



# Basic use of Inorganic Crystal Structure Database

**Some of the figures are not yet updated to ICSD version 2019**

# Search interface

- Open a web browser and go to <http://icsd.fiz-karlsruhe.de/> (works only from Aalto campus network or with Aalto VPN, see MyCourses -> Databases for details)
- Sometimes the Basic Search is enough, especially for simple composition-based searches. Generally, I recommend **Advanced search**

The screenshot shows the ICSD search interface. A red box highlights the 'Content Selection' section, where 'Experimental Structures only' is selected. Another red box highlights the 'Advanced search & retrieve' option in the navigation menu. A red arrow points from the 'Advanced search & retrieve' box to the 'Content Selection' box. A red text overlay reads: 'Make sure that "Experimental structures only" is selected (unless you know what you are doing)'. The interface includes a login section, a 'Basic Search & Retrieve' header, and various search filters such as Bibliography, Chemistry, Symmetry, and Exp. Info. & Ref. Data.

Welcome to ICSD Web. IP authenticated (130.233.85.107). Helsinki Univ of Technology

**Content Selection**

- Experimental Structures only
- Theoretical Structures only
- All Structures

**Advanced search & retrieve**

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

**Basic Search & Retrieve**

**Bibliography**

Authors  Year of Publication

Title of Journal

Title of Article

**Chemistry**

Composition  Periodic Table  Number of Elements

**Cell**

Cell Parameters

Cell Volume  Tolerance +/-  %

**Symmetry**

Space Group Symbol  Space Group Number

Crystal System  Centering

**Exp. Info. & Ref. Data**

New Data Only

PDF Number  Temperature  K

ICSD Collection Code  Pressure  MPa

Clear Basic Search  Count Basic Search

# The first ICSD query

- Choose **Advanced** -> **Chemistry**
- Set the search criteria as follows:
- Composition: **Na Cl** (the space inbetween Na and Cl is important)
- Number of elements: 2 (rule out other elements).
- Click "Count Chemistry Search". **Search Summary** shows, how many structures match your search (gives **27** on 2019-04-15)
- Next, click "Search Action -> Run Query" and ICSD will list all the structures
- Unique ID / Space group / Structural formula / Structure type / Original publication

<input type="checkbox"/>	Coll. Code ^	HMS ↕	Struct. Form. ↕	Struct. Type ↕	Title ↕	Authors ↕	Reference ↕	☆	
<input type="checkbox"/>	100633	F m -3 m	Na Cl	NaCl	A revised method of operat	Finger, L.W.; King, H.	American Mineralogist (197	☆	📄
<input type="checkbox"/>	165592	F m -3 m	Na Cl	NaCl	Solubility of Al2 O3 in some	Cherginets, V.L.; Baumer, V	Inorganic Chemistry (2006)	☆	📄
<input type="checkbox"/>	181148	F m -3 m	Na Cl	NaCl	Characterization of sodium	Fontana, P.; Schefer, J.; Pe	Journal of Crystal Growth (2	☆	📄
<input type="checkbox"/>	18189	F m -3 m	Na Cl	NaCl	Accuracy of an automatic d	Abrahams, S.C.; Bernstein,	Acta Crystallographica (196		📄
<input type="checkbox"/>	28948	F m -3 m	Na Cl	NaCl	Studies of Na Cl - K Cl Soli	Barrett, W.T.; Wallace, W.E	Journal of the American Ch		📄
<input type="checkbox"/>	41411	F m -3 m	Na Cl	NaCl	Electronic and thermal para	Strel'tsov, V.A. (Streltsov, V	Kristallografiya (1988) 33, ('		📄
<input type="checkbox"/>	41439	F m -3 m	Na Cl	NaCl	Structural and elastic prope	Srinivasa, R.B.; Sanyal, S.F	Physical Review B: Conden		📄
<input type="checkbox"/>	43434	P m -3 m	Na Cl	CsCl	Polymorphic transitions in N	Evdokimova, V.V.; Verashcl	Fizika Tverdogo Tela (Sank		📄
<input type="checkbox"/>	52232	F m -3 m	Na Cl	NaCl	Die Gitterkonstanten des N	Straumanis, M.E.; Jevins, A	Zeitschrift fuer Physik (1936		📄
<input type="checkbox"/>	52233	F m -3 m	Na Cl	NaCl	The effect of crystal-size or	Finch, G.J.; Fordham, S.	Proceedings of the Physica	3	📄

(1 of 3) 1 2 3 10

# ICSD detailed view

- Most of the NaCl structures are just the normal NaCl in space group *Fm-3m*
- Select one of the *Fm-3m* structures using the checkbox and click **"Show detailed view"**
- It good always to check the temperature and pressure
  - Don't use high-temperature (> 298 K) or high-pressure data (> atmospheric) unless you have a specific reason to do so!

**Summary** Collection Code 165592

Struct.formula	Na Cl			Author	Cherginets, V.L.; Baumer, V.N.; Galkin, S.S.; Glushkova, L.V.; Rebrova, T.P.; Shtitelman, Z.V.
Space Group	F m -3 m(225)			Title of Article	Solubility of Al <sub>2</sub> O <sub>3</sub> in some chloride-fluoride melts
Unit Cell	5.6573(7) 5.6573(7) 5.6573(7) 90. 90. 90.			Reference	Inorganic Chemistry (2006) 45, p7367-p7371
Cell Volume	181.06 Å <sup>3</sup>	Formula Units per Cell	4	Warnings & Comments	0 Warnings / 1 Comments
Temperature	290 K	Pressure	atmospheric		
PDF-numbers		R-value	0.138		
Remark					

Remark ★ High Quality Data

[Export CIF File](#) NaCl [Show Synoptic View](#) [Feedback to the ICSD Editor](#)

## Details

Expand All Collapse All

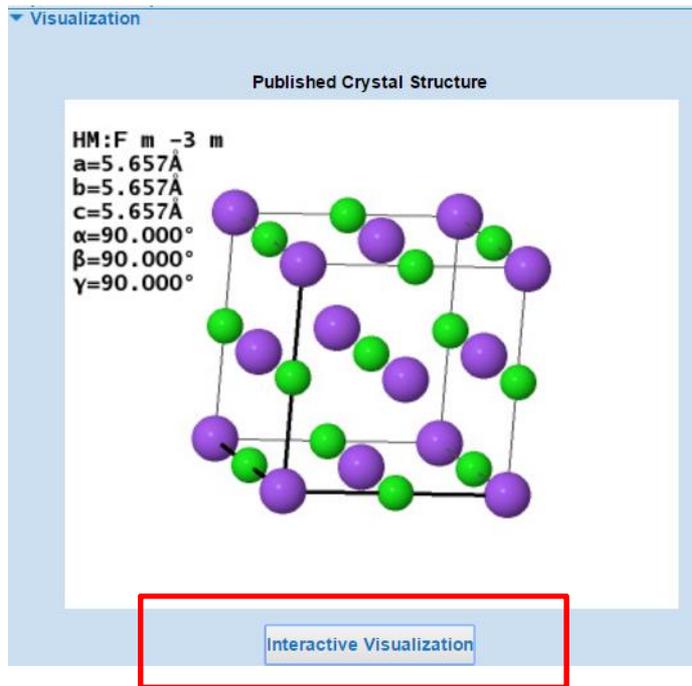
- ▶ Visualization
- ▶ Chemistry
  - ▶ Published Crystal Structure Data
  - ▶ Standardized Crystal Structure Data
  - ▶ Distances & Angles
  - ▶ Bibliography
  - ▶ Experimental Information
  - ▶ Warnings & Comments
  - ▶ Compare Published & Standardized Structure

Please have a look at all of these! (to learn what ICSD has to offer)

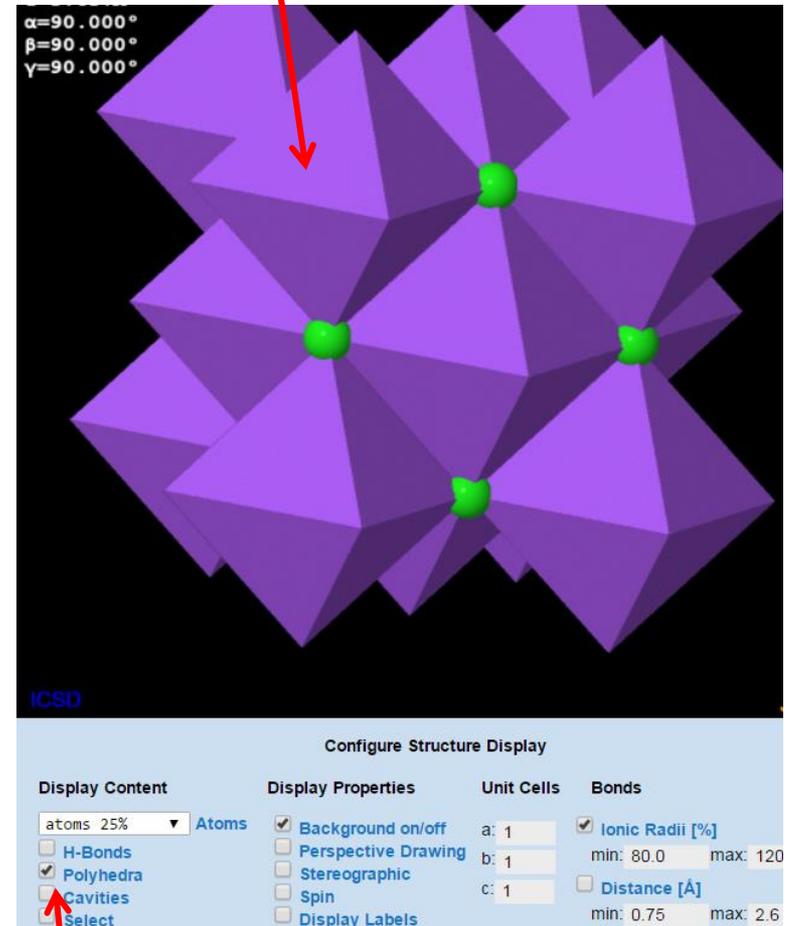
The next slide has more information on visualization

# ICSD visualization

The standard visualization is just a figure



Right-click for the JSmol menu!



Uncheck for ball-and-stick

Interactive Visualization with JSmol,  
the web-counterpart of Jmol!

JSmol is very convenient for quick visualization, but desktop Jmol is often even more convenient (larger display, faster). So, let's export a CIF file for Jmol (next slide)

# Exporting data from ICSD

- CIF files can be exported either from the detailed view (one structure at a time) or from the list view (many structures at a time)

Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Reference		
<input checked="" type="checkbox"/>	165592	F m -3 m	Na Cl	NaCl	Solubility of Al <sub>2</sub> O <sub>3</sub> in some chloride-fluoride melts	Cherginets, V.L.; Baumer, V.N.; Galkin, S.S.; Glushkova, L.V.; Rebrova, T.P.; Shtitelman, Z.V.	Inorganic Chemistry (2006) 45, p7367-p7371	
<input type="checkbox"/>	181148	F m -3 m	Na Cl	NaCl	Characterization of sodium chloride	Fontana, P.; Schefer, J.; Pettit	Journal of Crystal Growth (2011) 324 (1)	

- Now, export one CIF file with NaCl structure (space group *Fm-3m*) This works, too
- ***A comment on the data quality:***
- ICSD is a "curated" database and there should not be that many erroneous structures (but there still are some, we will see at least one example!)
- If you download a structure and use it for any serious work, you should always:
  - Check the "Warnings and comments" section
  - Find the ***original publication*** to see if the authors have included any additional information / warnings in there

# Further practical instructions

- Click "Back to query" and "Clear query" to reset
- ICSD -> Advanced search -> Chemistry -> Composition -> Periodic table
- The composition search is very powerful!

*Select periods*

*Select groups*

→ Metals      → Transition Metals      → Non-Metals

*Click on element or select period and/or group.*

Number of Elements       Units of Coefficients

El.Symb.	Co.(min)	Co.(max)	Ox.(min)	Ox.(max)
AND ▼ FEG	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
AND ▼ O	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

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

***"Number of Elements" = 2!***

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