Computer Program Abstracts

The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 of the June 1985 issue of the Journal [J. Appl. Cryst. (1985). 18, 189–190].

J. Appl. Cryst. (1994). **27**, 131

PSL + SEARCHER and *DIRECTER* – automatic structure analysis of organic compounds using a PC.

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The crystallographic problem: *PSL* selects one heavy-atom solving Patterson function and *SEARCHER* determines the positions of all the remaining atoms automatically. *DIRECTER* is based on the symbolic-addition method and automatically determines most atoms. In a single PC run, the user can determine the molecular fragments by inputting the atom symbols with no chemical assumptions or human intervention.

Method of solution: *PSL* and *SEARCHER* are used for organic compounds that include sulfur or a heavier atom. The *PSL* procedure is as follows: (i) read the cell constants, heavy-atom symbol, reflection data and Harker sets; (ii) calculate the Patterson function for all Harker sets or an asymmetric unit and store the peaks and heights (u, v, w, H); (iii) convert all peaks into coordinates, combine these coordinates and store them as atoms (x, y, z, H); (iv) remove the centers of symmetry [$(0, 0, 0)$, $(\frac{1}{2}, 0, 0), \ldots,$ $(1, 1, 1)$] and equivalent positions; (v) calculate the structure factors and refine each parameter (x, y, z, B) with full-matrix least squares; (vi) sort the final R factors so that heavy atoms are located with the lower R factor.

SEARCHER proceeds as follows: (i) read the cell constants, the number of input (NSF), total (NLS) and additional (NLH) atoms, the heavy-atom parameters, the reflection data and a maximum temperature factor (BCUT); (ii) calculate the structure factors and Fourier synthesis using the controlled reflection data by the combination of NSF and $(\sin\theta)/\lambda$; (iii) select the peaks (x, y, z, H), check for 'reasonable' interatomic distances between input atoms and peaks and add the NLH peaks to NSF atoms. If NSF is less than NLS, repeat step (ii); (iv) refine the parameters until ghost atoms are removed ($B >$ BCUT); (v) draw 2D projections of the molecules.

DIRECTER proceeds as follows: (i) read the cell constants, atom symbols, reflection data with $|F_o(\mathbf{h})|$; (ii) select three kinds of origin sets including enantiomorphs and Σ_1 reflections for which $P_+[E(\mathbf{2h})]$ are greater than 0.95; (iii) choose several potential members that can generate phases for more than 95% of the data; (iv) generate new phases by the tangent formula. The process is repeated to cover all combinations (run sets) of phases; (v) select the 'best five' run sets using the figures of merit R_{Karle}, Q_{Drew}, $\langle\alpha\rangle$ and $\langle t\rangle$ (Drew, Larson & Motherwell, 1971); (vi) calculate the 'best five' E maps, select 1.1 times peaks of one molecule and calculate the structure factors; (vii) draw 2D projections. If some fragments are obtained by *DIRECTER*, *SEARCHER* is a powerful tool to find the remaining atoms.

Software and hardware environments: These programs are written in standard Fortran77 and fully tested under MS-DOS™ 3.x. Only the standard option has been applied. These programs need 520 kbyte of memory and 2 Mbyte of disk space. A laser printer with HPGL emulation is needed for drawing.

Program specifications: These programs are part of the *DS*SYSTEM* (Okada & Koyama, 1991). Each program consists of a main segment plus *DS*SYSTEM* libraries totaling about 29 000 source-code lines. Run times are usually less than 30 min (*PSL* + *SEARCHER* and *DIRECTER*) and 1–7 h (*DIRECTER*) for a small structure by i486 + ODP (25MHz). The PC 1993 version is improved from 1991 by a change to the algorithms of peak summation in Fourier synthesis, which decreases calculation time.

Documentation and availability: WordStar™ 5.0 documentation and the latest executable files are available from the author.

Keywords: automatic structure determination, PC, organic compounds, heavy-atom analysis, direct methods, Patterson methods.

References

Drew, M., Larson, A. & Motherwell, S. (1971). *TANTWO: Generation and Refinement of Phases by the Tangent Formula.* Univ. of Cambridge, England.

Okada, K. & Koyama, H. (1991). *J. Appl. Cryst.* **24**, 1067–1070.

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Restructuring of the IUCr editorial office

Following the promotion of Mr Michael Dacombe from Technical Editor to Executive Secretary, it was considered an opportune time to restructure the editorial office to reflect better the greater variety of work now carried out and to clarify the responsibilities of the staff.

Mr Peter Strickland has been appointed as Managing Editor with overall responsibility for both the technical editing and the centralized checking. Mrs Sue King has been appointed as Technical Editor. Dr Amanda Berry has been appointed as Assistant Technical Editor with special responsibility for the centralized checking. There are three Senior Editorial Assistants and six Editorial Assistants. Mr Brian McMahon is the Research and Development Officer and his assistant is Dr M. Hoyland. The total number of graduate staff in the editorial office is 14.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.

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Structure of electrified interfaces. Edited by *J. Lipkowski* and *P. N. Ross.* Pp. x + 406. Weinheim: VCH Verlagsgesellschaft mbH, 1993. Price DM 196, £80.00. ISBN 3-527-28787-6.

This book aims to describe, to a broad audience, the current understanding of the metal–solution interface of electrochemistry. The clear objective in this field of interfacial electrochemistry is to replace or augment the thermodynamic continuum models of the classic electrochemical double layer with microscopic models that explicitly incorporate the roles and structures of individual atoms and molecules. The evolution of perspective from macroscopic to microscopic is clearly work in progress and the book provides an excellent overview of current theory and recent experimental advances.