

## Frank H. Allen (1944–2014)



Frank Allen died at the age of 70 on 10 November 2014. He leaves his wife Sandy, sons Andy and Stuart, and granddaughters Isabel and Eleanor. Frank and Sandy's eldest son, Ashley, was tragically killed in a road accident in 1988.

Frank was born in Reading and raised in Pangbourne, a village on the River Thames. He gained a First in chemistry and a PhD in crystallography at Imperial College, London, the latter under the supervision of Don Rogers. His first structures were of terpenoid derivatives, done the hard way with intensity measurement by eye (Sandy helped). He moved to Vancouver in 1968 to take up a NRC post-doctoral fellowship in Jim Trotter's group. One of the structures he and Jim solved was that of the notorious drug thalidomide. To everyone's great good fortune, Olga Kennard recruited Frank in 1970 to work for the fledgling Cambridge Crystallographic Data Centre. He remained there for the rest of his life, becoming Scientific Director and then Executive Director before retiring in 2008 to take on the role of Emeritus Research Fellow.

Searching the Cambridge Structural Database for 'F. H. Allen' yields 69 hits, but Frank drifted away from the diffractometer during his early years at Cambridge and turned to the computer. At a time when 'data' was not as fashionable as it is now, he worked with Sam Motherwell and others to write the programs that turned the CSD from a data library into a scientific instrument. It is easy to forget how innovative that software was. The CCDC was one of the pioneers of techniques such as chemical-name searching, two-dimensional and three-dimensional substructure searching, and structure- and substructure-sketching. Frank was also one of the first to use the CSD as a research tool in its own right, beginning with a study of the geometries of cyclopropane derivatives. He was one of the lead authors (Guy Orpen being the other) of two massive compilations of average bond lengths, which have now attracted some ten thousand citations. At the other extreme, his tongue-in-cheek letter on 'Retino-rectal connexions' has never been cited – until now: Allen, F. H. & Isaacs, N. W. (1971), *Nature*, **234**, 426.

Frank was a sportsman. He played cricket for his county at school level and opened the bowling for a strong University Chemical Laboratory team. A desire to play cricket was one of his stated reasons for wanting a return home from Canada! He was a mainstay of

Sawston hockey club, his CCDC colleague John Rodgers being a teammate there for a time. He sustained frequent injuries, including a broken nose, as is always a possibility when several men in close proximity to one another wave heavy sticks and propel hard spheres at high speed. In addition to these physical injuries, Frank had a lifetime of mental trauma as a long-suffering fan of Reading FC.

While Olga Kennard was shrewd and determined in attracting grants to support the ongoing maintenance of the CSD, it was always a concern that the next grant application might fail, leaving the CCDC in crisis. In the mid-1980s, as industrial interest in the CSD grew, the possibility emerged that the centre might become self-financing, supported by user subscriptions. The die was cast in 1987: the CCDC became an independent, not-for-profit company with its own new building. Frank was by then Principal Scientist in charge of R&D. He was convinced that CCDC's funding policy was the right one. It attracted some criticism because the CSD was not 'free' like the Protein Data Bank (in other words, it was not directly funded by taxpayers). But he argued that the CCDC model gave more stability and made it easier to draw up and execute long-term plans. He remained of this view to the end of his life, by which time the CCDC was in its fiftieth year.

Frank was the vigorous editor of *Acta Crystallographica Section B* from 1993 to 2002, highly valued by his co-editors for the astute advice he gave on difficult cases. He was also on the editorial boards of several other journals. Even more important to crystallographic publishing was his work with Syd Hall and David Brown on the crystallographic information file. Its dictionary-based format, well ahead of its time, allows exchange of crystallographic information in a standard, extensible and information-rich manner. Frank took responsibility for selecting and defining the 423 data items in the initial CIF dictionary, critical work that exploited his career-long interest in the management of crystallographic data. It is no overstatement that maintenance of the CSD would have become impossible without the CIF or something very like it.

An equable man, Frank could nevertheless get annoyed: for example, with the editors of two journals who refused to accept CSD-based research because 'reprocessing existing data isn't novel'. (Jack Dunitz pointed out that, on that basis, Mendeleev would not have got the Periodic Table published.) Annoyed, too, with those who thought the CSD could be maintained by a part-time post-doc and some clever software. The CCDC had very clever software – Frank wrote some of it – but he knew from experience that a great deal of manual effort was required to maintain a comprehensive database of high accuracy. From its beginning, Olga and David Watson had set high standards for the CSD. Frank shared and promulgated this view, knowing that it was essential if the database were to be suitable for top-quality research.

As Frank grew older and less able to terrorize opening batsmen and hockey goalkeepers, he took to more sedentary pastimes. He was very active in village life and served on the Governing Body of Impington Village College for many years, as its Chair from 1995 to 2001. With Sandy, he became quite expert at ornithology.

He won the RSC prize for Structural Chemistry in 1994 and the ACS Herman Skolnik Award in 2003, probably the highest accolade that can be awarded to a chemical information scientist. He was a Visiting Professor of Structural Chemistry at the University of Bristol, was on the International Advisory Board of the PDB (RCSB), a member of many commissions and committees of the IUCr, on the Council of the European Crystallographic Association, and Vice President of the British Crystallographic Association from 1997 to 2001. He was on the Board of Lhasa Limited, another not-for-profit scientific institution. He gave countless invited lectures and played his part as a conference organiser, including co-directing (with Judith Howard) the 1998 Erice School of Crystallography.

Frank was warm hearted, relaxed, totally reliable, sometimes emotional, always caring. He was naturally and unconsciously egalitarian. He would laugh with a visiting Nobel laureate and then walk over to the chemistry lab for lunch and make the same jokes to the young man at the sandwich bar. He treated everyone the same because it never occurred to him to do otherwise. Most of all, he loved to talk to his students, some based at the CCDC, others in the labs of long-term collaborators such as Judith Howard and Paul Raithby. He was passionate about research, producing a steady output of influential papers – over 200 in total – on a range of subjects: intermolecular interactions, structure correlation, conformational analysis, data-mining techniques, molecular recognition and the application of the CSD to chemical education. He wrote several highly cited reviews of the CSD, including one in a 2002 joint *Acta B/Acta D* special issue on databases that he put together with Jenny Glusker.

Frank, tunelessly whistling, coffee mug and notebook in hand, would wander into the CCDC seminar room where several people and an empty seat waited to start a meeting. He habitually met deadlines and was normally punctual, but always managed to be a little late for these meetings. Occasionally, this would elicit a moan from his grumpiest colleague. Frank would nod apologetically but both he and his admonisher knew that nothing would change. Now something has and there will be an empty seat at the CCDC for ever.

### Robin Taylor

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