

Dear Dr Le Bail

I have been reading the comments made in response to your petition addressed to the crystallographic database providers concerning the availability of individual CIFs. Existing responses indicate that many scientists may be unaware of the web facilities already offered by the CCDC in this area.

I should be grateful if you can make this note available through the COD website, since it will hopefully generate feedback directly to the CCDC that will extend and improve our current service. I will also arrange for this note to appear on appropriate electronic discussion lists.

Free Web availability of CIF datasets from the CCDC

For many years, the CCDC has made the data for individual crystal structures freely available. Originally this service operated via direct e-mail requests, but since January 2002 we have provided universal free Web access to our growing archive of deposited CIFs. You do not have to be a CSD subscriber to use this Web-based service, it is available to any scientist who wishes to use a CIF for *bona fide* research purposes. The 'Request-a-structure' service is accessible from our home page (www.ccdc.cam.ac.uk).

- The CCDC CIF archive currently contains more than 170,000 CIFs dating back to 1994, relating to organic and metal-organic structures. It grows daily.
- The Web form requires a journal reference together with either a CSD Deposition Number (published in many papers) or an author name.
- CIFs are returned to the enquirer via a plain text e-mail.
- 19,012 CIFs were supplied via the 'Request-a-Structure' form from 2002-date.

The CCDC is committed to improving its services to the scientific community, and we welcome feedback on the delivery of individual CIFs via the automated 'Request-a Structure' service. Please address this feedback to admin@ccdc.cam.ac.uk.

Availability of the full CSD System

I would also like to provide basic information about access to the full facilities of the CSD System. The full System not only provides access to individual structures, but also provides very extensive software facilities.

- The CSD System is available in > 1,000 institutions in 65 countries.
- The CCDC, working with a number of national governments, provide subsidies to developing countries so that any fees are minimal or zero. This covers full CSD System provision to institutions in e.g. Africa and South America, and elsewhere.
- Networked services are freely available to scientists in the UK, via the Daresbury Laboratory, and in Europe via CMBI, Nijmegen (see web information below).

We urge those who would like to access the full facilities of the CSD System to first look at our website (www.ccdc.cam.ac.uk/contacts/obtaining_products) and to contact us at admin@ccdc.cam.ac.uk.

I hope these comments are useful.

Frank Allen

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