

# Basic use of Cambridge Structural Database

# Cambridge Structural Database

- CSD contains primarily organometallic and organic structures
- Not of high importance for inorganic solid-state chemistry
- Still, currently the largest existing structural database and contains many “inorganic” structures, as well
- Let’s have a look at the extremely convenient **substructure search** of CSD
  - CSD naturally includes many other search techniques, text searches *etc.*
- Open a web browser and go to <https://www.ccdc.cam.ac.uk/structures/> (works only with Aalto VPN or from Aalto campus network, see MyCourses -> Databases -> Aalto VPN for details)



WebCSD

Sign In

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Simple Search

Structure Search

Unit Cell Search

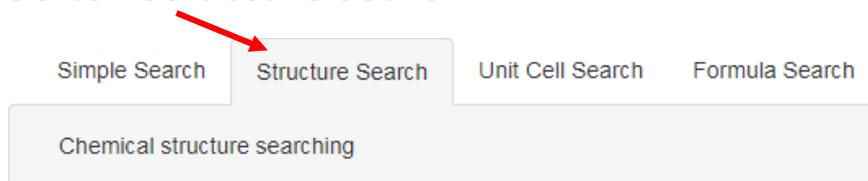
Formula Search

Simple text and numeric searching

Welcome to WebCSD. This service now includes the ability to search for inorganic structures through the CCDC's and FIZ Karlsruhe's joint Access Service using the Simple Search tab. Please use one or more of the boxes to find entries. If you enter details in more than one field the search will try to find records containing all the terms entered. [More information and search help](#)

# CSD Substructure search (1)

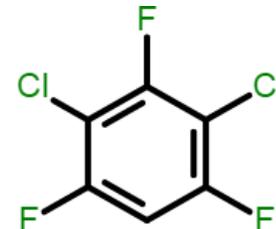
- Go to "Structure search"



- Set "Match condition" below the drawing area to "Substructure"

Match condition:  Exact  Substructure  Similarity

- Draw the structure shown on the right ( $C_6F_3Cl_2$ )
  - **Tip:** use the benzene ring as a template.
- Click the "Search" button in the bottom ("Substructure" has to be selected!)
- The search will take a while and return more than 70 hits
- All structures with a  $C_6F_3Cl_2$  "substructure" are included. This is very convenient if you want to find all structures with some certain ligand or structural motif!



# CSD Substructure search (2)

- Choose the structure **JOJPII** from the list on the left to get the following:
  - **3D structure** viewed directly in the browser using JSmol
  - Schematic **Chemical diagram**
  - Additional **details** on the crystal structure and the original publication
  - **Open** -> **CSD entry in external viewer** saves the shown molecule as MOL2 file (can be opened for example in Jmol)
  - **Download** button below the structure list on the left can be used to download the full crystal structure(s) as CIF file(s).

