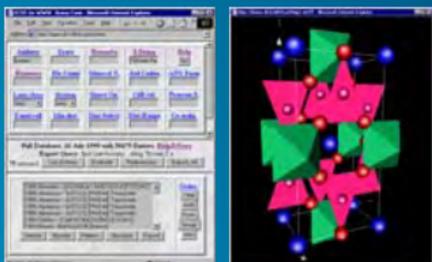# What's New with ICSD-for-WWW
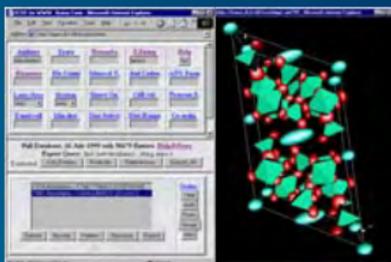
Alan Hewat, ILL Grenoble, FRANCE.

● 50,479 Inorganic Structures !

The 1999 version of the database from FIZ contains 50,479 entries. The full database is available to licensed users, with the 4% database available to everyone.
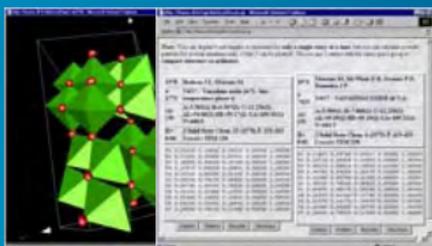
● 3D Display, anisotropic B-factors

Any of the 50,479 structures can be visualised in 3D with automatic display of co-ordination polyhedrae, anisotropic B-factors etc
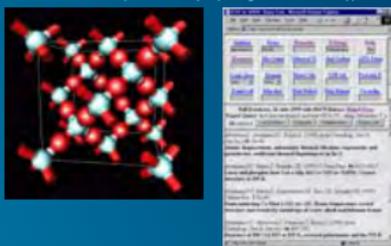
● Easily Compare Structures

Structures can be compared by displaying side-by-side lists of co-ordinates, bond-lengths, 3D-drawings etc.
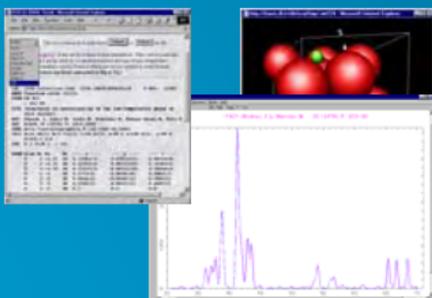
● Cut & Paste References

When you are writing a publication, you can cut-and-paste suitable references directly from ICSD-for-WWW. You can also construct your own reference database on your PC/Mac by exporting to the EndNote application.
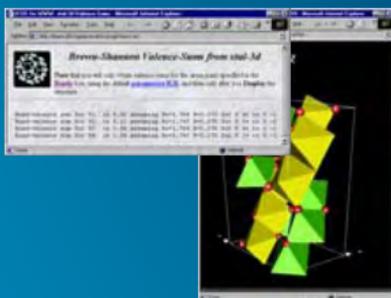
● Exporting to other Formats

You can export to CIF, Shel-X, GSAS, FullProf and other formats to rapidly provide starting points for structure refinement or display. You can also export multiple entries to Lazy PulverIx for pattern matching.
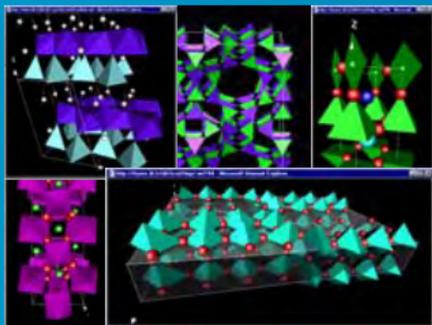
● Calculate Valence Sums

When you display the structure, the Brown-Shannon valence sums are automatically calculated. You can display them as a check of the correctness of the structure, and identify atoms in different valence states, such as in vanadates or cuprates.

● More ways to Display Structures

Co-ordination polyhedrae and bonds are constructed automatically whenever possible, so that you immediately see important structural features. All the usual types of structural models are available.

● National ICSD WWW servers

The full database is now available to academic users via national servers in several countries, including the UK, Spain, the Netherlands, China (Taiwan) etc.

- ILL/ESRF Grenoble France
- CDS UK (UK academic community)
- CCP14 Daresbury UK
- ICES Spain (Spanish Scientific Research Council)
- ORNL (Oak Ridge National Laboratory, USA)
- NIST Washington USA
- CAOS/CAMM Netherlands
- Nagoya University, Japan
- NCHC Taiwan (Taiwan national database)
- ...

● How can I try it ?

Just connect to one of the National servers, or to the ILL home site below. ICSD-for-WWW is also installed at Lachlan Cranswick's "Computing Fair".

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