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**

Make sure that only "Experim. inorganic structures" is selected (unless you know what you are doing)

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.

ICSD query for NaCl (2)

- Next, click **Search Action** -> **Run Query**

Search Action
| Run Query | Clear 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

		Coll. Code ▲	HMS ⇕	Struct. Form. ⇕	Struct. Type ⇕	Title ⇕	Authors ⇕	Cell Volume ⇕	Publication Year ⇕	✦ ▾	
☐		100633	F m -3 m	Na Cl	NaCl	A revised method of op	Finger, L.W.; King, H.	162.17	1978	✦	⬇
☐		165592	F m -3 m	Na Cl	NaCl	Solubility of Al2 O3 in s	Cherginets, V.L.; Baum	181.06	2006	✦	⬇
☐		181148	F m -3 m	Na Cl	NaCl	Characterization of sod	Fontana, P.; Schefer, J.	179.58	2011	✦	⬇
☐		18189	F m -3 m	Na Cl	NaCl	Accuracy of an automa	Abrahams, S.C.; Berns	177.50	1965		⬇
☐		28948	F m -3 m	Na Cl	NaCl	Studies of Na Cl - K Cl	Barrett, W.T.; Wallace,	179.41	1954		⬇
☐		41411	F m -3 m	Na Cl	NaCl	Electronic and thermal	Strel'tsov, V.A. (Streltso	177.50	1988		⬇
☐		41439	F m -3 m	Na Cl	NaCl	Structural and elastic p	Srinivasa, R.B.; Sanyal	179.79	1990		⬇
☐		43434	P m -3 m	Na Cl	CsCl	Polymorphic transitions	Evdokimova, V.V.; Vera	37.93	1962		⬇
☐		52232	F m -3 m	Na Cl	NaCl	Die Gitterkonstanten de	Straumanis, M.E.; Jevir	179.31	1936		⬇
☐		52233	F m -3 m	Na Cl	NaCl	The effect of crystal-siz	Finch, G.J.; Fordham, S	183.30	1936		⬇

For selecting

(1 of 3) |◀ ◀◀ **1** 2 3 ▶▶ ▶| 10 ▾

Three pages of structures, change the page here

Star = High-quality data

Download CIF

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ICSD detailed view (1)

- Most of the NaCl structures are just "normal" NaCl in space group *Fm*-3*m*
- Select the *Fm*-3*m* 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)

🔍 Back to Query	🔍 Show Detailed View **2.**	🖫 Export Data	🖨 Print	✧ Visualize Structure	✧ Visualize Powder Pattern ▾		☐ Column Selection	▼ Filter

	Coll. Code ▲	HMS ⇕	Struct. Form. ⇕	Struct. Type ⇕	Title ⇕	Authors ⇕	Cell Volume ⇕	Publication Year ⇕	✩ ▾	
☐	100633	F m -3 m	Na Cl	NaCl	A revised method of op	Finger, L.W.; King, H.	162.17	1978	✩	🔽
☐ **1.**	165592	F m -3 m	Na Cl	NaCl	Solubility of Al2 O3 in s	Cherginets, V.L.; Baum	181.06	2006	✩	🔽
☑	181148	F m -3 m	Na Cl	NaCl	Characterization of sod	Fontana, P.; Schefer, J.	179.58	2011	✩	🔽

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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

🔍 Back to Query | ☰ Back to List | ⏮ ◀ ▶ ⏭ | 💾 Export Cif | 🖨 Print | ✉ Feedback to Editor

Returns to the list of structures   **Downloads CIF file**

Summary   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 [Å³]	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.jcrysgro.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
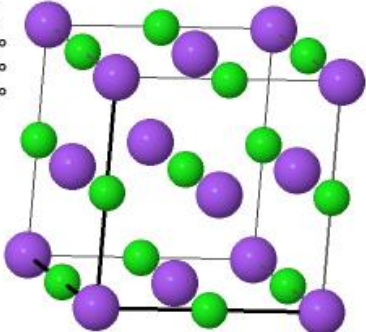
▸ Experimental information

▸ Additional information

ICSD visualization

The standard visualization is just a figure

Right-click the background for the menu

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

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

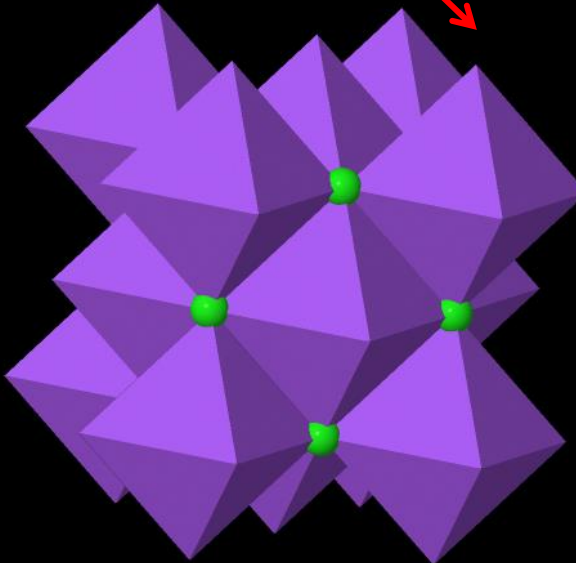💾 Save As Default   ↶ Restore Defaults   ↻ Reset To System

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).

Uncheck for ball-and-stick

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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!

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.* $Fe(CO)_5$)