International Union of Crystallography

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Notes for Authors

Revised *Notes for Authors* have been published in the January issue of *Acta Cryst.*, Section A, pages 174–186. Copies may be obtained from any of the editors. Appendix I in the *Notes* includes the criteria for publication of a paper in Section B; these are reproduced here for the benefit of authors:

1. The paper must contain a major structural element. This component may be an original determination of one or more structures (a single structure should generally have been studied under more than one condition of temperature or pressure), a theoretical structural investigation including new methodology, or a study of structural relationships based on a search of the literature. The calibre of this component should be at least as high as was previously required for acceptance in Section B up to 1982.

2. The paper should also present an experimental and/or theoretical contribution to one of the natural sciences that is novel, original and of high quality.

3. The paper should combine these two types of contribution to provide new structural insight for that science or for crystallography.

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Structure Reports

Volume 47A of *Structure Reports* has recently been published. It comprises four indexes (350 pages in all), covering the literature for metals and inorganic compounds for 1913–1980 (metal, inorganic and mineral indexes and, for 1971–1980, an author index). The price of the new volume is 51 Netherlands guilders for subscribers with standing orders. The full price for individual copies is 60 guilders but personal subscribers may buy a copy for their own use at 30 guilders. Orders for this publication may be placed direct with the publishers, D. Reidel Publishing Company, PO Box 17, 3300 AA Dordrecht, The Netherlands, with Polycrystal Book Service, PO Box 27, Western Springs, IL 60558, USA, or with any bookseller. Please note the new address of Polycrystal Book Service.

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Molecular Structures and Dimensions

The International Union of Crystallography and the Cambridge Crystallographic Data Centre have published Volume 13 of the series, entitled *Bibliography* 1980–81, *Organic and Organometallic Crystal Structures*. It contains bibliographic information on 3610 structures published during 1980–81. As in previous volumes the entries are arranged in 86 chemical classes and cover organic compounds, complexes and organometallic compounds. There are extensive indexes for authors, compound names, formulae and, for the first time, chemical diagrams. The new chemical diagram index should prove to be an invaluable tool for scanning the literature. The price of the new volume is 135 Netherlands guilders. Personal copies may be purchased at a reduced price of 101 Netherlands guilders.

Orders may be placed direct with the publisher, D. Reidel Publishing Company, PO Box 17, 3300 AA Dordrecht, The Netherlands, with Polycrystal Book Service, PO Box 27, Western Springs, IL 60558, USA, or with any bookseller. Please note the new address of Polycrystal Book Service.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

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Structural crystallography in chemistry and biology: benchmark papers in physical chemistry and chemical physics. Vol. 4. Edited by J. P. GLUSKER. Pp. xx + 421. Hutchinson Ross Publishing Co., distributed by Academic Press, New York, 1981. Price £33.00, US $50.00.

This book contains 59 key papers in X-ray crystallography from 1912 to 1977. It starts with the discovery of X-ray diffraction from a crystal of copper sulphate by von Laue, Friedrich and Knipping, and it ends with the structure of the protein disk of the tobacco mosaic virus by Anne Bloomer and others. This collection of papers is no substitute for a textbook of X-ray analysis, such as its author has already published [Glusker, J. & Trueblood, K. (1972). *Crystal Structure Analysis: A Primer*. Oxford Univ. Press], but it provides perspective for newcomers and refreshes the memories of old hands like me. The papers are grouped into 25 sections, each preceded by a lucid introductory text for the uninitiated and accompanied by references to further literature. The first seven papers deal with the history of structure determination by diffraction, the next 19 with

methods, the next 17 with X-ray structure analysis in chemistry and the last 16 with its role in biochemistry and biology.

Some of the historical details intrigued me. For example, von Laue concludes cautiously that Friedrich and Knipping's X-ray diffraction pictures *probably** exclude the corpuscular theory of X-rays that was then favoured by some physicists, notably W. H. Bragg (the father). He adds in brackets 'The light quantum theory of X-rays, *accepted by some investigators*,* can be included here under the description of corpuscular theory'. Did Laue really believe that diffraction of X-rays from crystals excluded the quantum theory of electromagnetic radiation? He continues: 'It still remains to be shown whether the periodic radiation is first generated in the crystal by fluorescence, or whether it is present in the primary radiation and is subsequently selected by the crystal'. W. L. Bragg's first contribution was the exclusion of the former possibility and the proof of the latter by his recognition that the focusing of the diffracted spots on the Germans' X-ray pictures was due to reflexion from successive lattice planes (Fig. 1). He had this remarkable insight at the age of 22.

I did know that as a young man Patterson had come to London to work with W. H. Bragg (the father) who had been the first to propose the application of Fourier series to X-ray analysis, but I did not realize that afterwards, at MIT, Patterson had frequently consulted Norbert Wiener, then one of the world's leading experts in Fourier series, before he formulated the function which is named after him. W. L. Bragg (the son) once told me that Patterson had applied to him for a lectureship that was vacant in his physics department at Manchester. This was at the time of the great depression in the 1930's; Bragg received over a hundred applications from British candidates to whom he felt he had to give preference. Suppose Patterson had got the job, instead of having to hang on at MIT without getting any pay, would he have formulated his famous function? Incidentally, Glusker gives an excellent introduction to her former teacher's great paper.

Glusker recalls that J. M. Robertson, after his successful use of isomorphous replacement with heavy atoms in the structure determination of the phthalocyanins, pointed out as early as 1939 that the replacement of the zinc atoms in zinc insulin crystals by mercury might allow the insulin phases to be determined. Bernal made a similar suggestion that same year. Why then did I wait until 1953 before trying isomorphous replacement on haemoglobin? Robertson's and Bernal's suggestions were just hunches which I did not take seriously, because it seemed unlikely to me that the scattering contribution from one mercury atom could alter measurably the combined contributions from 2500 atoms of carbon, nitrogen and oxygen in the asymmetric unit of haemoglobin. I did not then know the absolute intensity of reflexion from my crystals. In 1952, Bragg and I worked on a different kind of isomorphous replacement, that of salt solution by water in the lattice spaces between the haemoglobin molecules, in order to determine the transform of their external shape. To put that transform on an absolute scale I borrowed a primitive Geiger counter diffractometer built by W. Cochran and measured the absolute intensities of a few reflexions. The weakness of the absolute F's of even my strongest reflexions made me realize at last that >99% of the scattering contributions of the light atoms cancelled by interference, while those from the 80 electrons in a mercury atom would scatter in phase and would, therefore, have a marked effect on the diffraction pattern. I ought to have realized this ten years earlier by applying the statistics that A. J. C. Wilson developed while sharing a room with me at the Cavendish Laboratory, but at the time neither he nor I thought of their relevance to haemoglobin. Incidentally, I learnt from Glusker's book that Kaspar, Lucht and Harker, when solving the structure of decaborane in 1950, were oblivious of Wilson's paper and worked out his theory all over again.

In 1953, when I had obtained my first Fourier projection of haemoglobin on a centrosymmetric plane by a single isomorphous replacement with paramercuribenzoate, Dorothy Hodgkin drew my attention to Bokhoven, Schoone and Bijvoet's paper which showed that the phases of general reflexions could, in theory, be derived by double isomorphous replacement [Bokhoven, C., Schoone, J. C. & Bijvoet, J. K. (1951). *Acta Cryst.* **4**, 275–280]. It is a pity that Glusker neither reprints nor quotes that vital paper, but instead reprints an earlier one by the same authors [Bokhoven, C., Schoone, J. C. & Bijvoet, J. K. (1949). *Proc. K. Ned. Akad. Wet.* **52**, 120], which merely introduces what Blow and Rossmann later called the single isomorphous replacement Fourier [Blow, D. M. & Rossmann, M. G. (1961). *Acta Cryst.* **14**, 1195–1202], showing a superposition of the true structure with its mirror image.

I found a few other, minor, blemishes, which it is a reviewer's duty to point out, but which do not detract from the merit of Glusker's book. Röntgen discovered X-rays at Würzburg, not at Munich. Glusker describes Friedrich and Knipping as graduate students. This is true of Knipping, who was Röntgen's student, but Friedrich was more senior, being Assistant to Sommerfeld, the Professor of Theoretical Physics, who did his best to dissuade Friedrich from trying Laue's experiment. Paul Ewald worked at Stuttgart not Stuttgärt. In the section on anòmalous dispersion, Glusker does not explain the difference in phase change between normal and anomalous scattering. She lists the structures solved by W. L. Bragg in 1913/14, but omits that of copper, the first metal. Speaking of metals, I was intrigued to learn that Linus Pauling published the first alloy structure, Mg_2Sn, aged only 23.

Much in Glusker's book illustrates the profound truth of Karl Popper's dictum: 'I think it is a myth that the success of

* Author's italics.

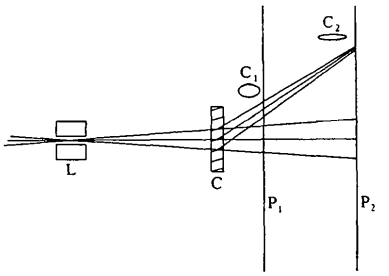

Fig. 1. Bragg's interpretation of the focusing of the diffracted spots observed by von Laue, Friedrich and Knipping which led to the formulation of Bragg's law: $n\lambda = 2d \sin \theta$. L, Lead screen; C, crystal; P_1P_2, positions of photographic plate; C_1C_2, cross sections of pencil of rays at P_1P_2. [From *Proc. Cambridge Philos. Soc.* (1913), **17**(1), 43.]

science in our time is mainly due to the huge amounts of money that have been spent on big machines. What really makes science grow is new ideas' [Elders, F. (1975). *Reflexive Waters*, p. 85. London: Souvenir Press]. For example, Patterson and Harker formulated their vector functions before any mechanized methods for the summation of Fourier series became available. E. W. Hughes introduced least-squares refinement in the structure analysis of melamine, when it took him 2 days to set up the normal equation for 18 parameters and 100 *h*0*l* reflexions on an IBM Hollerith punched-card machine and the machine took about 4 h to solve them. Crystallographers worked out phase relations many years before it became possible to use them effectively.

I quoted only part of Popper's dictum. The full sentence reads: 'What really makes science grow is new ideas, *including false ideas*.' I have had plenty of those, but it consoled me to find myself in good company.

In her 1928 paper on the structure of the benzene ring Kathleen Lonsdale writes: 'the benzene ring is almost if not quite flat ... The substitution, therefore, of a flat benzene ring for the puckered rings in naphthalene and anthracene would not affect the periodicity in the **c** direction which is one of the most striking features of those crystals'. An accurate structure of benzene was not published until 36 years later, when Curry and Wilson studied solid benzene by neutron diffraction, showing the positions of the H atoms and determining the C–C distances with an error of only 0·007 Å, at −135°C. At −3°C their mean C–C distance is 1·392 Å compared to Lonsdale's first estimate of 1·45 Å at room temperature. This paper immediately follows Lonsdale's, making one forget how much time had to elapse before this simple and important structure could be accurately determined.

Glusker's section on protein structures begins with Bernal and Crowfoot's famous note to *Nature* describing the diffraction pattern of wet pepsin crystals. They declare: 'Peptide chains in the ordinary sense may exist only in the more highly condensed or fibrous protein, while the molecules of the primary soluble proteins may have their constituent parts grouped more symmetrically around a prosthetic nucleus'. I wonder what they meant by that.

Glusker's book bears out not only Popper's views about science, but also my own: Money has its uses, but most progress springs from talent.

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Structural studies on molecules of biological interest. Edited by G. DODSON, J. P. GLUSKER and D. SAYRE. Pp. xviii + 610. Oxford: Clarendon Press, 1981. Price £39.00.

This volume is a *Festschrift* dedicated to Dorothy C. Hodgkin on her 70th birthday. In similar compilations the contents may be of variable quality but in this case the contributions have a very high standard. This is not an impression you only get immediately, laying your hands on the book. This review was delayed for various reasons and I had to read the volume a second time leaving me with my original opinion that this is an unusually good *Festschrift*.

The number of Dorothy's pupils and co-workers is remarkably large. The Editors have invited them to contribute to the volume. The fact that many have chosen not to take part may be taken as an indirect indication of its high quality. Only high-standard original papers are presented rather than hasty write-ups of old material.

On the other hand, it is essential that a volume of this nature should have a fair amount of historical background. All of us who have the privilege of knowing Dorothy will no doubt agree with the late Professor J. M. Bijvoet when he states in the beginning of this volume: 'one always rejoices at expressing feelings of admiration and affection. In no case in which I have felt this more clearly than at this moment now that I can contribute to the homage of Dorothy Hodgkin'.

M. Perutz leads off the section on history with an important chapter on the early days of crystallography in the UK, followed by interesting reminiscences by D. C. Philips, D. Parker-Riley – Dorothy's first research student – and the man taking care of the Oxford laboratory for many years, F. Welch. Recollections from work in the US and in China are given by L. Pauling and Tang You-chi respectively.

Dorothy's first major contribution to organic chemistry came through her work with C. H. Carlisle on cholesteryl iodide. Her research stimulated the whole field which is elegantly reviewed in the volume by J. Dunitz. The pioneering studies of J. M. Robertson are also described.

All of this of course leads up to Dorothy's famous work on vitamin B_{12} – a landmark in crystallography. J. P. Glusker gives an introduction to the subject and finally sums up the results obtained so far. The first studies are described by J. H. Robertson who gives a fascinating account of the Oxford laboratory at that time. The very interesting correspondence between Dorothy and K. N. Trueblood at UCLA is included. This illustrates well what crystallographers outside the US had to go through before computers were generally available. The vitamin B_{12} part also contains descriptions of the largely parallel work at Princeton (J. G. White).

Many chapters stem from studies not directly in line with Dorothy's main research. The work on gramicidin S was, however, performed mainly in her laboratory (M. M. Harding) and that on histamine (K. Prout and R. Ganellin) was performed in close cooperation with her.

Work on molecules of various nature is included, *e.g.* a description of an oxo-bridged binuclear iron(III) complex (B. Kamenar and B. Kaitner), of the conformation of amides (K. Venkatesan and S. Ramakumar), of nucleoside-5-diphosphate (M. A. Viswamitra, S. K. Katti and M. V. Holm) and of some mercury compounds (D. Grdenić). In this section there is finally a paper on pharmacological questions (E. Shefter).

A part is also included on methods in crystallography, starting with data collection for large molecules (R. A. Sparks). Several papers here deal with anomalous dispersion which was used extensively in Dorothy's research (S. Ramaseshan and R. Narayan), even on such large molecules as lysozyme (G. A. Bentley and S. A. Mason).

D. Sayre describes the early development of direct methods to which he made important contributions. His role in the introduction of FFT to crystallography is mentioned