



Basic use of Inorganic Crystal Structure Database

Three different ways to access ICSD

- Aalto Learning Centre remote access (**recommended, the easiest way**).
 - Open a web browser and go to <http://libproxy.aalto.fi/login?url=https://icsd.fiz-karlsruhe.de/>
 - After logging in with your Aalto account, you will be redirected to ICSD
- Aalto VPN
 - Instructions at MyCourses -> Databases -> Aalto VPN
 - Connect to VPN, open a web browser, and go to <https://icsd.fiz-karlsruhe.de/>
 - If you connect to VPN during a Zoom lecture you need to reconnect to Zoom
- Aalto campus network
 - Simply open a web browser and go to <https://icsd.fiz-karlsruhe.de/>

ICSD search interface

- Sometimes the Basic Search is enough, especially for simple composition-based searches. On this course, we use the **Advanced search & retrieve**

The screenshot shows the ICSD search interface. A red box highlights the 'Content Selection' section in the left sidebar, where 'Experim. inorganic structures' is checked. A red arrow points from the text 'Advanced search & retrieve' in the sidebar to the 'Basic Search & Retrieve' section. A blue arrow points from the 'Chemistry' section to the 'Composition' input field. A red text box with a blue arrow pointing to the 'Experim. inorganic structures' checkbox contains the text: 'Make sure that only "Experim. inorganic structures" is selected (unless you know what you are doing)'. The interface includes a 'Login' section, a 'Basic Search & Retrieve' section with various search criteria, and a 'Search Action' section with 'Run Query' and 'Clear Query' buttons. The top right corner shows 'FIZ Karlsruhe | Contact' and 'Close session'.

ICSD query for NaCl (1)

1. Choose **Advanced** -> **Chemistry** and set the search criteria as follows:
2. Composition: **Na Cl** (the space inbetween Na and Cl is important)
3. Number of elements: 2 (limit the search to Na and Cl).
4. Click "Count Chemistry Search".
5. **Search Summary** shows, how many structures match your search. In the figure below, there are 26 matches. You may see a few more.

The screenshot shows the ICSD Chemistry Search interface. The search criteria are set as follows:

- Search Type:** Chemistry (1.)
- Composition:** Na Cl (2.)
- Number of Elements:** 2 (3.)

The **Search Action** section includes buttons for "Run Query" and "Clear Query". The **Search Summary** (5.) table shows the following results:

Category	Count
Bibliography:	-
Cell:	-
Chemistry:	26
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-
Combined Results:	26

The **Query History** section shows "Number of queries: 0" and a "Clear Query History" button. The "Count Chemistry Search" button (4.) is highlighted in red.

ICSD query for NaCl (2)

Search Action

Run Query

Clear Query

- Next, click **Search Action** -> **Run Query**
- ICSD will now retrieve all matching crystal structures and list them
- *(Your listing may be bit different from the one below)*
- Unique ID / Space group / Structural formula / Structure type / Original publication

<input type="checkbox"/>	Coll. Code ▲	HMS ⇅	Struct. Form. ⇅	Struct. Type ⇅	Title ⇅	Authors ⇅	Cell Volume ⇅	Publication Year ⇅	☆	Download
<input type="checkbox"/>	100633	F m -3 m	Na Cl	NaCl	A revised method of op	Finger, L.W.; King, H.	162.17	1978	☆	Download
<input type="checkbox"/>	165592	F m -3 m	Na Cl	NaCl	Solubility of Al ₂ O ₃ in s	Cherginets, V.L.; Baum	181.06	2006	☆	Download
<input type="checkbox"/>	181148	F m -3 m	Na Cl	NaCl	Characterization of sod	Fontana, P.; Schefer, J.	179.58	2011	☆	Download
<input type="checkbox"/>	18189	F m -3 m	Na Cl	NaCl	Accuracy of an automa	Abrahams, S.C.; Berns	177.50	1965		Download
<input type="checkbox"/>	28948	F m -3 m	Na Cl	NaCl	Studies of Na Cl - K Cl	Barrett, W.T.; Wallace,	179.41	1954		Download
<input type="checkbox"/>	41411	F m -3 m	Na Cl	NaCl	Electronic and thermal	Strel'tsov, V.A. (Streltsc	177.50	1988		Download
<input type="checkbox"/>	41439	F m -3 m	Na Cl	NaCl	Structural and elastic p	Srinivasa, R.B.; Sanyal	179.79	1990		Download
<input type="checkbox"/>	43434	P m -3 m	Na Cl	CsCl	Polymorphic transitions	Evdokimova, V.V.; Vera	37.93	1962		Download
<input type="checkbox"/>	52232	F m -3 m	Na Cl	NaCl	Die Gitterkonstanten de	Straumanis, M.E.; Jevir	179.31	1936		Download
<input type="checkbox"/>	52233	F m -3 m	Na Cl	NaCl	The effect of crystal-siz	Finch, G.J.; Fordham, S	183.30	1936		Download

For selecting

(1 of 3) 1 2 3 10

Three pages of structures, change the page here

Star = High-quality data

Download CIF

ICSD detailed view (1)

- Most of the NaCl structures are just "normal" NaCl in space group *Fm-3m*
- Select the *Fm-3m* structure **181148** using the checkbox and click "**Show detailed view**" (or just directly click the structure ID number in the Coll. Code column)

(For downloading several selected structures at a time)

Results: List View # of Hits: 26 (1 selected) ?

2.

<input type="checkbox"/>	Coll. Code ^	HMS ⇅	Struct. Form. ⇅	Struct. Type ⇅	Title ⇅	Authors ⇅	Cell Volume ⇅	Publication Year ⇅	☆	
<input type="checkbox"/>	100633	F m -3 m	Na Cl	NaCl	A revised method of op	Finger, L.W.; King, H.	162.17	1978	☆	
<input type="checkbox"/>	1. 165592	F m -3 m	Na Cl	NaCl	Solubility of Al2 O3 in s	Cherginets, V.L.; Baum	181.06	2006	☆	
<input checked="" type="checkbox"/>	181148	F m -3 m	Na Cl	NaCl	Characterization of sod	Fontana, P.; Schefer, J.	179.58	2011	☆	

ICSD detailed view (2)

- It is always important to check the **temperature** and **pressure**
 - Do not use high-temperature (> 300 K) or high-pressure data (> atmospheric) unless you have a specific reason to do so!

Detailed View Entry 1 of 1 ?

[Back to Query](#) [Back to List](#) ⏪ ⏩ [Export Cif](#) [Print](#) [Feedback to Editor](#)

Summary	Returns to the list of structures	Downloads CIF file	Collection Code 181148
Struct. formula	Na Cl	Structure type	NaCl
Cell parameter	5.6418(2) 5.6418(2) 5.6418(2) 90 90 90	Space group	F m -3 m (225)
Cell volume	179.58 [Å ³]	Z	4
Temperature	room temperature	Pressure	atmospheric
Data quality	High quality	R-value	0.026
Author	Fontana, P.; Schefer, J.; Pettit, D.	Title	Characterization of sodium chloride crystals grown in microgravity
Reference	Journal of Crystal Growth (2011) 324, (1) p207-p211	DOI	10.1016/j.jcrysgr.2011.04.001

Details Expand all Collapse all ?

- ▶ Visualization **Please have a look at all of these details to learn what ICSD has to offer. The next slide has more information on visualization.**
- ▶ Chemistry
- ▶ Published Crystal Structure Data
- ▶ Standardized Crystal Structure Data
- ▶ Distances and Angles
- ▶ Bibliography
- ▶ Experimental information
- ▶ Additional information

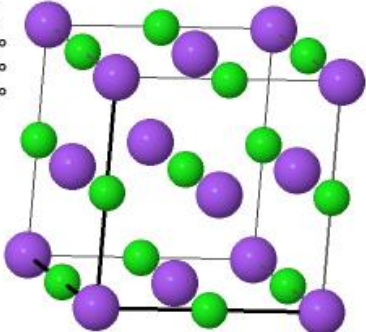
ICSD visualization

The standard visualization is just a figure

Visualization

Published Crystal Structure

HM: F m -3 m
a=5.642Å
b=5.642Å
c=5.642Å
α=90.000°
β=90.000°
γ=90.000°



Interactive Visualization

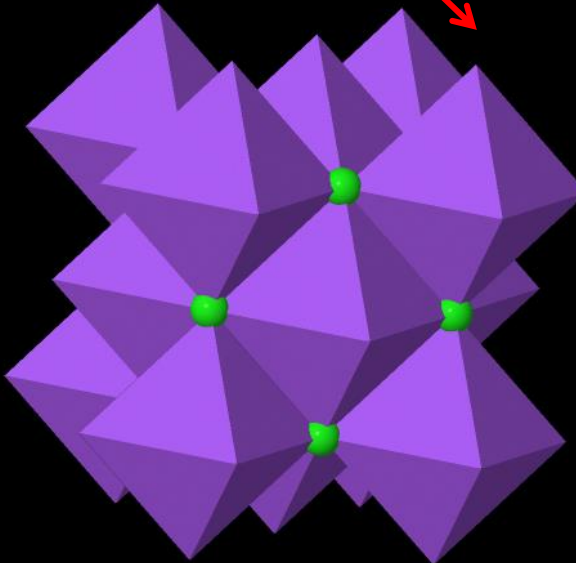
Interactive visualization with JSmol,
the web-counterpart of Jmol

JSmol is convenient for quick visualization,
but desktop Jmol is often more more
convenient (larger viewing area, faster).

Right-click the background for the menu

Coll. Code: 181148, Na Cl - 2011 Fontana P. Sc ...

HM: F m -3 m #225
a=5.642Å
b=5.642Å
c=5.642Å
α=90.000°
β=90.000°
γ=90.000°



ICSD

Align Explore Coordination Unitcell Distance/Ionic Radii Display Properties **Display Content**

Atoms: atoms 25% H-Bonds: No Polyhedra: Yes
Select/Mark Atom Site: No Cavities: No

Save As Default Restore Defaults Reset To System

Uncheck for ball-and-stick

Further practical instructions

- Click "**Back to query**" in the list view to return to the main page
- Click "**Search action**" -> "**Clear query**" on the main page to reset the query
- Click Advanced -> Chemistry -> Composition -> **Periodic table**
- The composition search is very powerful!

Search Chemistry Visual Search mode

Select groups

Select periods

→ Metals → Transition Metals → Non-Metals

Click on element or select period and/or group.

Number of Elements: Units of Coefficients:

AND	El.Symb.	Co.(min)	Co.(max)	Ox.(min)	Ox.(max)
AND	FEG				
AND	O				

Restrict total number of elements to selected number of elements

OK Cancel

The example here is for binary group 8 (iron group) oxides.

Binary oxide: One type of metal atom + oxygen

Note the setting "**Number of Elements**" = 2

This setting excludes other elements. Otherwise, the search would include **all** compounds that include iron group metal and oxygen (e.g. $\text{Fe}(\text{CO})_5$)