What's New with ICSD-for-WWW

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- **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.

- **National ICSD WWW servers**
  - The full database is now available to academic users via national servers in several countries, including:
    - UK: CDS-UK (UK academic community)
    - SCOPES (European Community)
    - ORNL (Oak Ridge National Laboratory, USA)
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- **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.

- **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 on a number of computers in Computing Services.
  - barns.ill.fr
  - www.ill.fr/dif
  - hewat@ill.fr