s9.m31.o3 **Maintaining the history of an X-ray laboratory**. Peter S White, *Department of Chemistry, CB#3290 Venable Hall, University of North Carolina at Chapel Hill, NC 27599-3290, USA. E-mail: pwhite@unc.ed*u

Keywords: Database; Validation; Archive

The X-ray laboratory at the University of North Carolina has been operating in its current format for over 15 years. In that time, structures have been determined using a variety of instruments, computer platforms and software packages. The data collection capabilities have expanded from dozens per year to hundreds per year and can only continue to increase. The result has been a volume of completed structures, many of which have not yet been published or deposited in the public databases. Over the years the computer data files have been saved, but little attempt, other than a reference number, has been made to allow users to search for old structures. This paper describes a project to save and categorize this data while the volume is still manageable, and provide a mechanism for future structures to be archived automatically. The main archive is a relational database with the choice of content based largely on the IUCr core CIF dictionary [1] augmented by a number of local fields. As a result, enough information is retained for each structure to permit the extraction of information required by journals with the most rigorous requirements. The main archive is only directly accessible to the system administrator and user access is via a software interface which exposes most of the database fields and a number of utilities that are based largely on the NRCVAX [2] software package. This permits the implementation of a security system which allows users to limit access to their structures as well as protecting the database from unauthorized or undocumented modification. As part of the archiving process a structure is passed through a validation procedure, similar to those employed by journals and public databases, which ensures consistency of the data and compares value ranges with those expected from a normal structure. This procedure also computes a number of fields that may be required, but are not normally produced by software, In order for the deposition to be finalized the user has either to correct any potential errors or provide an explanation which is stored with the entry. This ensures that if this structure is required at some point in the future for publication it will either pass any journal checks or the reason why not will be readily available. A number of tables are also generated that permit easy searching of the database for structures based on a number of structural or chemical criteria. The results of such a search permit an authorized user to extract the data for a structure. Utilities are provided to analyse such a structure and produce tables and graphics suitable for publication or inclusion in talks or presentations.

[1] IUCr, (October 2003) http://www.iucr.org/iucr-top/cif/cif_core/index.html
[2] Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S. (1989) *J. Appl. Crystallogr.*, **22**, 384—387.

s9.m31.o4 **CCP4 Molecular Graphics Project.** Liz Potterton and Stuart McNicholas, *University of York, UK. E-mail: ccp4mg@ccp4.ac.uk*

Keywords: Macromolecules; Program; Graphics

CCP4 are developing a graphics program to complement the existing suite of macromolecular software. The new program is intended to provide easy to use tools for crystallographic structure solution, structure analysis and comparison, and presentation graphics. It is also designed to enable other programmers to incorporate their applications into the program. The current program and future plans will be presented.