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Dorothy Crowfoot Hodgkin (1910–1994)

Within this world there are great scientists whose passing leaves the world saddened, but who gave so much to make the world a richer place. One of these, Dorothy Hodgkin, passed away on July 29, 1994. She was a dedicated scientist and a friend to all who knew her. In 1964 she won the Nobel Prize, unshared, in chemistry "for her determination by X-ray techniques of the structures of biologically important molecules." These include the structures of cholesteryl iodide (which showed the skeleton of steroids), the chemical formulae of penicillin, vitamin B_{12}, and vitamin B_{12} coenzyme, and, later, the three-dimensional structure of the protein hormone insulin. She had the courage, skill, and sheer willpower to extend the method of X-ray diffraction analyses of crystals to compounds that were far more complex than anything attempted before. Jack Dunitz, who worked in her laboratory for several years, wrote: "Dorothy had an unerring instinct for sensing the most significant structural problems in this field, she had the audacity to attack these problems when they seemed well-nigh insoluble, she had the perseverance to struggle onward where others would have given up, and she had the skill and imagination to solve these problems once the pieces of the puzzle began to take shape. It is for these reasons that Dorothy's contribution has been so special" (Dunitz, 1981).

Dorothy Crowfoot Hodgkin in 1970 when she came to the Fox Chase Cancer Center to describe the newly determined crystal structure of insulin in the first Patterson Memorial Lecture entitled, "X-ray analysis and the structure of insulin."

Dorothy was born Dorothy Mary Crowfoot on May 12, 1910, in Cairo, Egypt. Her father, John Winter Crowfoot, was an archaeologist and historian in the Egyptian Ministry of Education and subsequently the Principal of Gordon College at Khartoum and Director of Education and Antiquities in Sudan. Later he worked at the British School of Archaeology in Jerusalem. Her mother, Grace May (Molly) (née Hood), was an expert on the history of ancient textiles, and wrote a book on the flowering plants of Sudan. Dorothy, the eldest daughter, had three sisters with whom she remained close during her entire life. She lived with her family in Sudan for a time, but during the first World War, because of the fear of attacks on British colonies, Dorothy and her sisters were sent back to England. There she lived with her grandmother and attended a small private school. This experience, she believed, was the origin of her independent spirit. In 1918, as soon as the war was over, Dorothy's mother returned to England. Thereafter, both parents spent each summer in England, and the rest of the year in Sudan. Dorothy attended to a coeducational school, the Sir John Leman School, in Beccles, Suffolk, and her interest in science started early. She was encouraged by a family friend, Dr. A.F. Joseph ("Uncle Joseph"), a soil chemist at the Cairo branch of the Wellcome Laboratory. When Dorothy left Sudan, Dr. Joseph gave her a portable chemical laboratory complete with apparatus for mineralogical analyses. The archaeological studies of her parents also interested Dorothy. Just before going to college, Dorothy assisted her parents, who were living in Jerusalem, with excavations at Jerash in Transjordan. She was particularly intrigued by the elegant geometric patterns of the mosaic pavements that were found (McGrayne, 1993).

Dorothy obtained her undergraduate education in chemistry at Somerville College, Oxford, obtaining a Science Prize in 1930. Her X-ray crystallographic research career started with her studies of thallium dialkyl halides with H.M. ("Tiny") Powell, a demonstrator under H.L. Bowman, the professor of mineralogy and crystallography. This comprised the research part of her undergraduate degree (Powell & Crowfoot, 1932). She graduated from college with a B.A. degree with first-class honors and a B.Sc. degree. Then it was necessary for her to look for a position and "Uncle Joseph" introduced her to T. Martin Lowry, who advised her to work with John Desmond (JD) Bernal (affectionately called "Sage"). She took his advice and obtained a Ph.D. at Cambridge University in 1937, working with Bernal from 1932 to 1936. Her work there, in that very exciting laboratory, reinforced her lifelong interest in structural biochemistry. Somerville College was, however, eager for Dorothy to come back to Oxford. They awarded her a Vernon Harcourt Scholarship in 1932 and a Research Fellowship from 1933 to 1935, even though she was attached to Newnham College, Cambridge.

During her years in Bernal's laboratory Dorothy took many X-ray diffraction photographs. In 1934, Bernal and Dorothy

first reported on the diffraction pattern of a crystalline protein, pepsin, pointing out that in order to obtain good diffraction patterns, the crystals of proteins should not be dried, but should be studied surrounded by their mother liquor (Bernal & Crowfoot, 1934). Air-dried protein crystals gave very poor, if any, diffraction patterns, while those crystals that were kept in their mother liquor gave nice diffraction spots on photographic film. In fact, Dorothy was not in the laboratory on the day that the first X-ray diffraction photographs of a protein were obtained, because her parents had taken her to London to see a specialist about some health problems which were the beginning of rheumatoid arthritis. She subsequently took many X-ray diffraction photographs of proteins, and, in October 1934, obtained X-ray diffraction photographs of crystals of insulin (Crowfoot, 1935). Even though Dorothy corresponded with A. Lindo Patterson on his vector map method of analysis, the methods for interpreting these diffraction photographs could not, at that time, lead to a protein structure determination. In retrospect, she wrote of the Patterson maps of insulin that she had calculated: "These old patterns ... do correspond rather well to the pattern you get just from the main chain distribution in insulin, in spite of the complexity of the pattern" (Hodgkin, 1987).

While working in Bernal's laboratory Dorothy also became interested in steroids and their structures. Bernal had shown that X-ray diffraction photographs were not compatible with the then-accepted Windaus–Wieland formula because the latter could not be fit into the unit cell in the orientation indicated by the refractive index measurements (Bernal, 1932). Bernal's published note on the subject led to a revision of the chemical formulae of steroids. Dorothy, with Bernal and Isidor Fankuchen, studied crystals of over one hundred steroids and reported their unit-cell dimensions, refractive indices, and probable packing and hydrogen bonding (head-to-head or head-to-tail, for example) in a monumental study (Bernal et al., 1940).

It was then necessary for Dorothy to begin her own scientific career. In 1936, she became a Tutor and Fellow of Somerville College. She missed the camaraderie of Bernal's laboratory, however, and went back often during these early years. Oxford provided her with a scientific and intellectual environment free from most of the usual burden of administrative formalities, and she was given much moral support by the principal of Somerville College, hematologist Janet Vaughan. Dorothy was made a University Lecturer and Demonstrator in 1946, but did not become a University Reader until 1955. As was the Oxford tradition, she made students work hard and did not spoon-feed them. Somerville College admitted only women, but its students did laboratory work, attended lectures, and took examinations with all the other students, men and women, in various disciplines of study. The system at Oxford in the 1950s allowed women tutors to obtain Oxford University positions as lecturers and demonstrators, in addition to their appointments in the individual colleges. There were, at that time, 23 men's colleges and 5 women's colleges (most are now coeducational). Dorothy had students who were doing Part IIs (the fourth-year practical research part of the chemistry degree) and students who were doing D.Phils. One of her Part II students was Margaret Roberts, later Margaret Thatcher, Prime Minister of Great Britain and the only British Prime Minister with a degree in science.

Dorothy's laboratory in Oxford was in the Ruskin Science Museum, an old gothic building. The room where she worked was the room in which Thomas Henry Huxley successfully debated Bishop Samuel Wilberforce on the subject of evolution in an historic debate on June 30, 1860, at a meeting of the British Association for the Advancement of Science. The laboratory itself also had gothic qualities. Housed in a tiny gallery, the crystal mounting equipment and polarizing microscope were reachable only by ladder-like steps. Using the steps was hard for Dorothy, who was having trouble with arthritis, but she never lost a crystal while climbing up or down. Very soon she had two graduate students, both of them, by chance, male. Her first graduate student was Dennis Riley, who joined her in 1937. He was excited by a lecture she gave on steroids and wrote: "Here was I, a member of a prestigious college, choosing to do my fourth year's research in a new borderline subject with a young female who held no university appointment but only a Fellowship in a women's college" (Riley, 1981). Riley worked on preparing protein crystals and attempting to obtain diffraction patterns for lactoglobin, insulin, and several other proteins (Crowfoot & Riley, 1939).

During World War II Dorothy was joined by Bernal's collaborators, C.H. Carlisle and Dr. Kathe Dornberger-Schiff. Harry Carlisle was Dorothy's second graduate student and she interested him in the structure of steroids, another result of her work with Bernal. She now aimed to determine the molecular structure of cholesteryl iodide by locating each atom in the crystal structure. A crystallographic investigation of cholesteryl bromide and chloride had formed part of her Ph.D. thesis at Cambridge, but no molecular structure had yet come out of that work. Dorothy pioneered the use of Patterson maps in the determination of the structure of cholesteryl iodide, as she was always on the lookout for new and better ways to solve structures. The iodine positions were found from the Patterson map, and electron-density maps phased on these positions were then calculated. Dorothy had an uncanny ability to pick out a molecule from an electron-density map that contained symmetry-related artifacts, such as were present in maps of the crystal structure of cholesteryl iodide, and later, penicillin. Cholesteryl iodide was one of the first analyses based on three-dimensional calculations, and it established the relative stereochemistry at each carbon atom of the steroids (Carlisle & Crowfoot, 1945). This result was verified by other subsequent crystallographic studies of steroids (Crowfoot & Dunitz, 1948). Dorothy never published a result until she was sure it was right.

Dorothy had many other graduate students, including Barbara Rogers Low, Pauline Cowan Harrison, Monica Curzon Webster, Jenny Pickworth Glusker, Ted Maslen, Jennifer Kamper, David Dale, Roger Diamand, Carol Saunderson Huber, Anthony Cooper, Michael James, Frank Moore, C.E. Nockolds, Sofia Candeloro de Sanctis, Eric Edmond, H.R. Harrison, S.M. Cutfield, David Sayre, Marjorie M. Harding, Margaret Adams, and Judith Howard. Eleanor Dodson, who came from Australia, said of Dorothy's laboratory: "I loved the internationalness of it, feeling part of a world community. We all felt that we were equals – it was just that Dorothy knew more" (Ferry, 1994).

Dorothy's next big venture was the determination of the chemical formula of penicillin. This antibiotic changed the course of the management of human infectious diseases. Penicillin was discovered in a mold by Alexander Fleming at St. Mary's Hospital, London, in 1929. Then, at Oxford, Howard Florey and Ernest Chain proceeded to isolate the antibiotic from the mold. World War II, with its many casualties, was in progress and the

determination of the chemical formula of penicillin was vital. Chemists were working hard on the problem. Dorothy obtained crystals of penicillamine hydrochloride in the summer of 1942, and she and Barbara Rogers-Low studied crystals of several derivatives using the very antiquated equipment of Dorothy's laboratory. The correct determination of the molecular formula came from X-ray analyses of the sodium, potassium, and rubidium derivatives of benzylpenicillin by use of isomorphous replacement, optical analogues, and difference maps. This work was jointly reported by Dorothy and Barbara Rogers-Low from Oxford, and by Annette Turner-Jones and Charles Bunn from Imperial Chemical Industries (Crowfoot et al., 1949). They found that the formula contained a four-membered ring of three carbon atoms and one nitrogen atom. This was the β-lactam structure with which Sir Robert Robinson, the organic chemistry professor at Oxford at that time, disagreed because such chemical rings are generally unstable while penicillin seemed reasonably stable. John Cornforth, another organic chemist, is reported to have threatened to give up chemistry and grow mushrooms if the chemical formula was shown to contain a β-lactam ring. Dorothy did, indeed, determine the correct formula, but, fortunately for science, Cornforth did not keep his promise. This chemical formula served as the starting point for many chemical modifications that have been successfully used as antibiotics, such as the cephalosporins and thiostrepton for which Dorothy also later determined the crystal structures (Hodgkin & Maslen, 1961; Anderson et al., 1970).

Another chemical formula that Dorothy determined was that of the anti-pernicious anemia factor vitamin B_{12}. Pernicious anemia, a fatal disease, was found by Minot and Murphy in 1926 to be treatable by liver extracts, and, in 1948, the active factor was isolated from liver in crystalline form as beautiful, deep red crystals. E. Lester Smith brought these crystals from Glaxo Laboratories to Oxford so that Mary Porter and R.C. Spiller could study them and determine from their unit-cell dimensions and refractive indices if they were the same as those isolated by Karl Folkers at Merck Laboratories (Hodgkin et al., 1950). Dorothy was excited at the crystals' appearance and immediately measured their unit-cell dimensions and molecular weight. The subsequent crystal structure of the vitamin and several analogues took many years. It was achieved by use of heavy-atom methods and the detailed examination of many three-dimensional electron-density maps (that Dorothy was so good at). The possibility of studying so many three-dimensional maps came about because Ken Trueblood of UCLA approached Dorothy at a meeting and asked if she had diffraction data on any large crystal structures that he could use to test his computer programs. The programs he had written were for one of the largest computers of that time. Refinements of electron-density maps were done by an exchange of new maps and new atomic parameters between Oxford and UCLA. Dick Prosen and Bob Sparks assisted with the computational aspects. This collaboration boosted three-dimensional studies of crystal structures over the the less satisfactory two-dimensional studies that were common at the time due to computer limitations.

The structure obtained for vitamin B_{12} was that of a porphyrin-like ring with one bridging carbon atom missing so that two pyrrole rings were directly linked, and with each of the β-positions of these rings fully saturated (Brink et al., 1954; Hodgkin et al., 1955). Later Galen Lenhert showed in Dorothy's laboratory that the coenzyme contains a cobalt-carbon bond, making it the first known naturally occurring biologically significant organometallic compound (Lenhert & Hodgkin, 1961). The early work on vitamin B_{12} was done with June Broomhead Lindsey, Clara Brink Shoemaker, Jennifer Harrison Kamper, Ken Trueblood, John H. Robertson, Maureen Mackay, myself, John White at Princeton University, and many others. Crystals of a hexacarboxylic acid degradation product served to define precisely the atomic arrangement in that part of the vitamin that had eluded chemical identification. The crystals were grown by Jack Cannon in Alexander Todd's laboratory in Cambridge. W.L. Bragg, in *Fifty years of X-ray diffraction* (Bragg, 1962), described the B_{12} structure determination as "breaking the sound barrier," meaning that it led to new horizons in the field. This refers to the possibility of using heavy atoms as a means of determining the structures of biological macromolecules as suggested by J. Monteath Robertson (1939). Dorothy used the cobalt atom to phase the electron-density maps of the hexacarboxylic acid, even though everyone advised her that it would not work because the scattering power of the cobalt atom was too weak with respect to the rest of the molecule. Later vitamin B_{12} was synthesized by Robert B. Woodward and Albert Eschenmoser, thereby confirming the X-ray crystallographic result. Since Dorothy's method worked so well, people were then encouraged to tackle the crystal structures of proteins.

Dorothy took the first X-ray diffraction photographs of insulin in 1935 and, from that time, until 34 years later when the crystal structure was solved, she was confident that the molecular structure could be determined from the X-ray diffraction pattern. The sequence of amino acids in insulin, the first protein to be sequenced, was known from the work of Fred Sanger. In 1969, the structure of rhombohedral 2Zn insulin at 2.8 Å resolution was reported from Dorothy's laboratory. This showed the insulin hexamer as a trimer of dimers, and provided an atomic model of the protein. In China, Chinese crystallographers, led by Tang You Chi, also worked on the crystal structure of insulin. Dorothy and You Chi had met in California in 1947, and again, in China, in 1959, when Dorothy traveled there to compare and note differences (which mainly involved the side chains) between the electron-density maps of the two structure determinations. She also made a point of bringing the state of science in China to the attention of those in the West, since the Chinese at that time had no efficient way to communicate their scientific results throughout the world. In the insulin work Dorothy was assisted by Margaret Adams, Marjorie Harding, Ann Kennedy, Eleanor Dodson, Pauline Cowan Harrison, Guy Dodson, Siv Ramaseshan, Tom Blundell, M. Vijayan, Ted Baker, Beryl Oughton Rimmer, Dan Mercola, and many others (Dodson et al., 1966; Adams et al., 1969; Bentley et al., 1976).

Dorothy was made a Fellow of the Royal Society in 1947 (when she was only 37), and received an endowed professorship, the Wolfson Research Professorship of the Royal Society in 1960. She held this post until her retirement in 1977. She was then made fellow of Wolfson College, Oxford, 1977–1982. Dorothy received the Royal Medal of the Royal Society in 1957 and the Copley Medal in 1976. She won the Nobel Prize in Chemistry in 1964, the third woman to receive this prestigious award in the field of chemistry, following Marie Curie (1911) and Irene Joliot-Curie (1935), and the only British woman to do so. Dorothy served as President of the International Union of Crystallography, 1972–1975, and as President of the British Association for the Advancement of Science, 1977–1978. She received the

Order of Merit, the highest civilian honor in Great Britain, in 1965. She was the second woman to receive it, the other being Florence Nightingale in 1907. She was relieved that it was not the title of "Dame" which she said she would not have liked (Perutz, 1981). Dorothy had honorary degrees from many universities. She was Chancellor of Bristol University from 1970 through 1988, where, unlike most other Chancellors, she made a point of meeting students and talking to them. It is reported that, while giving her address at the University she told the graduates of the importance of education and research in this modern world, and then gave the advice to "live modestly and do serious things" (Dodson, 1994).

In 1937, Dorothy married Thomas Lionel Hodgkin, a tutor in adult education and later an historian of Africa. Thomas was Director of Extramural Studies in Oxford and was a Fellow of Balliol College. They had three children—Luke (1938), Elizabeth (Liz) (1941), and Toby (1946)—and both were loving and dedicated parents who took pains to let each child develop his or her particular talent. Thomas was a generous, interesting, and gregarious companion. Their home always had interesting visitors who gathered around the table for a meal cooked to perfection by Thomas. He did a lot of writing at home and helped looked after the children. Two neighbors, Edith and Alice, helped maintain the house when the children were young. Dorothy's sister, Joan, together with her five young children, joined the Hodgkin household. This home was always warm, inviting, chaotic, and interesting with Hodgkin children, relatives' children, and visiting children all over the place, as well as visitors from all over the world. Dorothy and Thomas had many grandchildren and great grandchildren. Sadly, Thomas died in Greece in 1982.

Like Thomas, Dorothy was interested in the social climate of the time and both worked hard to achieve her vision of socialistic paradise. This endeavor started for her, she once told me, as a result of her childhood experiences in the Girl Guides (Scouts). As a result she had many friends in the Soviet Union, China and Vietnam. Tom Blundell noted that "Dorothy saw politics as individual personalities, in terms of the people, not in terms of dogma or political convictions the way most people do" (McGrayne, 1993). In 1982 she was awarded the Mikhail Lomonosov Medal of the Soviet Academy of Sciences and in 1987 she was awarded the Lenin Peace Prize, partly, no doubt, because of her work to ease tensions between the East and West in the Pugwash Conferences on Science and World Affairs. The Pugwash organization, which is a fraternity of scientists interested in nuclear disarmament and improvements to life on earth, meets annually to discuss solutions to disarmament and the reduction of international tension. Dorothy was elected President in 1975. Her main service in these political activities was to keep open the possibility of a scientific dialogue between the countries that had such problems. Dorothy also had a great interest in African affairs, spurred by her upbringing and by her husband who traveled there often. In 1950 Kwame Nkrumah, the prime minister of Ghana, invited Thomas Hodgkin to establish an Institute for African Studies and to help change Ghana's University College into a full-fledged university. Dorothy spent several months each year with her husband in Africa, and she was with him in Accra, Ghana, when she received the news that she had won the Nobel Prize.

Dorothy retired in 1977 but continued her interest in science to the end. In the summer of 1993, aided by her daughter Liz and a grant from the Royal Society, she traveled to Beijing to attend the meeting of the International Union of Crystallography and to meet her Chinese friends. It was a joyous reunion and she made a point of listening to the plenary lectures particularly those on macromolecular structure. Her daughter Liz, as well as her other children, and her friends Jackie Hodgkinson, Judith Howard, and Eleanor Dodson, cared for her and visited her devotedly in the last years of her life when she was incapacitated. She died peacefully at home, surrounded by family and friends, on July 29, 1994 at Crab Mill, Ilmington, near Shipston-on-Stour, Warwickshire, England, in the old family home that had originally been a row of cottages and which retained the charm and friendliness of the Cotswolds.

Dorothy had the qualities of patience and optimism. She was physically slight and was increasingly frail in later years, bowed down with arthritis, although she refused to let this prevent her from working. Her arthritic hands have been portrayed by many famous artists, including Henry Moore. She was very generous with any scientific information she had available, and scientists such as Max Perutz did not hesitate to approach her for advice (Perutz, 1981). A quotation from the introduction to a volume in her honor, published in 1981, may help to give a picture of this remarkable lady: "In a world in which science is often performed in large impersonal groups, Dorothy has shown that absolutely first-class science may still be joined with a loving attention to individual values" (Dodson et al., 1981).

I first met Dorothy when, as an undergraduate, I applied to Oxford to study chemistry. I had promised my father I would go to medical school if I did not get into Oxford. Dorothy was concerned because I was young, but fortunately for me she accepted me and I was able to study chemistry as I had hoped. Through the years we became good friends and I enjoyed doing graduate work in her laboratory after a Part II research project in infrared spectroscopy. She taught me chemistry. She taught me by her example of never despairing or complaining even though she was profoundly crippled by arthritis. She taught me how she could manage a research program with low funding. She taught me to further the cause of women in science. At that time women lost fellowships and research grants if they married because the funding agency claimed they were now living "at home." Dorothy petitioned for each person to whom this happened, pointing out that two graduate students could not live on the stipend for one. This had to be done on a case-by-case basis, but she persevered. Margaret Adams wrote of her that she hummed in order to help her students cope with the frustration of science. But, Margaret added: "The nicest time I remember her humming was when I suddenly realized that what was being hummed was 'Through the night of doubt and sorrow'—that was actually quite supportive!" (Ferry, 1994).

If I were to paint a portrait of Dorothy I would not portray her crippled hands, even though she appreciated the compliment paid her by those that did. I would paint the great scientist beneath the frail and disabled exterior. She was slight, blond, blue-eyed, and pretty, excited by science, careful and precise in her experimental work, astounded by the beauty of the results of crystal-structure analyses, and thoughtful about the meaning of her results. She could be loving and gentle, yet stern, and cared deeply both for people and for the science that she advanced so greatly. Everyone listened at a meeting whenever she spoke up with her quiet but firm voice because they knew that what she had to say was important. She had an encyclopedic knowledge

of her field, and the contribution of her colleagues to it. But the most significant trait that Dorothy had was that she aimed for the highest peaks. She chose subjects of great importance which most scientists of the time felt were beyond the current state-of-the-art (Dodson et al., 1994). She had the imagination to insist that the problem she chose could be solved, even though she had to wait for many years for the answer. In fact Dorothy pioneered many of the methods of macromolecular structure determination that we now take for granted.

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