

Links between the CrystalWeb & ICSD-WWW database interfaces – Bob McMeeking & Dave Fletcher (r.f.mcmeeking@dl.ac.uk & d.a.fletcher@dl.ac.uk)

Providing ready access to major crystallographic data collections has always been a key task for the Chemical Database Service (CDS) [1], and to meet this requirement the Service has developed the CrystalWeb system over the last several years. CrystalWeb provides "one stop shop" web browser access to all our crystallographic data [2]. The aim has been to make such data readily useable by experts in a wide range of field without the requirement of any special crystallographic expertise [3].

At the same time other established modes of access continue to be supported. In particular we grant access to the Cambridge Structural Database (CSD) of organics and organo-metals via the ConQuest software and the Inorganic Structural Database (ICSD) using the ICSD-for-WWW developed by Alan Hewat and co-workers at the ILL Grenoble [4]. Like CrystalWeb ICSD-WWW is a web browser interface. However, it supports many valuable complementary features, having been built with inorganic structures specifically in mind.

A valuable option available in ICSD-WWW is having both atom (including thermal ellipsoid display) and polyhedron modes for its 3-D visualisation module [5]. There is also an interatomic distance calculator and an option to simulate and displaying neutron and X-ray powder diffraction patterns. The underlying calculations to generate the patterns are done by the program, Lazy, which uses Klaus Yvon *et al's* well established Lazy Pulverix code. The user, however, is shielded from most low level details, and all these facilities are accessed via easy-to-use web browser forms. In almost all cases ICSD-WWW can be used as a "black box" with no need for user manipulation of the retrieved entries.

Historically a problem remained for the relatively few entries where the crystal structure was reported in a "non-standard" crystallographic setting (e.g. A2/m or I2/m rather than C2/m for Space Group number 12). These were handled automatically by CrystalWeb from its inception, but traditionally have required manual intervention when using ICSD-WWW. Problem entries are flagged, and in most instances the user needed to find and add the correct space group operators in the appropriate format. In other cases it was necessary to apply a translational correction to the atom co-ordinations.

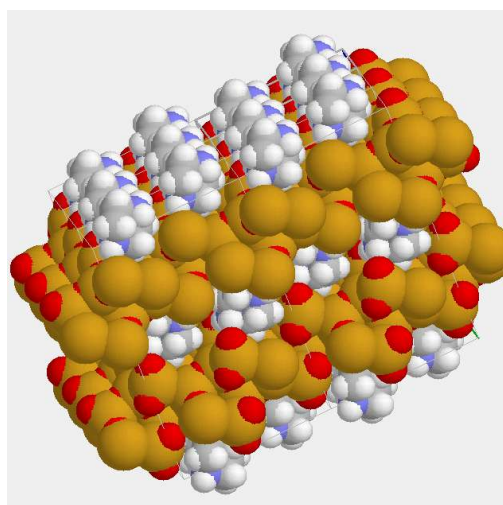
Here the cubic space group Pn3m (224) is the most troublesome. There are 4,500 such entries in the ICSD database, of which ~50% required a correction to their co-ordinates. To improve this situation we have made important modifications to the CDS implementation of ICSD-WWW so it can handle all problem structures properly without manual intervention. We have liaised

with Grenoble and hope that these changes will soon be added to the standard version of the ICSD-WWW system released to users worldwide.

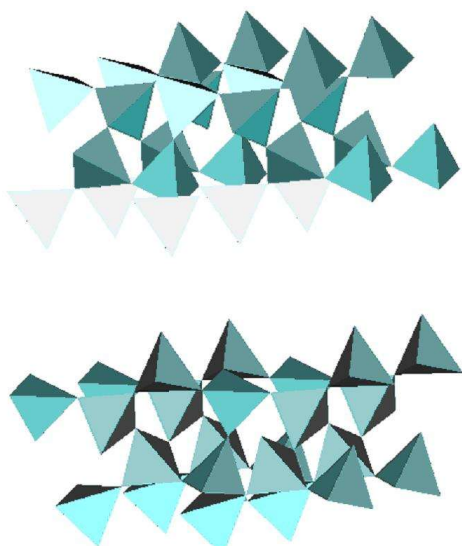
Below is a CrystalWeb hit display for one the 19 entries for Cuprite (Cu_2O) in the ICSD database with space group Pn3m (224). Structure determinations date back to 1915, but the example is for a synchrotron study from 1990. This retains the older, now "non-standard" setting, for this space group.

Hit number 10 of 19 Inorganic Crystal Structure Database Collection Code 52043	Reference	Cell data	
Copper(I) oxide Cu ₂ O	A. Kufel, K. D. Eichhorn, <i>Acta Crystallographica Section A, Foundations of Crystallography</i> , 46 (1990), p.71-784	Lengths	Angles
		a / Å 2.685	alpha 90
		b / Å 2.685	beta 90
		c / Å 2.685	gamma 90
		System: Cubic	
		Space group: Pn3m	
		Space group number: 224	
		R-factor=0.17	
		Z=2	
		Calculated cell volume=77.772	
			<input type="button" value="Display structure using Chrome"/> <input type="button" value="Download structure"/> <input type="button" value="Details from ICSD-WWW"/> <input type="button" value="Bond/angle calculation"/> <input type="button" value="Powder diffraction calculation"/> <input type="button" value="Xtal-3D structure display"/>

Another recent enhancement shown in the CrystalWeb hits display is that users can make a direct link between hits retrieved from their search and the various useful features provided by ICSD-WWW. This is available for entries from the CSD, CrystMet (metals, alloys and intermetallics), and the ICSD database itself. In the near future we plan to provide a direct link for ICSD-WWW hits to the CrystalWeb system. We will also add an option for users to upload their own co-ordinates sets and thus have access to the main features available of both CrystalWeb and ICSD-WWW. Screen shots showing a pyrazinium silicate structure [6] give some indication of display capabilities.

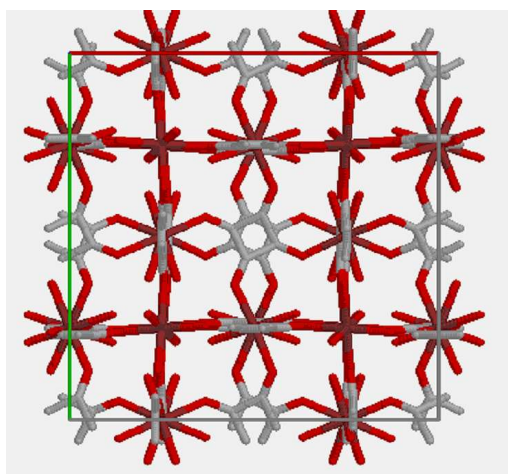


Here CrystalWeb highlights the silicate sheets with the pyrazinium moieties sandwiched between.



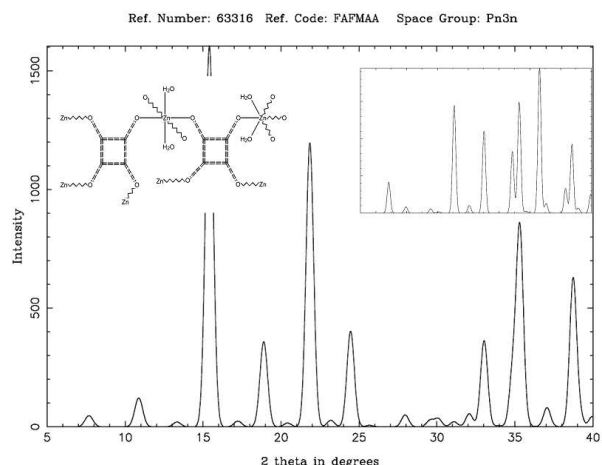
The link to ICSD-WWW allows the silicate part to be displayed using Xtal-3d in polyhedron mode.

Use of the new CrystalWeb/ICSD-WWW features is illustrated by another structure reported in a "non-standard" space group setting. Here we select an entry from the CSD which has the relatively rare space group Pn3n (222). This is an extended zinc "squarate" complex. It was described by the authors as a water/acetic acid clathrate, but the co-ordinates for these molecules were not determined.



A display produced by CrystalWeb gives an indication of the network structure of CSD Refcode entry FAFMAA.

The diagrams show the structural display using CrystalWeb and the simulated neutron and X-ray powder patterns available via the ICSD-WWW link. A later paper [7] recognised the possibility of sodalite networks for certain metal squarates complexes. These new structures are present in the ICSD database and can be found using CrystalWeb. It is then easy to display the structures and powder patterns and demonstrate the zinc compounds from both studies are indeed very similar.



ICSD-WWW was used to generate powder patterns. The main display is for neutrons in the range 2θ 5-40°. The X-ray pattern at the same wavelength above 25° is in the insert, which is aligned with the main pattern.

- [1] "The United Kingdom Chemical Database Service", D.A. Fletcher, R.F. McMeeking, D. Parkin., *J. Chem. Inf. Comput. Sci.* (1996), **36**, 746-749.
- [2] "The CrystalWeb database interface", Bob McMeeking & Dave Fletcher, *CDS Research Highlight 2002-3*, http://cds.dl.ac.uk/report/res_high.html;
- "The United Kingdom Chemical Database Service: CDS", B. McMeeking & D. Fletcher, in *Cheminformatics Developments: History, Reviews and Current Research* (Ed. J. H. Noordik), IOS Press, Amsterdam, Chapter 2, pp 37-67, 2004.
- [3] An example in archaeology is: "SR-XRD, Culture Heritage and the CDS database" Manolis Pantos, *CDS Research Highlight 2001*, http://cds.dl.ac.uk/report/res_high.html.
- [4] "ICSD for WWW", A.W. Hewat, *et al.*, <http://icsd.ill.fr/icsd>.
- [5] <http://www.ill.fr/dif/3D-crystals/xtal-3d.html>.
- [6] "Piperazine silicate (EU 19): the structure of a very small crystal determined with synchrotron radiation", S.J. Andrews M.Z. Papiz R. McMeeking A.J. Blake B.M. Lowe K.R. Franklin J.R. Helliwell M.M. Harding *Acta Cryst.* (1988), **B44**, 73-77.
- [7] "Sodalite networks formed by metal squarates", S. Neeraj, M.L. Noy, C.N.R. Rao, A.K. Cheetham, *Solid State Sciences* (2002), **4**, 1231-6.