

titative predictions are now possible. One should not forget, however, that, to paraphrase the famous statement by Mulliken, our ability to produce numbers does not necessarily imply that we can tell what the electrons in molecules are doing. Full understanding of the intricacies of chemical bonding can be attained only with the help of interpretative tools that facilitate analysis of the electronic wavefunctions obtained from quantum-mechanical calculations.

The concept of the atom is as old as chemistry itself. Like their predecessors, modern chemists find atoms indispensable in understanding and systematizing properties of molecules. Yet inspection of the postulates of quantum mechanics makes it clear that atoms cannot be identified in molecules unless additional assumptions are made. Although there are infinitely many distinct ways of dissecting molecular properties into contributions from individual atoms, the approach that achieves this end with a minimum degree of arbitrariness is obviously preferable.

The quantum theory of atoms in molecules, pioneered by Bader, is without doubt the most self-contained and general of such approaches. It takes advantage of the fact that, within the nonrelativistic Born-Oppenheimer approximation, partitioning of the Cartesian space into regions (called "attractor basins") demarcated by zero flux surfaces in the electron density results in open quantum-mechanical subsystems whose properties satisfy several fundamental relations, such as the (hyper)viral and Ehrenfest theorems. In other words, validity of such relations for the subsystems is the sole condition from which the partitioning ensues.

Bader's book covers a multitude of issues related to the concept of atoms in molecules. The topological properties of the electron density and the related topics of molecular structure and its change are discussed first. This is followed by an exposition of the quantum-mechanical properties of attractors in molecules. This part of the book is presented with mathematical rigor, but the fact that the theory of atoms in molecules actually consists of two overlying layers of interpretation seems to be largely ignored. Readers would benefit from the realization that, although the definitions of attractors, their basins, and the critical points in the electron density together with the associated attractor interaction lines are rigorous and supportable by quantum-mechanical arguments, their identification with atoms and bonds is a different matter. In fact, such identification is based on a purely empirical observation that the majority of molecules in their ground-state equilibrium geometries do not possess non-nuclear attractors. This

assumption is not always true, however. In fact, there are numerous known examples of molecules with either non-nuclear attractors or with unusual bond paths—many more than Bader would have us believe. Of course, this does not invalidate the first part of the theory, which deals with characterization and classification of molecules in terms of the properties of the critical points and the attractors. However, the decision whether the existence of such "anomalous" systems represents failure of the second part of the theory or of "chemical intuition" should be left to the reader.

Overall, *Atoms in Molecules: A Quantum Theory* is a very comprehensive monograph that I would strongly recommend not just to quantum chemists but also to anyone interested in a systematic and mathematically rigorous approach to understanding chemical and physical properties of molecules. Those who are not familiar with Bader's theory and manage to work through the formidable mathematics will appreciate its formal elegance and conceptual beauty. Those who know the theory and would like to have a convenient compendium with all the relevant equations and references handy will be equally satisfied. Those who expected a lot of new material not previously covered in the numerous publications by Bader and his co-workers probably will be slightly disappointed. One may hope that new editions with updated material (and possibly some exercises and answers for graduate students) will follow in the future.

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