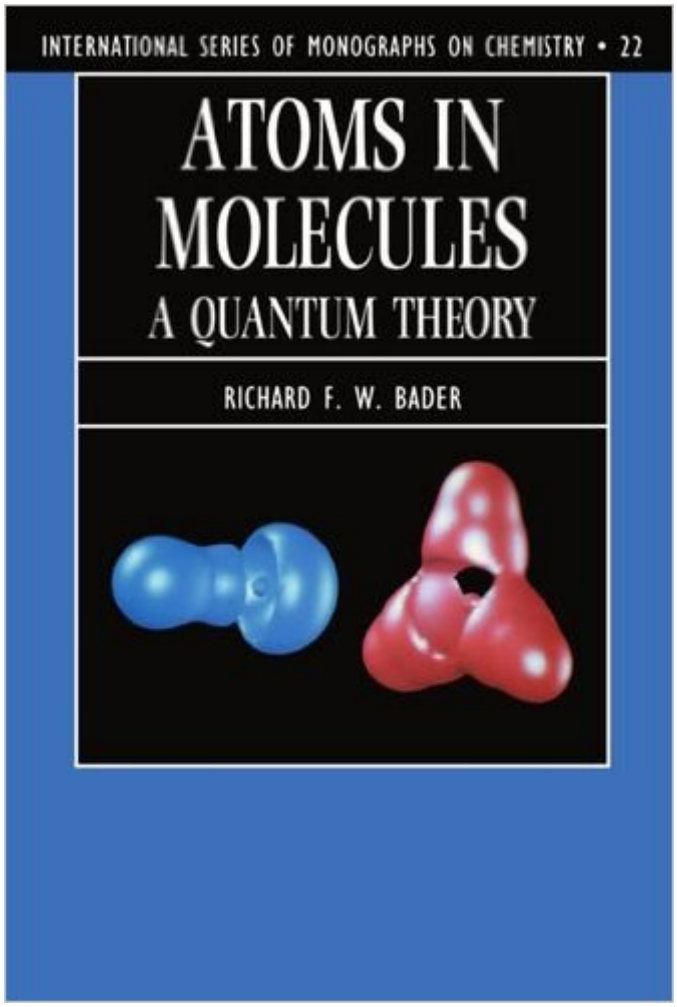
Atoms In Molecules: A Quantum Theory (International Series Of Monographs On Chemistry)



Synopsis

The molecular structure hypothesis--that a molecule is a collection of atoms linked by a network of bonds-- provides the principal means of ordering and classifying observations in chemistry. However this hypothesis is not related directly to the physics which governs the motions of atomic nuclei and electrons. It is the purpose of this important new book to show that a theory can be developed to establish the molecular structure hypothesis, demonstrating that the atoms in a molecule are real, with properties predicted and defined by the laws of quantum mechanics, and that the structure their presence imparts to a molecule is indeed a consequence of the underlying physics. As a result, the classification based upon the concept of atoms in molecules is freed from its empirical constraints and the full predictive power of quantum mechanics can be incorporated into the resulting theory--a theory of atoms in molecules. Eminently accessible and readable, the book will interest all scientists involved with experiment and observation at the atomic level, in addition to theoreticians.

Book Information

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Customer Reviews

The science of chemistry had always eluded me until I found this book. The author, Richard Bader, has, using computer graphics, quantum mechanics, and catastrophe theory created an approach to chemistry that is simultaneously rigorous, accurate, and, most importantly, understandable. Anyone with an elementary knowledge of physics and mathematics can read this book and come away with

a true understanding of chemical physics. Using the techniques pioneered by Bader and his students and colleagues, one can literally see the stability and reactivity properties of any molecule. And this is just the beginning. Laboring "against the dominant paradigms" for years, Bader's theories are now gaining wide acceptance as a new crop of younger, more graphics-oriented computational chemists are entering the workforce. Hardly an issue of any journal in chemical physics now gets published wthout at least one article citing this book. Indeed, Richard Bader has become the most-cited physical scientist in Canada. This is becoming the way to undertstand molecules, and I believe, over the next years, will become the way that theoretical chemistry is taught.

In the opinion of several world-class scientists, the author of this book should have received the nobel Prize in Chemistry for his work, of which this book is arguably his Magnum Opus. But, like Galileo, he was a bit too vociferous in his critique of the establishment. He writes lucidly, and has a riveting thesis - if you understand a bit about Physical Chemistry. Well worth the price. The book was mailed promptly, and is part of my permanent library.

I must admit that I bought this book several years ago but only now I feel confident writing a review about its content, the Quantum Theory of Atoms in Molecules (QTAIM) developed by Professor Richard Bader and coworkers. An important observation behind QTAIM is that the electronic charge density of any molecule or solid is an experimental observable which can be accurately determined with the aid of X-ray diffraction crystallography (see Prof. Coppens' book "X-Ray Charge Densities and Chemical Bonding" and Profs. Tsirelson and Ozerov's book "Electron Density and Bonding in Crystals: Principles, Theory and X-Ray Diffraction Experiments in Solid State Physics and Chemistry"). Experiments show that the electronic charge density is highest in regions where atoms (or better, nuclei) are located and lowest in the internuclear regions. It is the latter regions, however, which are important for chemical bonding. In other words, the accumulation of electronic charge density in the internuclear region is responsible for chemical bonding in molecules and solids. By analyzing the topological properties of the electron density, it is possible to quantitatively characterize atom-atom interactions on the basis of (quantum) physics. What turns out from the application of QTAIM to molecules is that the interactions or bonds which chemists have classified since the advent of X-ray crystallography differ only in the depth of their potential energy wells: the depth of a typical homo- or hetero-polar "covalent bond" is deeper than that of a Van der Waals interaction. Both, however, are characterized by an accumulation of electron density in the

internuclear region which can be computed with modern electronic structure methods. This important feature or property allows one to investigate any type of interatomic or intermolecular interaction while avoiding subjective interpretations based on the analysis of the wavefunction. In my opinion, QTAIM represents the ultimate theory of chemical bonding by employing which any scientist with an open mind can disclose the fascinating properties of atoms and molecules. An interesting book that may serve as an intoduction to QTAIM is Prof. Popelier's book "Atoms in Molecules: An Introduction" while the book of Profs. Matta and Boyd "The Quantum Theory of Atoms in Molecules: From Solid State to DNA and Drug Design" presents many contributions about the recent developments and applications of QTAIM.

Bader was an experimental physical organic chemist who taught himself quantum chemistry. He exercised great sway over many, who, like himself, never learned how to think critically. This accounts for his many citations, mainly by his bleating disciples who pay dutiful homage to their shepherd. He waged a near 50 year campaign against those he could not persuade. Not only did he not win a Nobel, he failed to win a single accolade of the physical chemistry community. A recent essay in Chemistry - A European Journal cautions that 'Chemists should protect themselves from the not uncommon argument: My argument is valid, other explanations should not be admitted' with specific reference to Bader and his followers. His 'theory' is to the undiscerning what SPSS is to non-professional statisticians. If you feel like this is how you want to masquerade as a quantum chemist, sign up, buy the book, and let the burlesque continue.One star is way too kind, two thumbs down is more fitting.

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