Paul von Ragué Schleyer

(1930–2014)

Chemist who launched the study of caged hydrocarbons.

The scientific career of Paul von Ragué Schleyer took off when, as a graduate student at Harvard University in Cambridge, Massachusetts, he discovered an astonishingly straightforward way to make adamantane, the simplest subunit of diamond and the simplest stable caged hydrocarbon.

In finding a way to synthesize kilograms of adamantane cheaply — by putting a compound called tetrahydrodicyclopentadiene into an acidic mixture — Schleyer paved the way for two best-selling drugs. One, memantine, improves cognitive abilities such as memory and attention in people with Alzheimer's disease. The other, saxagliptin, regulates insulin levels in people with diabetes. His work also launched a new field. The exploration of caged hydrocarbons led organic chemists, including Schleyer, to discover beautiful organic structures that no one had thought could be made, as well as leading to insights about chemical bonding.

Schleyer, who died on 21 November, was born in Cleveland, Ohio, in 1930, to parents of modest means. He obtained a degree in chemistry in 1951 from Princeton University in New Jersey, and then went to Harvard. By the time his adamantane paper was published in 1957, Schleyer was a faculty member at Princeton.

The next few years were taken up with experimental explorations of hydrocarbon rearrangements in organic molecules, and of the role of carbocations (positively charged organic ions) as reaction intermediates. When George Olah received the 1994 Nobel Prize in Chemistry for his research on carbocations, many of us felt that Schleyer might have received a share of the prize.

In 1969, Schleyer became Eugene Higgins Professor — Princeton's most prestigious chair in chemistry. He continued to produce experimental papers, but increasingly devoted his efforts to computational chemistry, in which mathematics, physics and computing are used to solve problems that are too difficult or dangerous to be solved experimentally.

In the 1960s, Schleyer began to make predictions about the molecular structures of known and unknown molecules using force-field methods — predictions that were later proved experimentally, in some cases by Schleyer himself. He treated molecules as mechanically connected systems of atoms,

and mapped their structures according to the energy of all the atom–atom interactions.

A turning point in Schleyer's career came when he started working with John Pople, then at the Carnegie Mellon University in Pittsburgh, Pennsylvania. Pople was using more-rigorous theoretical methods that factored in quantum mechanics.

Schleyer's entry into the young field of computational chemistry dismayed many of those who admired his experimental research. It also irritated a few theorists who falsely claimed that Pople's methods were not sufficiently reliable for real-world chemical problems, such as solving the structures of long-established, diatomic molecules. But most theorists, myself included, appreciated the attention and credibility that Schleyer brought to theoretical chemistry. Indeed, many in the field believe that without the collaborations with Schleyer, Pople might not have received the 1998 Nobel Prize in Chemistry.

In 1976, Schleyer horrified some by moving to a 'provincial' university: he left Princeton to take a post at the University of Erlangen-Nuremberg in Germany. At Erlangen, Schleyer continued to synthesize molecules that had never been made before. With exclusive use of a powerful computer on nights and weekends, he also devoted

more time than ever to computational chemistry. In 1983, Schleyer made the remarkable prediction that the seemingly bizarre carbon–lithium molecule CLi_6 could be made. The prediction was confirmed experimentally nine years later (H. Kudo *Nature* **355**, 432–434; 1992).

Schleyer loathed administration and officialdom. Instead of attending the endless committee meetings that assail professors at German universities, Schleyer spent time talking to his students and postdocs, writing papers and listening to classical music. His passion for research was contagious. By the time he left it in 1998, Erlangen had one of the most distinguished chemistry departments in Germany.

In 1990, Schleyer accepted a part-time appointment at the University of Georgia in Athens, where I had arrived three years earlier from the University of California, Berkeley. In 1998, he joined us permanently as a professor of chemistry and professorial fellow at the Center for Computational Quantum Chemistry.

Far from radically slowing down, Schleyer worked about 60 hours a week, instead of his previous 80. He collaborated with several of the faculty members, myself included, and published around 400 papers.

Everyone who worked in Paul's lab had to listen to classical music. He had an encyclopaedic knowledge of it and could identify the composer of any piece, and often the orchestra that had performed it. Paul could be intimidating to students and colleagues, but formed warm friendships with many. He was never bitter at having 'just missed' two Nobels.

Of the many tributes to Paul that I received after his death, that of Roald Hoffmann, who shared the 1981 chemistry Nobel for his theoretical work on chemical reactions, captures his essence best: "What Paul had to say was always so honest, so clearly imbued with a drive to understand, that his friends and colleagues valued every opportunity to talk to him, from the time of letters in real ink to e-mails." ■

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