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## 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).*

Professor **Alan Fredric Berndt** (1932–1984), Professor of Chemistry at the University of Missouri, St Louis, died of cancer May 1984. Dr Berndt, who was a graduate of Cooper Union School of Engineering in New York and received a doctorate from the California Institute of Technology in Pasadena, joined the UMSL faculty in 1965 as an assistant professor. He became an associate professor in 1967 and a full professor in 1971. From 1975 to 1978, he was Assistant Dean of the UMSL graduate school. A physical chemist with interests in solid state chemistry, inorganic crystal structures, thermodynamics and X-ray crystallography, Dr Berndt published 43 papers in chemical journals and was the co-author of a book, *Dental Fluoride Chemistry*.

Mr **J. K. Byron** died in Ottawa, Canada, after a short illness on 11 September 1984. For many years he had been assisting in the preparation of the Metals Section of *Structure Reports*. His contribution to this series was significant and greatly valued. Mr Byron worked to a meticulous and exacting standard and will be remembered as an able and conscientious colleague. He read widely and his wit and erudition will be missed by his friends.

**Jerry Donohue** died on 13 February 1985 aged 64. Born in Sheboygan, Wisconsin, he obtained his PhD in Linus Pauling's Laboratory at CalTech in 1947 and was a member of that remarkable group of scientists who were so instrumental in the development of modern structural

chemistry. Professor Donald Voet writes that, while at CalTech, Jerry began work on the structures of hydrogen-bonded compounds, a field in which he soon became the recognized authority. After leaving CalTech in 1952, he spent six months in Sir Lawrence Bragg's laboratory in Cambridge where he shared an office with James Watson and Francis Crick who were soon to discover the structure of DNA. However, as Watson and Crick have indicated, they would not have succeeded in doing so had Jerry not pointed out that the keto tautomers of the nucleic acid bases were dominant rather than, as was then generally accepted, the enol forms. Jerry was thus an indispensable participant in a discovery that is widely acknowledged to mark the birth of molecular biology. He accepted a position in 1953 at the University of Southern California where he rose rapidly to the rank of Professor. In the years 1963–1966 he was Chairman of its Chemistry Department. While at USC Jerry began work on the two other research themes for which he is best known, the structures of sulfur-containing compounds and the structures of the elements. He accepted a chair in 1966 at the University of Pennsylvania where he remained for the rest of his extraordinarily productive career. In 1974 Jerry published his book *The Structures of The Elements*. The remarkable aspect of this work was the way he went about writing it. When he came to information he thought might be in error, he often did the research necessary to clear up the confusion in the scientific literature. Like Mendeleev, his predecessor in characterizing the elements, a significant portion of the information he quoted stemmed from his own research. He was widely known for his valuable but not always appreciated service of policing the literature. He looked for and regularly found mistakes in the work of others and, to their chagrin, often redetermined the erroneous structures. Jerry's expertise was by no means limited to structural chemistry. He was an internationally recognized expert on sea shells who regularly pub-

lished on the subject in scholarly journals. In fact he was on the editorial board of one of them, *The Veliger*, and was also widely acclaimed as a horticulturalist who specialized in bromeliads. Jerry was an award-winning teacher of very nearly magical abilities. His students almost invariably thought he was among the best and most knowledgeable instructor that they had encountered. Many credited him with motivating them to continue their studies in chemistry or biochemistry. He will be sorely missed by them as well as by his family, his many friends and his colleagues.

Dr **Peter Gay** died suddenly on 2 March 1985 aged 57. Dr S. Fleet writes that Gay entered Sidney Sussex College Cambridge as an Exhibitioner from Sir Walter St. John School, Battersea, in 1945 and graduated in physics in 1948. Three years research in the Cavendish Laboratory followed, leading to a PhD in 1951 on the development and application of X-ray microbeam techniques in the study of microstructures of deformed metals. In 1951 he joined the teaching staff of the Cambridge Department of Mineralogy and Petrology (now the Department of Earth Sciences) where he spent the rest of his career, first as a University Demonstrator and then from 1956 as a University Lecturer. At this time he began his crystallographic work on minerals and in particular the feldspars. He published many papers elucidating the complexities of their crystal structure, crystal chemistry and phase relationships. He adopted a distinctive and empirical approach, working from readily observable X-ray diffraction phenomena characteristic of different members of the plagioclase feldspar solid-solution series, to derive information about chemical compositions and thermal histories. Subsequently he carried out a wide range of X-ray studies of other minerals including rare-earth silicates, pyroxenes, olivines, hydroxides and sulphates. His reputation as an X-ray crystallographer led to his selection by

NASA as a Principal Investigator for work on lunar rocks and minerals. He was awarded the ScD degree in 1971. Throughout his time in the Department, Gay undertook a full programme of teaching work. Many generations of Cambridge undergraduates had their first introduction to Crystal Physics, Crystal Chemistry and Crystal Optics from his lectures; and his two undergraduate textbooks, *Introduction to Crystal Optics* and *The Crystalline State* were models of clear presentation showing first-class judgement in the selection and coverage of material to match the background of the students for whom they were intended. Dr Gay was elected a Fellow of Downing College in 1959 and from that time onwards played an important role in College life. He was successively Tutor, Senior Tutor and Admissions Tutor. His own wide interests (he had himself represented his College at cricket, lawn tennis, badminton and squash as an undergraduate) made him an ideal tutor, and his approachability and understanding and sympathy for undergraduates helped him as Senior Tutor to pilot the College through the difficult period of national student unrest in the late 1960's. He became Vice Master in 1982, a role for which his long experience of University and College affairs suited him ideally. Members of the College at all levels relied on him for advice; finding his judicious and yet friendly approach of great value. Notwithstanding the full part he played in College affairs, Gay maintained his active involvement in research throughout his career. Those in the field of mineralogy and crystallography in which his work was internationally known will mourn his passing at a very early age.

**James Douglas McCullough**, Professor Emeritus of Chemistry at the University of California, Los Angeles, died at home on 28 January 1985. Known to his friends as Jimmy, he was born in Oskaloosa, Iowa on 17 May 1905 and grew up in Seattle, Washington before moving to California in the 1920's. Professor Kenneth Trueblood writes that Jimmy's first regular employment was with the Standard Oil Company of California as a junior clerk, then in a service station, as he worked toward a BS in chemistry at UCLA, which had been open less than a decade when he enrolled in the late 1920's. Upon graduation in 1932, he was described by the first department chairman as 'possibly the most outstanding man we have had in the Chemistry Department since we started giving instruction' and he was immediately appointed to the teaching staff. UCLA had no graduate program at that time, but it needed help in teaching undergraduates so Jimmy taught regularly in West Los

Angeles while doing graduate work at CalTech in Pasadena, first with Arnold Beckman and later with Linus Pauling. He initially chose a graduate research project in photochemistry, an interest developed during his undergraduate years. Beckman proposed that he work on the photolysis of H<sub>2</sub>Se but, since no photochemical equipment was available for several months, suggested that in the interim he study the thermodynamic relationships among the three crystalline allotropes of elemental selenium. X-ray diffraction seemed the only conclusive way to distinguish among them so he started by taking powder, Laue and rotation photographs of various selenium specimens. He quickly became hooked, both by the beauty of the crystals and of their diffraction patterns, and never returned to the photochemical problem. After he completed his PhD in 1936, Pauling and Sturdivant helped him set up an X-ray crystallography lab at UCLA by donating a rotation camera that was no longer in use at CalTech and by giving him plans for a new X-ray tube they were having built. From these modest beginnings grew the modern departmental X-ray laboratory at UCLA that was named in his honour at a ceremony that he and many of his family, friends and former students attended in April 1983. Jimmy's first published structure was that of selenium dioxide, and he continued research on the structural chemistry of selenium and tellurium throughout his lifetime. A man of strong principle and conscience, great loyalty and warm generosity, he played a major role in establishing the tradition of excellence in teaching that the UCLA Department of Chemistry has long cherished, and in the development of its strong graduate program. He taught introductory chemistry for many years and developed many of the laboratory experiments, demonstrations and thought-provoking problems still in use today. Those who knew him well during his long career at UCLA as student and faculty member relate hilarious accounts of his ingenuity in thwarting those who tried to get by in some devious manner. Following retirement in 1971, he continued to visit the department even in recent years when his health was not good, and he was still collaborating on a research paper during his last year.

Professor **André Guinier** has been awarded the 1985 Gregori Aminoff gold medal and prize for his fundamental experimental and theoretical studies of the dispersion of X-rays with application to the study of structures of condensed systems. This, the sixth such award, was presented to Professor Guinier at the Royal Swedish Academy of Sciences meeting on 8 May. Previous recipients of

the award are Professor **P. P. Ewald** (1979), Sir **Charles Frank** (1981), Professors **G. Hägg** (1982), **J. M. Robertson** (1983) and **D. Harker** (1984).

Professor **K. Łukaszewicz** of the Institute for Low Temperature and Structure Research, Polish Academy of Sciences in Wrocław, has been elected President of the European Crystallographic Committee. Professor G. S. D. King, of the Laboratorium voor Kristallografie of the Katholieke Universiteit Leuven, has been elected Vice-President and Dr G. Filippini of the Centro di Studio per le Relazioni tra Struttura e Reattività Chimica, of the CRN in Milan, has been elected Secretary, all these appointments being until 1987.

Dr **D. J. Smith** of Arizona State University has been awarded the Charles Vernon Boys Prize of the (UK) Institute of Physics, for his achievements in commissioning the Cambridge 600 kV high-resolution electron microscope and applying it to the elucidation of the atomic structure of materials.

Dr **B. E. Warren**, retired professor of physics from the Massachusetts Institute of Technology, has been made an Honorary Member of the American Ceramic Society, in recognition of his work on the study of amorphous solids by X-ray diffraction which has been a cornerstone of glass science.

## International Union of Crystallography

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### Guidelines for Computer Program Abstracts

*Computer Program Abstracts* is a new category of the *Journal of Applied Crystallography* that 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. Either the names and addresses of those people outside the author's laboratory who have used and tested the program(s) or a source code listing and test execution should be provided. These will be sent to the referee as supporting material but will not be published or deposited in any form. An Abstract should not exceed 500 words in length. The following format should be used. Section headings which are in bold type are intended to be used as such.