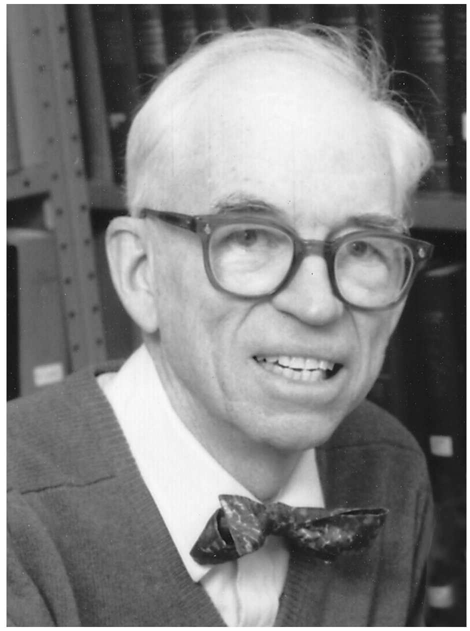
Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

David H. Templeton (1920–2010)



David died at the age of 90 at his house in El Cerrito near Berkeley, California. Just the evening before, he had enjoyed a pleasant dinner with his son Alan, who was visiting him. Although David tired easily, Alan certainly did not expect his father to leave us so soon. David survived his wife Lieselotte (Lilo), who died at the age of 91, by seven months.

I met David for the first time in 1972, in his office at the Lawrence Berkeley Laboratory, on the hill dominating the UC Berkeley campus. I arrived from Switzerland, shortly after obtaining my PhD from the ETH in Zürich, for a postdoctoral stay in David's laboratory. I immediately felt at ease around him; he spoke softly, had the manners of a gentleman and had the abilty to make others laugh with his funny stories. I was also happy to meet the senior members of his laboratory, Allan Zalkin, Helena Ruben and Lilo, who was also part of the research team. I greatly benefited from their help and advice.

David received his Bachelor of Science *summa cum laude* in 1941 from the Louisiana Polytechnic Institute. While working on his Master's degree in chemistry at the University of Texas, David was drafted in 1943 and served in the Army Corps of Engineers. He was, however, soon reassigned to the Manhattan Project in Chicago, where he met Glenn Seaborg, William Zachariasen and other leading scientists. It is certainly there where David got his first insight into crystallography and X-ray diffraction. I remember when David was discussing the time he spent in Chicago how impressed he was by the ability of Zachariasen, the author of the famous book, *Theory of X-ray Diffraction in Crystals*, to identify compounds from a simple inspection of their powder-diffraction patterns. Apparently the pre-computer scientists of that time did possess abilities that are missing today!

While in Chicago, Glenn Seaborg convinced David to come to Berkeley for his PhD once he had finished his Master's studies at Texas. David was apparently very successful in his research and completed his PhD in chemistry in 1947 after just three semesters at Berkeley. He then immediately joined the college faculty.

Shortly after the war, the accelerators for charged particles, cyclotrons, synchrotrons and other exclusive machines were the source of most of the newly discovered radionucleotides, and Berkeley was one of the most prominent centers in this field. David's first research studies were dedicated to radiochemistry. His publications with Isadore

Perlmann and Glenn Seaborg were dedicated to the fission of various heavy metals by high-energy particles to form artificial radioactive isotopes. Together, they discovered a dozen new ones. In 1949, David published as sole author *The Story of Radioactive Isotopes*, a review describing the production and properties of neutron-deficient isotopes produced by high-energy bombardment in the 184-inch cyclotron. In 1951 followed a review article with Glenn Seaborg as a second author (Seaborg won the Nobel Prize for chemistry that same year) concerning *Radioactivity and Nuclear Theory*, an obvious sign of recognition of David's expertise from Glenn.

The research on new materials produced at the Lawrence Berkeley Laboratory and the study of their properties could not be conceived without X-ray diffraction to characterize their crystal structures. David was soon given the assignment to start a crystallography laboratory. From this new unit, David and his graduate student, Allan Zalkin, published the first structural studies of a series of rare-earth tetraborides. In 1953, the two authors published one of their most cited publications – 258 citations with an average of approximately five per year – on the structures of yttrium trifluoride and related rare-earth trifluorides. This remarkable piece of work illustrates the quality of their studies from Weissenberg and powder-diffraction patterns recorded on films with visual estimation of the intensities.

Based on his experience working with heavy elements, David very soon realized the importance of obtaining precise atomic X-ray scattering factors close to certain absorption edges. In 1955, David published his first paper concerning the X-ray dispersion effects in crystal structure determination, which was immediately followed by his most cited paper (565 times) with Carol Dauben on the dispersion corrections for X-ray scattering by atoms from elements 20 to 96. These two papers dedicated to the topic of resonant (or anomalous) scattering marked a new orientation in David's career, which he pursued until the end of his scientific research activities.

The SPEAR ring at the Stanford Synchrotron Radiation Lightsource (SSRL) was constructed in the early 1970s, yielding intensive synchrotron radiation. This was the new source of X-rays that David was waiting for. The energy tunability of the source allowed crystallographers to extend their field of research by exploiting physical properties, which was not possible using conventional X-ray tubes. In collaboration with James Phillips and Keith Hodgson from the Department of Chemistry at Stanford University, David and Lilo published in *Science* their famous paper on the $L_{\rm III}$ absorption edge of caesium, where they showed that the change in scattering power was 'approximately equivalent to removing a rubidium atom from the structure' by appropriate tuning of the wavelength. The importance of dispersion, *i.e.* the dependence of the atomic scattering on X-ray energy, was immediately recognized as a powerful tool in phasing macromolecular structures. David's scientific curiosity and his deep knowledge of diffraction theory was at the origin of the observation of X-ray dichroism, a change in absorption depending on the polarization state of the incident beam, near the $L_{\rm I}$ and $L_{\rm III}$ edges of uranyl, platinate and aurate and the K edges of vanadium, bromate, bromide and iodate, properties that are closely related to the polarization anisotropy of resonant scattering and expressed in terms of second-rank tensors. David's continuous interest led him to discover some higher-order effects in the anisotropy of diffraction with the examples of potassium chromate and germanate, where non-negligible third-rank tensor effects could be measured. The last of David's studies dedicated to the anisotropy of resonant scattering was published in 1998. It is probably the increase in traffic congestion on the Bay Bridge between the Berkeley hills and the Stanford storage ring that brought to an end his fruitful contribution to this field.

David's interests in research were by no means limited to the field of resonant diffraction. To mention just a very short selection, he published several studies showing how to improve the calculation of Madelung's constant for the electrostatic energy of ionic crystals. He was also interested in the problem of least-squares and the fixing of the origin in polar space groups, and how to improve the calculation of the full matrix in least-squares refinements (David's last publication in 1999). His lifelong collaboration with Allan Zalkin was a success story. The number of interesting crystal structures published by the team included a few noble-gas compounds like XeF_4, XeF_5^+ and XeO_3, following Neil Bartlett's first syntheses. Studies of the structure and chemistry of the porphyrins were published with Melvin Calvin.

While I was preparing this article, I discovered a very interesting contribution by David to the field of mathematical puzzles. Indeed, in Martin Gardner's book *My Best Mathematical and Logic Puzzles*, the well known journalist for *Scientific American* mentions that David found a way to force a draw in the Hip game on an order-six board based on symmetry arguments, a typical sign of David's ability to put theoretical considerations into practice!

The quality of David's work can be estimated from some bibliometric indices. His articles were cited close to 11 000 times, a record. In the last 20 years, he was cited about 200 times each year!

David's scientific reputation attracted a large number of young crystallographers, doctoral students, trainees and postdoctoral fellows. He was very generous in giving advice and was at the origin of many innovative studies by several fellows who visited his laboratory. It is not an overstatement to characterize David's influence as the 'David Templeton School'. To cite just a few examples, Ivar Olovsson's collaboration with David and their studies on solid ammonia and various sodium chromate and sulfate polyhydrates were certainly at the origin of Ivar's lifelong interest in hydrogen bonds. Recently, the publication by Marc Schiltz and Gérard Bricogne entitled *Exploiting the anisotropy of anomalous scattering boosts the phasing power of SAD and MAD experiments* [*Acta Cryst.* (2008), D**64**, 711–729] was dedicated to David and Lilo's pioneering studies.

In 1982, I had the pleasure of inviting David to give a series of lectures at the Doctoral School of the Physics Department at Lausanne on the topic of anomalous X-ray scattering during the winter semester. One of the participants was Howard

Flack, who listened carefully to David's lecture on absolute configuration mentioning Roger's scale factor. The lecture was apparently well understood by Howard, who shortly afterwards published a description of what is now called 'Flack's parameter' for the estimation of the enantiomorph-polarity character of a structure. David's inspiring series of lectures describing his experiences with and the possibilities offered by synchrotron radiation was also at the origin of our laboratory's involvement in the creation of the Swiss–Norwegian beamlines at the European Synchrotron Research Facility (ESRF) in Grenoble.

David's remarkable contribution to scientific research and education was rewarded in 1977 by the degree of Doctor *honoris causa* by the University of Uppsala. In 1987 he obtained with Lilo the A. L. Patterson Award for his contribution to *Theory, Measurement and Use of Anomalous Scattering*. In 1988, he was also selected to give the G. N. Lewis Lecture of the College of Chemistry at the University of California, Berkeley.

David's management skills, diplomacy and sense of fairness helped him greatly in serving as Dean of the College of Chemistry between 1970 and 1975, a particularly tumultuous period on the Berkeley campus. He was also President of the Americal Crystallographic Association in 1984.

On the day before David died, his son Alan was able to confirm to his father that the University of California had received the final instalment of his contribution towards establishing an endowed Chair for the College of Chemistry at Berkeley that will be known as the Lieselotte and David Templeton Chair in Chemistry. The Hewlett Foundation equally matched his contribution, making it a substantial and fully funded Chair. Its purpose is to support a faculty member in chemistry, with a preference for a woman who has young children and who is trying to balance the demands of an academic career with raising a family – a challenge that was very familiar to David's family.

I would like to thank Alan Templeton, Allan Zalkin, Ivar Olovsson, Ken Raymond, Michael Barnes and Mindy Rex for their kind help in preparing this article, which also appears in the Fall 2010 issue of *RefleXions*, the Americal Crystallographic Association newsletter.

Gervais Chapuis

Federal School of Technology,
Laboratory of Crystallography,
BSP, 1015 Lausanne,
Switzerland