COMCIFS report to the IUCr Executive Committee for the year 2006.

Since 2005 was the year of the Florence Congress at which the future of CIF was examined in some detail, our report for that year looked back on the fifteen years of CIF development and usage, presenting the perspective of what COMCIFS had achieved and where it was going in the future. 2006 has been mostly a year of consolidation of these decisions.

The most far-reaching project that COMCIFS is currently pursuing is the development of the new Dictionary Definition Language with Methods, DDLm (previously referred to as DDL3). Its adoption in principle by COMCIFS during the IUCr Congress in Florence opened the way for the development of a DDLm dictionary which will shortly be presented to COMCIFS for adoption. On adoption it will be used to develop a new suite of CIFm dictionaries that incorporate innovative features such as methods (computer-readable algebraic algorithms). It is also designed to simplify dictionary maintenance and management. Most importantly, programs written to exploit the new features of these dictionaries will be able to read all previously written CIFs, both those using coreCIF and mmCIF which are currently mutually incompatible. The detailed work on DDLm has been undertaken by Nick Spadaccini, Syd Hall and John Westbrook, assisted by the visit of John Westbrook to Perth and a three-day workshop involving Brian McMahon, Syd Hall and David Brown held in Chester during the year, with financial support from the IUCr. Following the expected adoption of DDLm to complement the current DDL1 and DDL2, work will begin on preparing CIFm dictionaries. The approval of a coreCIFm dictionary will provide the materials essential for those interested in developing software for the new standard. As pointed out above, such software will be able to read all existing CIFs, ensuring the viability of the archive.

Work continues on the evolution of CIF dictionaries. The coreCIF Dictionary Maintenance Group continued working on the coreCIF dictionary revisions suggested by over a decade of extensive use, and it is coming within sight of the end of this project. Ilia Guzei and David Brown started developing a component of the coreCIF dictionary describing the constraints and restraints used in structure refinement, and Arie van der Lee and his colleagues have started work on a new dictionary for reflectivity measurements.

Herbert Bernstein and Robert Sweet organized a successful workshop in conjunction with the American Crystallographic Association annual conference in Hawaii to promote the implementation of the imgCIF dictionary in capturing images of diffraction patterns, primarily at synchrotron sources.

Howard Einspahr worked closely with John Westbrook, of the PDB, and IUCr editorial staff to develop streamlined procedures for incorporating structural data from PDB deposits in associated publications. This work has involved identifying mmCIF data items relevant to a full literature description, and the development of a tool for authors that will create experimental tables for

inclusion in manuscripts from mmCIF files.

The IUCr editorial office has released a public version of its publcif software. This software may be used to edit CIFs for publication. It combines dictionary-based CIF validation with a sophisticated collection of utilities that will assist prospective authors. These include active links to the checkCIF service, the ability to incorporate validation report forms (VRFs) generated by checkCIF, data entry wizards, table editors, previews of articles formatted in the styles of the different IUCr structural journals, citation sorting and checking, private databases of authors and citations, and dictionary browsing facilities. The software is being further developed to support publication of biological macromolecular structures.

With financial help from the IUCr, Herbert Bernstein and students have produced updated versions of standard software libraries and tools (the CIFTEST parser test and validation suite, CIFtbx3, cyclops, vcif2, and a new utility to fold and unfold long-line CIFs) that are compliant with the version 1.1 CIF specification.

The cif-developers list continues to act as a discussion list and opportunity for software developers to advertise their new software. The Python package PyCIFRW was described in a CIF applications paper in Journal of Applied Crystallography [Hester, J. R. (2006). J. Appl. Cryst. 39, 621-625].

Finally, but by no means least, the IUCr won the 2006 Award for Publishing Innovation of the Association of Learned and Professional Society Publishers (ALPSP) for its development of the Crystallographic Information Framework and the use of checkCIF in data exchange, quality assurance and integrated data publication.