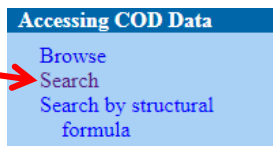


Basic use of
Crystallography Open Database

Search interface

- COD is open access, so anyone can use it without any licence fees
- Open a web browser and go to <http://www.crystallography.net/>
- Click **Search**
- The search interface is not that fancy, but basic queries are easy
- Let's start with NaCl
- **1 to 8 elements**: Na Cl
- **number of distinct elements min and max**: 2 2
- Without this setting, you will get structures including Na and Cl, but not excluding other elements. For example NaClO₃.
- Click **Send**



text (1 or 2 words)	<input type="text"/>
journal	<input type="text"/>
year	<input type="text"/>
volume	<input type="text"/>
issue	<input type="text"/>
DOI	<input type="text"/>
Z (min, max)	<input type="text"/> <input type="text"/>
Z' (min, max)	<input type="text"/> <input type="text"/>
1 to 8 elements	<input type="text" value="Na"/> <input type="text" value="Cl"/> <input type="text"/> <input type="text"/> <input type="text"/>
NOT these elements	<input type="text"/> <input type="text"/> <input type="text"/> <input type="text"/>
volume min and max	<input type="text"/> <input type="text"/>
number of distinct elements min and max	<input type="text" value="2"/> <input type="text" value="2"/>
filters	<input type="checkbox"/> has F _{obs} <input type="checkbox"/> include duplicates <input type="checkbox"/> include structures with errors <input type="checkbox"/> include theoretical structures
<input type="button" value="Reset"/>	<input type="button" value="Send"/>

Search results

- You will get the search results in the format below
 - In the case of NaCl, there are 34 structures in the database
- You can save the structure as a CIF file by clicking the **CIF** link of the structure
- You can view the details of the database entry by clicking the **COD ID** link

Search results

Result: there are 34 entries in the selection

[Switch to the old layout of the page](#)

Download all results as: [list of COD numbers](#) | [list of CIF URLs](#) | [data in CSV format](#) | [archive of CIF files \(ZIP\)](#)

Searching elements including Na, Cl number of elements between 2 and 2

◀◀ First | ◀ Previous 20 | Page 1 of 2 | [Next 20](#) ▶ | [Last](#) ▶▶ | Display 20 50 100 200 300 500 1000 entries per page

COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
1000041	CIF	Cl Na	F m -3 m	5.62; 5.62; 5.62 90; 90; 90	177.5	Abrahams, S C; Bernstein, J L Accuracy of an automatic diffractometer. measurement of the sodium chloride structure factors <i>Acta Crystallographica (1,1948-23,1967)</i> , 1965 , <i>18</i> , 926-932
2104025	CIF Paper	Cl Na	P m -3 m	2.86; 2.86; 2.86 90; 90; 90	23.394	Shiraki, Koichi; Tsuchiya, Taku; Ono, Shigeaki Structural refinements of high-pressure phases in germanium dioxide <i>Acta Crystallographica Section B</i> , 2003 , <i>59</i> , 701-708
2311042	CIF	Cl Na	F m -3 m	5.62; 5.62; 5.62 90; 90; 90	177.504	Juhás, Pavol; Farrow, Christopher L.; Yang, Xiaohao; Knox, Kevin R.; Billinge, Simon J. L. Complex modeling: a strategy and software program for combining multiple information source <i>Acta Crystallographica Section A</i> , 2015 , <i>71</i> , 562-568

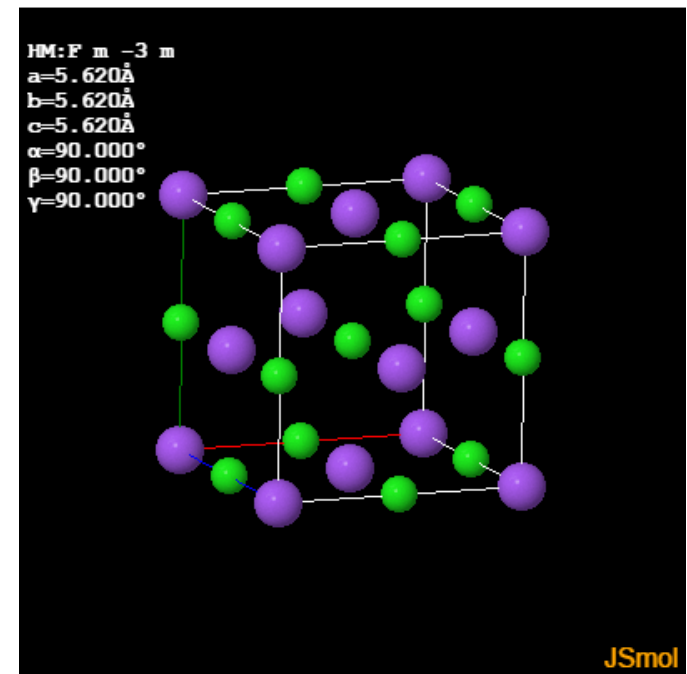
Quick visualization

- Click the first resulting COD ID 1000041
- The page includes a quick visualization implemented using JSmol
- Right-click for menu if you want to change settings (*e.g.* Symmetry -> Reload {1 1 1})
- A download link to the CIF file is also available (**Coordinates 1000041.cif**).
- You can also load COD structures directly to Jmol without downloading the CIF
 - Details in Jmol instructions ([link](#))
- Note: Please **don't** click "**Display in Jmol**" in COD: this will try to open the structure in a Jmol Java applet inside the browser. It most probably won't work.

Information card for 1000041

[1000040](#) << 1000041 >> [1000042](#)

Preview



Structure parameters

- For every database entry, COD shows the bibliographic information and other key information in a table below the quick visualization

▼ Structure parameters

Chemical name	Sodium chloride
Formula	Cl Na
Calculated formula	Cl Na
SMILES	[Na+].[Cl-]
Title of publication	Accuracy of an automatic diffractometer. measurement of the sodium chloride structure factors
Authors of publication	Abrahams, S C; Bernstein, J L
Journal of publication	Acta Crystallographica (1,1948-23,1967)
Year of publication	1965
Journal volume	18
Pages of publication	926 - 932
a	5.62 Å
b	5.62 Å
c	5.62 Å
α	90°
β	90°
γ	90°
Cell volume	177.5 Å ³
Number of distinct elements	2
Hermann-Mauguin symmetry space group	F m -3 m
Hall symmetry space group	-F 4 2 3
Residual factor for all reflections	0.022
Has coordinates	Yes
Has disorder	No
Has F _{obs}	No

Advanced COD topics (starting from Lecture 7)

Powder pattern matching with Crystallography Open Database

- COD (<http://www.crystallography.net/cod/>) has a large set of crystal structures
- Powder patterns have been simulated for all structures and collected into a database that can be used for pattern matching and phase identification
- Has been integrated in some commercial programs (Rigaku, PANalytical, Match!) and with free QualX2 program (<http://www.ba.ic.cnr.it/softwareic/qualx/>)
- Web search available at <http://cod.iutcaen.unicaen.fr/>
 - Try with ZnO (data in Materials -> Data files for lectures -> Lecture 07)

Figures: AJK

Diffraction pattern and sample composition

Upload diffraction pattern: ZnO_26170...owder.xy

Structures database: **Set to inorganic!**

Atomic elements in the sample: **Choose elements**

Threshold phase density: Maximum number of phases:

Crystallisation: **Limit to 4 or less**

Experiment details

Radiation:

X-ray tube:

Other: Wavelength (Å):

Instrument geometry:

Bragg-Brentano (theta-2theta)

Bragg-Brentano (2theta only), omega:

Debye-Scherrer

Transmission **Try medium first, then high**

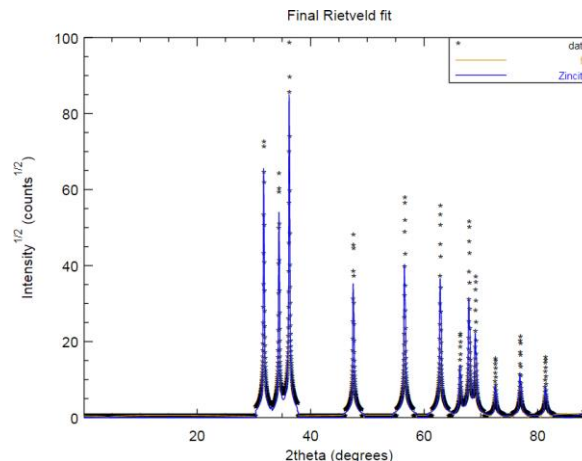
Instrument broadening function:

Found phases and quantification:

Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
9004181	Zincite	100	100	2758.64	0.000540488

Click to get the database entry →

Final Rietveld analysis, R_w: 0.503114, GofF: 3.75879



Information card for entry 9004181

[9004180](#) << [9004181](#) >> [9004182](#)

Preview

