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:

- *Organometallics*
- *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](http://cds.rsc.org/csd.asp) email: cds@rsc.org
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.

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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