

PEKPIK and **MODEL**. **GENEV** provides for the special treatment of weak reflection data, a general index-rescaling scheme, the application of inflexion-point least-squares to the Wilson plot, and the estimation of errors for the normalized structure factors. **GENSIN** generates both triplet and quartet relationships with a range of user controls. **GENTAN** provides for automatic starting set selection, permuted and random phase assignments, block and cascade phase refinement and different weighting schemes. The phase set having the best chance to yield the structure is selected using an absolute-measure-of-success (AMOS) parameter based on psi-zero triplets, negative quartets, $R(\text{Karle})$ and a combined figure of merit.

Software environment: The direct-methods programs are an integral part of the XTAL system, and are not intended for use as stand-alone routines. The distributed source code is in the pre-processor language RATMAC (Munn & Stewart, 1979) which is translated on site into the locally available Fortran (66 or 77). Programs are adapted to the local operating system and linking environment through the MACRO feature within RATMAC. The software currently runs on a wide range of machine types. For larger structures, **GENEV** requires either a VMS operating system or a random-access I/O facility.

Hardware environment: The current version of the XTAL system requires a minimum hardware configuration of 128 kbytes of memory; 32-bit integer and floating-point words and 20 Mbytes of offline memory (e.g. disk storage). **GENEV**, **GENSIN** and **GENTAN** have been implemented and tested on Control Data, Digital Equipment, IBM, Perkin Elmer and Univac computers.

Program specification: Reflection data are input via an XTAL binary file, and control parameters as free-format line data. Run times vary according to structure size and machine type. A typical example involving 120 non-H atoms/cell, 228 E values, 3121 triplets, 1497 quartets and 8 phase sets runs in 0:21, 4:58 and 3:56 CPU minutes on a DEC VAX 780, and 0:25, 6:40 and 4:80 minutes on a CDC Cyber 750/175. **GENEV**, **GENSIN** and **GENTAN** are 2010, 2490 and 4520 lines of RATMAC code, respectively.

Documentation: **GENEV**, **GENSIN** and **GENTAN** are documented as separate chapters in the *XTAL Users Manual* (Stewart & Hall, 1983). The program description and input instructions are detailed therein. The source code is fully commented.

Availability: These programs are distributed as part of the XTAL Crystallographic System. An information brochure on this system is available from Professor J. M. Stewart, Computer Science Center, University of Maryland, College Park, MD 20742, USA.

Keywords: Direct-methods software; Structure-invariant methods; Normalized structure factors; Tangent refinement; XTAL system.

References

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 Stewart, J. M. & Hall, S. R. (1983) Tech. Rep. TR-1364. Computer Science Center, Univ. of Maryland, College Park, Maryland.
 Stewart, J. M. & Hall, S. R. (1985). *J. Appl. Cryst.* **18**, 263.

Crystallographers

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This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England)

Dr **V. Cody**, an associate research scientist at the Medical Foundation of Buffalo, New York, USA, has been awarded the Faculty Research Award of the American Cancer Society for her study of the relationship between molecular structure and biological activity of drugs which inhibit tumour growth.

Dr **C. J. Humphreys**, of the Department of Metallurgy and Science of Materials at the University of Oxford, has been appointed to the Henry Bell Wortley Chair of Materials Engineering at the University of Liverpool. He is the Chairman of the Union's Commission on Electron Diffraction.

Gloria B. Lubkin has been appointed Editor of *Physics Today*, the monthly magazine of the American Institute of Physics which has a circulation of 80 000 and is written for physicists and those interested in the physical sciences. She has been on the staff of *Physics Today* for more than 21 years. She was elected a Fellow of the American Physical Society in 1973 and was a founding member of the APS Committee on Women in Physics in 1971.

Dr **D. Ringe**, Department of Chemistry, Maryland Institute of Technology, and Dr **B. Wallace**, Department of Biochemistry, Columbia University, have been named by the Biophysical Society as the first recipients of the Margaret Oakley Dayhoff Award. The award honours the memory of Dr Dayhoff, former President of the Biophysical Society, Professor of Biophysics at Georgetown University and Director of Research at the National Biomedical Research Foundation, and will be awarded each year to a junior woman scientist working in a field within the range of interest of the Biophysical Society.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication

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Industrial crystallization. By **S. J. Jančić** and **P. A. M. Groot-scholten**. Pp. xvi + 434. Delft University Press and D. Reidel Publishing Co., Dordrecht, 1984. Price US \$ 64.

The information explosion that has occurred over the past decade in virtually all of the areas relating to nucleation and crystal-growth kinetics, and in the analysis of particulate systems, is invoked by the authors to justify the comment that no single book can now offer a comprehensive text on the broad subject of industrial crystallization. They are probably right.

Accordingly, they have taken a slightly restricted view of the subject by confining their attention to crystallization from solution, which is still by far the major field of industrial activity. Their objective has been to exploit the links that are slowly being forged between theory and practice in order to be able to design, build and operate better crystallizers at all scales of operation. They have done a commendable job.

The first part of the book (nine chapters) entitled *Fundamentals of crystallization from solutions* deals with primary and secondary nucleation, crystal-growth kinetics, the population balance concept and its application to the MSMPR crystallizer. Methods of characterizing particulate systems, the laboratory measurement of crystallization kinetics and the assessment of transport phenomena in solid-liquid systems all get thorough treatment.

The second part (six chapters) entitled *Crystallizer design* covers the use of