

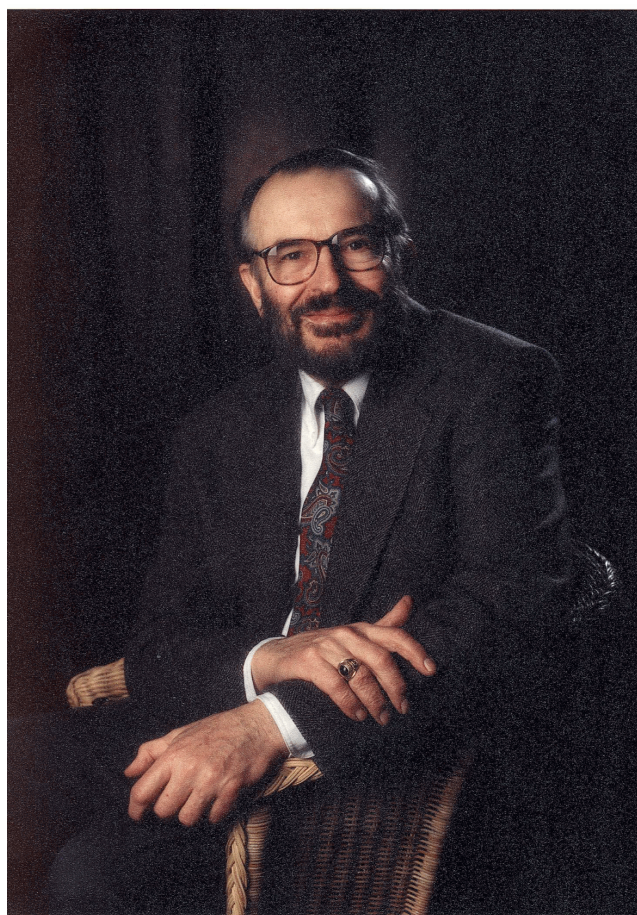
PREFACE

Paul von Ragué Schleyer

This Festschrift celebrates the 70th birthday of one of today's most remarkable chemists. Paul Schleyer was born in Cleveland, Ohio on February 27th 1930. As a child he persuaded his grandmother to help him buy chemicals for his experiments. All looked set for a career as an experimental chemist. Later, after his Ph.D. with Paul Bartlett in Harvard, Paul accepted a position as assistant professor in Princeton and began to establish his reputation as an experimental physical organic chemist. Always one to grasp new opportunities, Paul was an early exponent of the use of infrared spectroscopy to investigate hydrogen bonding. The synthesis of adamantane by Lewis-acid catalysed rearrangement was a highlight of this stage of Paul's career.

However, Paul's interest in understanding chemical bonding has always been the driving force behind his research. This and a sporting interest in breaking the rules (evident in other aspects of his life) led Paul to research areas that became more and more ambitious as his career advanced. On the drive from Philadelphia airport to Princeton when I arrived to postdoc with Paul in late 1975, he offered me the choice of three research projects; to synthesise a tetrahedrane, dodecahedrane or a perpendicular olefin. I chose the perpendicular olefin – probably because there were at least planar olefins – and became an organolithium chemist. I never made a perpendicular olefin, but did discover very quickly that Paul was enthusiastic about any interesting and unusual results. My first joint publication with Paul started life as a routine report after he had left Princeton for Erlangen in 1976 and I had stayed in Princeton for the rest of the year. Paul's reaction to my report of a cascade of deprotonation and hydride elimination reactions that eventually formed the heptafulvene dianion arrived in a letter that started "*I got quite excited about your results...*" and that included a first draft of a *Chemical Communication* in which I was obviously supposed to fill in the numerous missing details.

However, experiments are often indirect and the most interesting compounds are by nature difficult to make. Paul's involvement in the nonclassical carbocation debate had led him to search for ever more direct techniques to answer his questions about structure and bonding. John Pople described his interaction with Paul at this stage of their careers in his lecture in Erlangen at the symposium in honour of Paul's 60th birthday. He pictured his long and fruitful cooperation



with Paul as an experiment as to what would happen if one gave an organic chemist (a species with which John had had very little experience) *Gaussian 70* to play with. Unfortunately, John's experiment was flawed because he selected a very untypical organic chemist. Giving Paul a tool that removed the need to make the compounds that he invented and that gave him structures, electronic properties, energies and a host of other information was the start of a new direction in physical organic chemistry. The Pople/Schleyer partnership was to become one of the most fruitful and remarkable in the history of chemistry. I remember well the heady days of "STO-3G-lithium", a moderately electropositive strong π -acceptor that helped break van't Hoff and Lebel's

rules in just about every case. It hardly seems important that real lithium chooses not to behave quite like STO-3G-lithium. We learnt so much about bonding theory in those formative years that in retrospect it must be an omission of nature that there is no element that quite behaves like STO-3G-lithium.

This era also revealed one of the major features of Paul's career, his love of a good, no holds barred scientific discussion. His ongoing discussion with Andy Streitwieser about the degree of ionicity of the carbon-lithium bond still serves as an example of constructive and productive scientific dispute. The standing joke for years in Erlangen was that one of the questions in oral Ph.D. examinations remained constant ("*how ionic is the carbon-lithium bond?*") but that the answer was time-dependent. It still astonishes me how many of the techniques and arguments developed for and used in this discussion are second nature to today's computational chemists. Such discussions, of which there were (and are) many, never involved malice on Paul's side. Although such disputes could become very heated, Paul was always open to convincing arguments from the other side. He is for me exemplary in his commitment to scientific truth, rather than defence of his pet theory. This is not to say that he is easy to convince, but his opponents do have a chance.

The contributors to this issue come from many different phases of Paul's career, from the nonclassical carbocation

debate through to his recent work on magnetic properties and NICS. The most remarkable aspect of his career is perhaps that he has played such a major role in the development of so many different areas of chemistry. He has been closely associated with the very best chemists in every phase of his career and has always been able to "put the Schleyer stamp" on every one of his collaborations. When I was reading the contributions to this Festschrift, I was struck by a couple that were written in the unmistakable style of a Paul Schleyer paper. The effective, powerful English and the uncompromising accuracy of his best papers are unrivalled. Even today, my graduate students in Erlangen ask for Paul's famous seminars on "*How to write a scientific paper*" and "*How to give a good talk*". Paul freely admits that he doesn't stick to his own rules, but then he doesn't have to.

It is not without a little pride, and certainly with a great deal of pleasure, that we at the *Journal of Molecular Modeling* have produced this Festschrift. Our interaction with the authors has been characterised by their respect, admiration and friendship for Paul. It now only remains to wish Paul many more productive years of research, to hope that he will enjoy this tribute to one of the most remarkable and innovative chemists of the 20th century and to couple this hope with the confident expectation that he will continue to inspire, provoke and educate us well into the 21st.

Tim Clark

Erlangen, February 2nd 2000