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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

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CIF software in a DDLm world

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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

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

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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
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Keywords: CIF, DDLm, object-oriented

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The bilbao crystallographic server

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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

the subperiodic layer and rod groups (International Tables for Crystallography, Vol. E: Subperiodic groups) and their maximal subgroups. The symmetry information has been stored in XML and provisional CIF formats. For the extension of the existing CIF-core dictionary a list of data names has been developed which refer to the specific requirements of the subgroups and supergroups of space groups [2] and subperiodic groups. The accompanying software is divided into several shells according to its complexity and proximity to the information contained in the database core. Symmetry data as generators and general positions, Wyckoff-position data and maximal subgroups of space and subperiodic groups are retrieved directly from the databases by simple tools. There are a number of online applications for problems involving group-subgroup relations between space groups: subgroups and supergroups of space groups, graphs of maximal subgroups for an arbitrary group-subgroup pair, Wyckoff-position splitting schemes for group-subgroup pairs, etc. More specialized crystallographic software is also available and is distributed according to different topics: representation theory, solid-state physics and crystal chemistry applications.

[1] Aroyo, M.I et al. Z. Kristallogr. 221 (2006) 15.
[2] Wondratschek, H. et al. Abstracts of 17th Int'l Congress of IUCr, C-577, Seattle, 1996.

Keywords: bilbao crystallographic server, CIF, symmetry databases

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publCIF: A complete crystal structure publishing environment for authors

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The program system publCIF [1] is a fully-featured editor allowing authors to modify and add content to a Crystallographic Information File (CIF) for publication in an IUCr research journal, or in a number of other formats. The user interface offers synchronised WYSIWYG ('what you see is what you get') and raw file views of the CIF, with syntax and dictionary-based attribute validation. The editor has recently been enhanced in several ways. It allows interaction through web services with the online checkCIF validation system (including insertion, where appropriate, of a suitable validation reply form). Work is in hand to offer intelligent handling of graphics files supplied as illustrative figures to accompany an article. Most recently it has been developed to allow interactive three-dimensional visualization using the open-source application Jmol [2], including an editing toolkit to permit authors to create enhanced interactive figures and animation for online publication. Current developments are aimed at providing similar functionality to mmCIF submissions of biological macromolecular structure reports. To meet the specific requirements of the IUCr journals, the current software architecture of publCIF is largely procedural, but the development of an engine to validate dictionary attributes offers the possibility of increased methods-driven functionality with future versions of CIF. Meeting the requirements of publCIF would provide a useful development target for the new methods-based dictionary definition language DDLm.

References

[1] Westrip, S. P. (2008). publCIF - free software to edit and preview a CIF for publication. http://journals.iucr.org/services/cif/publcif/
[2] Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/

Keywords: CIF, publishing, software

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Performance of micro pixel gas chamber in small angle X-ray scattering experiments

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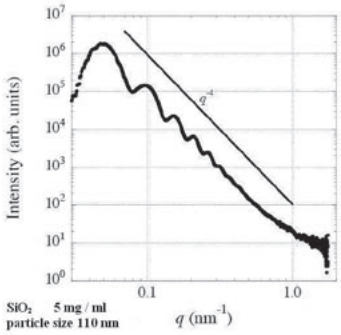
We report on the development a two-dimensional photon-counting detector based on a Micro Pixel Gas Chamber for high-resolution Small Angle X-ray Scattering (SAXS). The Micro Pixel Gas Chamber is a micro-pattern gaseous detector fabricated with printed circuit board technology. Here a 10 x 10cm Micro Pixel Gas Chamber was used, and we have demonstrated a position resolution of 120 um (RMS). Photon-counting detectors provide only statistical uncertainty as background. For this reason, photon-counting detectors are expected to achieve a higher dynamic range than CCDs and Imaging Plates. We performed SAXS experiments using nanoparticles (SiO_2) at SPring-8 and obtained a dynamic range of over 10^5. This result implies that our detector could provide high-resolution SAXS. The maximum counting rate of 5 MHz was achieved without saturation. We performed a time-resolved experiment at the KEK photon factory. We observed the dehydration reaction of pyromellitic acid hydrate. The transition state was observed for several seconds. We also report on the performance of a large Micro Pixel Gas Chamber with a detection area of 30 x 30cm.



Keywords: gas sensors, imaging detectors, X-ray detectors

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High speed readout of microgap X-ray detectors

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Since their introduction in 2004, microgap detectors have become a standard detector technology for powder diffraction and are now seeing increasing use for SAXS/WAXS and single crystal diffraction as well. Microgap detectors are true photon-counting detectors with quantum-limited sensitivity, zero noise, moderate energy resolution and zero readout deadtime. Compared to other photon-counting, imaging detector technologies, microgap detectors are significantly less expensive and also have the advantages of having no internal dead areas, not suffering from charge sharing at pixel boundaries and not requiring cooling. Because of their very high sensitivity they