New : COD (Crystallography Open Database)

In the IUCr Newsletter 10-4 (2002), Bill Duax (Letter from the President) wrote : "Emerging nations can benefit from the use of the powerful techniques of X-ray crystallography in order to analyze, understand and use the unique natural resources within their countries whether mineralogical, chemical, or biological in nature."

This generous wish would more easily be achieved by a free access to a global crystallography open database (inorganic/metallic/organometallic/organic) which is the purpose of a new web server located at http://www.crystallography.net/ and offering atomic coordinates in the IUCr CIF files format, together with a search engine.

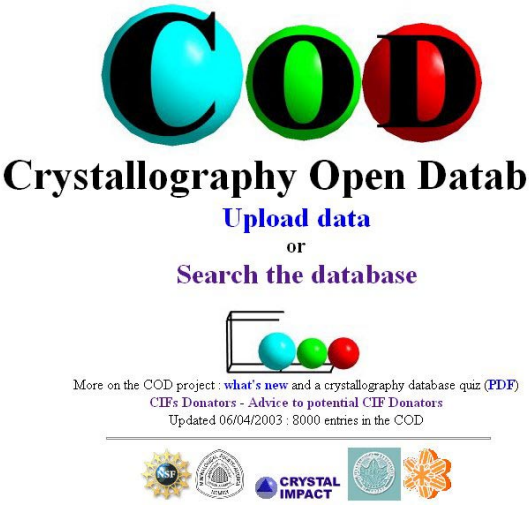

Fig. 1 - The http://www.crystallography.net/ Web page.

An international advisory board supervises that good practices are respected (M. Berndt, D. Chateigner, X. Chen, M. Ciriotti, L.M.D. Cranswick, R.T. Downs, A. Le Bail, L. Lutterotti, H. Rajan, B.H. Toby, A.F.T. Yokochi). Rather than to systematically copy the atomic coordinates from the literature, individual authors and laboratories are requested to send their own CIFs prior to (or after) publication, which is possible if you have not sold your experimental results exclusively (facts and raw scientific data are in principle not copyrightable). Thanks to a few major donators (the American Mineralogist Crystal Structure Database for 3725 entries, the Institut de Physique de la Matière Condensée -Grenoble- for ~1200 entries, the CRISMAT -Caen- for ~850 entries and the Laboratoire des Fluorures -Le Mans- for ~450 entries), as well as to many individual contributors, the COD can already propose more than 8.000 CIFs. This is however only 2 % of an expected total number close to 400.000 entries.

The search in COD is realized by two powerful options :

1 - by combining in the way you choose : text (2 words or parts of words), elements (1 to 8, with formula numbers or not), volume (min and max), and strict number of elements.

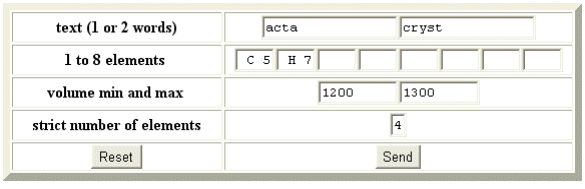

Fig. 2 - Part of the COD simple but powerful search form.

2 - By cell parameters ranges a_{min}-a_{max}, b_{min}-b_{max}, etc.

Given that the COD was built mainly for verifying if, knowing your sample cell, you are not redetermining an already known structure, these above search possibilities should fulfil basic needs (especially option 2 and using volume ranges in option 1, needing the cell knowledge). However, a real efficiency urgently requires completeness, so please upload your CIFs !

The whole COD system is based on open source software (Apache/MySQL/PHP) and can be downloaded by interested parties (contact cod@cristal.org). It is simple to install and would be quite useful to laboratories wanting to build their crystal database from their own crystal structure determinations, for either an intranet or an internet external access. Collecting all such laboratory fragments in the COD would serve invaluably the crystallographers community in the world and particularly in emerging nations. The CRYSTMET, ICSD and CSD commercial databases offer much more complete and powerful services than the COD which is limited to the minimum allowing a crystallographer to survive at low cost (though a not so cheap internet access is necessary).