Angewandte Chemie International Edition

Richard Bader (1931–2012)

R. Bader

Richard Bader, who developed the quantum theory of atoms in molecules, an edifice often called simply "Bader analysis", died on January 15 in Burlington, Ontario, Canada. He was 80.

Molecules are built from atoms, and the properties of a molecule are determined by the positions and identities of its composing atoms. This chemical creed is embodied by the periodic table, and the ubiquity of the periodic table in the halls of chemistry and minds of chemists attests to its utility. But this perspective was challenged by the advent of quantum mechanics. In the quantum mechanical description of a molecule, there is a molecular Schrödinger equation, involving the molecular Hamiltonian and a molecular wavefunction. Before Richard Bader's work, chemists had to choose between a precise mathematical treatment of molecules based on physics or a qualitative treatment with links to the historical language of chemistry. Wielding physics and mathematics, he showed how to slice molecules into atomic regions, leading to the quantum theory of atoms in molecules.

It is rare for any modern scientific method, much less a theory, to be almost wholly associated with one great mind. Richard Bader was not only the creator of the quantum theory of atoms in molecules (QTAIM), he was the driving force behind the theory for more than forty years. His office was the *sanctum sanctorum* of QTAIM, and almost every important discovery came from his research group. Richard Bader conceived QTAIM, defined and explored its physical and mathematically underpinnings, and vigorously pursued its development and extension. His association with the theory was so strong that QTAIM is often simply called "Bader analysis", a term he hated because he felt it made the theory sound like his personal philosophy of chemistry, obscuring the fact QTAIM defines a system of physics for open quantum subsystems like atoms and functional groups in molecules. His death is the cataclysm that ends an epoch in QTAIM.

Richard Bader's key insight was that chemists think of molecules and atoms in three-dimensional space, not the high-dimensioned space of electron configurations. Therefore it is more natural to partition molecules into atoms based on the three-dimensional function that quantifies the electron cloud, the electron density, and not the high-dimensional electronic wavefunction or its imperfect representation in terms of complex-valued and delocalized molecular orbitals. Armed with contour diagrams of the electron density, the idea of partitioning molecules into atomic regions in the same way that one assigns land to river basins is an elegant solution. Richard was not content with that: he learned the requisite mathematics and physics and developed this important insight into a quantitative theory that is an important tool for all those who seek insight, and not just numbers, from computations. Offshoots of his developments permeate modern chemical computation: in his zeal to compute atomic properties, he pioneered new approaches, techniques, and perspectives for molecular properties too.

Above the door of Richard's office, there was a sign: "If you cannot measure it or define it using physics, I do not want to discuss it." He forcefully challenged anyone he saw violating this exacting standard, which led to many contentious discussions. Nobody who ever argued with him will forget the experience. Richard saw himself as the advocate for the truth of physics against the quagmire of heuristic and ill-defined bonding models of chemistry, which he regarded as opiates that led to hallucinations and muddled thinking, rather than as stimulants of creative insight. He reacted with particular disapproval when his approaches and perspectives were viewed as complimentary to, and not substitutes for, the heuristic models of classical chemistry. He published many acerbic comments about work which did not meet his standard, and it required backbone for an opponent to withstand Richard's blasts. But this was like the fire that reveals the imperfections in one's own arguments—a purgatory for quite a few people, but not a hell. The spontaneous statement by one of us (G.F.) after learning about his death was: "He was a wonderful foe. Now God has someone to argue with."

Richard's principles influenced and inspired people developing ways of understanding molecular properties and reactivity. He, more than anyone else, is responsible for forcing this community to follow the precepts of physics, to be mathematically precise, and to focus on predicting and describing experimentally observable phenomena. After Richard's work on QTAIM, papers proposing conceptual methods for interpreting computations were expected, and even required, to contain a mathematical derivation of the method from first principles. Although it was sometimes perceived as truculence, his passionate defense of physics as the only acceptable source for chemical insight raised the standards and informed the discourse of chemistry. In the series of e-mails that the theoretical chemistry community exchanged upon the announcement of his death, scientists who persistently disagreed with him acknowledged how his skepticism forced them to hone their arguments and deepen their understanding. There was also recognition that he, by advocating molecular electron density as the cornerstone for chemical thought, catalyzed the acceptance of density functional theory (DFT) as a computational tool and as a leading topic of theoretical chemistry research in his home country of Canada.

Richard Bader was born in Kitchener, Ontario, Canada in 1931. He completed his BSc and Msc degrees at McMaster University before leaving to do his Ph.D. in physical organic chemistry with C. Gardner Swain at the Massachusetts Institute of Technology (MIT). Richard liked to remind his fellow theorists (most of whom would be hazardous to themselves and others in a laboratory) that he was a "practicing organic chemist", and he retained this perspective throughout his career. Many of his most important discoveries resulted from his attempts to find the physical basis for empirical rules of unquestioned utility in the chemical laboratory (for example, property additivity relationships and the valence-shell electron-pair repulsion (VSEPR) approach). After his stint at MIT, he moved to Cambridge for a postdoctoral fellowship with H. Christopher Longuet-Higgins before returning to Canada, first as a professor at the University of Ottawa (1959–1963) and later at McMaster University (1963–2012). Richard was always generous in acknowledging the contribution of others—not only his senior colleagues, but especially his students and postdocs—to his research. Especially early in his career, his studies of the electron density were facilitated by his association with Robert Mulliken and Clemens Roothaan. His attention was drawn to the Laplacian of the electron density during a 1968 visit to the theoretical chemistry group at ETH-Zürich; his interests in topological analysis and higher-order electron distribution functions were quickened during a 1972 visit to Raymond Daudel's group, in Paris. Among his McMaster colleagues, he had deep, rich, and long collaborations with his experimental colleagues (especially Ron Gillespie and Nick Werstiuk). Also at McMaster, he was a mentor and guide to one of us, constantly reminding P.W.A. that he should steer clear of "mathematical higgery-jiggery" and keep his feet on the ground, even if his head was in the clouds.

And that was how Richard lived his life and did science: with his feet grounded in the problems and language of practicing chemists, but with his mind in the pure and ethereal realm of physics. His desire for precision and rigor; his passion for chemistry and for life; his zeal for teaching and mentoring young scientists; his respect for experiment; his belief that experimental observables are the ultimate source of understanding; his unrelenting assault on the problem of defining chemical concepts with the language of physics: these are the traits that Richard Bader embodied, and that his quantum theory of atoms in molecules embodies still.

Paul W. Ayers
McMaster University, Hamilton (Canada)
Gernot Frenking
Universität Marburg (Germany)

DOI: 10.1002/anie.201201794