Software Engineering, MBDP M002, 35 Stirling Highway, Crawley, Western Australia, 6009, Australia, E-mail：Nick.Spadaccini@uwa.edu.au

Data items contained within a CIF file are currently defined in domain dictionaries using a data definition language (DDL1 or DDL2). The increasing complexity of data and the need for seamless integration across different sources creates demands that cannot be readily met by current definition capabilities. *DDLm* is an evolution of DDL1 and DDL2 that uses the same syntax but expands the attribute set so as to enrich the semantics of the data and class definitions. It maintains backward compatibility to existing CIF archives. The CIF syntax has been extended to describe more complex data structures, while maintaining the simple tag-value construct. *DDLm* supports a wider range of data types, including container classes such as lists, arrays, tuples and tables. Definitions for a domain, such as that of structural science, can now be modularised into separate dictionaries; each maintained by the relevant sub-discipline. *DDLm* provides for the real-time merging of modules, including the recognition of namespaces, and the resolution of namespace clashes. *DDLm* provides facilities for relating derivative data items via method expressions that are symbolic, easy to read as text, but are computer interpretable and executable [2]. Additionally user-defined processes can be used for data evaluation. The paper will describe the major features of *DDLm* highlighting its simplicity and importance for the more comprehensive definition of data items used in the discipline. The specification details are currently available for examination and comment by members of the crystallographic community [3].

[1] International Tables Vol. G (2005) Ed. S Hall and B McMahon. Springer.
[2] Spadaccini N, Hall SR, & Castleden IR (2000) *JCICS* 40 1289-1301.
[3] www.iucr.org/iucr-top/cif/ddlm/

Keywords: CIF, data representation, ontology

MS.96.2

Acta Cryst. (2008). A**64**, C160

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: crystallographic software development, CIF, data definition language

MS.96.3

Acta Cryst. (2008). A**64**, C160

Transition to object-oriented data representations: Interconversion between CIF and other formats

Herbert J. Bernstein
Dowling College, Dept. of Mathematics and Computer Science, 150 Idle Hour Blvd KSC 121, Oakdale, NY, 11769-1999, USA, E-mail：yaya@bernstein-plus-sons.com

The Crystallographic Information Framework [1] (CIF) has been very effective in codifying the vocabulary of crystallography, with two Dictionary Definition Languages, DDL1 for small molecules and DDL2 for macromolecules. The more than three-decade old PDB format and the new, remediated PDB format are critical to information management in macromolecular crystallography. There are many alternate representations, ASN.1, NeXus, CML, XML, etc. that convey much the same information with more or less structure, some more convenient for software or databases or for handling by humans, but, in most cases, these formats have focused on the nouns of our vocabulary. The work on a new DDL, DDLm [2], and related work on SBEVSL [3] have increased awareness of the need to deal with the verbs of our vocabulary, the actions that transform information, such as cell edge vectors into cell volumes, as well as the nouns, and raise the prospect of making CIF object-oriented.

[1] Hall, S. R., McMahon, B., eds., “International tables for crystallography, Volume G: Definition and exchange of crystallographic data,” International Union of Crystallography, Heidelberg: Springer, 2005.
[2] Hall, S. R., Spadaccini, N., Westbrook, J., “Dictionary Definition Language DDLm”, IUCr, 2007, http://www.iucr.org/iucr-top/cif/ddlm/index.html
[3] C. Westin, B. Hanson, H. J. Bernstein, I. Awuah Asiamah, D. Boycheva, G. Darakev, N. Darakev, J. Jemilawon, N. Jia, P. Kamburov, G. Todorov, P. A. Craig, S. Mottarella, “SBEVSL: Communicating scripts between molecular visualization programs,” Abstract E003, ACA 2007, Salt Lake City, UT, July 2007
Work supported in part by DOE, NIH, NSF and IUCr.

Keywords: CIF, DDLm, object-oriented

MS.96.4

Acta Cryst. (2008). A**64**, C160-161

The bilbao crystallographic server

Mois I. Aroyo, J. Manuel Perez-Mato, G. Madariaga, D. Orobengoa
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