



## Richard E. Marsh (1922–2017)

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**Keywords:** obituary; CRYM; PLATON; chemical crystallography.

Dick Marsh, Senior Research Associate in Chemistry, Emeritus, at Caltech, passed away on January 3, 2017, at the age of 94. He was born in Jackson, Michigan, in 1922. He entered Caltech in 1939 and graduated with a Bachelor's Degree in Applied Chemistry in 1943. He then joined the US Navy and degaussed ships on the Mississippi River in New Orleans. He was discharged from the Navy in 1946 and enrolled at Tulane University as a graduate student. During that period, he met two women who would influence the rest of his life: his future wife of 69 years, Helen, and a crystallographer, Rose L. Mooney. Mooney taught at Sophie Newcomb College, a girls' school across the street from Tulane, and had learned crystallography from W. H. Zachariasen (University of Chicago). After her course, Dick was hooked on crystallography. Tulane did not offer a graduate program in Chemistry, so he transferred to UCLA. He worked with James McCullough on crystallographic studies of organoselenium compounds and received his graduate degree in 1950. This was a period of immense growth in crystallographic computing that accelerated both structure determination and refinement.



Dick returned to Caltech in 1950 and remained there for over 67 years (for more information, see <http://www.amerocrystalassn.org/h-marsh>). Caltech was a mecca for crystallography, especially after the publication of *The Nature of the Chemical Bond* by Linus Pauling in 1948. Dick began his work with Linus Pauling on the structure of chlorine hydrate, a significant achievement since diffraction images were collected in a cold room using both powder and single-crystal intensity estimates. With continuing interest in proteins, and mentoring from Robert B. Corey, Dick shifted his interest to the structures of silk fibroin, amino acids, and nucleic acids. Other Caltech collaborators and researchers included Jerry Donohue on the structures of amino acids and peptides, David Shoemaker, and later Sten Samson, working on the structures of intermetallic compounds, Edward Hughes, developing methods for the refinement of crystal structures, Jack Dunitz, Leslie Orgel, and Alex Rich on ferrocene, Bill Sly on  $\beta$ -carotenes, Verner Schomaker, Bill Schaefer, Frank Herbstein, and countless others. Dick remained a colleague and collaborator with several members of the Caltech faculty throughout his long career.

In the early 1960s, Dave Duchamp developed an automated package for structure determination and refinement called *CRYM*; it was written in FORTRAN and

programmed to run on Caltech's IBM-7094. Dick contributed to corrections and improvements in the program for decades, assisted most ably by Jean Westphal, who modified the program code on the IBM-7094 and later on the Digital VAX/VMS we migrated to in 1982. Somewhat relatedly, as the determination and publication of crystal structures became more routine in the 1980s, Dick recognized dozens of errors in published structures, often resulting from a failure to recognize an inversion center in a noncentrosymmetric structure, or some other missing symmetry elements, leading to assignment of and refinement in the wrong space group. He published a series of papers correcting structural reports and systematically outlining classes of errors in space-group determination. This was nontrivial because the data were only available from the printed supplementary pages as  $F_o$  and  $F_c$  tables. Dick, Jean, Kirby (his daughter), or others would enter the data by hand, and he would then rerefine a structure in the corrected space group, and demonstrate the improvement. As evident from his publication list for this period, Dick corrected hundreds of crystal structures. The result was twofold, *i.e.* the potential threat to every crystallographer that you carefully determine every structure or be 'marshed' by his review, and the creation of a program *PLATON*, written by Ton Spek, that provided additional guidance for structure validation. Ton and Dick worked closely together for over a decade, and *PLATON* now serves as a standard tool for ascertaining the quality and validity of a small-molecule crystal structure. Dick continued to work on correcting the literature, with his last publication in 2014 surveying 100 000 entries in the Cambridge Structural Database and correcting errors in 156 crystal structures [*Some more space group corrections*; Henling, L. M. & Marsh, R. E. (2014). *Acta Cryst.* **C70**, 834–836].

Dick was an avid crystallographer, brilliant in his adoption of new techniques and advances over his career. He was modest, friendly, and always cheerful. His typical routine for decades was morning coffee at the 'Greasy Spoon' (Caltech cafeteria) with his group and the protein crystallographers (with Richard Dickerson and his group, before 1981), lunch with his colleagues, and afternoon coffee with his group and computing colleagues. He always wanted to know 'What's new?'. He loved teaching the X-ray crystallography course at

Caltech, as well as helping undergraduates, graduate students, and postdoctoral research fellows one-on-one. He was always approachable, interested, and generous with his time.

I can still recall in the early 1980s that I showed him a zero-level Weissenberg photograph of a new crystalline sample. (We still took photographs of all new crystal samples to obtain cell parameters, even though these were routinely determined by diffractometer data by this time.) Working with a new graduate student, he knew we had a metal dimer complex, and immediately determined the atomic coordinates of the metal by noting the modulation in the intensity pattern, wrote it down, and placed it in his desk drawer. A few days later, after data collection on the diffractometer, and processing was completed, we returned with our solution, and his coordinates matched ours to three places. All of those years of working with Patterson–Tunnell strips (for rapid Fourier summations) were still vivid in his memory!

In addition, he was an excellent tennis player and golfer. He and his family enjoyed their summers in Jackson, Michigan, at the family compound along Brown's Lake. I visited him and Helen a few months before his death, and he was still as keen on crossword puzzles, talking crystallography and science, and ready to critique a recent publication of interest. Once, when we were debating the potential outcome of an experiment, he exclaimed 'Oh good, I thought you were going to argue the other side; that would have been more difficult to defend.' He was unflappable, engaging, interesting, and charming. He was respected by all of his Caltech colleagues, and kept in touch with Linus Pauling and the family.

Dick served as President of the American Crystallographic Association in 1993, and was Co-Editor of *Acta Crystallographica* for the periods 1963–1971 and 1994–2004. He was the first recipient of the Kenneth N. Trueblood Award from the ACA in 2004, in recognition of his exceptional achievements in computational and chemical crystallography. He was one of the most remarkable crystallographers of his generation, and is sorely missed. He is survived by his wife, Helen, his four children Susan, Chip, Kirby, and Steve, eleven grandchildren, seven great-grandchildren, and countless friends from family, work, and his philanthropic interests. We all miss his infectious laugh and dedication to the craft of crystallography.