What is the ICSD?

The Inorganic Crystal Structure Database (ICSD) is a database of:

- > 160,000 inorganic crystal structures
- > 1,700 crystal structures of elements

The crystal structures present in the ICSD are taken from:

- > 1,900 periodicals
- Records from 1913 – present

How to search the ICSD

Ways to search the ICSD include:

- Chemical name
- Mineral name
- Chemical formula
- Bibliographic information
- Unit cell parameters
- Density
- Space Group Symbol

Alternatively, the Chemistry Visual Search can dictate the elemental composition of the compound.

Access the ICSD via the

Physical Sciences Data-science Service at www.psds.ac.uk email: info@psds.ac.uk
What information is given?

Each inorganic crystal structure features additional information:

- Structural formula
- Space group
- Unit cell
- Cell parameters and cell volume
- Experimental details (pressure, temperature, powder/single crystal)
- Bibliographic information

Visualisation of data

The 3D crystal structure and calculated Powder Pattern can both be visualised within your browser.

How do I access the ICSD?

Access to the ICSD is authenticated by IP address via [www.psds.ac.uk](http://www.psds.ac.uk). If working off-campus a PSDS username and password will be issued.

The ICSD is provided by academic IP address via the [PSDS at www.psds.ac.uk](http://www.psds.ac.uk). The ICSD is maintained by FIZ Karlsruhe GmbH. The Physical Sciences Data-science Service is funded by the EPSRC.

Access the ICSD via the

Physical Sciences Data-science Service

at [www.psds.ac.uk](http://www.psds.ac.uk)  
email: info@psds.ac.uk