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<th>Page</th>
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<td>Visualize Structure/Compare Structures</td>
<td>95</td>
</tr>
</tbody>
</table>
Visualize Powder Pattern/Compare Powder Pattern

Column Selection

Filter
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:

<table>
<thead>
<tr>
<th>Wildcard</th>
<th>Function</th>
<th>Example</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>*</td>
<td>Replace any number of characters</td>
<td>Sulf*</td>
<td>finds Sulfur, Sulfate, Sulfamic, ...</td>
</tr>
<tr>
<td>#</td>
<td>Replace either 0 or 1 character</td>
<td>Sul##ur</td>
<td>finds Sulfur and Sulphur</td>
</tr>
</tbody>
</table>

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 Structures Only
- Theoretical Structures Only
- All Structures

The default setting is “Experimental Structures Only”. 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 entries 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.

Bibliography

<table>
<thead>
<tr>
<th>Search Field</th>
<th># of entries</th>
<th>Format</th>
<th>Type</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Authors</td>
<td>Unlimited</td>
<td>Single entry</td>
<td>Text</td>
<td>Jansen</td>
</tr>
<tr>
<td></td>
<td></td>
<td>multiple entries</td>
<td></td>
<td>Fink Bolte</td>
</tr>
<tr>
<td></td>
<td></td>
<td>#, *</td>
<td></td>
<td>M##ller</td>
</tr>
<tr>
<td></td>
<td></td>
<td>“ “</td>
<td></td>
<td>Ander*</td>
</tr>
<tr>
<td>Title of Journal</td>
<td>Unlimited</td>
<td>Single entry</td>
<td>Text</td>
<td>Science</td>
</tr>
<tr>
<td></td>
<td></td>
<td>multiple entries</td>
<td></td>
<td>Angewandte Chemie</td>
</tr>
<tr>
<td></td>
<td></td>
<td>#, *</td>
<td></td>
<td>Crystallogr*</td>
</tr>
<tr>
<td>Title of Article</td>
<td>Unlimited</td>
<td>Single entry</td>
<td>Text</td>
<td>reactivity</td>
</tr>
<tr>
<td></td>
<td></td>
<td>multiple entries</td>
<td></td>
<td>magnetic structure</td>
</tr>
<tr>
<td></td>
<td></td>
<td>#, *</td>
<td></td>
<td>sul##ate</td>
</tr>
<tr>
<td>Year of Publication</td>
<td>1</td>
<td>Single value</td>
<td>Numeric</td>
<td>1913</td>
</tr>
<tr>
<td></td>
<td></td>
<td>&lt;, &lt;=, &gt;, &gt;=</td>
<td></td>
<td>&gt;2008</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-</td>
<td></td>
<td>2000-2006</td>
</tr>
<tr>
<td></td>
<td></td>
<td>&lt;=1940</td>
<td></td>
<td>&lt;=1940</td>
</tr>
</tbody>
</table>

Chemistry

<table>
<thead>
<tr>
<th>Search Field</th>
<th># of entries</th>
<th>Format</th>
<th>Type</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Composition</td>
<td>unlimited</td>
<td>Single entry</td>
<td>Text</td>
<td>Au</td>
</tr>
<tr>
<td></td>
<td></td>
<td>multiple entries</td>
<td></td>
<td>Na Cl O</td>
</tr>
<tr>
<td>Number of Elements</td>
<td>1</td>
<td>Single value</td>
<td>Numeric</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>&lt;, &lt;=, &gt;, &gt;=</td>
<td></td>
<td>4-5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-</td>
<td></td>
<td>&lt;=2</td>
</tr>
</tbody>
</table>
### Cell

<table>
<thead>
<tr>
<th>Search Field</th>
<th>Units</th>
<th># of entries</th>
<th>Format</th>
<th>Type</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell Parameters</td>
<td>angstrom, degree</td>
<td>6</td>
<td>Single value (\langle, \langle=, \rangle, \rangle)</td>
<td>Numeric</td>
<td>5 5 90 90 90 3.4 3.4 * 90 * 90 15.5-16 ** 90 &gt;=90 90 10 ** ** **</td>
</tr>
<tr>
<td>Cell Volume</td>
<td>cubic angstrom</td>
<td>1</td>
<td>Single value (\langle, \langle=, \rangle, \rangle)</td>
<td>Numeric</td>
<td>2400 1000-1100 &lt;=500</td>
</tr>
<tr>
<td>Tolerance(^1)</td>
<td>%</td>
<td>1</td>
<td>Single value</td>
<td>Numeric</td>
<td>3</td>
</tr>
</tbody>
</table>

\(^1\) Tolerances apply to Cell Parameters and Cell Volume

### Symmetry

<table>
<thead>
<tr>
<th>Search Field</th>
<th># of entries</th>
<th>Format</th>
<th>Type</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Space Group Symbol</td>
<td>1</td>
<td>Single entry, #, *</td>
<td>Text</td>
<td>P-1 P12#1 Fm*</td>
</tr>
<tr>
<td>Space Group Number</td>
<td>1</td>
<td>Single value (\langle, \langle=, \rangle, \rangle)</td>
<td>Numeric</td>
<td>14 &gt;225 83-145</td>
</tr>
<tr>
<td>Crystal System</td>
<td>1</td>
<td>-</td>
<td>Dropdown</td>
<td>-</td>
</tr>
<tr>
<td>Centering</td>
<td>1</td>
<td>-</td>
<td>Dropdown</td>
<td>-</td>
</tr>
</tbody>
</table>

### Experimental Info and Reference Data

<table>
<thead>
<tr>
<th>Search Field</th>
<th>Units</th>
<th># of entries</th>
<th>Format</th>
<th>Type</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>New Data Only</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Checkbox</td>
<td>-</td>
</tr>
<tr>
<td>PDF Number</td>
<td>-</td>
<td>1</td>
<td>Single entry, #, *</td>
<td>Numeric</td>
<td>01-077-1145 47-1360</td>
</tr>
<tr>
<td>Collection Code</td>
<td>-</td>
<td>1</td>
<td>Single value (\langle, \langle=, \rangle, \rangle)</td>
<td>Numeric</td>
<td>22333 &lt;=100000 600000-699999</td>
</tr>
<tr>
<td>Temperature</td>
<td>selectable</td>
<td>1</td>
<td>Single value (\langle, \langle=, \rangle, \rangle)</td>
<td>Numeric</td>
<td>100 &lt;=10 270-310</td>
</tr>
<tr>
<td>Pressure</td>
<td>selectable</td>
<td>1</td>
<td>Single value (\langle, \langle=, \rangle, \rangle)</td>
<td>Numeric</td>
<td>1.5 &gt;100000 0.01-</td>
</tr>
</tbody>
</table>
**Advanced Search and Retrieve**

**Bibliographic Search**

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

---

**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Authors’ name for the main (first) reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>

---

**Figure 1:** Bibliographic Search screen.
### Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>jAnSEn</td>
<td>Jansen</td>
</tr>
<tr>
<td>“Jansen, M.”</td>
<td>M. Jansen</td>
</tr>
<tr>
<td>Jans*</td>
<td>Jans[arbitrary rest], such as Jansen, Janssen, Jansson etc.</td>
</tr>
<tr>
<td>Mu#ller</td>
<td>Muller AND Mueller</td>
</tr>
</tbody>
</table>

### 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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Title of journal for the reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>““ exact term</td>
</tr>
</tbody>
</table>

**Examples:**

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

### 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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Title of article for the main (first) reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>““ exact term</td>
</tr>
</tbody>
</table>
Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>thio sulfate</td>
<td>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”</td>
</tr>
<tr>
<td>thiosul##ate</td>
<td>Thiosulfate or Thiosulphate, such as “Cadmium thiosulfate dihydrate” or “The crystal structure of anhydrous sodium thiosulphate”</td>
</tr>
<tr>
<td>“copper sulfate“</td>
<td>Finds exactly this phrase, such as “The crystal structure of spangolite, a complex copper sulfate sheet mineral”</td>
</tr>
</tbody>
</table>

**Year of Publication**

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Year of publication of an article in the reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, integer</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
</tbody>
</table>
| Wildcards   | - range; year1 – year2  
≤ range; ≤year  
< range; <year  
> range; >year  
≥ range; ≥year |

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>1974</td>
<td>1974</td>
</tr>
<tr>
<td>1974-1976</td>
<td>1974 or 1975 or 1976</td>
</tr>
<tr>
<td>&lt; 1915</td>
<td>1912 or 1913 (first structure published in 1912)</td>
</tr>
<tr>
<td>&lt;=1914</td>
<td>1912 or 1913</td>
</tr>
<tr>
<td>&gt;2005</td>
<td>2006 or 2007 or 2008 or 2009 or 2010 ...</td>
</tr>
<tr>
<td>&gt;=2006</td>
<td>2006 or 2007 or 2008 or 2009 or 2010 ...</td>
</tr>
</tbody>
</table>
### Volume

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

<table>
<thead>
<tr>
<th><strong>Description</strong></th>
<th>Volume of the journal in the reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type</strong></td>
<td>Numerical, integer</td>
</tr>
<tr>
<td><strong>Format</strong></td>
<td>Single value or range</td>
</tr>
<tr>
<td><strong># of entries</strong></td>
<td>1</td>
</tr>
<tr>
<td><strong>Wildcards</strong></td>
<td>- range; volume1 – volume2</td>
</tr>
<tr>
<td></td>
<td>&lt; range; &lt;volume</td>
</tr>
<tr>
<td></td>
<td>&lt;= range; &lt;=volume</td>
</tr>
<tr>
<td></td>
<td>&gt; range; &gt;volume</td>
</tr>
<tr>
<td></td>
<td>&gt;= range; &gt;=volume</td>
</tr>
</tbody>
</table>

**Examples:**

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>22</td>
<td>22</td>
</tr>
<tr>
<td>10-12</td>
<td>10 or 11 or 12</td>
</tr>
<tr>
<td>&lt;4</td>
<td>1 or 2 or 3</td>
</tr>
<tr>
<td>&gt;=67</td>
<td>66 or 67 or 68 or 69 or 70 ...</td>
</tr>
</tbody>
</table>

### Page

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

<table>
<thead>
<tr>
<th><strong>Description</strong></th>
<th>First page number of an article in the reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type</strong></td>
<td>Numerical, integer</td>
</tr>
<tr>
<td><strong>Format</strong></td>
<td>Single value or range</td>
</tr>
<tr>
<td><strong># of entries</strong></td>
<td>1</td>
</tr>
<tr>
<td><strong>Wildcards</strong></td>
<td>- range; page1 – page2</td>
</tr>
<tr>
<td></td>
<td>&lt; range; &lt;page</td>
</tr>
<tr>
<td></td>
<td>&lt;= range; &lt;=page</td>
</tr>
<tr>
<td></td>
<td>&gt; range; &gt;page</td>
</tr>
<tr>
<td></td>
<td>&gt;= range; &gt;=page</td>
</tr>
</tbody>
</table>

**Examples:**

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>197</td>
<td>197</td>
</tr>
<tr>
<td>197-199</td>
<td>197 or 198 or 199</td>
</tr>
<tr>
<td>&lt;65</td>
<td>64 or 63 or 62 or 61 or 60 ...</td>
</tr>
<tr>
<td>&gt;=121</td>
<td>121 or 122 or 123 or 124 or 125 ...</td>
</tr>
</tbody>
</table>
### Abstract

Search within the abstract (if available).

<table>
<thead>
<tr>
<th>Description</th>
<th>Abstract of the article</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
</tbody>
</table>
| Wildcards   | * any number of characters  
# 0 or 1 character  
“ “ exact term |

**Examples:**

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magnetic Proper*</td>
<td>magnetic [...] property (or properties, ...)</td>
</tr>
<tr>
<td>Supercond*</td>
<td>Superconductor, superconducting, ...</td>
</tr>
</tbody>
</table>

### 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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Keywords for the crystal structure (magnetic properties or spectroscopic methods)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
</tbody>
</table>
| Wildcards   | * any number of characters  
# 0 or 1 character  
“ “ exact term |

**Examples:**

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>ferromanget*</td>
<td>Ferromagnetic, ferromagnetism</td>
</tr>
<tr>
<td>Raman</td>
<td>Raman spectroscopy was applied</td>
</tr>
</tbody>
</table>
**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.

![Cell Search](image)

**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Cell length a or b or c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>range; cell_length; cell_length1 – cell_length2</td>
</tr>
<tr>
<td></td>
<td>&lt; range; &lt; cell_length</td>
</tr>
<tr>
<td></td>
<td>&lt;= range; &lt;= cell_length</td>
</tr>
<tr>
<td></td>
<td>&gt; range; &gt; cell_length</td>
</tr>
<tr>
<td></td>
<td>&gt;= range; &gt;= cell_length</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>10.0000</td>
</tr>
<tr>
<td>11.0-11.5</td>
<td>11.0000 – 11.5000</td>
</tr>
<tr>
<td>&lt;10</td>
<td>0.0000 – 9.9999</td>
</tr>
<tr>
<td>&gt;=100</td>
<td>100.0000 – 999999.9999</td>
</tr>
<tr>
<td></td>
<td>(currently the largest cell length in ICSD is more than 500 angstrom)</td>
</tr>
</tbody>
</table>

**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.
### Cell Angle

<table>
<thead>
<tr>
<th>Description</th>
<th>Cell angle $\alpha$ or $\beta$ or $\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>range; cell_angle; cell_angle1 – cell_angle2</td>
</tr>
<tr>
<td></td>
<td>range; $&lt;$ cell_angle</td>
</tr>
<tr>
<td></td>
<td>range; $\leq$ cell_angle</td>
</tr>
<tr>
<td></td>
<td>range; $&gt;$ cell_angle</td>
</tr>
<tr>
<td></td>
<td>range; $\geq$ cell_angle</td>
</tr>
</tbody>
</table>

**Examples:**

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>90</td>
<td>90.0000</td>
</tr>
<tr>
<td>110.0-115.0</td>
<td>110.0000 – 115.0000</td>
</tr>
<tr>
<td>$&lt;$100</td>
<td>0.0000 – 99.9999</td>
</tr>
<tr>
<td>$\geq$100</td>
<td>100.0000 – 179.9999</td>
</tr>
</tbody>
</table>

### 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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Cell volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>range; cell_volume; cell_volume1 – cell_volume2</td>
</tr>
<tr>
<td></td>
<td>range; $&lt;$ cell_volume</td>
</tr>
<tr>
<td></td>
<td>range; $\leq$ cell_volume</td>
</tr>
<tr>
<td></td>
<td>range; $&gt;$ cell_volume</td>
</tr>
<tr>
<td></td>
<td>range; $\geq$ cell_volume</td>
</tr>
</tbody>
</table>

**Examples:**

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>1000.0000</td>
</tr>
<tr>
<td>2000.0-2500.0</td>
<td>2000.0000 – 2500.0000</td>
</tr>
<tr>
<td>$&lt;$100</td>
<td>0.0000 – 99.9999</td>
</tr>
<tr>
<td>$\geq$100</td>
<td>100.0000 – 999999.9999 (largest cell volume in ICSD is over 350,000 Å³)</td>
</tr>
</tbody>
</table>
**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/cm³.

<table>
<thead>
<tr>
<th>Description</th>
<th>Calculated density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>&lt; br range; calculated density; density1 – density2 &lt; br &lt; range; &lt; density &lt; br &lt;= range; &lt;= density &lt; br &gt; range; &gt; density &lt; br &gt;= range; &gt;= density</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0000</td>
</tr>
<tr>
<td>2.0-20.0</td>
<td>2.0000 – 20.0000</td>
</tr>
<tr>
<td>&lt;1.0</td>
<td>0.0000 – 0.9999</td>
</tr>
<tr>
<td>&gt;=20</td>
<td>20.0000 – 99.9999</td>
</tr>
</tbody>
</table>

**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>This tolerance is applied to the cell parameters, volume and density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single value</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>none</td>
</tr>
</tbody>
</table>

**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Units of Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>
**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Specify the data used in the query</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

**Reduce Cell Parameters**

This checkbox defines the cell parameters specified in the search fields cell lengths a, b and c and the cell angles $\alpha$, $\beta$ or $\gamma$ 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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Transforms the specified cell parameters to the reduced cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Checkbox</td>
</tr>
<tr>
<td>Format</td>
<td>-</td>
</tr>
<tr>
<td># of entries</td>
<td>-</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Centering of the cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

**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 $\alpha$, $\beta$ or $\gamma$ to the reduced cell and displays it. This button becomes accessible only when the Reduce Cell Parameters checkbox is checked (Fig. 2).
<table>
<thead>
<tr>
<th>Description</th>
<th>Units of Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Button</td>
</tr>
<tr>
<td>Format</td>
<td>-</td>
</tr>
<tr>
<td># of entries</td>
<td>-</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

**Figure 2:** Display the Reduced Cell
Chemistry Search

With the Chemistry Search 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

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

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

Table 3: ICSD names for other chemical groups of elements

<table>
<thead>
<tr>
<th>Group</th>
<th>ICSD name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metals</td>
<td>MET</td>
<td></td>
</tr>
<tr>
<td>Transition metals</td>
<td>TME</td>
<td>not including f-block elements</td>
</tr>
<tr>
<td>Non-metals</td>
<td>NME</td>
<td></td>
</tr>
<tr>
<td>Lanthanoids</td>
<td>LAN</td>
<td>including La</td>
</tr>
<tr>
<td>Actinoids</td>
<td>ACT</td>
<td>including Ac</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Composition (including stoichiometric coefficients / oxidation numbers)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>- (excludes the following element/group (NOT))</td>
</tr>
<tr>
<td></td>
<td>() (includes at least one of the elements/groups specified (OR))</td>
</tr>
</tbody>
</table>
Examples:

<table>
<thead>
<tr>
<th>Composition</th>
<th># of Elements</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na Cl</td>
<td>2</td>
<td>NaCl</td>
</tr>
<tr>
<td>Na Cl Cl</td>
<td>3</td>
<td>e.g. NaClO₂, NaClO₃, NaMnCl₂, NaAlCl₄, Na₂ZnCl₄</td>
</tr>
<tr>
<td>Na Cl Cl O</td>
<td>3</td>
<td>NaClO₃, NaClO₂</td>
</tr>
<tr>
<td>Cl O Cl O</td>
<td>3</td>
<td>e.g. NaClO₃, KCIO₃, RbClO₃, Pb(ClO₃)₂, Hg₂(ClO₃)₂</td>
</tr>
<tr>
<td>TME Cl O Cl</td>
<td>3</td>
<td>Hg₂(ClO₃)₂, but not e.g. NaClO₃, Pb(ClO₃)₂ etc.</td>
</tr>
<tr>
<td>BEG Cl O Cl</td>
<td>3</td>
<td>Ba(ClO₃)₂, Sr(ClO₃)₂, but not e.g. NaClO₃, Pb(ClO₃)₂, Hg₂(ClO₃)₂ etc.</td>
</tr>
<tr>
<td>LIG FG O Cl</td>
<td>3</td>
<td>e.g. RbIIO₃, NaBrO₃, NaClO₄, Rb₃IO₅, CsI₄O₁₁</td>
</tr>
<tr>
<td>(Na K) Br</td>
<td>2</td>
<td>NaBr or KBr</td>
</tr>
<tr>
<td>-Na -K Br</td>
<td>2</td>
<td>all binary bromides except NaBr and KBr</td>
</tr>
<tr>
<td>-Na -K LiG:1:1 FG:1:1</td>
<td>2</td>
<td>all alkali metal halogenides except NaX and KX; will not include e.g. CsBr and Cs₂I₃</td>
</tr>
<tr>
<td>Cr:::4:4</td>
<td>2</td>
<td>all compounds with an oxidation number of +4 for Cr, such as CrO₂ or Cr₃B₄</td>
</tr>
<tr>
<td>Cr:1:1:4:4</td>
<td>2</td>
<td>all compounds with an oxidation number of +4 for Cr and exactly one Chromium, such as CrO₂, but not Cr₃B₄</td>
</tr>
</tbody>
</table>

**Number of Elements**

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Number of different elements in the composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, integer</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>- range; #ofelements1 – #ofelements2</td>
</tr>
<tr>
<td></td>
<td>&lt; range; &lt;#ofelements</td>
</tr>
<tr>
<td></td>
<td>&lt;= range; &lt;=#ofelements</td>
</tr>
<tr>
<td></td>
<td>&gt; range; &gt;#ofelements</td>
</tr>
<tr>
<td></td>
<td>&gt;= range; &gt;=#ofelements</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>binary compounds</td>
</tr>
<tr>
<td>2-3</td>
<td>binary or ternary compounds</td>
</tr>
<tr>
<td>&lt;3</td>
<td>elements or binary compounds</td>
</tr>
<tr>
<td>&gt;=5</td>
<td>compounds with at least 5 different elements in the composition</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for typical chemical groups</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
<tr>
<td></td>
<td>( ) exact term</td>
</tr>
</tbody>
</table>

Examples:

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

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for (parts of) the chemical name</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>sul##ate</td>
<td>e.g. Na2SO4, Na2SO4·10H2O, NaHSO4, Na2S2O3, NaMg2Fe5(SO4)7(OH)6(H2O)33</td>
</tr>
<tr>
<td>ammonium osmate</td>
<td>((CH3)4N)2(Os(NO)FI4), (((C4H9)4N)3(Se8(Re5OsCl6)))((C2H5)2O)2</td>
</tr>
</tbody>
</table>
## Mineral Name

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the mineral name</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>

### Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adamite</td>
<td>“Adamite” and “Adamite, cuproan”</td>
</tr>
<tr>
<td>Whitlock*</td>
<td>“Whitlockite”, “Whitlockite (heated)”, “Whitlockite, magnesian” and “Whitlockite, manganoan”</td>
</tr>
</tbody>
</table>

## Mineral Group

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the mineral group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>

### Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feldspar</td>
<td>Feldspar</td>
</tr>
<tr>
<td>per*</td>
<td>Perovskite and Periclase</td>
</tr>
</tbody>
</table>

## 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:
- \( \text{Fe}^{2+}(\text{Fe}^{3+})_2 \text{O}_4 \rightarrow \text{AB}_2 \text{X}_4 \)
- \( \text{Fe}^{2.6667+}(\text{Fe}^{3+})_2 \text{O}_4 \rightarrow \text{A}_3 \text{X}_4 \)

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: \( \text{AB}_2 \text{X}_4 \), not \( \text{A}_2 \text{BX}_4 \).

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>
<thead>
<tr>
<th>Chemical formula</th>
<th>ANX formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Mg}_3\text{Al}_2(\text{SiO}_4)_3 )</td>
<td>( \text{A}_2\text{B}_3\text{C}<em>3\text{X}</em>{12} )</td>
</tr>
<tr>
<td>( \text{Ca}<em>3(\text{Al}</em>{1.3325}\text{Fe}_{0.6675})\text{Si}<em>3\text{O}</em>{12} )</td>
<td>( \text{A}_2\text{B}_3\text{C}<em>3\text{X}</em>{12} )</td>
</tr>
<tr>
<td>( \text{Mg}<em>{2.7}\text{Fe}</em>{0.3}(\text{Al}<em>{1.7}\text{Cr}</em>{0.3})\text{Si}<em>3\text{O}</em>{12} )</td>
<td>( \text{A}_2\text{B}_3\text{C}<em>3\text{X}</em>{12} )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the ANX formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>““ exact term</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>N#</td>
<td>N, NO, NX</td>
</tr>
<tr>
<td>A*YZ</td>
<td>A2XYZ, AB2XYZ, ABXYZ and AXYZ</td>
</tr>
<tr>
<td>A<em>C</em></td>
<td>all formulae that have at least AnnBnnCnn in it. AX or ABX are not included.</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Chemical formula</th>
<th>AB formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li₂SO₄</td>
<td>AB₂C₄</td>
</tr>
<tr>
<td>H₂O</td>
<td>AB₂</td>
</tr>
<tr>
<td>K₂(O₂(SO₃)₂)</td>
<td>ABC₄</td>
</tr>
<tr>
<td>K₂(S₂O₃)</td>
<td>A₂B₂C₇</td>
</tr>
<tr>
<td>Na₆O(SO₄)₂</td>
<td>A₂B₆C₉</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABC</td>
<td>ABC, but not e.g. ABC₂</td>
</tr>
<tr>
<td>A#</td>
<td>A, AB</td>
</tr>
<tr>
<td>A*D</td>
<td>A0.33BCD, A0.47BCD</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Number of formula units per unit cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, integer</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td></td>
</tr>
</tbody>
</table>
- | range; #offormulaunits1 – #offormulaunits2
< | range; <#offormulaunits
<= | range; <=#offormulaunits
> | range; >#offormulaunits
>= | range; >=#offormulaunits
### Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>2·3</td>
<td>Compounds with two or three formula unit per cell</td>
</tr>
<tr>
<td>&lt;2</td>
<td>only compounds with exactly one formula unit per cell</td>
</tr>
<tr>
<td>&gt;=1</td>
<td>all entries in the database</td>
</tr>
</tbody>
</table>

### Formula Weight

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Formula Weight of the asymmetric unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, integer</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>- range; weight1 – weight</td>
</tr>
<tr>
<td></td>
<td>&lt; range; &lt; weight</td>
</tr>
<tr>
<td></td>
<td>&lt;= range; &lt;= weight</td>
</tr>
<tr>
<td></td>
<td>&gt; range; &gt;weight</td>
</tr>
<tr>
<td></td>
<td>&gt;= range; &gt;=weight</td>
</tr>
</tbody>
</table>

### Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>100-101</td>
<td>Compounds with a formula weight between 100 and 101</td>
</tr>
<tr>
<td>&gt;=1.0</td>
<td>All entries in ICSD</td>
</tr>
</tbody>
</table>
**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.
<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the space group symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-1</td>
<td>Space group number 2</td>
</tr>
<tr>
<td>„P – 1“</td>
<td>Space group number 2</td>
</tr>
<tr>
<td>fm-*</td>
<td>Space groups: Fm-3, Fm-3c, Fm-3m</td>
</tr>
<tr>
<td>p 1 2 # 1</td>
<td>Space groups: P121 and P1211</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Includes all alternative settings for the specified space group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Checkbox</td>
</tr>
<tr>
<td>Format</td>
<td>-</td>
</tr>
<tr>
<td># of entries</td>
<td>-</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the space group number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, integer</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>- range; spacegroupnumber1 – spacegroupnumber2</td>
</tr>
<tr>
<td></td>
<td>&lt; range; &lt;spacegroupnumber</td>
</tr>
<tr>
<td></td>
<td>&lt;= range; &lt;=spacegroupnumber</td>
</tr>
<tr>
<td></td>
<td>&gt; range; &gt;spacegroupnumber</td>
</tr>
<tr>
<td></td>
<td>&gt;= range; &gt;=spacegroupnumber</td>
</tr>
</tbody>
</table>
Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Space groups: P121 and P112</td>
</tr>
<tr>
<td>1-2</td>
<td>Space groups: B1, C1, F1, I1, P1 and A-1, B-1, C-1, F-1, I-1, P-1</td>
</tr>
<tr>
<td>&gt;=229</td>
<td>Space groups: Im-3m and Ia-3d</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Crystal system</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Centering</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the crystal class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>&quot; &quot; exact term</td>
</tr>
</tbody>
</table>
Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Td</td>
<td>Td (-4 3m in H-M notation)</td>
</tr>
<tr>
<td>4##</td>
<td>4, -4, 4/m, 422, 432, 4mm (H-M notation)</td>
</tr>
<tr>
<td>“m-3m”</td>
<td>m-3m in H-M notation or Oh in Schoenflies notation</td>
</tr>
</tbody>
</table>

**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Notation for the crystal class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the Laue class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for Wyckoff sequence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>““ exact term</td>
</tr>
</tbody>
</table>
Examples:

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

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

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

Description Search for the Pearson symbol

<table>
<thead>
<tr>
<th>Type</th>
<th>Search for the Pearson symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Format</td>
<td>Text</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>oF100</td>
<td>all orthorhombic, face-centered structures with 100 atoms in the unit cell</td>
</tr>
<tr>
<td>mS*</td>
<td>all monoclinic, side-centered structures with any number of atoms in the unit cell</td>
</tr>
<tr>
<td>cP##</td>
<td>all cubic, primitive structures with up to 99 atoms in the unit cell</td>
</tr>
</tbody>
</table>
**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Inclusion/Exclusion of an inversion center</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Inclusion/Exclusion of an inversion center</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>
**Crystal Chemistry Search**

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

**Figure 1:** Crystal Chemistry Search

<table>
<thead>
<tr>
<th>Interatomic Distances</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atom A</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>AND</td>
</tr>
<tr>
<td>AND</td>
</tr>
<tr>
<td>AND</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Minimum Distances</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atom A</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Crystal Structure is</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polytype Structure</td>
</tr>
<tr>
<td>Modulated Structure</td>
</tr>
<tr>
<td>Disordered Structure</td>
</tr>
<tr>
<td>Order/Disorder Structure</td>
</tr>
<tr>
<td>Mineral</td>
</tr>
<tr>
<td>Structure Type</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Defines the atoms for the interatomic distances</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Defines the oxidation number of the atoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

d\text{min} AB/ d\text{max} AB

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Defines the minimum/maximum distance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

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\text{min} AB,
- d\text{max} AB.
Atom A / Atom B

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Defines the atoms for the minimum distances</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

$d_{\text{min}} \text{AB} / d_{\text{max}} \text{AB}$

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Defines the minimum/maximum distances in the minimum distance search</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for predefined structure types directly</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Checkbox</td>
</tr>
<tr>
<td>Format</td>
<td>-</td>
</tr>
<tr>
<td># of entries</td>
<td>-</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>
**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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for structure types</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“” exact term</td>
</tr>
</tbody>
</table>

**Examples:**

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zeolite</td>
<td>all entries with this exact term, e.g. Zeolite-A-frame, Zeolite-ABW-frame, ...</td>
</tr>
<tr>
<td>Pe*</td>
<td>structure types containing a part starting with “pe”, e.g. pectolite, perrierite</td>
</tr>
<tr>
<td>&quot;Quartz,low&quot;</td>
<td>Structure type with this exact phrase</td>
</tr>
</tbody>
</table>

**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**

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the space group symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“” exact term</td>
</tr>
</tbody>
</table>
Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-1</td>
<td>Space group number 2</td>
</tr>
<tr>
<td>&quot;P – 1&quot;</td>
<td>Space group number 2</td>
</tr>
<tr>
<td>fm-*</td>
<td>Space groups: Fm-3, Fm-3c, Fm-3m</td>
</tr>
<tr>
<td>p 1 2 # 1</td>
<td>Space groups: P121 and P1211</td>
</tr>
</tbody>
</table>

**Wyckoff Sequence**

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for Wyckoff sequence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>

Examples:

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

**Pearson Symbol**

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the Pearson symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>oF100</td>
<td>all orthorhombic, face-centered structures with 100 atoms in the unit cell</td>
</tr>
<tr>
<td>mS*</td>
<td>all monoclinic, side-centered structures with any number of atoms in the unit cell</td>
</tr>
<tr>
<td>cP##</td>
<td>all cubic, primitive structures with up to 99 atoms in the unit cell</td>
</tr>
</tbody>
</table>
ANX formula

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for the ANX formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>*  any number of characters</td>
</tr>
<tr>
<td></td>
<td>#  0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>&quot; &quot; exact term</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>N#</td>
<td>N, NO, NX</td>
</tr>
<tr>
<td>A*YZ</td>
<td>A2XYZ, AB2XYZ, ABXYZ and AXYZ</td>
</tr>
<tr>
<td>A<em>C</em></td>
<td>all formulae that have at least AnnBnnCnn in it. AX or ABX are not included.</td>
</tr>
</tbody>
</table>

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.

![Structure Type Search](image)

**Figure 6:** All structure type descriptors can be specified
**Experimental Information Search**

The Experimental Information Search enables you to search explicitly for entries 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. Figure one corresponds to the “All Structures” choice and provides all possible search fields. Figure 2 (“Theoretical Structures Only”) shows only the search fields relevant for theoretically calculated structures. The last screenshot (Fig. 3) shows the mask for the default selection (“Experimental Structures Only”).

![Experimental Information Search Mask](image)

**Figure 1:** Experimental Information Search mask for the “All Structures” choice in the Content Selection
Figure 2: Experimental Information Search mask for the “Theoretical Structures Only” choice in the Content Selection

Figure 3: Experimental Information Search mask for the “Experimental Structures Only” choice in the Content Selection
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!

<table>
<thead>
<tr>
<th>Description</th>
<th>Temperature of the measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
</tbody>
</table>
| Wildcards   | range; temperature1 – temperature2
|             | range; ≤ temperature
|             | range; ≤= temperature
|             | range; > temperature
|             | range; >= temperature |

**Examples:**

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries (assuming K as unit)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-3</td>
<td>crystal structures measured between 2.0 K and 3.0 K</td>
</tr>
<tr>
<td>&lt;1.0</td>
<td>crystal structures measured at a lower temperature than 1.0 K</td>
</tr>
<tr>
<td>&gt;350</td>
<td>Crystal structures measured at temperatures above 350 K</td>
</tr>
</tbody>
</table>

Unit of Temperature

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Unit of temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

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!
<table>
<thead>
<tr>
<th>Description</th>
<th>Pressure during the measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>- range; pressure1 – pressure 2</td>
</tr>
<tr>
<td></td>
<td>&lt; range; &lt; pressure</td>
</tr>
<tr>
<td></td>
<td>&lt;= range; &lt;= pressure</td>
</tr>
<tr>
<td></td>
<td>&gt; range; &gt; pressure</td>
</tr>
<tr>
<td></td>
<td>&gt;= range; &gt;= pressure</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Unit of pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>

**Comments**

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Search for a comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single entry or multiple entries</td>
</tr>
<tr>
<td># of entries</td>
<td>Unlimited</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>
Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>F-Atoms</td>
<td>entries with the term in the comments, e.g. “F-atoms (AsF6) around As(4) were not determined.”</td>
</tr>
<tr>
<td>“F-Atoms (AsF6)”</td>
<td>entries with the exact phrase, e.g. “F-atoms (AsF6) around As(4) were not determined.”</td>
</tr>
<tr>
<td>cryst*</td>
<td>entries with this term starting with “cryst”, e.g. “Cell parameters from single crystal data.”</td>
</tr>
</tbody>
</table>

**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.

Only values between 0.00 and 1.00 are possible.

<table>
<thead>
<tr>
<th>Description</th>
<th>R-value of the refinement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, floating point</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td><code>- range; r_value1 – r_value2</code></td>
</tr>
<tr>
<td></td>
<td><code>&lt; range; &lt; r_value</code></td>
</tr>
<tr>
<td></td>
<td><code>&lt;= range; &lt;= r_value</code></td>
</tr>
<tr>
<td></td>
<td><code>&gt;</code> range; <code>&gt;</code> r_value</td>
</tr>
<tr>
<td></td>
<td><code>&gt;= range; &gt;= r_value</code></td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.015</td>
<td>structures with an R-value of exactly 0.015</td>
</tr>
<tr>
<td>0-1.0</td>
<td>all entries with a stored R-value</td>
</tr>
<tr>
<td>&lt;0.05</td>
<td>all entries with R-values smaller than 0.05</td>
</tr>
</tbody>
</table>

**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.

**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.

**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.

**Calculation Method**

This drop-down-box is only relevant for theoretically calculated structures. Here you can select the method used for the calculation.

<table>
<thead>
<tr>
<th>Description</th>
<th>Method used for the calculation of theoretical structures</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Dropdown box</td>
</tr>
<tr>
<td>Format</td>
<td>Single value, selectable, pre-defined</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>-</td>
</tr>
</tbody>
</table>
**DB Info Search**

Using the Database Information Search (Fig. 1) you can search for entries 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 entry in ICSD is assigned a collection code, which serves as a reference for this entry. Collection codes are not necessarily succeeding.

<table>
<thead>
<tr>
<th>Description</th>
<th>ICSD collection code</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, integer</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>range; collection_code1 – collection_code2</td>
</tr>
<tr>
<td></td>
<td>&lt; range; &lt; collection_code</td>
</tr>
<tr>
<td></td>
<td>&lt;= range; &lt;= collection_code</td>
</tr>
<tr>
<td></td>
<td>&gt; range; &gt; collection_code</td>
</tr>
<tr>
<td></td>
<td>&gt;= range; &gt;= collection_code</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>10203</td>
<td>crystal structure with CC 10203</td>
</tr>
<tr>
<td>1-10</td>
<td>all entries with CCs 1 – 10 (not necessarily 10 entries!)</td>
</tr>
<tr>
<td>&gt;=600000</td>
<td>all entries with CC 600000 - 9999999</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Description</th>
<th>PDF number as assigned by ICDD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Text</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>* any number of characters</td>
</tr>
<tr>
<td></td>
<td># 0 or 1 character</td>
</tr>
<tr>
<td></td>
<td>“ “ exact term</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>12-100</td>
<td>exact this PDF number 12-100</td>
</tr>
<tr>
<td>01-070-*</td>
<td>all PDF numbers in the range 01-070-0001 to 01-070-9999</td>
</tr>
<tr>
<td>01-07#-*</td>
<td>all PDF numbers in the range 01-070-0001 to 01-079-9999</td>
</tr>
</tbody>
</table>

Release Tag

Regular updates of ICSD are performed 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 entry in ICSD gets assigned a release tag when it is included in ICSD.

<table>
<thead>
<tr>
<th>Description</th>
<th>Release tag</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, integer, special format</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>- range; release_tag1 – release_tag2</td>
</tr>
<tr>
<td></td>
<td>&lt; range; &lt; release_tag</td>
</tr>
<tr>
<td></td>
<td>&lt;= range; &lt;= release_tag</td>
</tr>
<tr>
<td></td>
<td>&gt; range; &gt; release_tag</td>
</tr>
<tr>
<td></td>
<td>&gt;= range; &gt;= release_tag</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>2013.2</td>
<td>all entries that were newly included in release 2 in 2013</td>
</tr>
<tr>
<td>2012.1-2012.2</td>
<td>all entries included in the 2012 releases (not necessarily structures published in 2012)</td>
</tr>
<tr>
<td>&lt;2000.1</td>
<td>all entries included before 2000</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Recording date of an ICSD entry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, integer, special format</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>• range; recording_date1 – recording_date 2</td>
</tr>
<tr>
<td></td>
<td>• range; &lt; recording_date</td>
</tr>
<tr>
<td></td>
<td>• range; &lt;= recording_date</td>
</tr>
<tr>
<td></td>
<td>• range; &gt; recording_date</td>
</tr>
<tr>
<td></td>
<td>• range; &gt;= recording_date</td>
</tr>
</tbody>
</table>

Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>2012-02-1</td>
<td>all entries that were newly included on February 01, 2012</td>
</tr>
<tr>
<td>2000-01-01 – 2000-12-31</td>
<td>all entries included in 2000</td>
</tr>
<tr>
<td>&lt;2000-01-01</td>
<td>all entries included before 2000</td>
</tr>
</tbody>
</table>

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 entry 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.

<table>
<thead>
<tr>
<th>Description</th>
<th>Modification date of an ICSD entry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Numerical, integer, special format</td>
</tr>
<tr>
<td>Format</td>
<td>Single value or range</td>
</tr>
<tr>
<td># of entries</td>
<td>1</td>
</tr>
<tr>
<td>Wildcards</td>
<td>• range; modification_date1 – modification_date 2</td>
</tr>
<tr>
<td></td>
<td>• range; &lt; modification_date</td>
</tr>
<tr>
<td></td>
<td>• range; &lt;= modification_date</td>
</tr>
<tr>
<td></td>
<td>• range; &gt; modification_date</td>
</tr>
<tr>
<td></td>
<td>• range; &gt;= modification_date</td>
</tr>
</tbody>
</table>
Examples:

<table>
<thead>
<tr>
<th>Search term</th>
<th>will find the following entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>2012-08-01</td>
<td>all entries that were modified on August 01, 2012</td>
</tr>
<tr>
<td>2010-01-01 – 2010-01-31</td>
<td>all entries that were modified in January 2010</td>
</tr>
<tr>
<td>&lt;1990-01-01</td>
<td>all entries modified before 1990</td>
</tr>
</tbody>
</table>

**New Data Only**

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

<table>
<thead>
<tr>
<th>Description</th>
<th>Only entries added or modified in current release</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type</strong></td>
<td>Checkbox</td>
</tr>
<tr>
<td><strong>Format</strong></td>
<td>-</td>
</tr>
<tr>
<td><strong># of entries</strong></td>
<td>-</td>
</tr>
<tr>
<td><strong>Wildcards</strong></td>
<td>-</td>
</tr>
</tbody>
</table>
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).

![Manage Queries mask](image)

**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.

![Manage Queries Table]

**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.

![Manage Queries Table]

**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).
In 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.

![Create Combined Queries mask](image)

**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).

![Create Combined Query](image)

**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
- Report
- 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.

![ICSD Results: List View](image)

**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 choose 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.

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 entries have been selected the buttons Visualize Structure and Visualize Powder Pattern change to Compare Structures and Compare Powder Patterns, respectively.

The Report option generates a comprehensive pdf-file containing the List View, the comparison of the structures and simulated powder patterns and the Detailed View of the selected entries. Up to 15 entries can be included in a report.

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 entries are sorted in ascending (Fig. 2a) or descending (Fig. 2b) order.

**Figure 2:** Sorting by ICSD Collection Code. Ascending (left), descending (right), 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 entries or click on the checkbox in the title of the selection column to select/deselect all entries of the current page. The button “Show Detailed View” will be activated when at least one entry is selected (Fig. 1).

![Figure 1: Result set](image)

“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 entry 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 entry, to turn to the previous entry, to the next entry and to the last entry, respectively. The “Report”-button will generate a properly formatted pdf-file containing the complete information found for this entry in the Detailed View. And the “Feedback to Editor”-button provides an easy way to send us a feedback on the current entry.

2. The summary briefly describes the main features of the current entry, 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 entry 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 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.
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
  o background (on/off)
  o perspective drawing (on/off)
  o stereo (red/green) display
  o “Spin” will let the currently displayed structure rotate around the vertical axis
  o “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.
  o You can save preferred structure display settings with Jmol by pressing the "Save As Default"-button.
  o 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.
  o 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.

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. Toggling between line diagrams (checkbox “Intensities only”) and standard powder patterns (Gauß envelope) is possible, too. Once can also include or exclude dispersion.

  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. $\chi_{\text{min}}$, $\chi_{\text{max}}$, and $\chi_{\text{step}}$ 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**

<table>
<thead>
<tr>
<th>Sum Form</th>
<th>Structure</th>
<th>Number of Formula Units</th>
<th>Form. Unit</th>
<th>Cryst. Comp.</th>
<th>Chem. Comp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>O7 Sr2 Ta2</td>
<td>Sr2 (Ta2 O7)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dodecaborate</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Figure 6:** Chemistry details

The “Sum Form” field shows the sum formula 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.
Form." (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 would show C1 H12 Ca1 O9.

The chemical name, the mineral name and the mineral group are listed accordingly. The number of formula units (Z) shows how many times the unit cell contains the atoms in the field “Sum Form”.

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.

\[
\text{Fe}^{2+}(\text{Fe}^{3+})_2\text{O}_4 \rightarrow \text{AB2X4} \\
(\text{Fe}^{2.6667+})_3\text{O}_4 \rightarrow \text{A3X4}
\]

- 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

<table>
<thead>
<tr>
<th>Chemical formula</th>
<th>ANX formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg₃Al₃(SiO₄)₃</td>
<td>A2B3C3X12</td>
</tr>
<tr>
<td>Ca₃(Al₁₋₁₃₃₂₅Fe₀.₆₆₇₅)Si₃O₁₂</td>
<td>A2B3C3X12</td>
</tr>
<tr>
<td>(Mg₂₋₂₃₃Fe₀.₃)(Al₁₋₁₀₃Cr₀.₃)Si₃O₁₂</td>
<td>A2B3C3X12</td>
</tr>
</tbody>
</table>
The field “Published Crystal Structure Data” (Fig. 7, top) shows the crystallographic information as given by the author(s). Among the cell parameters, space group, crystal system, crystal class, Laue class and Pearson symbol you will find the cell volume, number of formula units (Z) and structure type information.

The list of atomic coordinates and, if available, the anisotropic displacement parameters are also contained.
The “Standardized Crystal Structure Data” (Fig. 7, bottom) is derived from the published data and gives information on the same fields as above. The standardization is done following the rules given by L. M. Gelato and E. Parthé in J. Appl. Cryst. (1987) 20, 139-143.

**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. 8) or from the atom position lists (Fig. 9).

![Figure 8: Distances and Angles screen: selection by elements](image)

![Figure 9: Distances and Angles screen: selection by atom positions](image)

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.
Figure 10: 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. 10). 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 subtracted 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. 11).
Figure 11: A text-only list of angles

Switching to the “Histograms” view (Fig. 12) 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 entry 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 12: Histograms of interatomic distances

Bibliography

Fig. 13 shows the “Bibliography” information of the current entry: Title and reference(s). The “Get full text” link provides a connection to the publication for the current entry.

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 to search for the article.
If an abstract is available for this entry it is displayed after the keywords.

**Experimental Information**

The section “Experimental Information” is divided into three subsections (Fig. 14):

1. **External conditions**

   The ambient pressure and temperature are given as published by the authors. Note: If no pressure or temperature were published, default values of 0.101325 MPa and 293 K are assumed and added. The corresponding fields for temperature and pressure will then contain "room temperature" and "atmospheric", respectively. The radiation type can be: X-ray, electrons, neutrons or synchrotron. The sample may either be a polycrystalline powder or a single crystal. The R values of a subsequent structure refinement are given if available.

2. **Additional Information**

   If published, the entry may additionally contain information about twinning of crystals, available temperature factors, available NMR data, performed Rietveld refinement, available magnetic structure, correction of earlier work, determination of absolute configuration, available anharmonic temperature factors, cell constants without standard deviations, assigned PDF numbers (either experimental or calculated), and/or that for a structure only the cell and the structure type were determined (coordinates are then derived from the corresponding structure type entry).

3. **Properties of Structure**

   This subsection shows whether or not the current structure is polytypic, disordered, a modulated structure, a mineral, a prototype structure type and/or a structure prototype was be assigned.
Figure 14: Experimental Information

Warnings and Comments

Figure 15: Warnings and Comments

The “Warnings and Comments” field informs you about (probable) inconsistencies (wrong coordinates, atoms too close etc.) of the current structure. Additional comments (stability of the compound etc.) are mentioned, too (Fig. 15).

Compare Published and Standardized Structure

Figure 16 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.
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
  o background (on/off)
  o perspective drawing (on/off)
  o stereo (red/green) display
  o “Spin” will let the currently displayed structure rotate around the vertical axis
  o “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.
  o You can save preferred structure display settings with Jmol by pressing the "Save As Default"-button.
  o 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.
  o The "Reset to System"-button will always restore the properties to the original defaults.
Figure 17: Interactive comparison of published and standardized structures

Export Data

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

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

![Figure 1: Result set](image)

Clicking on the button “Export Data” will show a dialogue as shown in Figure 2. Enter the base file name for the data sets to export. The other name fields will be updated accordingly.

![Figure 2: Export Data dialogue](image)
Exporting as a single CIF will lead to one file, in which the exported entries are sequentially listed. Multiple CIFs will result in individual files for each entry; 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.

Clicking on the download symbol in 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 entry. You may, of course, also change the suggested file name.
The Report button generates a comprehensive pdf-file containing List View (but currently only with the
default column selection), comparison of the crystal structures and powder patterns, and the Detailed View
of the selected entries (Fig. 1). The Report button is only accessible when one to 15 entries are selected.
**Visualize Structure/Compare Structures**

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

---

**Figure 1:** Result set
Figure 2: Compare Structures: Multiple plots of crystal structures

For each structure the collection and the structured formula is given in the title bar. The pace 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.

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
  
  o background (on/off)
  o perspective drawing (on/off)
  o stereo (red/green) display
  o “Spin” will let the currently displayed structure rotate around the vertical axis
  o “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.
  
  o You can save preferred structure display settings with Jmol by pressing the "Save As Default"-button.
  o 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.
  o 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 entry the button “Visualize Powder Pattern” becomes accessible, and it changes to the “Compare Powder Pattern” button as soon as a second entry is selected. Please note that either of the two buttons is only accessible when up to six entries 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. Toggling between line diagrams (checkbox “Intensities only”) and standard powder patterns (Gauß envelope) is possible, too. Once can also include or exclude dispersion.

  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. $x_{\text{min}}$, $x_{\text{max}}$, and $x_{\text{step}}$ 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.](image)

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

A post-query filtering has been implemented, which allows to further confine the number of hits from a query without having to rerun 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 entries from the current query.

Figure 1: The post-query Filter window with its options.
Figure 2: Checkbox for applying the selected filter options.