

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. (1993). 26, 144

XTALLAB and POWDER – computer assisted instruction in elementary crystallographic methods. By CATHERINE L. DAY and ROBERT A. JACOBSON, Ames Laboratory and Department of Chemistry, Iowa State University, Ames, Iowa 50011, USA

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The crystallographic problem. Addressing a significant part of the many facets of crystallographic methodology is not feasible in the undergraduate chemistry curriculum. Though X-ray diffraction has led the way to significant structural discoveries, crystallographic techniques receive, at best, only a cursory review during the undergraduate course of study.

Method of solution: POWDER and XTALLAB and their accompanying supplements were designed to provide the undergraduate junior or senior physical-chemistry student with computational experience using basic crystallographic methods to supplement knowledge obtained through course lectures.

Unlike other crystallographic laboratory exercises (Lessinger, 1988; Loehlin & Norton, 1988), these experiments require no previous computational experience or special crystallographic software. Each experiment can be run on a PC and can be performed in one 3h laboratory period. The experiments are each broken into two parts – a description of the crystallographic theory and calculations involved and an interactive computer program. Knowledge gained from the descriptive material is applied to the solution of a practical X-ray diffraction problem. POWDER helps the student index a powder photograph, decide the cubic lattice to which the crystal belongs and find the crystal's lattice constant. XTALLAB was designed to acquaint the student with the method of crystal structure determination based upon X-ray diffraction data

obtained with single crystals. To simplify calculations and viewing of the trial molecule, the structure determination is carried out on a relatively planar structure with a short cell axis which allows for two-dimensional analysis. Used in conjunction with each other, POWDER and XTALLAB combine to provide the student with an elementary understanding of crystal structure determination based upon X-ray diffraction data obtained from powder photographs and single crystals.

Hardware environment: POWDER and XTALLAB require a 286/386/486 IBM or clone PC, an EGA color monitor and a math coprocessor.

Availability: Programs and documentation are available from the authors.

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References

- Lessinger, L. (1988). *J. Chem. Educ.* **65**, 480-485.
Loehlin, J. H. & Norton, A. P. (1988). *J. Chem. Educ.* **65**, 486-490.

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 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).

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Professor **Mary F. Richardson**, Chemistry Department, Brock University, St Catharines, Ontario, Canada, was named Canadian Professor of the Year by the Council for Advancement and Support of Education, Washington, DC, on 15 June 1992. The citation states that she has focused on getting students, especially women, interested in chemistry. She led the committee that developed the women's studies programme at Brock University and also worked extensively with colleagues to review and revise the undergraduate curriculum for chemistry students. Additionally, she played a part in the design of an adjustable-height wheelchair so handicapped students could reach normal-height research equipment and library shelves. Professor

Richardson is also a national expert on the chemical composition of beer and beer making and periodically lectures on this topic.

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