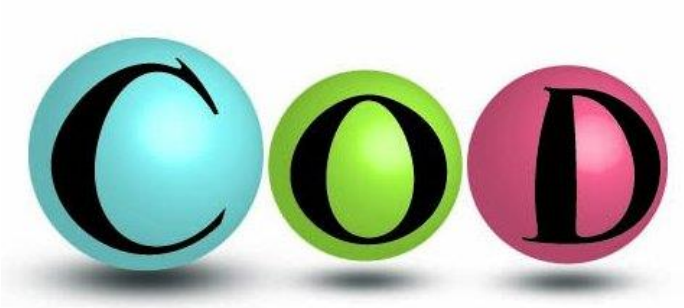
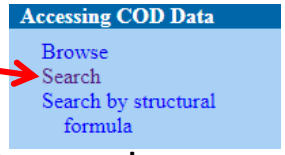


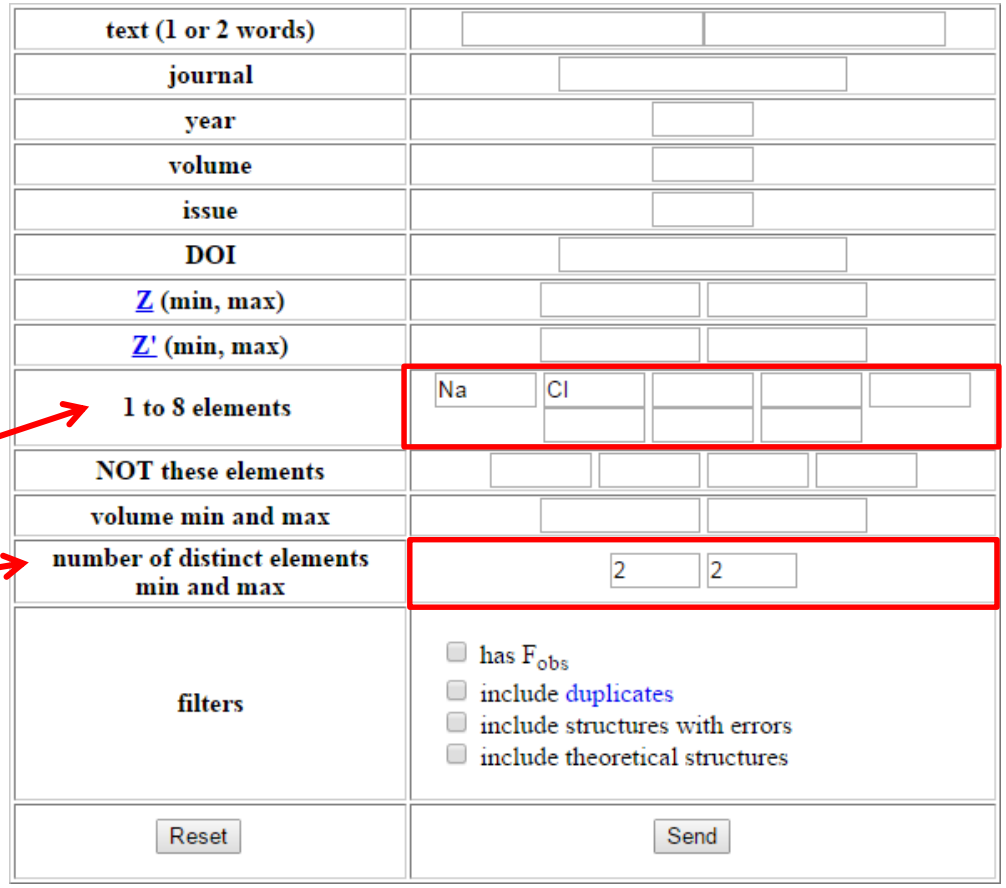
Basic use of Crystallography Open Database

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 $NaClO_3$.
- Click **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)

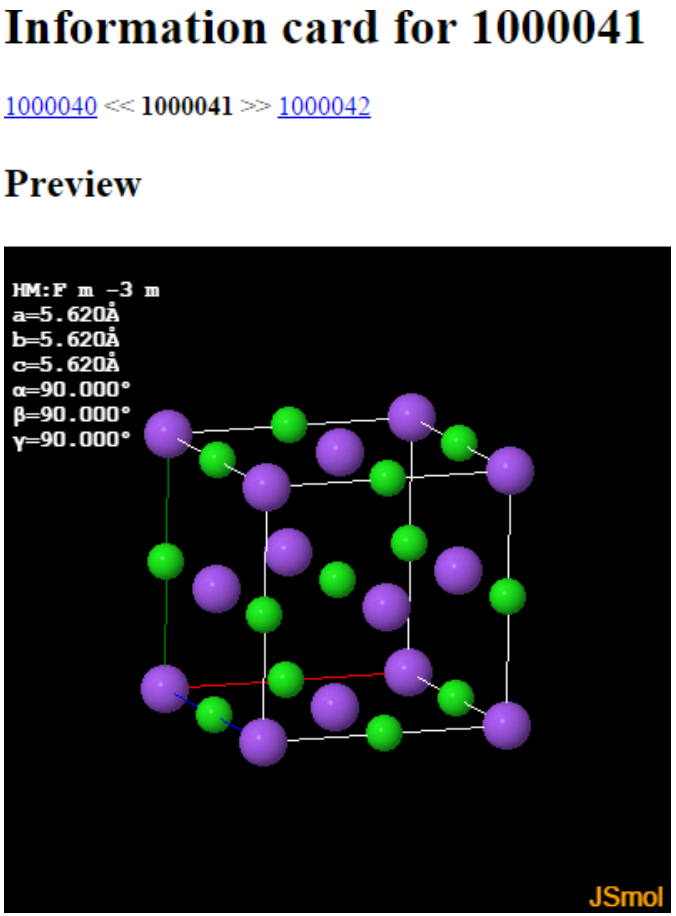
Searching elements including Na, Cl number of elements between 2 and 2

◄◄ First | ◄ Previous 20 | Page 1 of **2** | Next 20 ► | Last ►► | Display 5 **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 *Acta Crystallographica (1,1948-23,1967)*, **1965**, *18*, 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 *Acta Crystallographica Section B*, **2003**, *59*, 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 *Acta Crystallographica Section A*, **2015**, *71*, 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.



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