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The Teaching of Crystallography: a Historical Survey

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Abstract

The views of several well known crystallographers on how to teach the subject are presented with a description of teaching texts and schools available on a world-wide scale.

1. Introduction

The discovery in 1912 of X-ray diffraction by crystals and the use in 1913 of this physical phenomenon to find molecular structure are two events that have made it possible for us to view molecules in three dimensions. These structural results have had a profound influence on many scientific disciplines, putting each of them on a molecular basis. Fortunately for us, many famous crystallographers have also been inspired teachers, encouraging newcomers to share in their delight in the method and its application. All of us remember the joy of growing our first crystals, our amazement and awe on viewing our first X-ray diffraction photograph, and the excitement of having solved our first crystal structure and being able to analyze what this structure shows us. Such appreciations of the power of X-ray and neutron diffraction of crystals are what the teacher attempts to transfer to the students.

What is the essence of a teacher? It is to give the student the will and the means to learn about a subject so that he or she will have the groundwork and confidence to advance the subject, thereby providing new knowledge. In order to achieve these aims, the teacher needs a good grasp of the subject being taught, a personality that encourages collegial interactions with others, and a willingness to share knowledge, experience and expertise. The brightest students will merge what they have learned from their teachers with their own creativity, so that progress in the subject will result, to the credit of the teachers.

The theme that a primary role of a teacher is to enable the student to know how to find the required knowledge and then to use it productively, putting his own initiatives to work, has been echoed by many crystallographers. Bert Warren (Fig. 1), who was a staunch friend of Lindo Patterson and nurtured this famous crystallographer while he was developing the Patterson function, wrote "the best teaching is the kind that forces a student to teach himself, and thereby learn to think for himself." (Ewald, 1962, p. 667). This thought is also echoed by Martin J. Buerger, a prolific writer and respected teacher (Buerger, 1942), who wrote that students "need the teacher not only to guide them in technical matters, but to transmit a philosophy to them, partly by precept, partly by providing an appropriate atmosphere." (Ewald, 1962, p. 552). He also noted that "The close rapport between student and teacher makes it possible for the teacher to absorb from his students knowledge which has developed since the teacher was involved in formal study, or which the student, with his youthful viewpoint, has seen fit to cultivate . . . " (Ewald, 1962, p. 552). This stresses not only what the teacher can provide to the student, but also what the student can provide to the teacher.

Crystallography has blossomed in the 20th century so that we can now ask broader questions than we could 50 years ago; this is possible because experimental methods and techniques for analyzing the results are greatly improved. We can therefore now encourage students to analyze quite complicated scientific problems which 50 years ago could not have been contemplated. Crystallography in the 21st century will be even more exciting, provided we teach students in such a way that they are sufficiently well schooled to be able to take adequate advantage of the opportunities presented.

The sciences of crystallography and X-ray diffraction can be taught at various levels. Some teachers require

Jenny Glusker (née Pickworth) was born in England and educated at Oxford University, obtaining a DPhil with Dorothy Hodgkin as her supervisor. She was then a postdoc at Caltech working with Corey and Pauling. After that, she moved to Philadelphia to work with Lindo Patterson and has remained there at the Institute for Cancer Research, where she is a Senior Member. She has served as President of the American Crystallographic Association, and as Chairman of the US National Committee for Crystallography and of the IUCr Commission on Crystallographic Teaching. She is currently Editor of Acta Cryst. Section D, has co-authored some teaching texts and has taught at some of the schools mentioned in this article.

students to learn about the overall aspects of the science (the broad brush), while others aim to instruct students in the details of specific aspects of the science, making sure that experiments are properly performed and interpreted (pinpoint detail). Thus, some students will grow crystals and determine their three-dimensional structures and other crystallographic features, while other students (geologists, chemists, biochemists or molecular biologists, for example) merely want to know how the X-ray analysis is performed so that they can assess the results; they do not need most of the detailed information that practicing crystallographers do.

But the role of a teacher is not just to show that the results are interesting and significant, it is also to ensure that the student knows what to do in an analysis, why each stage of the analysis is needed, how the experimental conditions can be varied, how to ensure that the data are as precise as possible, how to interpret results correctly, how to avoid experimental pitfalls and, most important of all, how to design new experiments to test any derived hypotheses. Kathleen Lonsdale wrote "To be able to run an X-ray equipment, to measure and interpret X-ray photographs, to complete a structure analysis and write a paper on it is *not* a sufficient training for a modern crystallographer, any more than to carry out a complicated chemical analysis is sufficient training for a chemist" (Lonsdale, 1953). Thus, while the crystallographer may eventually, in his or her research, concentrate on one aspect of the method, it is important that an overall picture of the science first be presented.

Chemistry and biochemistry journals and textbooks contain so many illustrations of molecular structures determined by X-ray diffraction methods that the general reader now has an interest in the methods used to obtain the data on which these pictures are based. Since these structures are three-dimensional, they can be presented as stereodiagrams (so that the reader can obtain a three-dimensional image) or on a computer graphics screen (so that the diagrams can be rotated and viewed in any desired orientation). The methods for illustrating biological macromolecules, which contain thousands of atoms in each molecule, need simplification if structural information is to be clear. For example, the view of a protein molecule as a ball-and-stick diagram is so confusing to most that it is very difficult to find the overall folding of the backbone of the molecule. Therefore, it is usual when reporting the results of a protein structure determination to replace α-helical structures in the protein by spirals or cylinders and β-strand structure by flattened arrows. Such diagrams now appear regularly in the scientific literature and make it easier to compare folding patterns for diverse molecules. The methods used to obtain the input data to illustrations, that is, how the atomic positions were determined, need description.

Fig. 1. Bertram Eugene Warren.

Crystallography and X-ray diffraction studies of crystals do not just encompass molecular structure determination. There are many other aspects of solid-state structure that can be analyzed by crystallographers, such as molecular motion, diffuse X-ray scattering, the electron distribution within the molecule, solid-state reactions, molecular recognition and reactions at crystal surfaces. André Guinier wrote "If science is really to be opened up to a wider public, scientists themselves must make greater efforts to ease the passage through the barriers formed by the difficulties surrounding their territory. There are cliffs around our subjects that only expert climbers can scale." (Guinier & Jullien, 1989). He encourages us to carve out a path for nonscientists so that they can also enjoy the fruits of our science.

2. The teachers of crystallography and their methods

Crystallography has been rich in excellent teachers, and many of their students have continued this tradition. They have each fulfilled the requirements of a teacher listed in the *Introduction*. Selected examples of teachers, articles, books *etc.* are given here with regrets that the works of so many other excellent crystallographers, equally meritorious, could not be included because of space limitations.

An important attribute of a good teacher is the ability to present the material in as simple a way as possible. The Braggs, both father and son, were able to present very complex physical facts in simple terms with very clear illustrations in diagrams and words. The father, W. H. Bragg, (Fig. 2) gave some memorable 'Christmas Lectures' on the world of sound at the Royal Institution in 1919. E. N. da C. Andrade wrote of W. H. Bragg that "... his personal tone in lecturing which made each member of the audience think that the remark was intended for him, was also more reminiscent of the wise elder brother who was sharing with you the pleasure of a discovery, than that of the great sage who was instructing you. But he was a great sage." (Ewald, 1962, p. 326). He did not feel, writes Kathleen Lonsdale, that he should "produce research problems for ... [students or] ... have to tell them what to do next." (Ewald, 1962, p. 417).

W. L. Bragg, his son, pointed out that "X-ray analysis is a tool; it is in the results that the interest lies." (Bragg, 1975). The first publication of a crystal structure, that of sodium chloride, was made by the Braggs in 1913 (Bragg, 1913) and is commemorated on a British postage stamp (2 March 1977) as one of the great scientific discoveries of the century. What a good way to spread the word to young people, through their hobbies or everyday experiences in receiving letters! The first diffraction experiment that led to a structure determination excited W. L. Bragg and he hastened to explain in simple terms what he was doing. It always amazed me since my days as an undergraduate that the first demonstration of X-ray diffraction by Friedrich, Knipping and von Laue in 1912 was followed almost immediately by those works in which the atomic arrangement in some simple salts and elements were quickly determined and published in 1913 (Bragg, 1913). This happened because many understood deeply the principles of physics so that, when the discovery was made by von Laue and co-workers, their superb training in physics quickly came to the fore and could be utilized. No better reason for excellent teaching could be found in history.

The lecture demonstration is at the heart of the teaching of science, because otherwise the student might interpret the science as a purely theoretical exercise; new data are essential if a science is to survive. Some sterling tips on how to do this are provided in a delightful book by Charles Taylor (Taylor, 1988). The author, who is writing about an "illustration of a point in a lecture or lesson by means of something other than conventional visual-aid apparatus", stresses the importance of setting up demonstrations with care, but also gives some tips on what to do if the experiment fails or some other disaster takes place (his lecture emergency list). He writes, however, "I think there is a case for showing that experiments do not always work the first time and much could be learned by the students watching how the lecturer discovers the fault and corrects it". His overall advice is to "Tell them what they are going to see or hear and what to notice particularly; then do the demonstration; then remind them of what they should have seen or heard".

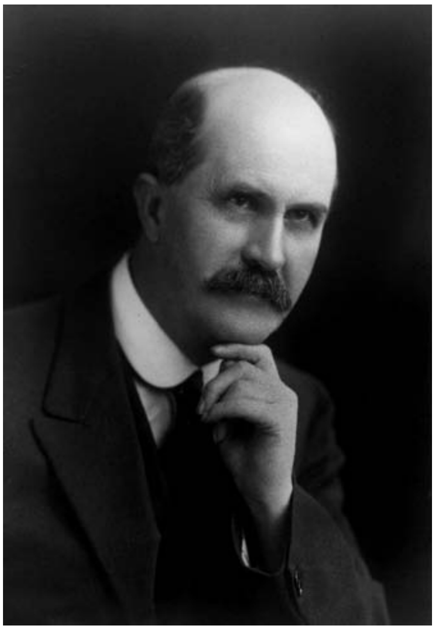

Fig. 2. William Henry Bragg.

From my own experience, I would say that one of the most inspiring lecturers that I heard as a student was Bill Astbury, who did so many fundamental studies of fiber structure (Astbury, 1933). He had found that what he called α-keratin was the normal form of the mammalian material, but that on stretching he could obtain the elongated β form which could be reconverted to the α form when the tension was released. Astbury was also involved in the production of tables of the 230 space groups, a publication that the Royal Society had to reprint, a rare event. J. D. Bernal wrote of Astbury (Ewald, 1962, p. 524) "At a time when there was no possibility of working out the structure of compounds much more complicated than naphthalene, he willingly attacked the totally unknown field of proteins where even chemical analysis was absent". P. P. Ewald wrote (Ewald, 1962, p. 354) that Astbury was "the soul and activator of the keen group of young workers that Sir William had brought together there. ... The reason for this lay in his unlimited enthusiasm for the new subject of crystal structure analysis, his temperamental approach, and the unexpected and perhaps provocative, but often most helpful turns in his conversation. ... Astbury's unsinkable optimism helped him along where more anxious scientists might have feared to tread". He projected this energy into his teaching with excellent results. I heard him give a lecture on only one occasion, but I can still remember its contents clearly. We need to emulate his teaching skills.

Another requirement of a teacher is that the subject should be concisely presented without too much verbiage. Writing of his own teacher, Walter H. Newhouse, Buerger said "Every student needs a wise and inspiring teacher. ... Newhouse has a feeling for relevance, and always stripped a matter of its extraneous wrappings and went directly to the core." (Ewald, 1962, p. 550). Len Muldawer wrote of Bert Warren (McLachlan & Glusker, 1983, p. 44): "He began with the fundamentals and developed the solution to the problem. ... with inexorable logic. There was never any fuzziness; only after the argument had been carried as far as possible were assumptions inserted. ... When we worked on problems for Warren, we were experimental and theoretical physicists". Ben Post wrote of

Fankuchen (Fig. 3) (McLachlan & Glusker, 1983, p. 54): "Fan's lectures were always clear and concise; they were delivered with enthusiasm, patience and humor. He managed to convey to his students a sense of scientific excitement and a feeling of participation in the research he discussed. . . . It is probably no exaggeration to state that as many as one half of the total membership of the American Crystallographic Association in the 1950's and early 1960's had, at one time or other, attended at least one of Fan's courses".

Another great teacher who gave memorable lectures was Linus Pauling, a crystallographer throughout his life time, who extended structural results to chemistry and biology with great flair, and also was one of the kindest and friendliest persons I have ever met. His book *The Nature of the Chemical Bond* (Pauling, 1960), which reflects his crystallographic background, has had an important influence on organic and inorganic chemistry and his work on protein structure revolutionized protein chemistry and led to an understanding of helical diffraction by others so that he can be considered a grandfather of the double helix of DNA first reported by Watson and Crick. Linus lectured at Caltech with a slide-rule tie clip which he would remove when needed and, with a big grin from ear to ear, would do a calculation and read the answer to four or five significant figures; his answer was always correct because he remembered what it should be. This little demonstration served to remind the student about significant figures, and impressed them with his super memory. Another memorable lecturer with a good sense of humor was Dan McLachlan who would always give well attended thought-provoking talks at meetings of the American Crystallographic Association "with the special sort of imagination and ingenuity that has characterized all of his work", as remarked by Betty Wood (Ewald, 1962, p. 443).

Fig. 3. Isidor Fankuchen.

The optimum content of lectures in the teaching of crystallography has been the subject of much debate. What exactly is 'crystallography'? Before the discovery that X rays could be diffracted by crystals there was an extensive science of crystallography, mainly involving mineralogists and geologists. Many nineteenth century teachers are listed by José Lima-de-Faria, who writes (Lima-de-Faria, 1990) "although the microscope was discovered early in the 17th century and applied with great success to the study of biological problems in the second half of this century, . . . it was not applied efficiently to minerals and rocks until the middle of the 19th century . . . ". The teacher of the 19th century would expound on the symmetry of crystals, Miller indices, crystal lattices, point groups, space groups and twinned crystals. An expert in this teaching in the 20th century was José Donnay, the maintainer of crystallographic standards. He used to stand up in crystallographic meetings and inform the speaker if, for example, the crystal axes in a diagram on the screen had been assigned in a non-standard manner, thereby reminding the entire audience of the importance of such standards. The newer crystallographers of the 20th century learn about the details of the experimental systems that must be set up to detect X-ray diffraction (powder cameras, diffractometers, Laue methods, devices for measuring diffraction at low temperatures, apparatus at synchrotron sources *etc.*), how to measure intensities (a rapidly changing field originally involving photographic film but now utilizing sophisticated devices such as charge-coupled detectors) and index each, how to calculate structure factors and how to determine and refine the structure (now greatly simplified by the advent of high-speed computer systems). Henry remarked "a division between the 'old' and the 'new' in crystallography still persists, although it ought to disappear with the development of a modern syllabus of crystallographic education" (Henry, 1953). The International Union of Crystallography has worked hard to help the merging of these two branches of crystallography into one by encouraging the publications of books and articles in their journals and the various activities of the Commission on Crystallographic Teaching. Now, at the end of the 20th century, we can appreciate the multi-dimensional nature of modern crystallography. It is far more extensive than the determination of molecular structures by X-ray diffraction, even though the sizes of molecules and their complexes that can be studied are impressive. Crystal growth, physical properties and electron distribution within the crystal are among the many aspects now under investigation and available for description in a course on crystallography.

A main problem in teaching about crystal structure determinations is making clear to the student the connection between the diffraction pattern and the electron-density map. This hurdle was overcome for me when I read J. M. Bijvoet's book (Fig. 4). In it he noted that "the harmonic density wave of period d/n gives only an nth-order reflection" (Bijvoet *et al.*, 1951, p. 105). This concept can be developed to teach the relationship between the electron density and the diffraction pattern and between Fourier analyses and Fourier syntheses. An alternative way of viewing this (Bragg, 1944) has been wonderfully shown by Charles Taylor and Henry Lipson in volumes containing pictures of a wide variety of arrangements of holes in diffraction masks and the resultant diffraction pattern (Taylor & Lipson, 1964; Harburn *et al.*, 1975). Photographs in this book accentuate the optics of diffraction, and also show the relationship between structure and the diffraction pattern.

Mentoring is also an important component of teaching; it can provide trustworthy and experienced counsel, and a life-time friendship. W. H. Bragg, father of W. L. Bragg, introduced many women to the science of crystallography and encouraged them to pursue this science. Probably the most famous of W. H. Bragg's women students is Kathleen Lonsdale (Fig. 5). She ultimately became a star in the field and determined the crystal structure of hexamethylbenzene in 1928 (Lonsdale, 1928) using a precursor to direct methods to do so; this was the experiment that showed that the benzene ring has a regular planar hexagonal structure. While she was doing this work and raising a young family of three children, W. H. Bragg arranged for her to receive a grant to pay for a housekeeper to look after the children so that she could work in the laboratory (Ewald, 1962, p. 599). In a similar way, J. D. Bernal, who inspired many and was known as 'Sage', encouraged Dorothy Hodgkin, who went on to win a Nobel Prize in chemistry. These mentors set examples that many followed.

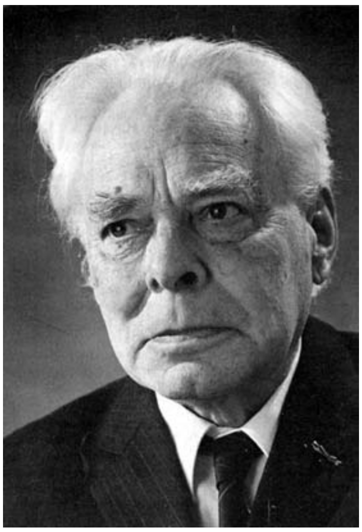

Fig. 4. Johannes Martin Bijvoet.

The mentoring talents of some of the great teachers were evident at scientific meetings. Isidor Fankuchen was particularly good at this and the ACA teaching award is given in his honor. Lindo Patterson used to approach young crystallographers giving their first presentations at a meeting, and congratulate them, telling them how well they did – a very positive experience for the young scientist. Dorothy Hodgkin made a point of attending talks for which the audience was small and encouraged her students to do likewise. Sometimes interactions in the discussion periods at meetings between well known scientists provide food for thought. I remember W. L. Bragg gently chastising Kathleen Lonsdale at a meeting because it was obvious that the student who was presenting the paper had not been instructed in how to derive a heavy-atom position in the structure of a small molecule simply by looking at the diffraction photograph. 'Do you mean,' he said, 'that you do not teach your students how to do this?' Most students nowadays cannot do this, often because their structure is more complicated that those studied by W. L. Bragg, and also, possibly, because they do not spend time examining X-ray diffraction photographs.

3. The dissemination of crystallographic information

Worldwide teaching can take place in a variety of ways. One of these is the publication of books on subjects that crystallographers need to know about. The Commission on Crystallographic Teaching of the International Union of Crystallography also produces pamphlets on specific subjects for teachers to use in their courses. These were originally the idea of Professor Charles Taylor and they are concise, mainly stressing the essentials of a particular subject, together with a list of additional sources of information on the subject. The International Union of Crystallography has also published a brief but very useful teaching edition of Volume A of *International Tables for Crystallography* (Hahn, 1993), which contains

Fig. 5. Kathleen Lonsdale.

symmetry information on the 17 plane groups (which all students should find helpful to work through) and examples of the common space groups. A second method of dissemination of information is *via* electronic media. Videotapes are not entirely satisfactory for this because there are no worldwide standards for them so that a video cassette that can be read on an instrument in one country may not be readable with the commonly used equipment of another country (unlike audio tapes which are universally readable). On the other hand, much information on crystallographic techniques and results is now available on the World Wide Web. Many students now start their research there rather than in the library.

Books and web-site information are very useful to students, but it is best to have teachers who can instruct students in a person-to-person environment. The Commission on Crystallographic Teaching of the International Union of Crystallography has tackled the problem of how to teach students on a worldwide scale, making state-of-the art instruction available to all, no matter what part of the globe they live in. Two mechanisms have been used to facilitate this. Teaching Schools have been held in various countries and an effort has been made to bring as many students as possible to these schools from neighboring countries. A set of lecture notes is prepared beforehand by each teacher and a text is made from them by the organizers after the meeting and is given to each student that attended. The second mechanism has been by way of the Visiting Professorship Programme, originally suggested by Professor Henk Schenk, in which a teacher or group of teachers is sent to a particular university, anywhere in the world, that has requested this. A series of lectures, tutorials, and demonstrations on crystallographic topics on the subject requested by the host institution is given over a period of a week or longer. The host institution provides one co-tutor per 15 students to work in cooperation with the Visiting Professor(s), particularly in the practical experimental classes. This is helpful in ensuring that the students, who are generally not native English speakers, fully understand what they have heard in lectures. The teacher, therefore, travels to the student rather than the other way round as for the Teaching Schools. These two mechanisms are sometimes merged so that Visiting Professors can take part in Teaching Schools when appropriate.

The overall aim of the Visiting Professorship Programme is to provide high-level teaching to students throughout the crystallographic world. All who have performed this have found it to be a very rewarding experience and have enjoyed their interactions with dedicated and lively students. Visiting Professors have traveled to Vietnam, the People's Republic of China, Sri Lanka, Russia, Egypt, Argentina and Venezuela, to name a few. The International Union of Crystallography covers travel and insurance and the host organization provides food and appropriate lodging. Sometimes there are challenges for the Visiting Professors, such as equipment that does not work, or is lacking. On the other hand, the first Visiting Professor was reported in a letter from the university he taught at to have "won the hearts of our students with his extremely lucid and clear approach to teaching an otherwise difficult subject". As for all teaching, time spent trying to make the subject 'crystal clear' is time well spent.

Some Teaching Schools have taken place at Erice, Italy, a lovely medieval hilltop town that serves as a wonderful milieu for the mixing of students from various parts of the world. International Union of Crystallography Teaching Schools have also been held in Tianjin (China), Bangkok (Thailand), Madras (India) (Schenk *et al.*, 1987), and many other places throughout the world. The most recent one was held 5–11 April 1997 in Suez, Egypt (El-Sayed & Ramadan, 1997). Dedicated teachers, such as Ken Trueblood (Fig. 6) and Bob Sparks, also organize independent teaching schools in their own country.

There are many books on details of the subject of crystallography. Some are general and cover wide aspects of the subject. A series of books on the crystalline state, edited by W. L. Bragg, was important for early understanding of crystallography (Bragg, 1949). So was the book by Kathleen Lonsdale (which was my personal introduction to crystallography) (Lonsdale, 1948). Charles Bunn (1961) wrote a book that helped many of us understand the intricacies of X-ray structure analysis in more detail. These books highlighted the importance of simplicity in getting the message across to as many readers as possible. A book that dealt with the subject in greater depth was the information-packed text on the optical physics of X-ray diffraction by R. W.

Fig. 6. Kenneth Nyitray Trueblood.

James (1958, 1965). This was generally viewed by students as a difficult book to read, but many students found that if they put some effort into reading it they gained much new insight into diffraction by crystals. Methods used to determine crystal structures in the mid-1950s, together with many of the molecular structures so found, were presented by J. Monteath Robertson in a book that we all treasured (Robertson, 1953). Jack Dunitz, who studied under Robertson, later wrote a much used text that contained detailed mathematical and physical explanations for the processes invoked by X-ray crystallographers together with overviews of some of the chemical and conformational results so obtained (Dunitz, 1995). Many other books on broad aspects of crystallography have resulted (Lipson & Cochran, 1953, 1966; Nyburg, 1961; Wheatley, 1968; Sands, 1969; Bacon, 1975; Steadman, 1982; Glusker & Trueblood, 1985; Paufler, 1986; Stout & Jensen, 1989; Vainshtein *et al.*, 1992; Ladd & Palmer, 1995).

Some wonderful books on more specific aspects of crystallography are also available. The history of the subject can be used to teach how crystallographic methods were developed through the years and the scientific principles on which they were based (Burke, 1966; Bijvoet *et al.*, 1969, 1972; Schneer, 1977; Bragg, 1975; Glusker, 1981). Crystal growth has been a favorite occupation of school-age children, particularly the recipes in the book by Holden & Singer (1960), which have provided so many ideas for 'science fairs'. More recently, information can be obtained from books by McPherson (1982) and Ducruix & Giegé (1991); the latter book contains some specific recipes such as for the growth of lysozyme crystals. When teaching about the geometry of crystals, books such as that by Phillips (1971) have been found to be very useful. Optical properties of crystals are described by Shubnikov (1960), Wood (1977), Wahlstrom (1979) and Nye (1985). A superb source of information on diffraction is contained in the set of lectures by Feynman, himself a renowned teacher of physics (Feynman *et al.*, 1963). Several good books and articles have been written to help explain Fourier series to students (Waser, 1968; Glasser 1987*a*,*b*; Steward, 1987). Structure determination by direct methods is difficult to teach, but help can be obtained from various volumes on the subject (Woolfson, 1961; Ladd & Palmer, 1980). There are many excellent books on macromolecular crystallography ranging from details of the method to illustration of the results (Holmes & Blow, 1966; Rossmann, 1972; Blundell & Johnson, 1976; Drenth, 1994; Helliwell, 1992). Finally, analyses of the overall significance of the results have been gathered in many books and articles (Wells, 1962; Kitaigorodsky, 1973; Desiraju, 1989; Bürgi & Dunitz, 1994).

There are also some books for the general public, such as photographs of snowflakes (Bentley & Humphreys, 1931) and of minerals (Gramaccioli, 1986) and illustrations of symmetry in which the works of artists such as M. C. Escher are featured (MacGillavry, 1976; Heilbronner & Dunitz, 1993). Books such as *The Path to the Double Helix* (Olby, 1974) and *The Eighth Day of Creation* (Judson, 1979) are examples of studies of DNA from both a historical and a scientific point of view and make good reading for the student because the background to the work is so eloquently presented. The description of the Patterson function in *The Eighth Day of Creation* is the best that I have yet seen. More general books, such as *The Structure of Matter: from the Blue Sky to Liquid Crystals* by André Guinier, provide a general overview of molecular structure, ranging from the crystalline state to gases ('plastics, rubber, concrete and even mayonnaise' as he says in the Foreword) (Guinier, 1984).

4. The impact of crystallography on the teaching of chemistry, biochemistry, biology

General texts in chemistry, biochemistry, biology, geology and solid-state physics are full of diagrams of molecular structures determined by X-ray diffraction. Illustrations are becoming increasingly improved and more instructive with time. But the main impact of crystallography on biology is the information that it has given on three-dimensional structure so that we now know the stereochemistries of the active sites of many enzymes, the manner by which substrates and inhibitors bind to them, the structures of nucleic acids and their modes of interaction with proteins, and the structural organization of viruses. Excellent examples can be found in the biochemistry text by Voet & Voet (1995) which combines biochemistry and crystallography. Organic and inorganic chemistry texts have also profited from X-ray diffraction results. These have provided the chemical formulae of natural products and the modes of metal coordination to complexing agents. Chemists now teach about symmetry (Cotton, 1971) and the sizes of atoms and ions (Cotton & Wilkinson, 1988). Biochemists learn about hydrogen bonding (Jeffrey, 1997), nucleic acid structure (Saenger, 1983), α-helices, β-strands and protein folding in general (Brändén & Tooze, 1991), the stereochemistries of enzyme reactions (Dickerson & Geis, 1969; Voet & Voet, 1995) and the multimolecular complexes involved in DNA transcription (Steitz, 1993).

A main modern development in communication and provision of information to chemists, biochemists and biologists lies in the World Wide Web. For example, this now provides a simple way to access the atomic positions of atoms in proteins in the Protein Databank. As a result, molecules can be displayed on a computer graphics system by the use of programs developed from the early program *ORTEP* used to display small molecules (Johnson, 1965, 1971). Macromolecular structures can be viewed by programs such as *Molscript* (Kraulis, 1991) and *Rasmol2* (Sayle, 1994). The molecules so displayed can be rotated, colored in various ways, inspected, labeled and truncated at will. This provides a superb way for students to analyze molecular structure themselves, sitting at a computer console.

Finally, interesting trends that will be further developed in the 21st century include the visualization of protein reactions by Laue techniques, studies of reactions on the surfaces of crystals and studies of electron distributions in molecules, which lead to an understanding of the chemical reactivity of the molecule. In the last 50 years, since *Acta Crystallographica* was started, the science of crystallography has greatly advanced. There is still room for further advancement – for the manufacture of X-ray lenses and the use of holography to aid in this – and the teaching of the early 21st century must prepare students for these and other as-yet unpredicted advances in the field.

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