

Professor **P. Coppens**, Chemistry Department, State University of New York at Buffalo, New York, USA, received a Doctor Honoris Causa degree from the University of Nancy, France, in December 1989 in recognition of his scientific accomplishments, primarily in the fields of materials research and crystallography.

Professor **B. K. Vainshtein**, Institute of Crystallography, USSR Academy of Sciences, Moscow, USSR, has been awarded the Ewald prize for his contributions to the development of theories and methods of structure analysis by electron and X-ray diffraction and for his applications of his theories to structural investigations of polymers, liquid crystals, peptides and proteins. The first Ewald Prize was awarded jointly to Professor J. M. Cowley and Dr A. F. Moodie.

New Commercial Products

Announcements of new commercial products are published by the Journal of Applied Crystallography free of charge. The descriptions, up to 300 words or the equivalent if a figure is included, should give the price and the manufacturer's full address. Full or partial inclusion is subject to the Editor's approval and to the space available. All correspondence should be sent to the Editor, Professor M. Schlenker, Editor Journal of Applied Crystallography, Laboratoire Louis Néel du CNRS, BP 166, F-38042 Grenoble CEDEX, France.

The International Union of Crystallography can assume no responsibility for the accuracy of the claims made. A copy of the version sent to the printer is sent to the company concerned.

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New XRF Wafer Analyser from Philips

Philips Analytical has announced a new **X-ray fluorescence wafer analyser**, designed specifically for use in process control in the manufacture of integrated circuits.

The analyser, a member of the PW1480 series, is ideal for use in a clean-room environment, where it can be employed for a variety of applications in wafer analysis.

These include composition and layer thickness of BPSG passivation layers; layer thickness of Ti and alpha silicon in Ti silicide; P, As and Sb implantations; Cl and F plasma etching residues; and Cu and Si levels in Al metallisation layers.

Automatic measurement of multi-spot patterns can be made on wafers up to 200 mm (8 in) in diameter, giving

highly accurate information on composition and layer thickness. The system is capable of analysing elements from boron upwards. Results can be archived automatically, with operation supervised by a special version of Philips X40 analytical software, currently in use with more than 500 of the company's X-ray installations worldwide.

Philips Analytical, York Street, Cambridge CB1 2QU, England

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New Release of Chem-X QSAR Module

The January 1990 release of Chem-X sees major enhancements to **ChemStat**, the specialist **QSAR module** within the Chem-X molecular modelling system.

ChemStat uses a combination of automatic parameter generation and statistical analysis to help users determine the structural features of a molecule which are responsible for its biological activity (*i.e.* to find quantitative structure-activity relationships or QSARs). Developed because it can be very time consuming (and not always very effective!) to study the effects of selected structural parameters one by one, ChemStat automatically evaluates a large number (100+) of user-specified parameters for a predefined set of molecules (20-2000+) and stores the results in a database. The parameters may include distances, angles, energies, charge distributions, dipole moments, electron densities, superdelocalizabilities, surface areas and any other parameter defined in Chem-X or by a user-written routine. This approach enables a vast amount of data to be collected quickly and easily, and also minimizes the possibility that crucial factors may be overlooked. ChemStat's powerful built-in statistics routines may then be used to identify the parameters which correlate most strongly with activity. This information may be used in the design of new more efficacious drugs or agrochemicals.

In the January 1990 release, ChemStat's built-in statistics routines have been extended to include principal components analysis (PCA). This is a form of data reduction in which the data table is transformed such that a small number of fields in the new table describes most of the variance in the

original. Data reduction is important because in most cases the amount of data in the table is too great for immediate regression analysis. ChemStat then uses multiple linear regression or principal components regression to derive relationships between structural parameters and activity.

ChemStat now reports additional information that can be used to help establish the statistical validity of the regression equation. Values reported include the standard deviation, the square of the correlation coefficient (r^2) and the F value for the regression equation, together with the standard deviation, confidence intervals and the results of t tests for the coefficients. These data can be automatically recorded in the Chem-X electronic notebook for future reference.

With the introduction of an interface to RS/1, ChemStat now interfaces to all the major statistics programs requested by customers. The new interface allows the user to transfer the contents of a database directly into RS/1 for further statistical analysis.

ChemStat may also be used in conjunction with the new 3D database search module, ChemDBS-3D, to add new parameter fields to the database and to analyse 3D search results.

Chemical Design Ltd, Unit 12, 7 West Way, Oxford OX2 0JB, England

Books Received

The following book has been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

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Crystal chemistry. By *Howard W. Jaffee*. Pp. xii + 336. Cambridge: Cambridge University Press, 1989. Price £55.00 or \$75.00. ISBN 0521369851. A review of this book, by A. M. Glazer, has been published in the June 1990 issue of *Acta Crystallographica*, Section B, page 447.

Inorganic crystal structures. By *B. G. Hyde* and *Sten Anderson*. Pp. xviii + 430. Chichester, New York: John Wiley, 1989. Price £41.55. ISBN 0471628972. A review of this book, by R. O. Gould, has been published in the June 1990 issue of *Acta Crystallographica*, Section B, page 448.