Acta Cryst. (2002). A**58** (Supplement), C254

CRYSTAL STRUCTURE OF ETHYL-(2-AMINO-4-PHENYL-5-THIAZOLYL) ACETATE

P. Dyavegowda M. K. Kokila N. M. VN Veerammana Hally Narayanappa M. V Kulkarni G. K. Rao J. S. Prasad Javare Gowda
Bangalore University Department of Physics Bangalore University, Jnanbharathi Campus BANGALORE KARNATAKA 560 056 INDIA

Thiazole-5-acetic acid derivatives have been a useful class of non-steroidal anti-inflammatory agents. The aryl groups in thiazoles have been of vital importance in minimizing the toxic effects of many anti arthritic drugs. 2-amino-thiazolidinone-5-acetic acids have served as model compounds to study the S¨O interactions in solid state. The title compound has been investigated for its antimicrobial and anti inflammatory activity.

The molecule is non-planar. The phenyl ring is twisted by an angle 45° with respect to thiazole ring where as the side chain ethyl acetate is oriented at an angle of 60°. These two groups are almost eclipsed with a dihedral angle of 15°. The carbonyl carbon and methyl groups are anti-periplanar and the ester group is in cis arrangement about the C-O bond. The molecules are held by N-H¨O, N-H¨N and C-H¨O hydrogen bonds.

The Structure analysis of the title compound has been done by X-ray methods. The three-dimensional intensity data were collected on an Enraf-Nonius CAD-4 diffractometer using Cu-Kα-radiation. The structure was solved by direct methods and refined by full-matrix least-squares methods using SHELXL-97 program.

Keywords: THIAZOLE, NON-STEROIDAL ANTI-INFLAMMATORY AGENT, THIAZOLYL ESTER.

Acta Cryst. (2002). A**58** (Supplement), C254

CRYSTALLOGRAPHIC COMPUTING: WHERE DO WE GO NOW?

D. Watkin
Chemical Crystallogrpahy Laboratory, OXFORD, UK.

Traditionally, crystallographic software has been developed in the 'public domain', and distributed freely. The maintenance has been done by the authors, at their institutions expense. Many of the authors of significant programs are now approaching retirement. Many institutions are being forced to make harsh cost-analyses. The world is changing and there are issues to be faced. 1. Is there a problem emerging, or will 'cultural evolution' ensure survival of the best? 2. How can Crystallographic Software be financed and maintained? 3. What role can government institutions (EPSRC,CNR,CNRS,NSF etc) play in software projects? 4. Who should 'own' academic software, and what provisions can be made for its maintenance? 5. What can companies do with software which becomes unprofitable? 6. Is there a future for academic software? 7. Is there a risk of us loosing 'software diversity'? 8. Is software moving towards 'the best possible', or 'the lowest acceptable' level? 9. Is it worth preserving legacy software, and if so, who should pay?

This list is not comprehensive - there is no strategy evolving which can optimize the needs of funding agencies, educational and government research, commercial enterprises and individuals. The role of computers in research is now inescapable, but there is no good model to explain who is going to pay for the software we all need. It may be evident from this note that my own vision of the future is rather pessimistic - it would be good to have some optimistic analyses!

Keywords: COMPUTING COMMISSION SOFTWARE ARCHIVE PROGRAMMING

Acta Cryst. (2002). A**58** (Supplement), C254

FORTRAN ARCHAEOLOGY: AN ISSUE FOR A KNOWLEDGE ORGANIZATION LIKE THE IUCr?

H. Flack
University of Geneva Laboratoire De Cristallographie 24 Quai Ernest-Ansermet GENEVA CH-1211-4 SWITZERLAND

The International Union of Crystallography is an archetypal knowledge organization. By way of its multifarious activities in: journal, reference works and book publishing; teaching support; nomenclature; data standards; scientific projects; it has from its inception been engaged in knowledge creation and management. Current thinking on knowledge organizations reminds us that to the above tangible assets one should also add the accumulated know-how of its members. Knowledge management then seeks the ways and the means to capitalize on these assets, and to develop and preserve them for the future. Early on crystallographers understood the potential of computers for scientific calculation and in recent times the IUCr has made very good use of modern information technology for its activities in electron publishing, online news service and online directory of crystallographers. The e-publishing activities have engendered a whole host of problems unknown to the IUCr in the print on paper era. The major ones relevant to this open commission meeting are those of preservation and archiving of digital information. Indeed these problems are common to many institutions and are seen to be of a truly global scope. There has been considerable research effort in this area throughout the world and operational systems for digital preservation and archive are now beginning to come on stream.

It is against this background of the IUCr as a knowledge organization and recent research in digital preservation and archiving that it is beneficial to analyze the impending crisis in crystallographic software identified by the IUCr's Commission on Computing.

Keywords: ARCHIVING PRESERVATION SOFTWARE

Acta Cryst. (2002). A**58** (Supplement), C254

SHELX: 30 YEARS OF OPEN SOURCE EXPERIENCE

G.M. Sheldrick
Universitaet Goettingen Lehrstuhl Fuer Strukturchemie Tammannstrasse 4 GOETTINGEN D-37077 GERMANY

The SHELX system of programs for structure determination from single crystal diffraction data has been distributed and supported since the early seventies of the last century and is still evolving. The author will describe his experiences and lessons learnt from this 'open source' project. Recent developments affecting intellectual property rights could severely complicate and restrict this approach in the future, with adverse long-term consequences for scientific progress.

Keywords: COMPUTER PROGRAMS OPEN SOURCE SHELX