David Sayre

(1924–2012)

Crystallographer who pioneered methods of X-ray imaging and modern computing.

David Sayre, who died on 23 February, was a pioneer in crystallography and diffraction imaging, a visionary in X-ray microscopy and an architect of modern computing. A superb scientist, deep thinker and wonderful mentor, he could have built a scientific empire. But that was not his style. He was driven by the desire to do pure and original science.

Sayre was born on 2 March 1924 in New York. His father was an organic chemist whose ancestors helped to found the town of Southampton, New York, in the sixteenth century. His mother was the daughter of Jewish immigrants. Sayre was educated at Yale University in New Haven, Connecticut, graduating in 1943 at the age of 19 with a bachelor's degree in physics. The Second World War was at its height, so Sayre worked on radar at the Radiation Laboratory at the Massachusetts Institute of Technology in Cambridge.

In 1946, guessing biology would be the next exciting field, Sayre became a graduate student in biology at the University of Pennsylvania in Philadelphia and then at Harvard University in Cambridge. He was not initially interested in what he was learning, but in 1947 Sayre came across an article about X-ray crystallography that changed his life. He joined Raymond Pepinsky's crystallography laboratory at Auburn University in Alabama, where he used a mathematical operation known as the Fourier transform to analyse the structures of crystals probed with X-ray beams.

That year, Sayre married Anne Colquhoun, a fiction writer. She took a teaching position at the Tuskegee Institute, but her involvement in the school, which enrolled black students, was controversial in the Deep South at that time, and the Sayres soon left. They moved to Oxford, UK, where Sayre completed his PhD in the lab of Dorothy Hodgkin in 1951.

Sayre produced his most profound papers during this period, solving the 'phase problem' in crystallography — the loss of phase information in the measurement of diffraction intensity. In 1952, he proposed atomicity — the fact that atoms are small and discrete points relative to the space between them — as a constraint for determining the phases of crystals of small molecules, giving rise to what is now called Sayre's equation. Atomicity is the key concept behind the direct methods used for crystallography today, although Sayre did not share the 1985 chemistry Nobel prize awarded for


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it. In 1952, Sayre also realized that, even in the absence of regular crystal structure, information could be gleaned from the fine sampling of diffraction patterns.

Sayre saw early on that solving complex crystal structures would require substantial computational resources. In 1956 he joined IBM's Watson Research Center in New York, and eventually became assistant manager of the team that wrote the original FORTRAN compiler. He became corporate director of programming, and later head of the IBM programming research group. In 1969, he and his team proved the efficiency of virtual memory in computing.

In 1972–73, Sayre took a sabbatical, returning to Hodgkin's lab and to crystallography. It was during this time that one of us (J.K.) met the Sayres, forming a lasting friendship and collaboration. Anne Sayre also wrote the influential book *Rosalind Franklin and DNA*, about the outstanding crystallographer and Sayre family friend who had died of cancer at an early age.

After returning to IBM, Sayre became interested in X-ray microscopy. His 1971 idea of how to fabricate Fresnel zone plates for focusing X-rays became a reality through the use of IBM's nanofabrication technology and with the advent of synchrotron radiation sources such as the National Synchrotron Light Source at Brookhaven National Laboratory in Upton, New York. X-ray microscopy based on zone plates is now used in synchrotron-radiation facilities worldwide.

Around 1990, Anne developed scleroderma, a debilitating disease, and David retired from work to care for her. But he continued working to realize his 1952 dream: the reconstruction of molecular structures without the use of crystals. The idea came to fruition almost 50 years later, with the publication in 1999 of the first reconstruction of a non-crystalline model object from its diffraction pattern (which was J.M.'s PhD project). This paper established coherent diffraction imaging (CDI), also called lensless imaging or diffraction microscopy, as the most promising form of high-resolution X-ray imaging. CDI is now one of the fastest-growing fields in X-ray science.

Anne died in 1998, and in the last decade of his life David suffered from Parkinson's disease. But he continued to participate in research and to offer advice. A researcher with exceptional intuition, David lived for science. His passing is a huge loss for all of us. ■

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