

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).

J. Appl. Cryst. (1990). **23**, 349–350

J. Monteath Robertson, 1900–1989

Professor J. M. Robertson, who died on 27 December 1989, was a key figure in the development of X-ray crystallography as the definitive approach to molecular structure. In several classic papers published between 1935 and 1940 he described the first determination of the structure of a sizeable molecule by isomorphous replacement and the heavy-atom method and established these as realistic procedures for the study of large and complex molecules.

Monteath Robertson was born at Nether Fordun Farm, near Auchterarder in Perthshire, Scotland, on 24th July 1900 and was educated at Perth Academy and Glasgow University. His research training at Glasgow was in organic chemistry and his PhD degree was awarded in 1926 for a thesis entitled 'The Structural Relationship of Certain Members of the Bicyclic Sesquiterpene Series'.

During his PhD research it became clear to him that the chemical procedures available at that time were inadequate to deal with the complex three-dimensional molecules of natural products. Aware of the progress that was being made in the study of inorganic crystal structures by X-ray diffraction, he sent a sample of the chloride of caryophyllene alcohol, one of the few crystalline materials he had obtained in his research, to W. H. Bragg at the Royal Institution, London, and shortly afterwards went there himself with a Carnegie Fellowship, hoping to work on these crystals and elucidate the structure of his compound. It was to be thirty years later, and back in Glasgow, that he accomplished this task. He spent two years at the Royal Institution, with W. T. Astbury, J. D. Bernal, K. Lonsdale, A. Muller and G. Shearer, and two subsequent years in the USA with a Commonwealth Fellowship preparing for a career in X-ray crystallography.

In 1930 Robertson returned to the Royal Institution and embarked on a series of studies of organic compounds: naphthalene, anthracene, hexamethylbenzene, dibenzyl, stilbene, tolane, resorcinol, benzoquinone, oxalic acid

dihydrate,.... At that time the only computational aid available was an adding machine, hence X-ray studies were confined to two-dimensional projections and Robertson recognized that only flat molecules are likely to yield an unobscured crystal projection. His early training in organic chemistry gave him the background to choose important two-dimensional molecules and to circumvent the crystallographic phase problem by trial-and-error intuitive procedures. The molecular dimensions that he obtained served to underpin developments in theoretical chemistry by Pauling and Coulson. These results, obtained largely without assistance, would have justified international recognition. A more important project, however, was to secure his place in crystallographic history.

The dark blue pigment phthalocyanine, $C_{32}H_{16}N_8$, was discovered at the Grangemouth Factory of Scottish Dyestuffs in 1928. The compound is crystalline, extraordinarily stable, and forms a series of metal derivatives. The potential commercial importance of these materials led to intensive chemical investigation by Linstead and his assistants at Imperial College and late in 1933 Robertson obtained specimens of the crystals. The phthalocyanine compounds crystallize in the monoclinic space group $P2_1/a$, with two molecules in the unit cell. The metal atom is therefore at the centre of symmetry and a comparison of the intensities of corresponding reflections from free phthalocyanine and the nickel derivative enabled Robertson to derive the phase constants for the $h0l$ reflections of free phthalocyanine. For the comparison, the intensities had to be placed on the absolute scale and this was achieved by the direct determination of a few of the strongest reflections on an ionization chamber and also photographically by comparison with known standards on a two-crystal moving-film spectrometer. The resulting Fourier analysis of the $h0l$ zone of the metal-free compound produced an electron-density contour map which unequivocally showed the molecule in full detail. In the case of the platinum derivative, the presence of an atom of atomic number 78 at a centre of symmetry made it realistic to take all phase angles as 0 and a Fourier summation with all terms positive gave a picture of the molecule without any prior structural assumptions and quite independent of the work of the organic chemists.

The determination of phase constants by substitution (method of isomorphous replacement) had been applied to some simple inorganic structures, notably the alums, by Cork and by Beevers and Lipson, but Robertson's

analysis of phthalocyanine was much more direct and complete and represented the first direct determination of the structure of a sizeable molecule by X-ray methods. Robertson realized the potentialities of isomorphous replacement and the heavy-atom method and as early as 1939 suggested that the replacement of the zinc atoms in insulin by mercury atoms could lead to the determination of the structure of this protein.

In 1942, Robertson was appointed to the Gardiner Chair of Chemistry at Glasgow University and after the end of the war built up what was probably the leading centre for the study of organic molecules by X-ray diffraction methods. Until the late fifties computational limitations caused him to emphasize the careful study of fairly simple molecules: polycyclic aromatic hydrocarbons, carboxylic acids and other hydrogen-bonded materials. In 1958, however, Glasgow University obtained one of the early commercial electronic computers, DEUCE, and full three-dimensional X-ray analysis became feasible. In the next few years Robertson and his students revolutionized structural organic chemistry. Terpenes, alkaloids and other natural products with complex structures and stereochemistries were elucidated rapidly and unambiguously by the heavy-atom approach and a steady stream of important new results appeared in *Proceedings of the Chemical Society*. When he retired in 1970 he had published nearly 300 papers.

Robertson was elected to the Royal Society in 1945, was the George Fisher Baker Lecturer in Chemistry at Cornell University in 1951, and was President of the Chemical Society 1962–1964. He was awarded the Davy Medal of the Royal Society in 1960, the Longstaff Medal of the Chemical Society in 1966, the Paracelsus Medal of the Swiss Chemical Society in 1971, and the Gregori Aminoff Medal of the Royal Swedish Academy in 1983.

He was very successful in developing the talents of his students and many went on to set up crystallographic laboratories in the UK, USA, Canada, Australia and Europe. His laboratory provided a stimulating and happy environment in which to be introduced to research.

At the end of November 1989 Mrs Robertson formally opened the new J. M. Robertson Protein Crystallography Laboratory in the Chemistry Department of Glasgow University. Professor Robertson was too ill to attend but we hope that he was pleased that the crystallographic school that he established at Glasgow continues to flourish.

G. SIM

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.

J. Appl. Cryst. (1990), **23**, 350

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

J. Appl. Cryst. (1990), **23**, 350

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.

J. Appl. Cryst. (1990), **23**, 350

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.