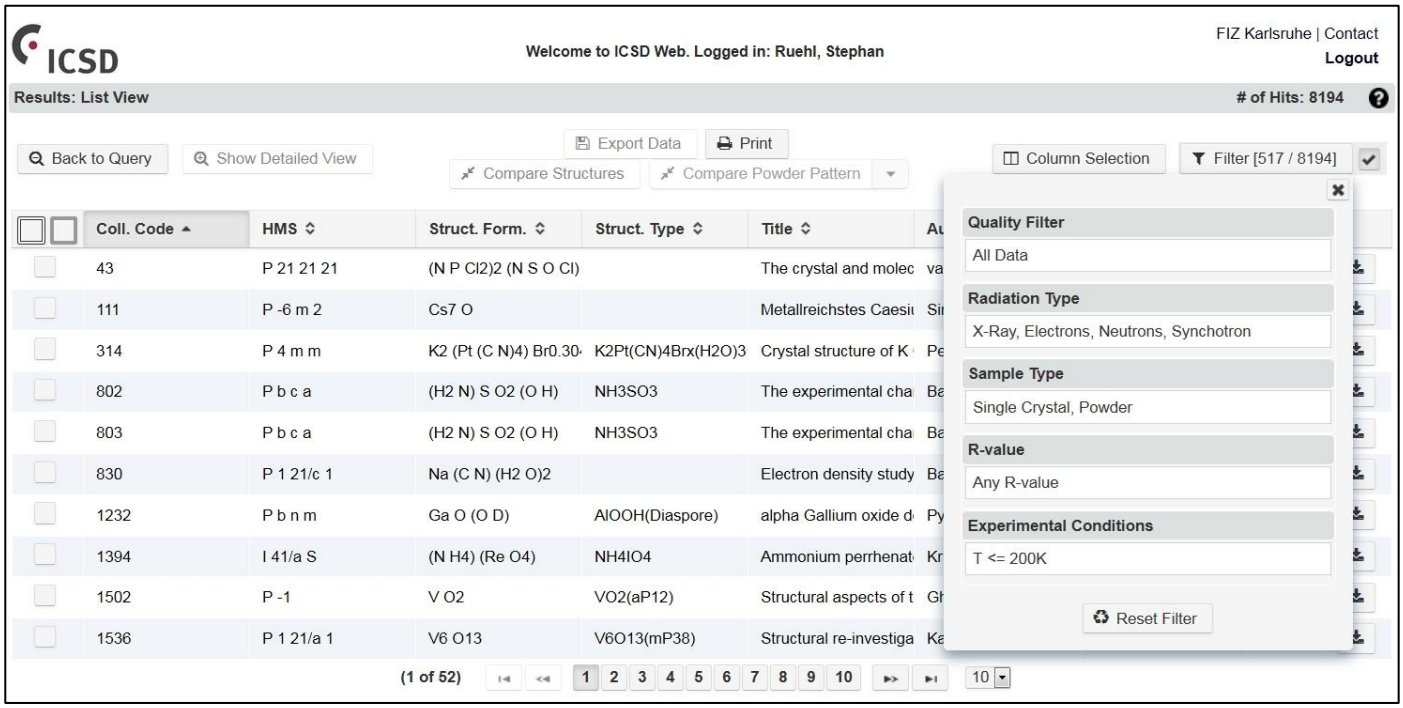


Figure 2: Checkbox for applying the selected filter options.