crystallographers

JOURNAL OF APPLIED CRYSTALLOGRAPHY

Volume 50 | **Part 2** | April 2017 | Pages 666-667
https://doi.org/10.1107/S1600576717002862
Cited by 3

ISSN: 1600-5767

Howard D. Flack (1943–2017)

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Keywords: obituary.

What is it about?

Howard D Flack revolutionised the determination of the absolute structure of crystalline materials by X-ray diffraction, and hence the absolute configuration of crystalline molecular materials. The significance of his insight was such that a parameter quantifying absolute structure very quickly became universally known as 'The Flack Parameter'. The sudden death of Howard D Flack in the spring of 2017 after a short illness was a shock to the crystallographic community. This obituary outlines some of his other major contributions to crystallography.

Why is it important?

The importance of The Flack Parameter over shaddowed his many other contributions to X-ray crystallography. In particular, his very early enthusiasm for sharing experience and information by electronic means played an important role in the advancement of crystallography (http://www.iucr.org /people/crystallographers/flack_ep).

Howard Flack died quite suddenly on Thursday 2 February 2017 from pneumonia contracted during treatment for recently diagnosed mesothelioma.

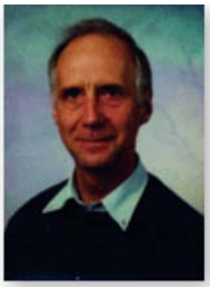

Figure 1
Howard D. Flack (1943–2017).

There can be no doubt that the direction of his life-long research interests was formed while he was studying under Kathleen Lonsdale at University College London. His PhD project, *Studies of disorder in anthrone and in mixed crystals of anthrone–anthraquinone*, exposed him to the need for a deep understanding of the diffraction process and its mathematical treatment. The introduction to his paper *Calculation of dimensions of ordered regions in triclinic and monclinic pseudosymmetric crystals from the intensity of diffuse scattering* (Flack, 1970) reveals a train of thought that was to reemerge a decade later in his work on absolute structure determination, and his desire to provide a detailed mathematical explanation of physical processes.

After gaining his PhD, Howard moved to Cambridge (England) to work as Research Assistant in Surface Physics in The Cavendish Laboratory. It was at this time, 1971, that he started walking out with a Swiss girl, Evelyne, who had been sent to Cambridge by her employer in order to improve her English. Who better to teach her the Queen's English than Howard? It had been his intention to continue his studies in one of the Commonwealth countries, perhaps Australia or Canada, when by happy coincidence an opportunity opened to work with Erwin Parthé as Maître-assistant in the Laboratoire de Cristallographie at the University of Geneva, Switzerland. Howard moved to Switzerland in January 1972, and by the summer he and Evelyne were married. His arrival in Geneva coincided with a new start of crystallography in western Switzerland. Parthé's interdisciplinary Crystallography Laboratory was a new central facility serving the Faculty of Science of the university. A year later, an Institute of Crystallography was newly created at the University of Lausanne, while the Universities of Neuchâtel and Basel gradually developed structure determination services. Howard generously collaborated with all these start-ups and was involved in their success. For many years, the *X-RAY76* program system (Stewart, 1976) was developed jointly at Geneva and Lausanne. Howard contributed code to *X-RAY76* until its slow demise in the 1990s. Except for short periods spent elsewhere, he was to remain in Geneva until his retirement. He was employed as part of the technical staff, but his brilliance, wit, courage, and generous unselfish services to the Swiss and international crystallographic communities outshone his humble professional position.

From 1981 to 1990 he was secretary of the Swiss Society of Crystallography. His work with Parthé on highly absorbing crystals of $SmAu_6$ ($\mu R = 5.9$) made him realize that the approximations made in the absorption corrections of North *et al.* (1968) and Kopfmann & Huber (1968) were inappropriate. The problem was resolved by representing the absorption profile as a Fourier series, an idea which has since been developed to use spherical harmonics. This and all subsequent non-analytical absorption corrections essentially reduce the sample to a sphere, which will have an effect which cannot be corrected for experimentally. Alternative suggestions for dealing with this residual error are given in the paper *Automatic absorption correction using intensity measurements from azimuthal scans* (Flack, 1974). The computations were implemented in the computer program *CAMEL JOCKEY*, an early example of his anarchic sense of humour. The absorption algorithm was extended and appeared as the program *CAMEL JOCKEY WITH THREE HUMPS*, also compatible with the *X-RAY76* software system.

Howard continued to have a deep interest in the problems associated with obtaining the best quality experimental data, especially as a result of his growing interest in the determination of absolute structure by X-ray diffraction. Prior to Rogers' introduction of his η refinement, absolute structure estimation had depended on the careful examination of a small number of carefully measured reflections. Rogers' idea, related to earlier attempts to experimentally determine anomalous (resonant) scattering factors, introduced a refinable parameter into the main structure refinement (Rogers, 1981). Howard realized that the η parameter became singular midway between its extreme theoretical values, and that the problem could be better posed by regarding the sample as a twin containing x and $1 - x$ twin fractions of the two enantiomers (with x a refinable parameter) (Flack, 1983) in an analogous way to his 1970 treatment of disorder. This elegant solution to the problem of absolute structure determination proved to be enormously popular, with the twin fraction x quickly being called the Flack parameter. Technical difficulties with its robust implementation were eventually resolved through practical experience and a reorganization of the algorithm (Parsons *et al.*, 2013).

Having opened Pandora's box, Howard was even more in demand as a speaker and authority on absolute structure determination. Since he was a good lecturer and he enjoyed direct interaction with other crystallographers, he accepted invitations as often as he could. He particularly enjoyed being with students and would take every opportunity to get them to talk about their own work. However, it sometimes seemed that he was disappointed that his work on chirality overshadowed other projects. He was saddened that concepts in the paper *On the definition and practical use of crystal-based azimuthal angles* (Schwarzenbach & Flack, 1989) were not widely adopted as a mechanism for sharing diffraction data. The paper *Merohedral twin interpretation spreadsheet, including command lines for SHELXL* (Flack & Wörle, 2013) seems to have attracted less attention than it deserves. As we noted earlier, Howard was always keen to provide a sound mathematical background to his ideas, and some of this has been published in papers on the intensity statistics of Friedel pairs (*e.g.* Shmueli & Flack, 2009), though these papers too have not attracted a large audience.

Howard saw, very early on, the contribution modern computer-based communication systems could make to the dissemination of crystallography. His contributions to the digital publication of IUCr material, to the structured archiving of data and to the crystallographic community warrant their own description and are detailed at http://www.iucr.org/people/crystallographers/flack_ep.

Howard's knowledge of the early crystallographic literature repeatedly led him to reinvestigate old problems. His very recent paper on the Patterson function (Flack, 2015) returns to the use of the resonant difference Patterson function, something he had briefly visited in *Practical applications of averages and differences of Friedel opposites* (Flack *et al.*, 2011). In that paper he wrote `The Fourier transform of *D* has never been used in structure solution but a simulation by Woolfson (see *International Tables for Crystallography*, Vol. B, *Reciprocal Space*, ch. 2.3, pp. 235–263) confirms that it has interesting properties.' Naturally, Howard could not leave anything with `interesting properties' alone for long.

Howard was in the middle of active collaborations when he fell ill, but he was determined not to let his condition interfere with his dreams. Just a few weeks before he died, he had drastically reorganized a draft manuscript and changed the prosaic title to `*HUG and SQUEEZE*:' *etc.* One could not help remembering the *CAMEL JOCKEY*, with or without the humps.

With Howard, we have not only lost an influential scientist and teacher, we have also lost a widely interested and cultured person. He was well read and familiar with, for example, Tristram Shandy as well as with the lore of Middle-earth. He loved music, opera and concerts. With Evelyne he assembled and restored an impressive collection of vintage toy trains and railway accessories produced by the British firm Hornby between 1920 and 1963. He was a good down-hill skier and horseback rider. And he was a wonderful companion with a fresh humour, funny and fair. He is survived by his wife Evelyne, his son Patrick and his daughter Christine.

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ISSN: 1600-5767