Oral Contributions

[MS10] General interests of single molecule crystallography, both large and small

Co-Chairs: Thomas Schneider (DE), Kirsten Christensen (UK)

[MS10-01] Recent developments in SHELX.

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SHELX [1] dates from about 1970 but was first released in 1976. The program, consisting of about 5000 Fortran statements, was then distributed in compressed form, together with test data for five small structures and an unpacking program, as a box of 2000 punched cards. The 2013 version consists of eight somewhat larger (but still Fortran) programs and may be downloaded by registration at the SHELX homepage http://shelx.uni-ac.gwdg.de/SHELX/ This homepage is also a source of extensive tutorials, documentation and background information. The programs are provided free for academic use, and are available in compiled form for modern Windows, Mac and Linux systems. A strict zero dependency philosophy is employed: the stand-alone programs are statically linked and require NO libraries, dlls, other files or environment variables, so they are particularly simple to install and use.Three of the programs already exploit the presence of multiple CPUs efficiently. The structure solving program SHELXD, which is used both for *ab initio* direct methods of small molecules and for the location of heavy atom sites in macromolecular phasing [2], runs about 29 times faster on a 32CPU computer. There was a major new release of the least-squares refinement program SHELXL in 2013, primarily for small-molecule applications, partly driven by the demands of CIF for archiving and validation but also to implement many new features, for example new restraints for anisotropic displacement parameters [3] and new facilities for refinement against neutron diffraction data. Other recent changes include the extension of the density modification and protein tracing program SHELXE so that it can be used to evaluate and extend molecular replacement solutions as well as for experimental phasing, and the program AnoDe [4] for the analysis of anomalous maps of macromolecules. Although the programs may be run from a command line, younger users find that GUIs such as shelXle [5] for small molecule refinement and hkl2map [6] for experimental phasing of macromolecules are a very convenient way of running SHELX. The SHELX programs have been incorporated into many pipelines for macromolecular structure determination, for example ARCIMBOLDO [7] and AMPLE.[8]

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Keywords: SHELX, Computer programs, Crystal structure solution, Crystal structure refinement.