



**Report from
Dowling College, Oakdale, NY, USA
to the International Union of Crystallography, Chester, England
concerning provision of new and upgraded CIF software to facilitate publication in
IUCr journals**

2 April 2005

The Executive Secretary of the IUCr
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This is the 4th bimonthly progress report on the IUCr funded project at Dowling College to support the evolving needs of the community for new and upgraded CIF software to facilitate publication in IUCr journals.

I. Project Summary

Dowling College is providing to the IUCr the services of Professor Herbert J. Bernstein as project director (PI/PD) and certain of his students to modify existing software and to create new software as detailed in section I below in order to support the evolving needs of the community for new and upgraded CIF software to facilitate publication in IUCr journals. This is a major set of inter-related projects, expected to take more than two years to complete. However, a phased release to the Chester office of the IUCr of partial preliminary versions of all of these packages is expected before the end of the first year, and feedback from the Chester office of the IUCr will be used to guide completion of the packages.

As versions of these packages mature they will be released to the community as open source software without charge to encourage wide use. The software will be released using the GNU GPL or a similar license. "CIF Applications" articles will be submitted to help make the community aware of these new and upgraded tools, and the IUCr will be given first refusal in publication of such articles produced from the work of this project.

II. Description of goods and services to be delivered to the IUCr

These include:

- (1) CIFTTEST – Creation of a new and extended test file suite and test protocol for validation of CIF parsers.
- (2) vcif2 – an extended version of vcif (a program used to validate the syntax of CIF files). vcif2 will verify compliance with CIF 1.0, CIF 1.1 or mmCIF file formats. vcif2 will also accept an arbitrary list of layered DDL1 and DDL2 dictionaries against which units, enumerations, parent–child relationships and category integrity will be checked.
- (3) CIFFOLD – a new utility to fold and unfold long-line CIFs to allow existing CIF 1.0 applications to work with CIF 1.1 files.
- (4) CIFtbx3 – a new release of CIFtbx to provide support for CIF 1.1 (as well as CIF 1.0 and mmCIF) for Fortran applications and to provide extended integrity checking comparable to that in vcif2.

III. Timetable

The agreement started 1 August 2004. The Agreement will terminate when the work under Item I is complete and this will be no later than 31 July 2006.

IV. 2 April 2005 Status

Overview: The project started on time on 1 August 2004, and has continued to date. This is a report for the work done from 31 January 2004 through 2 April 2005. The project is fully staffed and operational and in this period the major effort was on finishing the GUI version of CIFFOLD for release and resolution of the performance issues with the long line version of CIFtbx. The progress-status web site has been updated.

Staffing: The PI/PD is Professor Herbert J. Bernstein. The students working on the project are Kostadin Mitev and Georgi Todorov. Isaac Asiamah, Ricky Chachra and Stavros Louris have assisted in testing.

Funding and Administration: Cash flows and burn rates are appropriate to the needs of the project.

Project Activities: In this project period the focus has been on getting packages ready for release at the IUCr Congress in Florence, starting with CIFFOLD and CIFtbx3. At Brian McMahon's request we are exploring the possibility of releasing at least some of the packages this month for possible inclusion in the ITVG CDROM. In order to accomplish this goal, we have narrowly focused our efforts on finishing the two packages closest to being ready for release: CIFFOLD and CIFtbx3. The internal project web site at <http://arcib.dowling.edu/~bernsteh/.cifucr> has been updated for these two packages.

CIFtbx: H. J. Bernstein has continued working on coding changes in CIFtbx. The performance issue uncovered in the last cycle has been reasonably well addressed. The code for text and comment folding is written and the code for comment unfolding is written. Work has started on modifications to cif2cif to support folding and unfolding. With the addition of the code for text unfolding, this version of CIFtbx with cif2cif, cyclops and cif2xml may be ready for release and inclusion in the ITVG CDROM this month. The patch to generate the CIFtbx code to date is available on the web site.

CIFFOLD: K. Mitev has prepared a full GUI release for testing. The release is being actively tested by others in the lab to see if it can be gotten ready for release and for inclusion in the ITVG CDROM this month. A tar for others who wish to test this prerelease is available on the web site. The work has been done by K. Mitev and G. Todorov, with testing so far by H. Bernstein, G. Todorov, R. Chachra, Isaac Asiamah and Stavros Louris.

CIFTEST: Nothing new to report for this period.

vcif: Nothing new to report for this period.

Summary: The project continues on track.

Respectfully Submitted,

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Professor of Computer Science

Cc: Brian McMahon
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