

## 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.

The screenshot shows the 'Search Chemistry Visual Search mode' interface. At the top, there is a 'Switch to Quick Search mode' button. Below this is a periodic table where elements are highlighted in blue, indicating they are selected for the search. The selected elements include H, Li, Be, Na, Mg, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Al, Si, P, S, Cl, Ar, B, C, N, O, F, Ne, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, Ga, Ge, As, Se, Br, Kr, Cs, Ba, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, In, Sn, Sb, Te, I, Xe, Fr, Ra, Rf, and Ha. Below the periodic table, there is a section for search parameters: 'Number of Elements' (input field), 'Units of Coefficients' (dropdown menu set to 'Moles'), and 'El.Symb.' (input field). There are also fields for 'Co.(min)', 'Co.(max)', 'Ox.(min)', and 'Ox.(max)'. Below these are two search entries: 'AND N' and 'AND As', both with a red 'X' next to them. At the bottom, there are two buttons: 'Clear Chemistry Search' and 'Count Chemistry Search'. There is also a checkbox labeled 'Restrict total number of elements to selected number of elements'.

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](mailto:info@psds.ac.uk)

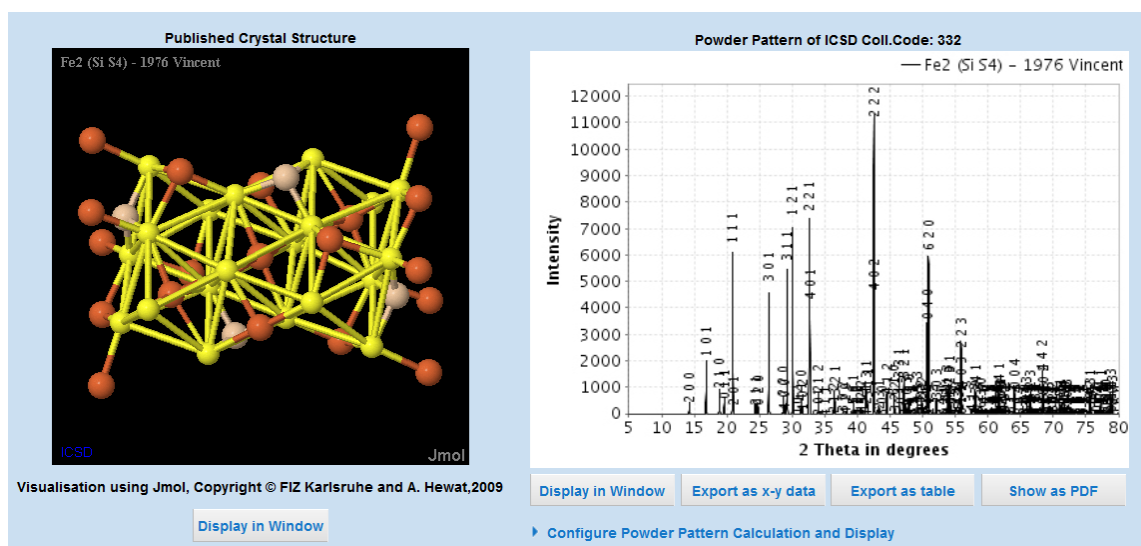
## What information is given?

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](mailto:info@psds.ac.uk)