

## A Reflection on Paul von Ragué Schleyer

The world of chemistry suffered a great loss with the passing of Paul Schleyer on November 20, 2014, at age 84. Active to the end, Paul was one of the greatest physical organic chemists of all time. He was an incredibly stimulating person, always full of exciting, novel ideas. There was never a meeting with Paul when one was not energized.

Paul grew up in Cleveland, graduated from Princeton, and received a Ph.D. with Paul D. Bartlett at Harvard. He began his independent career at Princeton in 1957. His early work included experimental carbocation chemistry and hydrocarbon chemistry, including a remarkable synthesis of adamantane by Lewis-acid catalyzed rearrangement of tetrahydro-cyclopentadiene dimer. Simultaneously, Paul helped pioneer molecular mechanics calculations on hydrocarbons. This led him to become increasingly interested in computational chemistry, which was his dominant activity after he left Princeton in 1976 for the University of Erlangen. He interacted significantly with Lee Allen at Princeton, then with John Pople, leading to many publications on molecular energetics, especially for carbocations. Paul completely embraced *ab initio* quantum mechanics, and from 1998, he was a member of the Center for Computational Chemistry, which also includes Lou Allinger and Fritz Schaefer, at the University of Georgia.

I was an undergraduate at Princeton during 1967–70. In my second year, Paul and Ted Taylor were my professors for introductory organic chemistry. They were both great, but Paul really resonated with me owing to his enthusiasm and his covering the more physical topics. Paul was a dashing figure, which was accompanied by exotic rumors. As an alumnus, I was disappointed that Paul left Princeton. A key issue appeared to be computer access. People with endless ideas and energy like Paul are rare; they provide the pillars of academic chemistry departments. There was always a storm of activity around him.

My next contact with Paul was at the time of my book with Lionel Salem (1973); Paul loved the orbital pictures, reflecting the strong visual aspect of organic chemists. We stayed in touch, and after I became an Assistant Professor at Purdue, Paul arranged for me to spend a month in Erlangen during the summer of 1978. Paul and Inge were incredibly generous, allowing numerous visitors to stay at the large house that they were renting, the “Wagner Villa”. Marty Saunders was there too, and Clayton Heathcock was staying nearby. During this trip, I met Jayaraman Chandrasekhar, who became one of my most productive co-workers. It was also my first exposure to the World Cup, which was viewed en masse at the Wagner Villa. It was a stimulating time. Paul also made several trips to Purdue to visit Herb Brown, where they worked on the book “The Non-Classical Ion Problem”. Paul wrote a spirited rebuttal section after Herb’s chapters. I was delighted to interact with Paul on these occasions and provide airport transportation. In 5 minutes with Paul, anyone would realize that they were with an incredibly bright and informed scientist, who was happy to engage in vigorous, but fair, debate. Paul loved to travel, and he provided the epicenter for innumerable meetings and conferences around the world.

Paul published more than 1200 papers. They are striking in their sense of excitement in probing novel phenomena. Paul was very interested in unusual bonding including planar tetracoordinate carbon and organometallics. I had an early paper (1976) with him, John Pople, and Yitzhak Apeloig on dilithioacetylene. Paul revolutionized the understanding of lithium chemistry. He also had endless fascination for aromatic systems and measures of aromaticity, for example, NICS. Additionally, he never lost interest in carbocations, especially 2-norbornyl. In the last two years, he coauthored two superb joint computational and experimental studies of gas-phase rearrangements of 2-norbornyl cation and of its crystal structure as an  $\text{Al}_2\text{Br}_7^-$  salt. Like Paul, 2-norbornyl cation has always been nonclassical.

All who knew Paul miss him deeply. He was a truly dynamic, exciting person. His spirited love of chemistry remains an inspiration.

**William L. Jorgensen\***

Department of Chemistry, Yale University, New Haven, Connecticut 06520-8107, United States

### ■ AUTHOR INFORMATION

#### Corresponding Author

\*E-mail: [william.jorgensen@yale.edu](mailto:william.jorgensen@yale.edu)

#### Notes

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