

Chapter 6.1.1

SHELXL-97

Introduction

George W. Sheldrick
Dept. of Structural Chemistry
Tammannstraße 4
37077 Göttingen, Germany
email: gsheldr@shelx.uni-ac.gwdg.de

1. General Introduction to SHELX-97

The first version of **SHELX** was written at the end of the 1960's. The gradual emergence of a relatively portable FORTRAN subset enabled it to be distributed (in compressed form including test data as one box of punched cards) in 1976. **SHELX-76** survived unchanged - the extremely compact globally optimized code proved difficult to modify - until major advances in direct methods theory made an update of the structure solution part necessary (**SHELXS-86**). Rewriting and validating the least-squares refinement part proved more difficult but was finally achieved with **SHELXL-93**. **SHELXS-86** and **SHELXL-93** were as far as possible upwards compatible with **SHELX-76** (for example the format of the reflection data file was unchanged) and are now employed in well over 50% of all small-molecule structure determinations. A commercial version including interactive reciprocal and real space graphics is available in the form of the Siemens **SHELXTL** system.

A further release of **SHELX** in the current millenium was never intended, but the increased (mis)use of the programs by macromolecular crystallographers, and some changes to CIF format, have unfortunately made it necessary to release this new version of the complete package as **SHELX-97**. This also provided an opportunity to update the structure solution algorithms, to fix various bugs, and to improve the documentation.

Various beta-test versions were made available to selected guinea-pigs in 1996; these should be referred to as **SHELX-96**, and the final release (in 1997) as **SHELX-97**.

For the latest news the **SHELX** homepage at <http://linux.uni-ac.gwdg.de/SHELX/> should be consulted.

1.1 Programs

SHELX-97 contains the following six executable programs:

SHELXS - Structure solution by Patterson and direct methods.

SHELXL - Structure refinement (**SHELXH** for refinement of very large structures).

CIFTAB - Tables for publication via CIF format.

SHELXA - Post-absorption corrections (for emergency use only).

SHELXPRO - Protein interface to **SHELX**.

SHELXWAT - Automatic water divining for macromolecules.

The structure solution program **SHELXS** now includes more powerful direct methods (Sheldrick, 1990) and the use of the Patterson vector superposition method (Sheldrick et al., 1993) - completely different to the naive Patterson interpretation algorithm used in SHELXS-86 - for the automatic location of heavy atoms. This new Patterson interpretation routine is not only effective for small structures, but is also useful for the location of heavy atom sites from isomorphous or anomalous ΔF data of macromolecules.

The refinement program **SHELXL** includes many new features to make it easier to use for macromolecules, even at moderate resolution (say better than 2.5Å). It also incorporates a large number of small improvements suggested by small-molecule users of SHELXL-93.

In view of the fact that users were encouraged to adapt the 1993 version of **CIFTAB**, which produces tables from the CIF format files generated by SHELXL, only minor corrections have been made to this program.

An anonymous user has kindly donated the program **SHELXA** that can be used to make an 'absorption correction' by fitting the observed to the calculated intensities (like DIFABS). This is intended for emergency use only, e.g. when it is impossible to apply proper absorption corrections because the world's only crystal has been lost before measurements of crystal faces or azimuthal scans could be made. It would be quite unethical to submit a structure processed in this way for publication, and the anonymous donor does not wish to be cited in this non-existent publication since it would ruin his scientific reputation!

A new feature in SHELX-97 is an interactive interface program **SHELXPRO** that is specific to protein applications; SHELXS and SHELXL are very general and in no way specific to certain types of crystal structure. SHELXPRO handles problems of communication with other widely used protein programs; for example it can convert PDB to SHELX format, adding appropriate restraints etc., and can generate sigma-A maps etc. for map interpretation programs such as O. SHELXPRO also displays the refinement results in the form of Postscript diagrams, and facilitates deposition of the refined structure with the PDB.

SHELXWAT is a shell program that calls SHELXL iteratively to locate and refine solvent water atoms in macromolecules.

1.2 Distribution

SHELX-97 is provided in the form UNIX and VMS sources, plus precompiled versions for MSDOS, LINUX, AIX and IRIX. The programs are written entirely in a very simple

subset of FORTRAN. The UNIX versions are highly portable, but sometimes it will be necessary to replace the routines that return the time, date and CPU time with the alternatives provided. Documentation in WINWORD 6.0, HTML and Postscript form, plus examples and test files, are included in the release. The programs are currently available by ftp and on ZIP diskettes or CDROM.

The programs are available free to academics (there is a small charge for ZIP diskettes and CDROMs) and for a license fee (because it is necessary to cover all the costs of distributing and supporting the programs) to for-profit institutions. The license agreement covers the use of the programs for an unlimited time on an unlimited number of computers at one geographical location.

1.3 Support

The author (gsheldr@shelx.uni-ac.gwdg.de) is always interested to receive suggestions and comments, and tries to provide advice on installing and using the programs. Email may be quicker than reading the manual, but all emails asking the questions in Chapter 18 (Frequently Asked Questions) will be ignored! The programs are provided on the understanding that the author is in no way liable for any consequences of errors in the programs or their documentation.