

Pioneers of Quantum Chemistry, ACS Symposium Series 1122, E. Thomas Strom and Angela K. Wilson, Eds., Washington, DC, American Chemical Society (distributed by Oxford University Press), 2013, xi+330 pp, ISBN: 978-0-8412-2716-3, \$150 (hardback; e-book also available).

With the development of powerful desktop computers and commercial software packages, sophisticated quantum chemistry calculations have become accessible and relatively simple to perform so it is easy to forget the long struggle that brought us to this point. Thankfully, scholars are turning their attention to documenting the history of quantum chemistry. This collection of articles based on presentations at an ACS symposium held on March 28, 2011, in Anaheim, CA, is a welcome addition to that literature. The articles describe important early developments in quantum chemistry and profile the pioneers in the field and their accomplishments.

The lead article by Klaus Ruedenberg and W. H. Eugen Schwartz is a whirlwind tour of ideas about atoms and molecules from the Greeks to the present. This is followed by a survey of more modern developments. A particularly valuable section of the chapter by Istvan Hargittai is a discussion of the Soviet resonance controversy, an example of politics interfering with science. The remaining chapters mainly focus on the contributions of notable figures in the history of quantum chemistry, some of whom are nearly forgotten.

I found the chapter by E. Thomas Strom, one of the editors of the collection, on George W. Wheland to be particularly interesting. Originally from Chattanooga, Tennessee, where his father ran a foundry, Wheland had a stellar academic career, beginning with a bachelors degree from Dartmouth, a doctorate from Harvard where he worked with James Bryant Conant, and a postdoctoral stint at Caltech with Linus Pauling where he co-authored three seminal papers on resonance theory. He spent the remainder of his career at the University of Chicago where he wrote influential books on the theory of resonance and advanced organic chemistry. Wheland suffered from multiple sclerosis and became unable to function as a faculty member at about age 50 in the early 1960s, cutting short a brilliant career. There are also chapters on other pioneers including Michael J. S. Dewar, H. C. Longuet-Higgins, and John Pople, all members of the so-called British School of Quantum Chemistry. Each provides the personal perspective of the author on the scientist and his contributions.

Quantum chemistry came into its own with the development of the high speed digital computer and the requisite software to perform calculations. Some of those developments are highlighted in chapters entitled, "The Golden Years at LMSS and IBM San Jose," and "Quantum Chemistry Program Exchange, Facilitator of Theoretical and Computational Chemistry in Pre-Internet History." The first of these is a history of two important research groups, the Laboratory of Molecular Structure and Spectra at the University of Chicago presided over by R. S. Mulliken and C. C. J. Roothan, and the ALCHEMY project at IBM San Jose headed by Enrico Clementi, where talented scientists took advantage of developing computer technology to develop programs to carry out high-level (for the time) quantum chemistry calculations. While the San Jose group had access to the latest IBM mainframe computers, before 1960, members of the Chicago group had to fly to Dayton, OH, to use the computer at Wright-Patterson Air Force base. In the early 1960s, they obtained permission to use the IBM 704 computer at Argonne National Laboratory. Eventually, the University of Chicago got its own computer, an IBM 7090. The 7090 was the first transistorized computer and cost several million dollars. Results were checked by hand using electric desk calculators. This chapter reminds the reader that in the early 1960s, the calculation of a square root was not routine. The first electronic desk calculators became available in the late 1960s. Only the most expensive of them could automatically calculate a square root.

The Quantum Chemistry Program Exchange (QCPE) which was housed at Indiana University is a distant memory, but in its heyday it was a repository for the latest in software for computational chemistry. Individual researchers would contribute their source code, usually written in FORTRAN, and for a nominal fee, anyone could obtain a copy to use. Early on, if you wanted a program it would be shipped as boxes of IBM cards. Later, magnetic tape was used. QCPE also organized workshops to introduce researchers to computational methods and published a regular newsletter. QCPE was a remarkable example of scientific cooperation. The programs were all donated by the developers. The whole operation was run on a shoestring from an office or two in Bloomington, but it had an enormous impact. At its zenith, QCPE distributed as many as 2500 programs per year. With the development of commercial packages, such as Gaussian, and the ability to download software quickly from the internet, QCPE became irrelevant and disappeared so it was a pleasure to read this history and remember a gentler time.

Because of the nature of this volume as a collection of articles, it is not a systematic history of quantum chemistry. Such histories are being written, for example, *Neither Physics nor Chemistry: A History of Quantum Chemistry*, by Kostas Gavroglu and Ana Simões (1), but the individual contributions in this book do add to our knowledge of the history of this important area of contemporary science. *Pioneers of Quantum Chemistry* is enriched by a large number of historical photographs: George Wheland in his Baylor Military School uniform, Robert Mulliken working at his messy desk at the LMSS, and Linus Pauling lecturing at Moscow State University

in 1984, for example. Historians of chemistry will certainly want to peruse this book although its rather high price may mean that it will not find its way into a large number of personal libraries.

(1) Kostas Gavroglu and Ana Simões, *Neither Physics nor Chemistry: A History of Quantum Chemistry*, MIT Press, Cambridge, MA, 2012. Reviewed in *Bull. Hist. Chem.*, **2012**, 37, 103.

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A Festival of Chemistry Entertainments, Jack Stocker and Natalie Foster, Eds., ACS Symposium Series 1153, Washington, DC, American Chemical Society (distributed by Oxford University Press), 2013, xiii+118 pp, ISBN: 978-0-8412-2716-3, \$150 (hardback; e-book also available).

If the phrase “chemistry entertainments” strikes you as an oxymoron, then this book is not for you. I suspect, however, that the phrase makes perfect sense to many readers of the *Bulletin*, as well as to readers of the “Newsreports” column of *Chemical and Engineering News*, collectors of chemistry trivia, and aficionados of science-themed songs, verse, and puzzles. The authors and editors of this volume have all shown the capacity to be entertained by chemistry and they endeavor here to entertain other like-minded chemists, chemistry students, and chemistry fans.

The book is based on a symposium organized by Jack Stocker at the 235th National meeting of ACS in New Orleans in April 2008. Stocker was a long-time professor of chemistry at the University of New Orleans and an extraordinary collector of chemistry memorabilia. As an ACS tour speaker, Stocker was willing to travel anywhere to share his collection, which he called “chemage” (a portmanteau of chemistry and garbage). He gathered quite an assembly of raconteurs, collectors, aficionados, and composers of puzzle and verse to share their enthusiasm for the whimsical in chemistry. This volume is one result of that occasion.

For those who were there, the symposium (and by extension the volume) evokes two bittersweet impressions. One is of resilience, as ACS met in New Orleans for the first time since Katrina. Stocker had lost much of his collection, but he was still sharing it with others as well as sharing his enthusiasm for chemistry and for his city. The other is of loss, for Stocker passed away the following year at the age of 85. One need not have been at the symposium or known Stocker, though, to appreciate the book, which stands on its own as a miscellaneous collection of metachemical fun.

One of the book’s chapters has “history” in the title: “ACS History in Personal Debates, Both ‘political’ and ‘Political.’” Former ACS President Mary Good writes about some of the politics within and outside ACS during her long years of service to the organization. She touches on matters ranging from the small-scale diplomacy of arranging for scientists who did not get along well to share the same stage, to some scientific fallout from the large-scale geopolitics of the Cold War. Her chapter makes for both interesting reading and raw material for further historical inquiry.

Another chapter that is rich in personal recollection is Mary Virginia Orna’s, “Always a Cross(ed) Word.” It is a delightful memoir that describes the development of her love for Latin and chemistry in high school. The latter became her career, while the former turned into a serious avocation in crossword puzzles. As a puzzle constructor, Orna has published in the *New York Times*,