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Editorial

The Publications of Howard Flack (1943–2017)

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Abstract: Howard Flack was a driving force in the development of modern crystallography. Today "the Flack parameter" has entered into the common parlance of crystallography but his influence was far wider. This article provides an overview of his scientific output and a full bibliography.

Keywords: crystallography; Howard Flack

1. Introduction

This short article provides a bibliography of the publications of Howard Flack. This is not the place to provide an appreciation of the contributions of this outstanding crystallographer, but rather to provide a convenient point of reference for his life's work. Excellent overviews of the contribution of Howard Flack are to be found in this volume and elsewhere [1,2]. The short accompanying text groups the output by theme. Published conference abstracts are included for completeness. The bibliography is as complete as I have been able to compile, but as always, the author is responsible for any omissions (and apologizes for any such omissions in advance).

2. The Scientific Output

2.1. Properties and Structure of Solid State Inorganic Materials

A number of publications or conference presentations appeared concerning the crystal, mechanical and electronic properties of solid state materials such as MoS_2 [3], $NbSe_2$ [3], HfS_2 [3], $SmAu_6$ [4], Ga_xSe_{1-x} [5], TiC [6,7], TiN [6,7], VN [8,9], Al_2O_3 [10], $Mo_4Ru_2Se_8$ [11], $Mo_{1.5}Re_{4.5}Se_8$ [11], MNi_3Al_9 (M = Y, Gd, Dy, Er) [12], TiGePt [13], Nb_3Si [14] and Nb_3As [14]. Another reported structure of an inorganic material is the "simple" salt, $MgSO_3{\cdot}6H_2O$ [15]. One publication from 2003 entitled "Anti-wurtzite reoriented" [16] is noteworthy as it provides a link to the earliest studies of zinc sulfide in which the Friedel pairs were shown to have different intensities [17,18].

Two very early studies were concerned with the properties of crystalline polytetrafluoroethene [19,20].

2.2. Structural Studies on Discrete Species

Although Flack is not widely thought of as a service crystallographer, a number of small molecule structures determined by him have been reported, including $[Cl_2(SEt_2)_2Ir(\mu\text{–}Cl)_2IrCl_2(SEt_2)_2]$ [21], $[Cl_3(SEt_2)Ir(\mu\text{–}Cl)(\mu\text{–}SEt_2)IrCl_2(SEt_2)_2]$ [22], $[Ir(NCS)(NH_3)_5]Cl_2$ [23], $[Ir(NCS)(NH_3)_5](ClO_4)_2$ [24], MeOC(Ph) = C(Ph)OH [25], (+)-8β-acetoxy-12-(4-bromobenzoyloxy)-13,14,15,16-tetranorlabdane [26] and other chiral organic [27] and inorganic [28] species.

2.3. Crystallographic Publications

2.3.1. Disorder

A number of early publications describe types of disorder in anthrone crystals [29–31] and present a general description of X-ray diffraction by such disordered crystals [32]. A body of publications

commencing in the 1970s is concerned with new methods for making absorption corrections in diffraction measurements [30,33–37]. The crystallographer's obsession with the "ideal" spherical crystal also attracted his attention at this time [36,38–42].

2.3.2. Improving Data Quality

There is a significant body of work concerned with general aspects of improving the quality of collected crystallographic data [43–48]. Flack also made a number of additional contributions to the use of statistical methods in crystallography [49–53] including a review of the standard work by Shmueli and Weiss [54].

2.3.3. Absolute Configuration, Absolute-Structure Refinement and the Flack Parameter

Probably the most important paper published by Howard Flack was the 1983 work "On enantiomorph-polarity estimation" in which he derived an expression for the determination of the absolute structure of crystals and, therefore, the absolute configuration of any chiral molecules contained therein [55]. Flack included a parameter which he called "x", but which the community now knows as 'The Flack Parameter'. He subsequently published numerous articles on the theory and practice of solving absolute structures [56–82]. Related work dealt with the origins of chirality [83] and general reflections on the use and misuse of symmetry and chiral descriptions in chemistry [84–88].

One additional interesting publication is a review of planar-chiral five-membered metallacycles [89].

2.3.4. Technical Contributions and Software

By its nature, crystallography is a technical and sometimes mathematically demanding and intense subject and Flack made a wide range of contributions to fundamental aspects of crystallography [90–98]. A 2017 book chapter presented a concise state-of-the-art view of chemical crystallography [99].

Flack was also involved in the new knowledge culture, and contributions entitled "Crystallographic publishing in the electronic era" [100], "Internet resources for crystallography" [101] and "World Wide Web for crystallography" [102] attest to this, as does a 1996 workshop "Surfing the Crystallographic Net (CRYSNET) workshops" [103]. Another conference contribution entitled "Is your crystal representative of the bulk?" addressed one of the fundamental issues for a synthetic chemist relying on crystallography [104].

He was a co-author of many software programs including DIFRAC [105] and HUG [106], X-RAY 76 [107] X-RAY 76 (the first System offering all the software needed for an X-ray analysis) and its successor, XTAL [108,109].

Finally, I should note that one of his last publications testifies to the breadth of his engagement with, and commitment to, crystallography in its broadest sense [110]. The web-site http://crystal.flack.ch/ maintains an up-to-date publication list and links to other sources commemorating his work.

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