Acta Cryst. (1992). A**48**, 1-3

Obituary

David Harker
1906–1991

Dr David Harker died of complications due to heart disease and pneumonia in Buffalo, New York on 27 February 1991 after a long illness. Harker was born into a scientific and medical family on 19 October 1906. Both of his parents were MD's. His mother graduated from Vassar in 1898, taught chemistry and physics and 'boasted of being the first woman in New Brunswick, New Jersey to go to college, wear trousers, ride a bicycle and smoke a cigar'. His father obtained his MD without graduating from college, taught school in Hawaii and fought in the Spanish war of 1898. Harker grew up on the side of Mount Tamalpais in Mill Valley near San Francisco within view of the bay end of the Golden Gate, a scene of great activity in those days before the opening of the Panama Canal.

Although his father died when David was 5 years old David could recall him making plaster molds of his patients' feet and hammering copper into precise forms for arch supports on their front porch, memories that David associated with an early interest in form and structure. Mrs Harker gave up her career in order personally to take charge of the education of David and his brother up to the fourth grade. In later years, together with faculty members from Berkeley, his mother taught classes in exchange for free tuition at a high school he attended together with William Randolph Hearst.

David read Ira Remsens text on chemistry when he was twelve and developed 'a tendency to arrange objects in symmetrical patterns'. He graduated with honors in chemistry from the University of California at Berkeley in 1928 where he was exposed to a brilliant chemistry faculty that included Hildebrand, Latimer, Bray and Branch. While an undergraduate he toured Japan by bicycle with his brother one summer and undertook a 200 mile hike along the Old Spanish coast trail, a mule pack trail that is now Highway 1 from Carmel to St Luis Obispo. In 1930, Harker married Katherine de Savich, the daughter of the Imperial Prosecutor under the last Tzar, who fled Russia in 1917.

He entered graduate school at the California Institute of Technology in 1933 to work in Linus Pauling's group on the determination of crystal structures of minerals using X-ray diffraction. Early structure determination depended upon developing models that would produce calculated spectra to match observation. Harker was unable to conceive of suitable models for the subject of his dissertation

problem, the structures of 'ruby silvers' proustite ($Ag_3A_5S_3$) and pyrargyrite (Ag_3SpS_3). Harker has written,

'This problem baffled me for a long time. There were six unknown parameters in the description of the structure - more than could be found rigorously by the methods then known, and I was desperate to get my Ph.D. and a good job in science. Then at one of the weekly seminars of Pauling's students, A. L. Patterson's famous paper of 1934 on the "Patterson Function" was presented. A few nights later I awoke in the dark, sat up in bed and yelled "It's going to work!". I had seen that the relationships between symmetrically related atoms would produce peaks in the Patterson function on certain planes or along certain lines only. The structure of proustite and pyrargyrite were quickly deduced by using the Patterson function in this way.'

This conception of the Harker sections influenced the development of X-ray crystallography for the next 50 years, and it still finds application in structural analysis, particularly for crystals containing a small number of heavy atoms.

From 1936 to 1941 David Harker taught and conducted research at Johns Hopkins University in Baltimore, Maryland. While at Johns Hopkins he became acquainted with J. D. H. Donnay and together they developed a correlation between the internal structure and the external face development of crystals that mineralogists refer to as the Donnay-Harker law.

In 1941, Harker accepted a position in the Metallurgy Division of the Research Laboratory of the General Electric Company in Schenectady, New York where he published papers on grain shape and grain growth, developed an X-ray method for finding the orientation of quartz fragments so that oscillation plates could be cut from them and started work on the design of X-ray diffraction equipment in which the diffracted intensity would be measured with a Geiger-Müller or particle counter.

While at the General Electric Laboratory, David Harker and John Kasper discovered the first inequalities among crystal structure factors and used them to solve the molecular structure of decaborane, $B_{10}H_{14}$, a problem that had defeated their best efforts for some time. This achievement demonstrated that contrary to universally held beliefs the diffraction intensity data contained information about the phases of the intensities and stimulated heated debate at early gatherings of crystallographers in the US.

The Harker-Kasper inequalities relate the complex structure factors with their magnitudes, and impose a limitation on their values. This work of Harker and Kasper served as the inspiration for the development of a major branch of X-ray crystallography, the so-called direct methods, which has made possible the routine determination of tens of thousands of molecular structures using the techniques of X-ray diffraction.

Moving to the Polytechnic Institute of Brooklyn, in 1950, Harker opened yet another frontier embarking on the determination of the three-dimensional structure of the protein ribonuclease. At the same time, together with Thomas Furnas Jr, he designed and built an instrument that would usher in a new era in X-ray diffraction data collection.

Commenting on his choice of a protein to study Harker said,

'We picked ribonuclease as the protein on which to work because it could be had relatively pure at a reasonable price, could be crystallized, and had a quite small molecular weight. Dr M. V. King crystallized this substance in fourteen different modifications eventually. He also invented the method of attaching heavy atoms to specific sites in the protein crystals by "dyeing" the crystals with specially synthesized dyes, the molecules of which contained heavy atoms. I worked out a scheme of phase determination for protein structure factors which involved using the intensities from three isomorphous crystals - one undyed, the other two dyed with heavy atoms in different arrangements. It turned out that Professor Bijvoet of Utrecht had found the same princple a few years before, but had not emphasized it in his papers.'

While engaged in this challenging protein study, David Harker took his research team to Roswell Park Memorial Institute in Buffalo where in 1967 his structure determination of ribonuclease, an enzyme vital to genetic control of growth and development, was completed and earned front-page coverage in the *New York Times*. Although this was the first time that a protein structure had been solved in the United States, it was not the first protein structure to be determined. Working in Cambridge, British crystallographers, John Kendrew in 1960 and Max Perutz in 1961, had determined the structures of the proteins myoglobin and hemoglobin; and for this work they received the Nobel Prize in 1962.

After his retirement from RPMI in 1976, Harker continued his crystallographic studies as a Research Scientist Emeritus at the Medical Foundation of Buffalo. He worked there until the end of his life making important contributions to the theory of colored space groups, an aspect of crystallographic symmetry which he found particularly fascinating. Only a month before his death his last paper on a novel class of infinite polyhedra was published in the Proceedings of the National Academy of Sciences.

David Harker was a consultant on X-ray crystallography to the Carborundum Company and the General Electric Corporation. He played a leading role in the establishment of the International Union of Crystallography and its adhering body in the United States, the US National Committee for Crystallography. In 1946, as the President of the American Society for X-ray and Electron Diffraction, ASXRED - one of the two societies that merged to form the American Crystallographic Association in 1950 - he led the American delegation to the London Conference where the formation of an International Union of Crystallography was proposed. He was joint chairman with Sir Lawrence Bragg of the 'Provisional International Crystallographic Committee' and served as US representative on the Interim Executive Committee that was left in charge of the affairs of the International Union before formal elections were held. David was a member of the first National Committee of the US, the adhering body of the US to the IUCr in 1948, and a member of the USA National Committee for Crystallography, the official National Research Council Committee that subsequently became the adhering body to the IUCr, from its inception in 1950 through 1956, serving as Vice-Chairman in 1953 and Chairman in 1954 and 1955. He again served as a member of the Committee from 1958 through 1963.

David Harker had a passion for lively debate, mystery novels, the proper use of language and the poetry of Rudyard Kipling. When Herbert Hauptman and Jerome Karle were awarded the Nobel Prize in Chemistry in 1985, Dr

Hauptman invited David Harker to accompany him to the award ceremonies in Stockholm, Sweden, in recognition of the critical contributions that David Harker's early work had made to the development of direct methods.

David Harker was a founding father of modern crystallography. His scientific breakthroughs contributed directly to current knowledge of the molecular structure of drugs, hormones, proteins and antibiotics, and the molecular basis for chemical and biological processes. His work had a direct bearing upon a wide range of industrial and medicinal advances.

A Special Seminar in memory of David Harker held at the annual meeting of the American Crystallographic Association in Toledo, Ohio, on 22 July 1991 was attended by his second wife Deborah Anne Maxwell Harker and many friends and acquaintances of the Harkers. One of the speakers in that session was Herbert Hauptman who said of Harker.

'He was courteous and unpretentious, but honestly so. He was a warm and friendly man, concerned to be helpful, particularly to younger colleagues; and his teaching was unsurpassed. He was one of the greatest crystallographers of this century but he was never patronizing to others, young or old. He was kind and gentle and, at the same time, a man of uncompromising honesty and integrity. He was a tireless seeker of the truth, wherever he could find it, and in this quest he succeeded as few others have.'

In 1988, on the occasion of his 82nd birthday, an endowment fund was established in Dr Harker's name at the Medical Foundation of Buffalo. The fund is intended to support research and lecturers in crystallography.

WILLIAM L. DAUX
Medical Foundation of Buffalo, Inc.