## 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 exisiting 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].*

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### *XENVIEW* – an interactive program to display and analyze electronic area detector data.

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**The crystallographic problem:** It is desirable to be able to display X-ray diffraction data acquired by electronic area detectors at various stages of a structural analysis. This is useful for following changes in the quality of the diffraction and detecting problems incurred during data collection. When integrated data are obtained, viewing reflections in reciprocal-lattice planes assists in space-group determination. In addition, simultaneous viewing of reciprocal-lattice planes of native and heavy-atom-derivative data scaled together facilitates qualitative evaluation of potential derivatives for use in structure determination by the multiple isomorphous replacement method. This is also useful for any other isomorphous data in which diffraction pattern differences are expected.

**Method of solution:** A program has been written to display diffraction images of crystals of biological macromolecules recorded using a Siemens† electronic area detector. Single diffraction images or composite images, obtained by summing successive frames, can be displayed on a Silicon Graphics 4D workstation. The predicted location of diffraction spots calculated by the *XENGEN PREDICT* computer program (Howard *et al.*, 1987) can also be superimposed on the diffraction images.

The program can also produce pseudo-precession pictures of selected reciprocal-space lattice planes from the integrated reflections files produced by the *XENGEN* program system. It also allows the comparison of selected lattice planes of two different diffraction data sets, after scaling them together using a modification of the program *AMALG* (John Moult, personal communication). The same lattice plane from each data set can be displayed simultaneously along with the 'difference' plane. The color and contrast of the diffraction images may be altered by simple manipulation of the mouse.

**Software environment:** The programs are written in ANSI C and Fortran 77. They are controlled by a unix *C*-shell script operating under the IRIX 3.2 Silicon Graphics operating system. The graphics calls are made to the IRIS 4D graphics library.

**Hardware environment:** The program is implemented for Silicon Graphics IRIS 4D workstations.

**Program specification:** All of the program functions are controlled through the use of pull-down menus. Menu selection and positioning of the diffraction images on the Silicon Graphics workstation screen are controlled with the mouse. The source contains about 2000 lines of code.

**Documentation:** Documentation for installation and operation is provided. Sample data for testing is also included.

**Availability:** The *C*-shell script, executable and source code files of the program are available from the authors. One cartridge tape, for either high- or low-density Silicon Graphics format, is required.

**Keywords:** oscillation photograph, electronic area detector, *XENGEN*, precession photograph, heavy-atom derivative, Silicon Graphics 4D display.

#### Reference

Howard, A. J., Gilliland, G. L., Finzel, B. C., Poulos, T. L., Ohlendorf, D. H. & Salemne, F. R. (1987). *J. Appl. Cryst.* **20**, 383–387.

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† Certain commercial equipment, instruments and materials are identified in this paper in order to specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

## Crystallographers

*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 Editoral 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).*

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Dr **Vivian Cody,** Molecular Biophysics Department, Medical Foundation of Buffalo, Buffalo, New York, USA, has been re-elected ACA Secretary for 1991, 1992 and 1993.

Ms **Judith L. Flippen-Anderson,** Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, DC, USA, is the President of the American Crystallographic Association for 1991.

Professor **D. Grdenic,** Laboratory of General and Inorganic Chemistry, Zagreb University, Yugoslavia, has been elected Honorary President of the Yugoslav Centre of Crystallography, in recognition of his 25 years service as President of that Centre. The new President is Professor **B. Kamenar,** of the same laboratory.

Professor **Yury T. Struchkov,** Head of the Crystallographic Centre, Chemical Division, Academy of Sciences of the USSR, Moscow, USSR, and a newly elected member of the Executive Committee of the International Union of Crystallography, has been elected a Corresponding Member of the Academy of Sciences of the Soviet Union. He is well known for his contributions to X-ray crystallography, in particular for his systematic studies of organic and organometallic compounds.

Dr **Keith D. Watenpaugh,** Physical and Analytical Chemistry, The Upjohn Company, Kalamazoo, Michigan, USA, has been elected ACA Vice-President for 1991. He will then assume the office of ACA President on 1 January 1992.

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