MICHAEL MARK WOOLFSON
9 January 1927 — 23 December 2019
MICHAEL MARK WOOLFSON

9 January 1927 — 23 December 2019

Elected FRS 1984

BY KEITH S. WILSON* AND ELEANOR J. DODSON†

York Structural Biology Laboratory, Department of Chemistry, University of York, York YO10 5DD, UK

Michael Woolfson contributed enormously to the theory and practice of X-ray crystallography for almost 60 years. He extended the theory of ‘direct methods’, which provided a general solution of the crystallographic phase problem from the measured diffraction data alone, and provided tools to exploit this theory. Software developed in his laboratory, such as the computer package MULTAN, was responsible for about half of the structures determined around the world in the 1970s and 1980s. His parallel work on the origin of the Solar System renewed interest in the Capture theory, and he contributed numerous stimulating ideas to the general study of the origin and dynamical evolution of the Solar System.

Michael was a great educator and mentor for both undergraduates and young researchers, and many of these went on to make significant scientific contributions.

EARLY LIFE AND EDUCATION‡

Michael was born in Hackney in 1927. His father worked as a furrier, his mother as a dressmaker, and times were hard during the Depression years. Both parents valued education and encouraged him to study. In 1938 he was one of three boys from his class who won places at the local grammar school, which was so unusual that the headmaster declared a

* keith.wilson@york.ac.uk
† eleanor.dodson@york.ac.uk
‡ Much of this material is taken from Michael’s autobiographical article written in 2014 (39).
§ Numbers in this form refere to the bibliography at the end of the text.
day’s holiday for the whole school! When war was declared in 1939 the school was evacuated from Inner London, so Michael finished his secondary schooling via an accelerated study programme at Wellingborough Grammar School. He said that throughout all his schooling he had done well but never been top of the class, which had taught him that one can always ‘do better’. Another important skill gained at Wellingborough was rugby; Michael was tall and well-built and became a ‘useful forward’. He claimed that some later opportunities were awarded to him, not for academic excellence, but because he would be a valuable member of the local rugby team.

In 1944, still only 17 years old, he won a scholarship to Jesus College, Oxford, to study physics, where his tutor was Dr Claude Hurst. He complained later that the syllabus was old-fashioned; neither relativity nor quantum mechanics was even mentioned. However, there was plenty of time for rugby and enjoying life, and he graduated in 1947 with a respectable second-class degree, but without much enthusiasm for further study. (Later, when he applied to study for a PhD, his college reference claimed ‘This young man is quite unsuited for research’—luckily ignored by his supervisor-to-be.)

Like the rest of his generation, on graduating Michael was conscripted into the army for two years and sent for officer training. He was selected for the Royal Engineers Survey Establishment to learn the skills required for accurate mapping. (He found later that his principal qualification for selection was indeed his ability at rugby—the Colonel prided himself on his unit’s sporting prowess.) The procedures were highly technical, but crucially dependent on having accurate distance measures between pre-positioned theodolites. In rough terrain this required a good deal of hard footwork, so while on leave Michael designed a system for using ‘speed-of-light’ measurements to get better results with less effort. Nowadays this is routine practice using laser beams, but in 1948 it was deemed ‘interesting but impracticable’. However, it rekindled Michael’s interest in science, and he decided that after his stint in the army he would try to do research. He was not fussy about which field to follow, but his application to the X-ray crystallographer Henry Lipson (FRS 1957) was accepted, so that decided his future (39).

**University of Manchester Institute of Science and Technology, 1949–1952**

Henry Lipson was head of the Physics Department at the Technology Faculty for the University of Manchester Institute of Science and Technology (UMIST). The majority of its activities provided practical training, and Lipson had built up his crystallographic school in a practical way, constructing an optical instrument to simulate X-ray diffraction. Possible models of simple chemical structures were manufactured, and their optical diffraction compared with that obtained by X-ray diffraction. Michael expected to help with this project, but in fact it was already functioning by 1949, so he was directed to build a different analogue device: a photoelectric structure factor machine. This was a laborious task and after a year there was still much to do. A description of it was published (1), but in fact as computers became more functional it was rarely used in anger.

Michael used the optical apparatus to ‘solve’ the crystal structure of 1:1:6:6 tetraphenylhexapentaene, verifying that the chemist’s expectations matched the observed X-ray intensities (4). The distribution of intensities did not fit the theoretical curve, but knowing
the compound contained an internal centre of symmetry, he was able to derive a new formula for the expected distribution from a hypercentric structure, and publish his first theoretical paper (2). This persuaded him that being a theoretician had great advantages over building equipment!

In 1952 a set of seminal papers appeared in the fifth volume of *Acta Crystallographica* (Cochran 1952; Hauptman & Karle 1952; Sayre 1952; Zachariasen 1952). Each outlined similar ideas for determining the signed phases of the strongest X-ray reflections for centrosymmetric structures. Michael followed up this methodology and presented the results in his PhD thesis. On the basis of this interest, Lipson suggested he apply for a research assistant post with William Cochran (FRS 1962) in Cambridge. Michael was fortunate to enter the field at that time. The literature was awash with ideas, and he was able to join the debates and contribute important insights himself for the rest of his career. It will be simpler to outline the principal developments and then highlight Michaels’s contributions chronologically in the text.

**A BRIEF OUTLINE OF THE DEVELOPMENT OF DIRECT METHODS FOR PHASING CRYSTAL DIFFRACTION**

This summary is chronological, but for any reader who is interested in the fundamental principles, an excellent outline is presented by Peter Main using a matrix approach (Main 1975). Michael himself wrote several review articles and the theory is outlined in his books (see supplementary material).

**Crystallographic terminology**

The aim of X-ray crystallography is to provide a 3-dimensional (3D) image of a molecule, showing the relative positions of all the constituent atoms (figure 1).

Atoms are typically separated by about 1.5 Å, and X-rays can be generated with a wavelength comparable to this. X-rays are scattered from each atom independently, but if the molecules can be crystallized this scattering is concentrated to points on a diffraction grid. A parallel beam of X-rays is directed onto the sample and a diffraction pattern is recorded. For a single molecule the diffraction would be very weak, but the signal is greatly amplified by using a 3D crystal. This is equivalent in principle to the magnification obtained using an optical microscope (figure 2a,b).

Atoms are recorded at fractional positions \( r = (r_1a + r_2b + r_3c) \) along these axes; i.e. at positions \( h = (ha^* + kb^* + lc^*) \) where \((h, k, l)\) are integers and \( hr = hr_1 + kr_2 + lr_3 \). There are two sets of information inherent in the diffraction pattern. First, the spacing between the Bragg reflections is inversely related to the dimensions of the unit cell. Second, the intensities of the Bragg reflections are related to the positions of the atoms in that cell.

**The structure factor equation \( F_h \)**

If the atomic positions \( r_j \) were known, then the 3D vector sum over all \( N \) atoms in the unit cell could be calculated, where \( f_j \) is the theoretical scattering from that atom type, \( T_j \) an associated
Temperature factor correction and $g_j = f_j T_j$. 

$$F_h(\text{calc}) = \sum_{j=1}^{N} g_j \exp(2\pi i \mathbf{h} \cdot \mathbf{r}_j) = F_h \exp(i \phi_h), \quad [1]$$

giving both the amplitude $F_h$ and the phase $\phi_h$ for each Bragg reflection. If the atoms are correctly placed, the calculated amplitude $F_h(\text{calc})$ should agree with the observed $F_h(\text{obs})$. $F_h$ is a complex number with magnitude $F_h$ and phase $\phi_h$.

For the first structures of rather elementary compounds, such as simple salts, the solution was found by manually adjusting the positions of the few atoms in the crystal, taking account of known chemistry and symmetry, until the calculated structure factors agreed with those observed.

For any given crystal diffraction pattern, there are a few reflections for which phases can be assigned values to govern the choice of origin and hand according to a set of rules related to the symmetry of the space group. These are known as structure invariants.

The electron density equation $\rho(xyz)$

The inverse of equation [1] generates the electron density at each grid point $(x, y, z)$ in the crystal unit cell:

$$\rho(x) = \frac{1}{V} \sum_{h,k,l} F_h(\text{Obs}) \exp[i \phi_h] \exp[-2\pi i (hx + ky + lz)]. \quad [2]$$

If $F_h$ and the phase $\phi_h$ are those calculated in equation [1], then the electron density map $\rho(xyz)$ will have resolved peaks at the atomic positions. If the atomic positions are not known, then $F_h$ can be replaced by the experimentally observed value, but more ingenious methods are required to estimate $\phi_h$. This is the ‘phase problem’—meaningful electron density cannot be calculated until some phase information has been acquired. Solving this problem lies at the
heart of crystallography, and it is in practical solutions to this where Michael Woolfson made ground-breaking contributions.

**Normalized structure factors: $E_h$**

Owing to interference between electrons from different parts of the atom, the X-ray scattering from an atom falls off with the resolution $d^*$, and hence the expected measured X-ray intensity $I_h$ is weaker for high resolution reflections than for low. Corrections can be applied to ensure that the mean scattering is constant for all resolutions. The normalized structure factor is defined as $E_h = K(d^*) F_h$, where $K(d^*)$ is the scale factor chosen to make the mean $(E_h)$ approximate to $I$ over the whole resolution range. An equal atom electron
density map calculated using $E_h$ rather than $F_h$ has sharp peaks at the atomic sites, all with approximately unitary peak height.

**‘Direct methods’ for phase determination—Sayre’s equation**

Several papers outlining ‘direct methods’ for determining phases from relationships between different reflections had been published in 1952. All led to similar equations, but the conceptually simplest description was given by Sayre (1952), who derived an equation linking phases providing the following conditions hold for the electron density:

(i) Positivity: the electron density $\rho(x)$ should always be positive.
(ii) Atomicity: each atom should be represented by a single, discrete, non-overlapping peak.
(iii) Equal atoms: all atoms in the structure should contain the same number of electrons and hence have the same scattering power for X-rays.

Given a crystal structure represented by $\rho(x)$, we can construct a ‘squared structure’ expressed as

$$\rho(x) \cong K \times \rho(x)\rho(x).$$

Since all normalized atoms have a peak height of 1, using $E_h$ instead of $F_h$ should give a map

$$\rho(x) \cong \rho(x)\rho(x),$$

and this means it is possible to derive a relation between the phases of three reflections, $E_h$, $E_{h'}$ and $E_{h-h'}$ (Cochran 1955):

$$\phi_{-h} + \phi_{h'} + \phi_{h-h'} \cong 0.$$

Hence, if there is an estimate for $\phi_h$ and $\phi_{h'}$, then a value for $\phi_{h-h'}$ can be estimated. If there are several values of $h'$ generating such triplets, then a better estimate of $\phi(h)$ can be derived from the tangent formula (Karle & Hauptman 1956):

$$\tan(\phi_h) = \frac{\sum_{h'} |E_{h'}E_{h-h'}| \sin(\phi_{h'} + \phi_{h-h'})}{\sum_{h'} |E_{h'}E_{h-h'}| \cos(\phi_{h'} + \phi_{h-h'})}.$$

It is important to have a probability weighting for this. A formula was given by Michael (5) and more generally by Michael with Cochran (6), which states that the probability distribution for a structure with $N$ equal atoms is:

$$P(\Phi_3) = [2\pi I_0(\kappa_{h,h'})]^{-1} \exp(\kappa_{h,h'} \cos \Phi_3),$$

where $\kappa_{h,h'} = 2N^{-1/2} E_h E_{h'} E_{h-h'}$

Note that this probability is higher the larger the values of $E$, but reduces as the number of atoms increases.

**How best to use these equations to extend phases?**

All methods essentially involved the following steps:

(a) Select a starting set of three or four phases with the strongest amplitudes $E_h$. 
(b) Identify all triple products where a pair of strong reflections $E_{h'}E_{h-h'}$ could be associated with $E_h$.

(c) Assign multiple sets of test phase values to a subset of these—for instance, 0° or 180° for a centric reflection, or four possible values of 45°, 135°, 225°, 315° for a non-centric reflection.

(d) Use the tangent formula from these starting phases to generate more phases for strong $Es$.

(e) Identify which of the many sets of derived phases is most likely to be correct using an appropriate figure of merit. (This is key to successful application of direct methods.)

(f) Calculate an electron density map with this phase set using a weighting factor, and interpret the structure.

**Cavendish Laboratory, Cambridge, 1952–1955**

This was a seminal period for Michael’s research, and introduced him to many aspects of crystallography. The group in the Physics Department was led by W. L. Bragg FRS and included theoretical crystallographers led by William Cochran, the protein crystallographers Max Perutz FRS and John Kendrew (FRS 1960), and Francis Crick (FRS 1959) and James D. Watson (ForMemRS 1981), who were focused on the structure of DNA.

Michael’s first task was to determine the structure of adenylic acid, a component of RNA (3). He completed this in a few weeks, so Cochran and he were then able to concentrate on investigating phase relationships. They realized that electron density maps calculated with generated phases needed a weighting term to reflect the estimated phase probability. A formula for equal atom structures was established by 1954 (5) and extended for structures with unequal atoms (6). By 1955 Cochran had extended the formulation of triple phase relationships to include non-centric phases (Cochran 1955). An early and rather primitive digital computer, EDSAC, was available in Cambridge, so Cochran, working with computer expert Sandy Douglas, produced a program for generating sign relationships to give possible solutions in two dimensions (Cochran & Douglas 1955). This program was the forerunner of the many more powerful ones that were to revolutionize crystallography.

**University of Manchester Institute of Science and Technology, 1955–1965**

Michael was very happy in Cambridge, but he had a wife and son to support and no permanent position. In 1955 Lipson suggested he apply for a lectureship back in the UMIST, a position that would give him long term security. An added bonus was that University of Manchester had some computing facilities (the only other university in the UK with these at the time) and Michael realized how crucial this would be for his research. So he applied, was offered and accepted the position, but not without regrets—in 1956 Cochran wrote sadly to say how he was missed in Cambridge, ‘Now I have no-one to talk to...’, and Michael replied, ‘Me neither’.

He continued to publish work he had started in Cambridge, investigating the reliability of phases based on the Karle–Hauptman equations (8) and deriving a formula for the protein crystallographers to weight structure factors phased by the heavy atom method (7), but applying the new methods was a painfully slow task without the aid of computers. In 1958,
when David Sayre, who was now at the IBM centre in New York State, invited him to spend a year there to develop user-friendly software written in the new computer language Fortran, he accepted with alacrity. The results were presented at the 1960 Symposium on Computer Methods (10).

However, although the year was agreeable socially, the IBM computing resources were so entangled with red tape that Michael realized he could work more effectively within the University of Manchester environment and was happy to return. In 1960 he was very fortunate to be allocated Peter Main as a research student, which led to a lifelong collaboration. Michael said later: ‘In the first year I taught him, in the second we collaborated and by the third he was doing his own independent research.’ Together, and later with Gabriel Germain, they began to develop the required software to automate structure solution.

OTHER INTERESTS

Colour vision

While at IBM Michael read about, then met, one of the founders of polaroid photography. He was puzzled by the apparent simplicity of generating colour images using very few filters, and investigated methods for modelling colour perception. His interest continued after returning to Britain, and he even marshalled volunteers to test their response to different images, but after some time he realized there were not enough hours in the day to diversify so far from his main research interests (9,12,13,16).

Astronomy: the Capture theory of the origin of the Solar System

His position in Manchester required that Michael teach a variety of courses, and this helped stimulate his interest in other areas of physics. An astronomy textbook discussed theories on the origin of the Solar System, none of which seemed completely satisfactory, so Michael designed a model that he christened the Capture theory (11,15). It invoked a mechanism for the formation of the Solar System involving a tidal interaction between a condensed Sun and a collapsing protostar with the capture of protostar material by the Sun. The hypothesis was tested by computer modelling and found to be plausible (13). He continued to be fascinated by this puzzle throughout his life (18,23,25,28). His co-worker, John Dormand, has provided this summary of the fundamental ideas:

Any theory of the origin of the solar system must obey the basic laws of physics, particularly those relating to energy conservation. Michael Woolfson found that in the 1960s almost all theories failed to explain the solar system’s distribution of angular momentum. He noted that the sun, with 99.87% of the mass of the system, spins very slowly so that it contains less than 0.5% of the total angular momentum, and that in all the major planet-satellite systems, most of the angular momentum is contained in the rapid planetary spin. Cosmogonists proposing that the sun and planets originated from the collapse of a single body were unable to identify a plausible mechanism which would ensure transfer of angular momentum to the planets. Michael’s Capture Theory avoids that difficulty by proposing planets derived from the tidal disruption of a diffuse young protostar in a close encounter with the Sun. The tidal filament of the protostar, captured by the sun, fragments to form the major planets, and the angular momentum of the planets is derived from the hyperbolic orbit of the protostar. To test the theory the capture event was subjected to computer simulation. This requires solution of the equations of motion of the bodies involved and, at the time of the proposal, sufficiently powerful computers had only
recently become available. The orbits of the newly formed planets were very much more eccentric than those of today, but this feature gave orbital periods long enough to allow the initially diffuse protoplanets to collapse sufficiently to avoid disruption at the second perihelion passage. There would be much uncondensed material forming the medium in which the new planets moved. The gravitational effects of this medium would serve to round-off the planetary orbits. Some of this medium would be accreted but most of it removed by solar radiation.

A fairly obvious objection to the theory is due to the rarity of encounters between stars. But the capture event postulated here would take place in the star cluster in which both the sun and the protostar were formed. Such clusters are known to undergo very dense phases in which encounters would be common. Michael estimated the chances of an encounter as between 1% and 15%. The theory described so far has covered only the formation of major planets, but there are also the terrestrial planets and other phenomena which need to be explained. Since the early planetary orbits are eccentric and subject to rounding-off at varying rates, the chances of a planetary collision are quite favourable. The parameters of such a catastrophe are very speculative but Michael suggested that two of the terrestrial planets are the cores of the colliding planets and that the others may be ex-satellites.

The Capture Theory proposed in the 1960s underwent considerable refinement over a period of 50 years. The amount of observational data on our solar system is now much greater, and it is now known that planetary systems are quite common and that their configurations vary greatly. Over the years Michael made some changes in the parameters of the capture event to maintain its consistency with observation. Computer modelling has always been important to the theory. At first it was only possible to handle 3-body systems, but this progressed to extended bodies composed of modified mass points, and, in recent times, the smoothed particle hydrodynamics technique allowing realistic physical properties to be simulated.

**University of York, 1965–1994**

In 1965 Michael was appointed professor of theoretical physics in the newly-founded University of York, and this became his base until his retirement and beyond.

**Undergraduate teaching**

There were many exciting challenges in setting up a new department, and the young staff threw themselves into designing a course that combined practical and theoretical studies and was relevant to the whole body of students. Michael had already written a thoughtful article about the issues (14). To paraphrase from this:

What is the prime cause of the failure of physics students? It is clear that their single greatest difficulty is the lack of proper understanding of mathematics—an inability to grasp its significance and to be able to apply it to a physical problem.

Another difficulty for many students is that they never acquire a perspective view of the subject. It is taught in neatly labelled parcels, and the interdependencies of one part to another are never made clear.

A third important cause of difficulty is illogical ordering of the lecture courses. The lecturers should plan the whole course together and a uniform nomenclature be agreed so that previously derived results may be recognizable.

On the whole it seemed the York staff succeeded in these aims. John Helliwell, now a professor emeritus himself, has written about his experience as a student with Michael:
I was one of 32 undergraduates in the physics department from 1971 to 1974. Michael Woolfson taught three courses in our third year: X-ray Crystallography, Astrophysics and Advanced Quantum Mechanics. He was a marvellous lecturer providing clear and rigorous presentation. There were advantages to being in a small class, it was straightforward to approach a lecturer when we had questions. I had launched the York University Astronomical Society, and we were enthralled by Michael’s lectures on theories about the formation of the planets. Michael and his wife Margaret came along with us on a coach trip to Scarborough to visit the planetarium there.

Post-graduate teaching: NATO and Erice courses for direct methods in crystallography

Michael and Peter Main were organizers of a number of very influential direct method schools—in Parma (1970), York (1971), Erice (1974), York (1975), Erice (1978) and York (1980)—attended by many of the then leading crystallographic theoreticians. The school in 1974 at Erice brought together the experts in the field plus a cohort of students. By the next school there, in 1978, five of the 14 speakers had been ‘students’ in 1974 (figure 3). Carmelo Giacovazzo, in his book *Phasing in crystallography* (Giacovazzo 2013), writes: ‘We must acknowledge Michael Woolfson and his group (among whom I recall Peter Main and Gabriel Germain) for their extraordinary contribution: They led the way from old to modern phasing procedures.’

Michael also contributed to several volumes of the book series entitled ‘Computational Crystallography’, which published papers from summer schools organized by the International Union of Crystallography (IUCr). It is interesting to look back at these; many complex ideas are described, (often in extremely complex ways!), but Michael’s insightful articles are always a model of clarity (24,26).

Crystallographic research

Direct methods:

In 1964 Isabella and Jerome Karle had extended a method that they called ‘symbolic addition’ to solve both centrosymmetric and non-centrosymmetric structures. Phases were represented by letter symbols, and, by a great tour-de-force and virtually by hand, in 1964 they solved the non-centrosymmetric 14 atom structure of L-arginine dihydrate (*Karle & Karle 1964*).
Gabriel Germain, a crystallographer from Louvain, had joined Michael’s group in Manchester in 1964, and moved with him to York. They set out to design a computer-based multi-solution symbolic addition method. Although the computer at York was primitive by today’s standards, the resultant program, LSAM (Logical Symbolic Addition Method), was successful in solving centrosymmetric structures (17, 22). They then moved on to program in Fortran a multi-solution method for non-centrosymmetric structures, working with Peter Main, who had been appointed to a lectureship in York in 1967. They introduced an innovative procedure to avoid the use of symbols. The origin fixed reflections were assigned fixed phases. A small number (n) of reflections with large $E$ magnitudes were assigned one of four phases, $\pm \pi/4$ or $\pm 3\pi/4$. Multiple trial phase sets (i.e. $4^n$) were generated, and the tangent formula used to predict more phases. The trials were ranked by several figures of merit, and the most promising used to generate maps and yield peak lists for manual inspection. If the peaks showed a structure that made chemical sense, then the problem could be deemed as solved. The developers were happy to share their software, and publish their findings, so there was a great deal of informal collaboration. There were still many problems to consider, but each success helped hone the decision-making algorithms, and by 1971 the group was ready to distribute their program, MULTAN (21).

For the next decade MULTAN was used to solve most small non-centrosymmetric structures worldwide. It was (and is) a prime example of good programming technique. The program was modular, meaning that for instance if a more sensitive figure of merit was discovered, it was simple to add it or replace existing ones. The crystallographic library routines were well designed, well documented and rigorously tested, functional for all space groups, and reusable in other applications. The results were clearly presented and for portability the programming language used was the most basic Fortran.

One example of the software’s versatility was demonstrated by one of us (KSW); while a graduate student in Oxford he applied MULTAN to the analysis of isomorphous derivatives of proteins, despite the limited resolution and accuracy of the data. Heavy atom sites are typically well separated, so the concept of ‘atomicity’ is conserved. The figures of merit pinpointed the best phase set, and the method gave the correct sites for almost all his tests (Wilson 1978).

As the decade progressed, computing power increased and it became possible to solve ever larger structures, providing there were atomic resolution data. New ways to assign the initial phase sets were explored, and a particular focus was on finding optimal figures of merit to identify the best solution. Many visiting scientists spent time in York, sharing their approaches to solving the phase problem and benefitting from the stimulating open atmosphere of the laboratory. The authorship affiliations for the long series of papers entitled ‘On the application of phase relationships to complex structures I–XXXV’ (1968–1994) are evidence of this; Britain, Germany, Belgium, Italy, France, Russia, Argentina, Brazil, China, Egypt and India are all represented. The collaboration with Germain and his Louvain colleagues continued, and Michael was able to raise funds from the Royal Society to support several Russian and Chinese workers. The Russian contacts stopped abruptly in 1984 after one visitor defected. There were angry exchanges with Russian diplomats, who suggested Michael had connived with the plan, but this view was not shared by the scientists themselves, as is clear in the cheerful picture taken in 1990 of Michael and his wife Margaret with Professor Vainshtein, head of the Moscow Institute of Crystallography (figure 4).
Macromolecular studies:

Two developments probably helped to stimulate Michael’s interest in applying his expertise towards phasing larger molecules. First, in 1976 Guy Dodson (FRS 1994) had been appointed to the York chemistry department to establish a protein crystallography group. At that time protein crystallographers derived their first phases from multiple sets of imperfect experimental measurements, struggled to build a preliminary model into imperfect electron density, then refined that model to improve the phasing; in contrast, direct methods practitioners assumed the diffraction data were perfect and complete, and relied on the formalism to provide near-perfect phases from which to generate near-perfect, clearly interpretable electron density maps. There were frequent discussions between the two research groups, and a growing understanding of the strengths and weaknesses of each aspect of structure solution, which in time led to very fruitful collaborations.

The second event was almost accidental. The 1978 IUCr triennial meeting in Warsaw was the first international meeting that Chinese scientists had been allowed to attend after the fall of the Gang of Four in 1976, and the whole delegation came on to visit York, primarily to compare results on insulin research. Not all the members were particularly interested in that topic, and one, Professor Fan Hai-fu, has written this account of his visit:

I met Michael for the first time at the reception party (in the Dodson house!) I told him of an idea of mine for using direct methods to deal with the problem of phase ambiguities arising from pseudo crystallographic symmetries. Michael immediately said: ‘Tomorrow I was planning on using the morning to talk about the work done here in York. But now I would like to leave half the time for you to talk about your work done in Beijing’. This was the beginning of a long friendship and a very fruitful collaboration.
In 1980 Michael made his first visit to China, and in 1981 I visited York for a month. We had just succeeded in solving a few superstructures using a Sayre-equation based process. Michael suggested automating that method so my colleague Jia-Xing Yao and I began using the platform MULTAN.

In 1985, we signed a formal agreement for collaboration on methods of solving crystal structures, especially proteins. This became one of the longest international collaborations supported by the Royal Society and the Chinese Academy of Sciences. Jia-Xing Yao finally settled in York and continued working very productively with Michael for many years (31–33).

A pleasing fall-out from the exchange visits contributed greatly to Michael’s well-being. He had suffered from gastric upsets for many years, variously assigned by different medics to causes such as stress, overwork, fatigue, etc., but after one visit Michael realized that (a) he had been perfectly healthy while in Beijing, (b) he had eaten only Chinese food, and (c) this could be a clue that he suffered from coeliac disease; and, indeed, that proved to be so. Once Margaret mastered the art of providing gluten-free bread, his health greatly improved.

Other visitors continued to spend time in York and test new ideas, but the afore-mentioned series of papers ‘On the application of phase relationships to complex structures I–XXXV’ moved from having sub-titles such as ‘Getting a good start’ (20) to ‘Phase extension for small proteins’ (27) as his interests changed.

The new developments depended crucially on increasing computer power, which allowed the exploitation of ‘dual space’ procedures. These algorithms refine structure factor phases by iterative modifications of the current model in direct space (electron density) and reciprocal space (structure factors) and it is the alternation between the two spaces that is crucial. These ideas revolutionized macromolecular structure determination. The applications used fast Fourier transforms to test many modifications quickly and benefitted from the more complete experimental measurements available from synchrotron sources.

During the 1980s, protein crystallographers were realizing that, although the limited data and poor initial phase estimates obtained for proteins could not yield density that showed ‘atomicity’, i.e. not all atom peaks could be resolved, their maps did possess other global features, such as solvent boundaries, which allowed sensible density modifications (Wang 1985). Michael and his Chinese colleagues were exploring these ideas, and by the late 1980s Peter Main and his research students Kam J. Zhang and Kevin Cowtan were providing software combining sophisticated density modification in real space with direct methods style phase improvement. The programs were distributed with CCP4 (Collaborative Computing Project 4) (Winn et al. 2011) and widely used (Main 1990; Zhang & Main 1990). Other excellent software packages using these approaches also became available, such as Shake-and-Bake (Miller et al. 1994) and SHELXE (Sheldrick 1997).

Before discussing Michael’s contributions in more detail, it is important to appreciate that there were also rapid advances in the acquisition of X-ray experimental data. By the 1990s it was sometimes possible to collect atomic resolution data from macromolecular crystals, and this meant that, in principle, well phased maps using such data would satisfy Sayre’s equation requirements of ‘positivity’ and ‘atomicity’, and that it might be possible to exploit the ‘direct methods’ phase relationships. However, there was a snag: the probability of any phase being correctly estimated involves a factor of $1/\sqrt{N}$, which reduces rapidly in value as the number of atoms increases.
Synchrotron radiation for X-ray data collection: the Woolfson Report

These facilities provided much better experimental data than any laboratory source. One of the first synchrotron beam lines for protein crystallography was set up at LURE in 1979. In 1990 the Hamburg resource was providing the best facilities for protein crystallography and showing that it was feasible to collect atomic resolution data sets from these large molecules (Dauter et al. 1996). It was partly the access to higher resolution data from protein crystals that encouraged the direct methods practitioners to consider these problems.

As a physicist, Michael was cognisant of the technology and very aware of the value of such a resource—three of his appointees to the physics staff became leaders in the field: Keith Wilson (a lecturer in York seconded to Hamburg in 1985), Zbigniew Dauter (a scientist from Poland also at Hamburg and finally at Argonne, USA) and John Helliwell (an academic in York from 1985 to 1988 who was responsible for some design aspects of the new UK Synchrotron, which finally became the Diamond Light Source.

In November 1991 the Science and Engineering Research Council (SERC) commissioned its second six-yearly review of synchrotron radiation science:

A multidisciplinary panel, to be chaired by Professor M. M. Woolfson FRS, has been established to undertake this review. The task of this panel is to assess and report on the UK community’s needs for access to synchrotron radiation facilities in the next century and the form they might take.

In April 1993 the ‘Woolfson Report’, as it became known, was published. The report recognised the quality, volume and diversity of science being carried out at synchrotron radiation facilities and put forward a number of recommendations for continued support. Among these was the major recommendation that a new medium-energy X-ray source be constructed to replace the UK’s existing one. [https://publications.parliament.uk/pa/cm199900/cmselect/cmsctech/82/9121503.htm]

The UK Research Councils accepted the scientific and technical case for this in 1994, although Michael was to be retired well before it was completed in 2007! But, as the largest single scientific infrastructure project for many decades, it is fair to say that the Woolfson Report of 1993 had a truly major impact on science in the UK. The availability of data from such synchrotron sources was crucial to his next major research initiative, carried out after his retirement.

Astronomy interests:

Michael continued to supervise graduate students in this field, and to collaborate with the mathematician and physicist John Dormand. In 1971 their calculations were only able to approximate the Solar System with three bodies, but by the 1980s they could exploit increasing computer power to extend the theory first to the larger planets and then build it into a coherent self-consistent model of the whole Solar System, incorporating minor planets and their satellite moons. In 1989 they published a book together expounding their ideas: The origin of the Solar System: the Capture theory (28). This gave rise to a set of interesting intellectual exchanges with other astronomers, some of whom had conflicting theories.

New evidence was becoming available about a surprisingly wide range of deuterium/hydrogen ratios in the Solar System, varying from $2 \times 10^{-5}$ for Jupiter to $1.6 \times 10^{-2}$ for Venus. These differences allowed estimates of the internal temperatures generated by the
masses of specific solar collisions and provided another source of precise information for the theoretical calculations (Roueff et al. 2000; Loinard et al. 2000).

Michael with his colleagues contributed regularly to the *Monthly Notices of the Royal Astronomical Society* using this information to extend their analysis of planet formation and the Solar System (34,35).

**RETIREMENT, YORK 1994–2019**

After his retirement in 1994 Michael was relieved from many of his administrative duties, although he carried on teaching the Physics Department astronomy courses for the next seven years. This gave him more time for his research projects, and he continued to publish extensively, collaborating with many visitors. Crystallographic ideas poured out; there were papers discussing the use of anomalous scattering (31), new figures of merit (32), new ways of modifying density, the feasibility of *ab initio* phasing. Importantly, he was still able to fund the work of his colleague Jia-Xing Yao.

One particularly powerful idea they pursued in collaboration with the present authors is coded into the program ACORN (named from the song—*Mighty oaks from little acorns grow*). This is a dual-space phasing procedure that needs near-atomic resolution data, extended to 1 Å simply by adding $E$ values all with the expected unit mean intensity for the resolution range (33,37). This data extension idea has been christened by George Sheldrick (FRS 2001) as the ‘free lunch syndrome’ (Usón et al. 2007). Phases are calculated for the strong $E$ values using as a starting point some correctly placed coordinates, such as heavy atoms or the sulfur sites placed using anomalous differences, or an $\alpha$-helix positioned by a molecular replacement search, or even a randomly placed test atom site. These phases are refined using the tangent formula and a map calculated using only the strong $E$ values. This is modified using a very simple algorithm: all density below a certain sigma level is set to zero and high values are pruned. Then structure factors are regenerated for all reflections, and a simple but robust scoring system is used to indicate whether there is progress. The correlation coefficient between the observed and calculated magnitude for the set of ‘medium’ $E$ values not used for the map calculation should increase, and when this does occur the procedure can quickly generate an extremely accurate set of phases for all reflections. ACORN is distributed through CCP4 and is widely used (Gordon et al. 2001; McAuley et al. 2001; Whelan et al. 2019).

**AUTHORSHIP**

Michael wrote clearly and fluently and had written or co-authored a number of valuable textbooks before 1994 (19,29,30). As his mobility decreased with age, he got a lot of pleasure from writing, and completed 15 books during his retirement! Several were essentially textbooks, but presented in a style that made them accessible to a wide range of students, others deal with various astronomical issues, often with a historical slant, and provide a delightful introduction to the subjects under discussion, e.g. (36,38) (see full bibliography in online supplementary material).
Awards

Michael was awarded many honours. He was elected a fellow of the Royal Society in 1984, and received the Royal Society Hughes Medal in 1986. He received the Patterson Award from the American Crystallographic Association in 1990 and was thrilled to receive the Gregori Aminoff Prize from the Royal Swedish Academy of Sciences in 1992 (this is seen as a ‘runner-up’ to the Nobel Prize, which had been awarded to Karle and Hauptman in 1985). In 1997 he was awarded the Dorothy Hodgkin Prize by the British Crystallographic Association, and in 2002 the Ewald Prize by the International Union of Crystallography for outstanding contributions to the science of crystallography. In 1999 he was elected an Honorary Fellow of Jesus College, Oxford.

Three citations are:

Royal Society Hughes Medal in 1986, for ‘the creation of algorithms including MULTAN and SAYTAN which are used world-wide to solve the majority of reported crystal structures’.

Gregori Aminoff Prize from the Royal Swedish Academy of Sciences in 1992, for ‘your development of direct methods for statistical phase determination of crystal structures’.

Ewald Prize by the International Union of Crystallography in 2002, ‘awarded to Professor Michael M. Woolfson for his exceptional contributions in developing the conceptual and theoretical framework of direct methods along with the algorithm design and computer programs for automatic solutions that changed the face of structural science, and for his contributions to crystallographic education and international collaboration, which have strengthened the intellectual development of crystallographers worldwide’.

Public service

To quote Michael: ‘I believe that those who receive the benefits of the ancillary activities of science should be willing to serve their community in any way they are able. True, it detracts from the time one can spend doing science, but unless someone does these things the overall amount and quality of science that is done will be much diminished’ (39).

Astronomy

He was a valued member of numerous Royal Society committees, and was chairman of the Subcommittee on Planetary Sciences for many years, and vice president of the Royal Astronomical Society, and sat on the Astronomy and Planetary Science Board of the SERC. He was also president of the local York Astronomical Society for many years.

Crystallography

He contributed greatly to the crystallographic community, both in Britain and internationally. As outlined above he was an expert and dedicated teacher, willing to give his time and expertise at numerous workshops and conferences.
International Union of Crystallographers (IUCr):

This organization was established in 1947 to stimulate collaboration between nations, rich and under-developed, and to provide journals to both publish crystallographic theory and report structures. One of the founders was Henry Lipson, Michael’s PhD supervisor, and Michael’s early career was fostered by the publications and debates reported in the journal *Acta Crystallographica*. In time he too became an important contributor. As well as being a prolific subscriber, he was book review editor from 1968 to 1975, and a co-editor for *Acta Crystallographica A* and *B* from 1977 to 1980. He participated in all the triennial meetings until his old age, and his warmth and friendship contributed greatly to their success (figure 5).

He was a member of the IUCr Commission on Crystallographic Computing from 1972 to 1975 and led several, and attended all, of their workshops.

He was a member of the IUCr Executive Committee from 1981 to 1984, during which he served as the first convener of the IUCr Finance Committee. This was a very challenging role—at that time the IUCr publication costs in Sweden had virtually bankrupted the IUCr, and Michael was part of the team that re-established the journals in Chester, UK, where they continue to thrive to this day.

British Crystallography Association (BCA):

Michael was one of the founding fathers of the BCA. This had a somewhat complicated gestation. In British universities, crystallographers were included in both chemistry and physics departments. Each group had their own fiercely independent society, so there was no simple mechanism for joint meetings. By the end of the 1970s, after convoluted negotiations, it was agreed to form a BCA, but it was still not clear how it could be financed. Finally, in
1982 David Blow FRS suggested inviting established crystallographers to become ‘founder members’ on payment of a life membership fee of £100. Michael was one of these founder members—you can see his signature in figure 6. The BCA has held annual meetings in the UK, several organized at York, and Michael continued to attend and enjoy these into his old age.

Yorkshire Philosophical Society

In the early nineteenth century, many ‘philosophical societies’ were founded in the north of England. The minutes from the Newcastle Society outline their objectives: ‘The Literary and Philosophical Society . . . to consist of ordinary and honorary members; the former to be local persons . . . The meetings of the Society to be held . . . at which religion, the practical
branches of law and physic, British politics, and indeed all politics of the day, are deemed prohibited subjects of conversation.' (Anonymous n.d.).

A Yorkshire society was formed in 1822. Michael Woolfson joined in 1965 as soon as he moved to York and was always a committed member (figure 7). The intellectual and secular constitution fitted his own ethos perfectly. He was chairman of the Education Committee for a time, which provided lectures for local schoolchildren and prizes for school project competitions, then was president from 1985 until 1999. His last lecture to the Society, ‘On the origin of planets’, was in 2009.

**Personal life**

Margaret had agreed to marry Michael while he was still doing his PhD; they survived the lean years very happily and indeed were together for 67 years. By the time they moved to York they had three children, all still at school. The university students were accommodated in colleges—not architecturally distinguished, since all buildings were assembled from prefabricated CLASP concrete slabs—but very successful as student residences. Michael became the first provost of Goodricke College in 1968, so for the next few years the family lived on campus and was closely involved with student life. He was proud that he had persuaded the administration to name ‘his’ college Goodricke, after an eighteenth-century York astronomer.

Michael always thoroughly enjoyed the chance to interact with young people. In the early 2000s when we were collaborating, he would come to the laboratory once a week, always making sure he was in time for the communal coffee session. He would be welcomed as an old friend by the receptionist, talk to the graduate students and then only when the group dispersed would we settle down to check how last week’s ideas had panned out and discuss what could be tried next. His three granddaughters also gave him great pleasure—he was
delighted that his eighty-first birthday card from them referred to him as a ‘perfect square’ and boasted that at least one of them must be an arithmetician!

He was a very happy traveller, excited by new cultures and by the international comradeship that marked his scientific career. One of their retirement pleasures was to go on ‘educational’ cruises; Michael said ‘there is ALWAYS someone interesting to talk to’. He saw himself as a ‘cultural Jew’, part of the Jewish community without being religious. He was very proud to be included in Wikipedia’s list of British Jewish scientists.

**CONCLUSION**

Michael is of course remembered for his important contributions to science, as an inspiring teacher and mentor, but also more personally as an unrepentant intellectual, always excited to learn more about the world we live in and taking great pleasure from making new friends and discussing new ideas. He continued to work and think until his death, submitting his last book a few months before he died. His son Malcolm acknowledged this:

Dad was a ‘people’ person, enjoying talking to everyone about their own interests and general matters. He welcomed moving to assisted accommodation—he said, ‘And now I can make new friends’.

**ACKNOWLEDGEMENTS**

We would like to thank all Michael’s colleagues who have read these memoirs and contributed their own recollections; in particular John Dormand, for his help with the astronomy sections, John Helliwell, who was taught by Michael, Fan Hai-Fu, for details of the Chinese–UK research projects, and Malcolm Woolfson, for his personal insights. The frontispiece portrait was taken in 1985 and is © Godfrey Argent Studio.

**AUTHOR PROCFILES**

*Professor Eleanor Dodson FRS*

Eleanor Dodson learnt crystallography in Oxford in Dorothy Hodgkin’s group, where she contributed to developing software for macromolecular crystallography. In 1976 the University of York established a small crystallography group in the chemistry department, led by Guy Dodson, and soon they were collaborating with the group in physics, led by Michael Woolfson. As Michael’s interest in structure solution of proteins grew, the collaboration became closer and mutually beneficial.
Keith Wilson started his crystallography career by doing a final year project in Oxford with Dr Keith Prout, before moving on to do his DPhil with Louise Johnson (FRS 1990) in molecular biophysics. His external thesis examiner was Michael Woolfson. He was briefly a lecturer in Michael’s physics department in York, 1983–1985, before taking up the post as head of the European Molecular Biology Laboratory Outstation in Hamburg. He returned to the York Structural Laboratory in 1995 and collaborated with Michael and Eleanor in the following years.

REFERENCES TO OTHER AUTHORS

Anonymous. The beginnings of the Lit & Phil. Lit. Phil. See https://www.litandphil.org.uk/blog/posts/2021/february/the-beginnings-of-the-lit-phil/ (accessed 25 July 2021).

Bialek, W, Krzywda, M, Jaskolski, M. J., Szczepaniak, A.. 2009 Atomic resolution structure of reduced cyanobacterial cytochrome c6 with an unusual sequence insertion. FEBS J. 276, 4426–4436. (doi:10.1111/j.1742-4658.2009.07150x)

Cochran, W. 1952 Relations between the signs of structure factors. Acta Cryst. 5, 65–67. (doi:10.1107/S0365110X52000149)

Cochran, W. 1955 Relations between the phases of structure factors. Acta Cryst. 8, 473–478. (doi:10.1107/S0365110X55001485)

Cochran, W. & Douglas, A. S. 1955 The use of a computer for the direct determination of crystal structures. Proc. R. Soc. Lond. A 227, 486–500. (doi:10.1098/rspa.1955.0025)

Dauter, Z., Lamzin, V. S & Wilson. K. S. 1996 Proteins at atomic resolution. Curr. Opin. Struct. Biol. 3, 784–790. (doi:10.1016/0959-440X(95)80011-5)

Giacovazzo, C. 2013 Phasing in crystallography: a modern perspective. Oxford, UK: International Union of Crystallography/Oxford University Press.

Glusker, J. P. & Trueblood, K. N. 2010 Crystal structure analysis: a primer, 3rd edn. Oxford, UK: Oxford University Press.

Gordon, E. J., Leonard, G. A., McSweeney, S. & Zagalsky, P. F. 2001 The C1 subunit of α-crustacyanin: the de novo phasing of the crystal structure of a 40 kDa homodimeric protein using the anomalous scattering from S atoms combined with direct methods. Acta Cryst. D 57, 1230–1237. (doi:10.1107/S0907444901009362)

Hauptman, H. & Karle, J. 1952 Crystal-structure determination by means of a statistical distribution of interatomic vectors. Acta Cryst. 5, 48–59. (doi:10.1107/S0365110X52000125)

Karle, J. & Hauptman, H. 1956 A theory of phase determination for the four types of non-centrosymmetric space groups P222, 2P22, 3P2, 2P22. Acta Cryst. 9, 635–651. (doi:10.1107/S0365110X56001741)

Karle, I. I. & Karle, J. 1964 An application of the symbolic addition method to the structure of l-arginine dihydrate. Acta Cryst. 17, 835–841. (doi:10.1107/S0365110X64002250)

Loinard, L. A., Castets, A., Ceccarelli, C., Caux, E. & Tielen, A. G. G. M. 2001 Doubly deuterated molecular species in protostellar environments. Astrophys. J. 552, 163–166.

Main, P. 1975 Matrix approach to the phase problem. In Crystallographic computing techniques, Proc. Crystallographic Computing Summer School of the IUCR, 28 July–5 August 1975, Prague (ed. F. R. Ahmed), pp. 165–175. Prague. Copenhagen, Denmark: Munksgaard.

Main, P. 1990 The use of Sayre’s equation with constraints for the direct determination of phases. Acta Cryst. A 46, 372–377. (doi:10.1107/S0108776789012146)
McAuley, K. E., Yao, J. X., Dodson, E. J., Lehmebeck, J., Astergaard, P. R. & Wilson, K. S. 2001 A quick solution: \textit{ab initio} structure determination of a 19 kDa metalloproteinase using ACORN. \textit{Acta Cryst. D} \textbf{57}, 1571–1578. (doi:10.1107/S090744490101335X)

Miller, R., Gallo, S. M., Khalak, H. G. & Weeks, C. M. 1994 SnB: crystal structure determination via Shake-and-Bake. \textit{J. Appl. Cryst.} \textbf{27}, 613–621. (doi:10.1107/S0021889894000191)

Roueff, E., Tine, S., Coudert, L. H., Pineau, G., Fulgarone, E. & Gerin, M. 2000 Detection of doubly deuterated ammonia in L134N. \textit{Astr. Astrophys.} \textbf{354}, 63–66.

Sayre, D. 1952 The squaring method: a new method for phase determination. \textit{Acta Cryst.} \textbf{5}, 60–65. (doi:10.1107/S0365110X52000137)

Sheldrick, G. M. 1997 Direct methods based on real/reciprocal space iteration. In \textit{Recent Advances in Phasing: Proc. CCP4 Study Weekend (DL-CONF-97-001)} (ed. K. S. Wilson, G. Davies, A. S. Ashton & S. Bailey), pp. 147–158. Warrington, UK: Daresbury Laboratory CCLRC. See https://legacy.ccp4.ac.uk/courses/proceedings/1997/g_sheldrick/main.html.

Usón, I., Stevenson, C. E. M., Lawson, D. M. & Sheldrick, G. M. 2007 Structure determination of the \textit{O}\textsubscript{\textsuperscript{-}}-methyltransferase NovP using the ‘free lunch algorithm’ as implemented in SHELXE. \textit{Acta Cryst. D} \textbf{63}, 1069–1074. (doi:10.1107/S0907444907042230)

Wang, B. C. 1985 Resolution of phase ambiguity in macromolecular crystallography. \textit{Methods Enzymol.} \textbf{115}, 90–112. (doi:10.1016/0076-6879(85)15009-3)

Wilson, K. S. 1978 The application of \textit{MULTAN} to the analysis of isomorphous derivatives in protein crystallography. \textit{Acta Cryst. B} \textbf{34}, 1599–1608. (doi:10.1107/S0567740878006135)

Winn, M. W. \textit{et al.} 2011 Overview of the CCP4 suite and current developments. \textit{Acta Cryst. D} \textbf{67}, 235–242. (doi:10.1107/S0907444910045749)

Whelan, F. \textit{et al.} 2019 Defining the remarkable structural malleability of a bacterial surface protein Rib domain implicated in infection. \textit{Proc. Natl Acad. Sci. USA} \textbf{116}, 26 540–26 548. (doi:10.1073/pnas.1911776116)

Zhang, K. Y. J. & Main, P. 1990 The use of Sayre’s equation with solvent flattening and histogram matching for phase extension and refinement of protein structures. \textit{Acta Cryst. A} \textbf{46}, 377–381. (doi:10.1107/S0108767389012158)

The following publications are those referred to directly in the text. A full bibliography is available as electronic supplementary material at https://doi.org/10.6084/m9.figshare.c.5575594.

(1) 1951 A photoelectric structure-factor machine. \textit{Acta Cryst.} \textbf{4}, 250–253. (doi:10.1107/S0365110X51000830)

(2) 1952 (With H. Lipson) An extension of the use of intensity statistics. \textit{Acta Cryst.} \textbf{5}, 680–682. (doi:10.1107/S0365110X52001854)

(3) 1953 (With D. M. Brown, G. D. Fasman, D. I. Magrath, A. R. Todd & W. Cochran) The structure of adenylic acids \textit{a} and \textit{b}. \textit{Nature} \textbf{172}, 1184–1187. (doi:10.1038/1721184a0)

(4) 1953 The structure of 1:1:6:6 tetraphenylhexapentaene. \textit{Acta Cryst.} \textbf{6}, 838–841. (doi:10.1107/S0365110X53004265)

(5) 1954 (With A. S. Douglas) The statistical theory of sign relationships. \textit{Acta Cryst.} \textbf{7}, 61–64. (doi:10.1107/S0365110X54000102)

(6) 1955 (With W. Cochran) The theory of sign relationships between structure Factors. \textit{Acta Cryst.} \textbf{8}, 1–12. (doi:10.1107/S0365110X55000017)

(7) 1956 An improvement of the ‘heavy-atom’ method of solving crystal structures. \textit{Acta Cryst.} \textbf{9}, 804–810. (doi:10.1107/S0365110X56002187)

(8) 1957 The critical examination of a weak sign relationship between structure factors. \textit{Acta Cryst.} \textbf{10}, 635–638. (doi:10.1107/S0365110X57002224)

(9) 1959 Some new aspects of color perception. \textit{IBM J. Res. Dev.} \textbf{3}, 312–325. (doi:10.1147/rd.34.0312)

(10) 1960 A multi-solution direct method programme for the IBM 704 computer. In \textit{Symp. Computer Methods, Glasgow 1960}. Oxford, UK: Pergamon Press.
(11) Origin of the solar system. *Nature* **187**, 47–48. (doi:10.1038/187047a0)
(12) 1964 Colour vision. *Sci. Progr.* **52**, 177–190. See [https://www.jstor.org/stable/43418978](https://www.jstor.org/stable/43418978).
(13) Colour associated with scotopic vision. *Nature* **202**, 485–507. (doi:10.1038/202278a0)
(14) Lower entropy courses in physics. *Phys. Bull.* **15**, 107–109. (doi:10.1088/0031-9112/15/5/002)
(15) A capture theory for the origin of the Solar System. *Proc. R. Soc. Lond. A* **282**, 485–507. (doi:10.1098/rspa.1964.0247)
(16) 1965 Colour vision. *Royal Society of Health J.* **85**, 197–199. (doi:10.1177/146642406508500407)
(17) 1968 (with G. Germain) On the application of phase relationships to complex structures. *Acta Cryst. B* **24**, 91–96. (doi:10.1107/S0567740868001743)
(18) The evolution of the solar system. *Rep. Prog. Phys.* **32**, 135–185. (doi:10.1088/0034-4885/32/1/303)
(19) 1970 An Introduction to X-ray Crystallography. Cambridge: University Press.
(20) 1970 (With P. Main & G. Germain) On the application of phase relationships to complex structures. II: Getting a good start. *Acta Cryst. B* **26**, 274–285. (doi:10.1107/S056774087000225X)
(21) 1971 (With G. Germain & P. Main) MULTAN: a computer program for the automatic solution of crystal structures. York, UK: University of York.
(22) 1972 (With P. Main & G. Germain) LSAM: a system of computer programs for the automatic solution of crystal structure. York, UK: University of York.
(23) 1974 (With J. R. Dormand) The evolution of planetary orbits. *Proc. R. Soc. Lond. A* **340**, 349–365. (doi:10.1098/rspa.1974.0156)
(24) 1976 In Crystallographic Computing Techniques (ed. F. R. Ahmed, K. Huml & B. Edlacek), pp. 85–114. Copenhagen: Munksgaard.
(25) 1977 (With J. R. Dormand) Interactions in the early Solar System. *Mon. Not. R. Astr. Soc.* **180**, 243–279. (doi:10.1093/mnras/180.2.243)
(26) 1982 Computational crystallography. In *International Summer School on Crystallographic Computing* (ed. D. Sayre), pp. 110–120. Oxford, UK: Clarendon Press.
(27) 1988 (With J.-X. Yao) On the application of phase relationships to complex structures. XXVII: Phase extension for small proteins. *Acta Cryst. A* **44**, 410–413. (doi:10.1107/S0108767388001552)
(28) 1989 (With J. R. Dormand) The origin of the Solar System: the Capture theory. UK/USA: Ellis Horwood/Prentice Hall.
(29) 1995 (With Fan Hai-fu) *Physical and Non-Physical Method of Solving Crystal Structures*. Cambridge: University Press.
(30) (With G. J. Pert) *An Introduction to Computer Simulation*. Oxford: University Press.
(31) (With others) Direct phasing of one-wavelength anomalous-scattering data of the protein core streptavidin. *Acta Cryst. D* **51**, 342–346. (doi:10.1107/S0907444994012266)
(32) 2000 (With J. Foadi, E. J. Dodson, K. S. Wilson, Yao Jia-Xing & Zheng Chao-de) A flexible and efficient procedure for the solution and phase refinement of protein structures. *Acta Cryst. D* **56**, 1137–1147. (doi:10.1107/S090744490000932X)
(33) (With J.-X. Yao, E. J. Dodson & K. S. Wilson) ACORN: theory and practice. *Z. Kristallogr.* **217**, 636–643. (doi:10.1524/zkri.217.12.636.20655)
(34) 2003 (With S. Oxley) Smoothed particle hydrodynamics with radiation transfer. *Mon. Not. R. Astr. Soc.* **343**, 900–912. (doi:10.1046/j.1365-8711.2003.06751.x)
(35) 2004 (With S. Oxley) The formation of planetary systems. *Mon. Not. R. Astr. Soc.* **348**, 1135–1149. (doi:10.1111/j.1365-2966.2004.07417.x)
(36) 2013 (With G. H. A. Cole) *Planetary Science: the science of planets around stars*. Institute of Physics: Bristol.
(37) 2005 (With J.-X. Yao, K. S. Wilson & E. J. Dodson) A modified ACORN to solve protein structures at resolutions of 1.7 Å or better. *Acta Cryst. D* **61**, 1465–1475. (doi:10.1107/S090744490502576X)
(38) 2007 (With M. S. Woolfson) *Mathematics for Physics*. Oxford University Press: Oxford.
(39) 2014 (With M. M. Woolfson) Structural crystallography and direct methods: from rock salt to proteins. *Phys. Scr.* **89**, 108001. (doi:10.1088/0031-8949/89/10/108001)
(40) 2019 (With M. M. Woolfson) Planet formation and the evolution of the Solar System. *Physica Scripta.* **94**, 108001.