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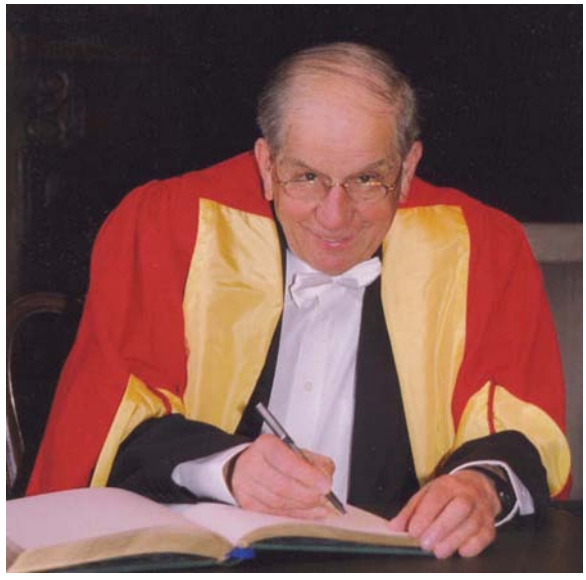
Durward William John Cruickshank (1924–2007)



Crystallography in general and the International Union of Crystallography (IUCr) in particular owe much to Professor Durward Cruickshank FRS, the eminent crystallographer and structural chemist of high mathematical ability, who died peacefully on 13 July 2007 in his Alderley Edge home near Manchester. He 'retired' as Professor of Theoretical Chemistry at the University of Manchester Institute of Science and Technology (UMIST) in 1983 but continued to collaborate very actively with one of us until his death, with his last paper appearing in *Acta Cryst*. (2007), D**63**, 906–922.

Durward Cruickshank transformed the precision of molecular structure determination in three dimensions by X-ray diffraction with research publications that span 60 years and that directly influence at least some 450000 chemical structures, the number currently held in the Cambridge Structural Database alone. Research on the precision and refinement of proteins dominated his attention throughout his last decade, and the Cruickshank Diffraction Precision Index (DPI), an indicator of the precision of a protein structure, is now generally included regularly both in published protein three-dimensional structures as important information and in depositions at the Protein Data Bank (PDB) files.

His first paper in *Acta Cryst*., on 'The accuracy of electron-density maps in X-ray structure analysis', published with Gordon Cox in Volume 1, pp. 92–93, proved to be an indicator of one of his major future interests. His concern for accuracy led him to a critical examination of many crystal structure determinations from which further important information could be retrieved. In consequence, applying more powerful correction, refinement and analysis techniques, he was able to use previously published experimental data to extract higher level information from over 20 structures, including naphthalene, anthracene, pentaerythritol, allokainic acid and [18]-annulene. In the latter molecule, for

example, he and his coauthors were able to show that the difference between the 12 inner and 6 outer C—C bond lengths, deemed in previous work to be of high significance, was in fact due to partial but overlooked disorder at the 80 K measurement temperature, hence that the $4n + 2$ π-electron [18]-annulene molecule is indeed aromatic, as expected. He also successfully solved and refined a number of inorganic structures including Na_2GeO_3, $(NH_4)_2CrO_4$ and α-$Na_2Si_2O_3$ in addition to several others by electron diffraction in the gas phase.

Another of Cruickshank's seminal contributions to the increasing power of X-ray analysis concerned benzene, the structure of which was published in 1958. John Robertson, a former colleague at Leeds University who died 2003, wrote 'A really good electron density map was obtained in Leeds that confirmed the planarity of the ring and allowed the carbon–carbon (C—C) bond length to be determined with good precision. However, this result revealed a problem and Cruickshank's solution to it resulted in a major theoretical advance. The crystal structure analysis gave C—C bonds that were shorter than the spectroscopic measurements with a discrepancy that exceeded the estimated limits of error. It seemed a nasty problem but the embarrassment vanished when he realised that molecular libration was the cause of this apparent shortening'. He was thus able to add one more new and valuable mathematical tool to the crystallographer's kit. He was also able, that same year, to relate the molecular amplitudes of crystalline hydrocarbons at different temperatures to their entropy, which he showed were comparable to the values derived calorimetrically. In his final paper on a very different topic, he provides definitive light on the factors required to determine quantitatively the protonation states in proteins.

Cruickshank was an early pioneer in the use of digital computers. He would travel from Leeds to Manchester, where Ferranti Ltd had commercialized the first stored-program digital computer, to work all night running crystallographic computations. Next day, back in Leeds, he would scrutinize the results in preparation for further computational analysis that night. He attended the 1950 Cambridge Summer School on Programme Design for Automatic Digital Computing Machines, which was amongst the world's first summer schools on electronic computing and which introduced him to the principles of computer programming, machine order codes and binary arithmetic.

The 'state of the art' in crystal structure refinement during the late 'forties and early 'fifties depended on the estimated relative intensities of the diffraction amplitudes as captured on X-ray film. Such visual estimates, often made by use of multiple film packs for Cu $K\alpha$ or packs interleaved with absorbing material for Mo $K\alpha$ radiation, provided the most common means by which a trial structure could be 'refined', either by successive Fourier series or, less commonly, by least squares. Computations generally relied on hand-operated mechanical calculators, usually Marchant, Monroe or Facit machines equivalent in size and as noisy as standard mechanical typewriters. Fourier series evaluation was tedious but feasible with Beevers & Lipson's $A \sin f(x)$ strips available in nearly all crystallographic laboratories. In stark contrast to this prevailing technique, Cruickshank's early introduction to high-speed digital computers and their successful initial use by several crystallographers in evaluating both difference Fourier series and three-dimensional least-squares refinements inspired him to take a more general approach. His masterly series of three papers in 1956 provided the formalisms by which anisotropic rigid-body translational and rotational thermal vibration molecular tensors, the anisotropic thermal motion of atoms in crystals, and the variation of these amplitudes with temperature could be determined, and each became widely used.

In his 'retirement', Durward joined with John Helliwell who, together with Keith Moffat, Marjorie Harding, their students and postdocs, along with Daresbury Laboratory software specialists Mike Elder, Pella Machin, John Campbell and colleagues, were engaged in developing the synchrotron Laue method. Mike and Pella died tragically in a climbing accident in Scotland on 7 March 1987. Moffat had been the overall initial investigator with Don Bilderback and Dolothea Szebenyi at the Cornell High Energy Synchrotron Source (*Science*, 1984). Louise Johnson, Janos Hajdu and colleagues made important seminal contributions to time-resolved enzyme crystallography using monochromatic and then Laue methods notably at the Daresbury synchrotron. Durward brought mathematical rigour to efforts aimed at defining the multiplicity and angular distribution of reflections in Laue patterns, especially over wide wavelength bandpass ranges from the zero, *i.e.* monochromatic, case to the infinite fully polychromatic limit. The theoretical analyses, backed up by computer simulations, showed that Sir Lawrence Bragg's views of the difficulties of using the Laue method were unduly pessimistic. Harnessing the gnomonic projection was a particular initiative. A special highlight of this period was its direct connection with Linus Pauling's use of the Laue method for analysing numerous small-molecule structures. The emphasis on the important relevance of white X-ray and neutron sources attracted the interest of the wider crystallographic community and related initiatives unfolded in instrumentation and applications. The latter included sub-nanosecond time-resolved diffraction studies of proteins, led by Keith Moffat, at the European Synchrotron Research Facility and neutron Laue diffraction of small and large (*i.e* protein) molecules at the Institut Laue Langevin. David Blow's important reformulation of the DPI [*Acta Cryst.* (2002), D**58**, 792–797], casting it in terms of experimental resolution parameters that vary to the power 5/2 and approximately linearly with the completeness of the diffraction data, was very pleasing to Durward during his last decade.

Thus, all the hallmarks of his style that were evident at his outset carried through to his 'retirement', and resulted in 80 papers published in *Acta Crystallographica*. In a 2002 personal collection of his own science publications, Durward defined his categories of scientific interest as follows: (i) crystallographic refinement theory, errors, computation, vibrational analysis and protein structure precision, with 31 articles published; (ii) vibrations in crystals, 9 publications; (iii) reviews of structural chemistry, 5 articles; (iv) crystal structure determinations, 18 publications, (v) tetrahedral oxyanion and related compound crystal structures, 29 articles; (vi) gas phase electron diffraction studies, 14 papers; (vii) semi-empirical and *ab initio* quantum chemistry, mostly in chemical journals but one in *Z. Kristallogr.*, 20 articles; (viii) Laue diffraction and synchrotron protein crystallography, 9 articles; (ix) history and biography, 6 articles. A Web of Science check in August 2007 reveals a citation impact involving approximately 9000 citations overall, an '*h* index' of 44 and an average citation per publication of 64. His top three most cited publications have more than 500 citations each, and are (i) 'The accuracy of electron density maps with special reference to dibenzyl' [*Acta Cryst.* (1949), **2**, 65–82]; (ii) 'The analysis of anisotropic thermal motion in crystals' [*Acta Cryst.* (1956), **9**, 754–756] and (iii) with E. G. Cox and J. A. S. Smith, 'The crystal structure of benzene at −3°C' [*Proc. R. Soc. London Ser. A* (1958), **247**, 1–21]. Ten of his publications have over 200 citations each. His most prolific publication year was 1964, with 14 papers; 30% of his publications have him as their sole author.

His career started at Loughborough College, now Loughborough University, as an engineering student. He received an external degree from London

University in 1944, then worked until 1946 for the Admiralty on Naval Operations Research. He subsequently studied mathematics at Cambridge, 'learning at the feet of Bondi, Hoyle, Boys and Dirac' as he would put it, and was successively awarded his BA (1949), MA (1954) and finally DSc (1961). His entry into the world of crystal structures began in 1946 when he joined E. G. Cox's chemical crystallography group at Leeds University; he later acknowledged Cox as a great and encouraging influence on his career. Durward presented his PhD thesis, entitled 'A theoretical study of some of the interpretational methods used in crystal structure analysis' to the University of Leeds in 1952.

His first academic appointment, as Lecturer in Mathematical Chemistry at the University of Leeds, was in September 1950. He became Joseph Black Professor of Chemistry at Glasgow University from 1962 to 1967. In furtherance of his wife Marjorie's career, it became necessary to return to the Manchester region and he was invited to UMIST in 1967 as Professor of Theoretical Chemistry. Upon retirement in 1983, he became Emeritus Professor at UMIST and, latterly, at the University of Manchester. He became Visiting Honorary Scientist at the SERC Daresbury Laboratory in 1983 and Visiting Honorary Professor at the University of York in 1985. He was appointed Deputy Principal of UMIST, 1971–1972, made a Companion of UMIST in 1992, and awarded an Honorary Degree by UMIST in 2004. He also received an Honorary DSc from Glasgow University in 2004, on which occasion the photograph above was taken, and which named its Diffraction Laboratories after him.

His major contributions were formally recognized by the Royal Society through his election as a Fellow in 1979. He initiated a Royal Society Discussion Meeting held in 1992 on 'Time-Resolved Macromolecular Crystallography' whose proceedings were published, edited by Durward, John Helliwell and Louise Johnson. Durward's achievements were recognized also by other Prizes and Awards. Notably, he won the Chemical Society (now Royal Society of Chemistry) Award for Structural Chemistry in 1978 and the first Dorothy Hodgkin Prize of the British Crystallographic Association (BCA) in 1991. He delivered the prestigious Bragg Lecture, a large fraction of which was a memorial by Durward to Sir Gordon Cox, at Leeds University during the annual BCA Conference of 1997 and to the public at The Royal Institution in London, the latter where both Braggs, father and son, had worked. The Braggs are still the only father and son to be jointly awarded a Nobel Prize (in Physics, 1915, 'for their services in the analysis of crystal structure by means of X-rays').

Cruickshank devoted much effort to the IUCr. He was elected IUCr Treasurer in 1966 at the General Assembly and Congress in Moscow for the period 1966 to 1969. The office of Treasurer was combined with that of IUCr General Secretary at the General Assembly and Congress in Stony Brook, NY, in 1969, to which joint office he was elected to serve from 1969 to 1972. Under his guidance, the total financial assets of the IUCr grew steadily over his two terms to double their value until his final year, when the rising costs of publication and editing and a small erosion of the subscription base resulted in a small loss. The two offices together demanded and received an unusually high level of time and thought. His sage advice was subsequently sought by the IUCr on a variety of occasions. Cruickshank also served as an Editor, with H. J. Juretschke and Norio Kato, of the 1992 IUCr Memorial Volume *P. P. Ewald and his Dynamical Theory of X-ray Diffraction* commemorating Paul Ewald, the founding father of the IUCr. Cruickshank's first contact with the international crystallographic community was at the small symposium held in 1948 in Leeds that attracted many

participants from the X-ray Analysis Group conference held some days previously in London and which led to the formation of the IUCr; he is visible in the photograph in *Acta Cryst.* (1989), A**45**, 585.

Cruickshank also served the British Crystallographic Association (BCA) as Vice President 1983–1985, was admitted an Honorary Member of the BCA in 2003, and continued to contribute enthusiastically to BCA activities until his death.

Durward Cruickshank was always upbeat, kind and helpful, courteous and gracious. He inspired the love and affection of family and colleagues, was utterly trustworthy and sincere, and could always be turned to for advice. His deep insight into science extended to its history. He liked to emphasize, as his 80th birthday celebration notes show, that there had been relatively few years over which modern science had arisen, *i.e.* (his examples) between Newton's theory of gravitation, Dalton's atomic theory and Watson and Crick's DNA double helix model. Newton, he also noted, was the first person with the mathematical capability of comprehending space flight. Looking to future major advances, he highlighted molecular biology and drug discovery, areas which he judged were still in their infancy. He could also be quite firm. At the BCA's AGM in York in 2003, for example, the question of introducing the category of 'Fellow of the BCA' arose. Durward spoke successfully against the motion, saying that such a hierarchical membership structure would put the egalitarian nature of crystallography in jeopardy if introduced.

He was a keen golfer and an enthusiastic member of the Manchester Literary and Philosophical Society. His interest in his family tree, renewed in retirement, led him to visit the extensive genealogical archives in Salt Lake City. He then became interested in retracing the Arctic routes of a 19th century whaling ancestor, also in visiting the Antarctic where he noted numerous islands and other features that were named after crystallographers by the responsible authority, primarily to commemorate prominent pioneers in techniques that elucidated Antarctic problems, particularly the structure of ice.

Durward's wife Marjorie predeceased him and he is survived by a son and a daughter and five beloved grandchildren. He died of cancer and will be sadly missed by the whole community.

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