when executing and a word size of 32 bits. Output is partially 132 columns wide. No other special peripherals are needed.

Program specifications: At present the program is restricted to structures containing no more than eight different atom types, each having no more than 50 positions in the asymmetric unit. The total number of output reflections is only limited by disk space. Polarization is considered to be of no influence. Much of the correctness of the intensity calculation depends on the accurate knowledge of the energy dependence of the primary-beam intensity and detector efficiency, which should be measured, although some suitable distributions are supplied. A provision is made for the user to easily update the file containing these data. No correct value for the intensity can be expected for peaks that coincide with an emission line of the X-ray tube, an escape peak, a sample fluorescence line, a sample element absorption edge or the K absorption edge of the Ge detector. Run times on a mainframe Siemens vary from 3 s for NaCl (two light atoms, eight reflections) to 68 s CPU time for α-Pu (eight heavy atoms, 234 reflections). The program, including 12 subroutines and two utilities, contains some 3200 lines of code. The data files have 14450, 430 and 280 80-character lines of data respectively.

Documentation: A detailed description of the theoretical background, the methods used to calculate the various factors, the outline of the program together with the description of input and output (illustrated with an example) can be found in a EURATOM Report (Hovestreydt, Parthé & Benedict, 1987), available from the authors, preferably UB, or the publisher.

Availability: Copies of *ENDIX* are available on request either on 9-track magnetic tape in one of the common formats (800/1600/6250 bpi, ASCII/EBCDIC code), or by network. Applications should be forwarded to the authors, preferably EH (EARN: bj02 at dkauni48).

Keywords: Simulation, energy-dispersive, powder-diffraction, synchrotron, diagram.

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Crystallographers

J. Appl. Cryst. (1988). **21**, 283–284

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).

Edward Wesley Hughes 1904–1987

Edward Wesley Hughes, Emeritus Senior Research Associate at Caltech, died on 25 December 1987, aged 83. Eddie, as we all knew him, was born in Wilkes-Barre, Pennsylvania, on 22 March 1904 and obtained a BChem in 1924 and a PhD in Chemistry at Cornell University in 1935. He then went to Caltech as a Research Fellow from 1938 to 1943. He was, during the war, a Research Chemist at Shell Development Corporation from 1943 to 1946 and then returned to Caltech where he remained for the rest of his life, apart from a sabbatical in Leeds in 1951–1952 where he met his wife. His interest in crystallography was stimulated by contact with two famous Baker lecturers, W. H. Bragg (1933–34) and Linus Pauling (1937–38). Eddie felt remarkably fortunate that, while a graduate student at Cornell, he was assigned as Bragg's assistant for a term and doubly fortunate because Linus Pauling had the astuteness to bring him back to Caltech in 1938. What a boon the Baker lectureships are!

Eddie will be chiefly remembered as the person who introduced the least-squares method of refinement to crystallographers. This method is now used routinely because high-speed computers are now available to carry out the tedious tasks involved. Hughes was working on the crystal structure of melamine in 1941 and attempted to adjust the approximate atomic coordinates by a least-squares refinement in two dimensions. It took him two eight-hour days to set up the 105 linear observational equations (from 105 measured reflections) with 18 unknowns (two parameters per atom). Since no computer was available to him he used some mechanical bookkeeping equipment and his calculations took eight hours. The method was then applied to methylammonium chloride. Eddie introduced the paper on melamine with the words: 'In the trial and error method one makes small adjustments of the parameters, chosen in such a way as to improve as many of the outstanding discrepancies as possible and then recalculates all the Fs. The process is repeated until the best possible agreement is thought to have been obtained. However, to make all possible combinations of small displacements in a multiparameter structure and show that the agreement is best for the parameters proposed would seem to be an impossible task. The situation seems to call for the use of the method of least squares.'

Eddie knew that his work was important. He wrote, with amusement, in 1978, 'Some time ago I had a letter from the Institute for Scientific Information, publishers of the "Citation Index", stating that the melamine paper had been cited nearly 600 times since 1961 and asking me to write a "Citation Classic" comment for the "Current Contents." Upon investigation I found they had classified the paper as "Biological!" Getting it reclassified took some time.'

Eddie was President of the American Crystallographic Association in 1954. He also served in place of Bill Lipscomb at the Pasadena meeting in 1955 when Lipscomb, who was on sabbatical, 'drove to the harbor at Le Havre to find no boat at all. There was a strike.' Lipscomb continued 'I missed the 1955 meeting in Pasadena where my good friend and first teacher of crystallography, E. W. Hughes, filled in my duties.' Eddie also served as a Co-editor of *Acta Crystallographica* from 1956 until 1963.

He also did much early work on direct methods and on peptide structure. To the end he continued his great interest in crystallography and helped with the book *Patterson and Pattersons*, insisting that a paper in Pepinsky's book be reproduced there, writing an article that put it in context and including a humorous note entitled 'How I first learned of the Patterson function and Bragg's second law'.

To his wife, Ruth, we extend our deep sympathy. Crystallography has lost one of its pioneers.

J. P. GLUSKER

H. P. Rooksby 1906–1986

It is extraordinary that most of us seem not to have heard of the death, in retirement, of H. P. Rooksby on 12 February 1986. He had been a pioneer of the applications of X-ray powder diffraction in industry, and a prominent and active member of the British Institute of Physics and the International Union of Crystallography.

Harold Percy Rooksby was born on 8 September 1906 and educated at Harrow County School in the northwest outskirts of London. He entered the nearby Research Laboratories of The General Electric Company at Wembley in 1924 as their first student assistant, taking a London University BSc General Honours Degree in Science by part-time study at the then Sir John Cass College. That became a good route into industry in those days and Rooksby was always to be a little sceptical about the value in industry of the too academic education, especially the full-time PhD that gave no initiation into the scientific world outside.

I believe that X-ray diffraction studies of materials were started at Wembley in the 1920s by Dr Goucher, in connection with tungsten lamp filaments. Certainly some of Rooksby's earliest publications were, with the metallurgist C. J. Smithells, on the reactions of incandescent tungsten with nitrogen and water vapour, and on the deformation of tungsten crystals by rolling and drawing.

In the 1920s and 1930s, though maintaining an active interest in tungsten, Rooksby also made important contributions to the study of clay minerals and the changes occurring in the manufacture of refractories used as linings in glass-making furnaces. And with J. T. Randall, also at the GEC laboratories at that time, he worked on the structural nature of glasses, especially selenium ruby and opal glasses.

There was much interest in the 1930s in the nature of thermionic cathode coatings and it was this work that under Rooksby led to the discovery of the cubic or pseudo-cubic R_3MX_6 class of alkaline-earth-metal oxides of the cryolite type but with valencies doubled.

In the early years of the war L. A. Thomas had joined Rooksby. But the need for synthetic quartz became urgent since natural supplies were cut off, and Thomas was deployed to develop methods for making large crystals of quartz and other piezoelectric materials. Graduating from King's College at that time, I was sent to GEC by C. P. Snow in his war-time role as Head of the Science Section of the Government Central Register's work in directing scientific manpower. The Director of the laboratories at Wembley, C. C. Paterson, decided that I should fill the gap with Rooksby who, like most others there, was then engaged in work of national importance.

Rooksby's stamina and enthusiasm for work were prodigious throughout the sixteen years that I worked with him. In the daily life of the laboratory he would not tolerate a powder camera standing idle. After a camera exposure an assistant or we ourselves had to unload the camera but not develop the film until the specimen had been changed, the camera reloaded and the next exposure started. Not only was there a large amount of analytical service work but there were numerous lines of self-motivated research which often stemmed from the service work. He was a great believer in cross-fertilization of ideas, and with good reason, for there were many examples of its value to the company. In all this work he received much encouragement from J. W. Ryde who, during my time at the laboratories, held the overall position of Chief Scientist.

Rooksby had the knowledge and intuitive skill to get to the essentials of an analytical problem and solve it where others would hardly know where to start, whether it be corrosion, stones in glass, faulty deep-drawing of metal sheet, luminescent materials development, electrodeposits, to name a few examples that spring to mind.

During the years that I worked with him his major contributions were so diverse and numerous that justice cannot be done to them here. They included the formidable detailing of the Al–O and Fe–O systems, and the discovery of small structural temperature-sensitive deformations in some transition-metal oxides which pre-dated the discovery of their antiferromagnetic properties.

With young colleagues whom he recruited in those years he also elucidated (a favourite word of his), from powder photographs, the structures of compounds of alkaline-earth oxides with tantalum and niobium, the relations between the structures of phases in the Pt–Mo system, and the occurrence of intermetallic phases in commercial beryllium. His long-standing interest and experience of studying imperfections in large single crystals paved the way to the expansion of this field by the team at GEC in the years after I left.

In Rooksby's hands and under his guidance, powder photographs were routinely obtained of a quality that was the envy of all. The same can be said of his skill in interpreting powder patterns, particularly in sorting out components in a mixture and in the wielding of Hull–Davey charts. His great knowledge of inorganic chemistry and metallurgy bore fruit in the exploration of new compounds prepared by firing dry mixtures in small platinum boats after much grinding with pestle and mortar.

The X-ray laboratory at GEC gained international recognition and respect early on and Rooksby was approached for help by workers in many fields in the UK and abroad. One example that pleased him especially was his study, in collaboration with W. E. S. Turner, of the opalizing agents in ancient glass relics, including minute fragments from the Portland Vase in the British Museum. His interest in ceramics in general spanned his whole career and from a year before his retirement from GEC in 1971 until 1974 he was External Professor within the Department of Ceramics at Leeds University.

In addition to writing a vast number of papers (always drafted with pencil and rubber incredibly clearly both in content and legibility) for a wide variety of journals, and the thousands of internal reports, Rooksby found time to give lectures about his work and the X-ray apparatus and techniques he developed to the professional societies concerned with the many fields to which he contributed. His contributions to books included co-editorship of *X-ray Diffraction by Polycrystalline Materials* (Institute of Physics, 1955). At various times he was a member of the Royal Society's British National Committee for Crystallography, Chairman of the Clay Minerals Group of the Mineralogical Society and member of its Council, and member of the Council of the Basic Science Section of the British Ceramic Society. He was a prominent member of the Institute of Physics, served on its Board and numerous committees, and did much to revive the Institute after the war. From 1954 to 1957 he was Chairman of the X-ray Analysis Group and in 1969 was awarded the Institute's Charles Vernon Boys Prize for his work in X-ray crystallography.

Widely liked and respected, Rooksby was prominent among those who worked for the formation of the International Union of Crystallography, served on its Apparatus Commission from 1948 to 1957 and the Data Commission from 1957 to 1963 and was an untiring and meticulous co-editor of the *Journal of Applied Crystallography* from its foundation in 1967 until 1972.

I have seldom met anyone to equal Rooksby's total integrity in all his dealings.

Rooksby's family was very important to him. That was where he found relaxation, and in music. He was an accomplished pianist and a keen concert and opera goer.

An exceptionally talented man, he was (alas) formally less recognized by the scientific community, for example the Royal Society, for his outstanding skills and wide-ranging achievements than some whose contributions to science may perhaps have been deeper though resulting – by who can tell to what extent – from having certainly been narrower.

E. G. STEWARD

Dr **Isabella Karle**, Laboratory for The Structure of Matter, US Naval Research Laboratory, Washington, DC, USA, has been awarded the 1988 Gregori Aminoff gold medal and prize for her eminent crystallographic studies of complicated natural products. This, the ninth such award, was presented to Dr Karle at the Royal Swedish Academy of Sciences meeting on 27th April 1988.

Previous recipients of the award are Professor P. P. Ewald (1979), Sir Charles Frank (1981), Professors G. Hägg (1982), J. M. Robertson (1983), D. Harker (1984), A. Guinier (1985), E. F. Bertaut (1986) and O. Kratky (1987).