CSD

Organic and organometallic crystal structure database at the Chemical Database Service

What is the CSD?

The Cambridge Structural Database (CSD) is a collection of >600,000 small-molecule **organic and organometallic crystal structures** that can be visualised and downloaded using a host of software applications, including:

WebCSD	A browser-based interface to the CSD data
ConQuest	For searching and retrieving CSD data
Mercury	A range of 3D structure visualisation tools

Where are the crystal structures from?

The 3D crystal structures which make up the CSD are derived from the **published literature** and **directly deposited data**. Each structure is validated and cross-checked by experts to ensure the CSD remains a **highly curated database**.

The 6 most featured journals are:

Inorg. Chem.	*Organometallics*
Dalton & J. Chem. Soc., Dalton Trans.	*J. Am. Chem. Soc.*
Acta Crystallogr., Sect E	*Acta Crystallogr., Sect C*

WebCSD - access the CSD in your web browser

WebCSD allows **searching and visualisation** of the CSD **within a web browser**. 3D structures can be exported in *.cif, *.sdf or *.mol2 format.

Search by:

- Structure / substructure
- Reduced cell
- Structural similarity
- Bibliographic information, compound name

Access the CSD via the Chemical Database Service at cds.rsc.org/csd.asp

email: cds@rsc.org

CSD Organic crystal structure database

ConQuest

The ConQuest application allows the user to search the CSD by:

- **Compound name**, formula, bibliographic information
- **Compound structure** / substructure with chemical constraints (charge, cyclicity)
- 3D **molecular constraints**, conformational preferences
- Non-bonded contacts, **intermolecular interactions**

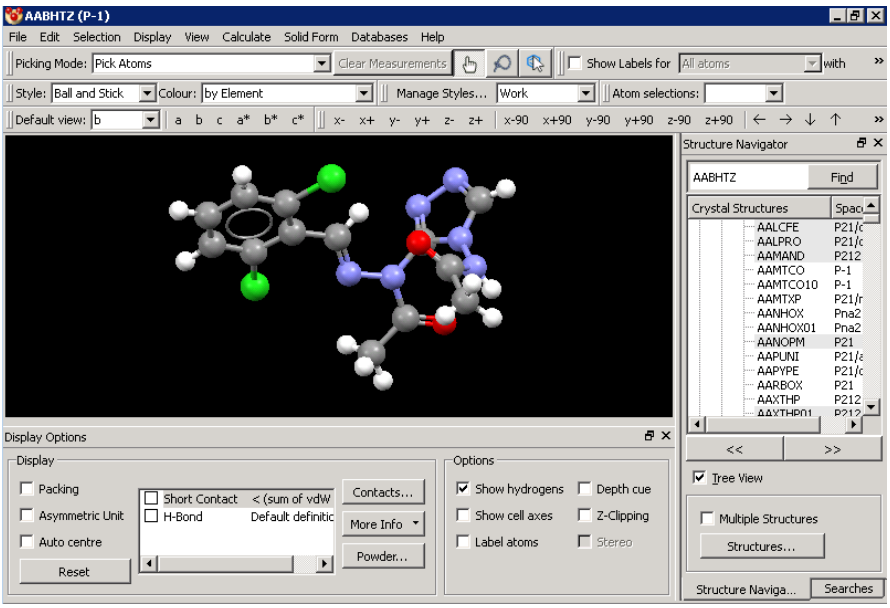
For advanced 3D visualisation, **export the hit list to Mercury.**

Mercury

The Mercury application is used for **advanced 3D visualisation** and export of crystal structures. **Distances**, **angles** and **dihedrals** can be measured.

Many properties can be calculated, including:

- **Packing**
- **Contacts**
- **Powder pattern**
- **Intermolecular potentials**



How do I access the CSD?

Access to the browser-based **WebCSD** is authenticated by **IP address**. If working off-campus a Chemical Database Service username and password will be issued. The applications **ConQuest** and **Mercury** (and others) are accessed via a **Remote Desktop Connection**. Signup for this at **cds.rsc.org/csd.asp**.

The CSD is developed by the Cambridge Crystallographic Data Centre (CCDC), and is provided to the UK academic community via the **Royal Society of Chemistry-hosted Chemical Database Service** at **cds.rsc.org**. The Chemical Database Service is funded by the EPSRC.

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