CIF software in a DDLm world

James R Hester
Bragg Institute, PMB 1, Menai, NSW, 2234, Australia, E-mail : jamesrhester@gmail.com

Although CIF dictionaries store crystallographic knowledge in a machine-readable form, there has been relatively limited run-time use of DDL1/2 dictionaries in CIF software. This is attributable to the small added value of the primarily descriptive DDL1/2 attributes compared to the cost of implementing a dictionary-aware system. In other words, CIF syntax and DDL1/2 attributes are simple enough for software creators to produce (with occasional errors) and read conformant CIF data files simply by referring to the dictionaries at program creation time. The new DDLm standard enhances DDL1/2 descriptive capabilities while also introducing dictionary-based synthesis of derived data values by including dREL algorithms in data item definitions. While algorithms are usually also implemented as part of program creation, several orders of magnitude more time is involved in developing a correct algorithm compared to a typical DDL1/2 task of specifying a dataitem name and type. A DDLm dictionary gains considerable practical value for this reason. This value is potentially compromised by the work involved in making a DDLm algorithm available to the software. Two practical paths exist: (i) communication with a separate dictionary processing package, or (ii) automatic rewriting of the dREL algorithm into the language of choice. Both approaches are amenable to provision by the IUCr of openly-available tools, which coupled with the clear added value of having tested, standard algorithms will help overcome the implementation barrier experienced by the DDL1/2 standards, a barrier which is even higher for the more complex DDLm standard.

Keywords: CIF, DDLm, object-oriented

The bilbao crystallographic server

Universidad del Pais Vasco, Fisica de la Materia Condensada, Apartado 644, Bilbao, Vizcaya, E-48080, Spain, E-mail : mois.aroyo@ehu.es

The Bilbao Crystallographic Server is a free web site with crystallographic databases and programs available at http://www.cryst.ehu.es [1]. The server is built on a core of databases that include data from International Tables for Crystallography, Vol. A: Space-group symmetry and Vol. A1: Symmetry Relations between Space Groups. There is an access to the crystallographic data for...