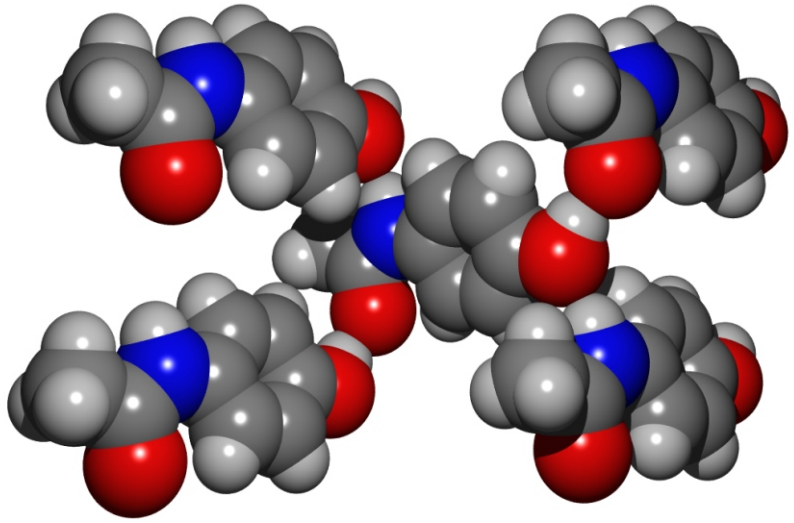
THE NEXT X-STEP 32



X-STEP32 software suite is STOE´s new X-ray structure evaluation package and the successor of the well known X-STEP.

As a pure 32bit application, it takes advantage of the full power and speed of modern PC technology for rapid structure solution and refinement. The interactive software is a powerful tool not only for routine structural work but also supports the user in solving special difficult problems.

The software package is running under Windows 95, 98 and Windows NT, it fully supports remote calculations on any computer connected via a TCP-IP network.

X-STEP32 offers a friendly graphic user interface with on-line help. It supports the well known programs SHELX 97* and SIR 97*.

Reflection files collected on the STOE´s Imaging Plate systems as well as from STADI4 and STADI4 CCD are loaded automatically and can be used for the actual solution and refinement process.

Distinct interactive graphic routines provide a clear and detailed overview of the obtained results, leading to a better and straight forward structure solution and refinement. The program also supports the user with sophisticated error handling due to a systematic backup procedure.

Thus X-STEP32 is an easy data handling and modification suite for X-ray structure evaluation for both the newcomer and the experienced user.

*These programs are available from the authors
SIR 97, http://www.ba.cnr.it/IRMEC/sirware.html
SHELX97, http://shelx.uni-ac.gwdg.de/SHELX

After the data collection …

a powerful, variable and easy-to-use structure evaluation software helps the user in his everyday structural work.

STOE is not only a manufacturer of excellent X-ray equipment, it supports the scientific community with state-of-the-art crystallographic software.
The X-STEP^{32} software is one of the crystallographic tools developed by STOE to guide a newcomer through a successful structure determination and to support the experienced user in analysing and solving complex problems.

A graphic user interface leads to an easy set-up and is designed to minimise possible user mistakes. Extensive on-line help completes this task.
Various graphic modes like ball-and-stick or thermal ellipsoids together with continuous rotation, including all atom labels, offer a clear and distinct view of the structure.

Assistance for a deeper knowledge of the structural model is given by symmetry checks, colour-coded peak heights, temperature factors, visualisation of fourier peaks etc..

The results of the structure evaluation can be automatically saved into a compressed archive, to assist the user in saving his work in clearly arranged files. Various interfaces to other programs

New Features

- True 32bit application, taking full advantage of modern PC technology
- Modern, user friendly graphic user interface
- New stereo plot utility
- Open GL support
- Support of BIND and FREE commands of SHELX 97
- Use of SIR 97
- Up to 10 different orientations of the structural model can be saved
- Choose and display of single symmetry operations
- Use of graphical elements for clear presentation of the structure
- Remote control via TCP-IP network
- STRUPLO, POV, SCHAKAL, PLUTON interface
- Automatic compression of all files into one ZIP archive

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