

## Instinct for success

**The Right Place at the Right Time.** John D. Roberts. American Chemical Society, Washington, DC, USA. 1990. 390 pp

Among the basic sciences, chemistry has not produced its share of 'great communicators'. It is obviously difficult to attract and inspire new talent if the intellectual challenges of the field and the excitement of the people who work in it are not adequately propagated. However, there is good news. The American Chemical Society plans to publish 22 volumes in a series entitled 'Profiles, Pathways, and Dreams: Auto-biographies of Eminent Chemists', edited by J. I. Seeman. Colourful personalities in chemistry have been asked to write about the whys and hows of their efforts as well as about the overall developments in their field. The book by John D. Roberts is among the first to appear in this series.

Professor Roberts is an admirable choice to recount the major technical and methodological developments that have taken place in organic chemistry over the last 50 years. He has been an active and innovative participant in many of these developments. Going through the book, it is easy to see why he is the personal hero for generations of physical organic chemists.

In the early part of his career, Roberts made significant contributions to the chemistry of small ring compounds. The work led him to the famous formulation of the bicyclobutonium structure for the  $C_4H_7^+$  ion, the first 'nonclassical' carbocation. The concept as well as the term 'nonclassical' caught on rapidly, but led to one of the most bitter controversies of organic chemistry. Having taken enormous trouble to elucidate the subtle features of structure and reactivity in some of these systems, Roberts has little patience for (over)simplified representations. He makes no attempt to be polite about H. C. Brown's contributions in this area.

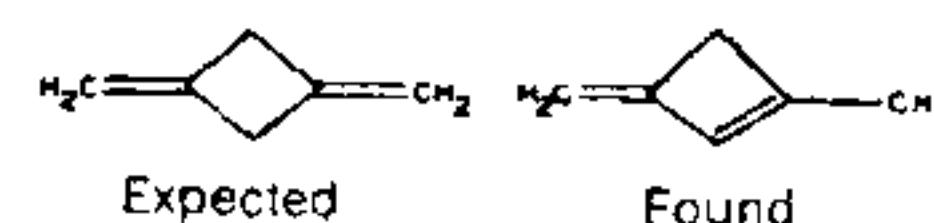
The intelligent use of isotopes for studying reaction mechanisms brought Roberts unqualified success. His proof for the intermediacy of benzyne (another name he coined) in nucleophilic aromatic substitution reactions of halobenzenes

(before the days of modern analytical techniques) is simply astounding. Somewhat less known, but equally impressive, are his other mechanistic studies, e.g. on the structure of Grignard reagents and on the degree of concertedness of Diels-Alder reactions.

Roberts was one of the first organic chemists to have realized the usefulness of molecular orbital theory. Having taught himself Huckel theory (not an easy task for someone who had never taken any course in quantum chemistry; in fact, had not done any course work at all in his graduate programme in those good old days), he proceeded to publish several applications and spread the message widely by lecturing about the method at numerous places. He even wrote a book on the topic (a tip for all students: questions on Huckel theory are generally taken from this little paperback to this day).

Roberts was also the first organic chemist to widely propagate the use of nuclear magnetic resonance as a routine analytical tool. At the half-way mark in the book, he begins this fascinating story. With relatively little knowledge of the method, but with the information that Du Pont had acquired a spectrometer because of its chemical utility, Roberts wants CalTech to be the first university to own a commercial NMR spectrometer. The division chairman Linus Pauling agrees, but feels it should go to a chemical-physics type'. Rebuffed, Roberts rethinks his strategy, collects contributions from fellow organic chemists, uses the punch line 'with NMR, we can investigate the borderline between resonance and tautomerism' with Pauling, and is finally successful in getting 'a complex mass of electronic equipment with the most meagre of instruction books'. When the Varian installer, James Shoolery, asks for a sample to check the machine, Roberts gives some 1,3-dimethylenecyclobutane, which his student had just made for the first time! After twirling the knobs for a long time and staring at the CRT traces (the spectrometer was not stable enough to permit recording), Shoolery announces that 'the compound had a methyl group and a single hydrogen on a double bond, plus other groups'. Naturally Roberts is flabbergasted and dismayed. But he soon realizes that the assignment was correct after all. The compound which he claimed to have made had in

fact rearranged in the last step of the synthesis:



The episode redoubles his respect for NMR as a structural tool for organic compounds. So he 'gave up everything else and lived at the machine'.

What follows is a fine documentation of developments in NMR instrumentation and methodology, and of numerous applications to structural chemistry over the last four decades: natural-abundance NMR, both  $^{13}C$  and  $^{15}N$ ; conformational analysis of organic rings; rotational barriers; inversion barriers; enzyme structures, etc.

The human side of scientific endeavour comes out well in this book. The frustrations of a guide who cannot get any student to work on his 'best' project (in the case of Roberts, what turned out to be a classic study of field effects of substituents across bicyclo[2.2.2]octyl systems); the challenge of having to teach chapter 19 of Eyring, Walter, and Kimball's *Quantum Chemistry* without going through the previous 18 chapters; the pleasure and the pain of getting a bright idea and being told by a graduate student that he has already found it to be wrong a week back; the empty feeling on being told after obtaining a beautiful solution that the problem itself was wrong in the first place, and a host of other emotions should prove to be of general interest.

Several affectionate portraits of people who made significant contributions (e.g. Paul Bartlett, Saul Winstein, Max Rogers), occasionally irreverent descriptions of some of the high and the mighty (e.g. Pauling, Woodward, Robinson, Ingold), and a ruthless attack on H. C. Brown provide attractive fare for all those interested in the personal interactions among the major contributors to chemistry over the last six decades.

Most importantly, Roberts succeeds in showing that solving chemical problems can be a great intellectual challenge and a lot of fun.

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