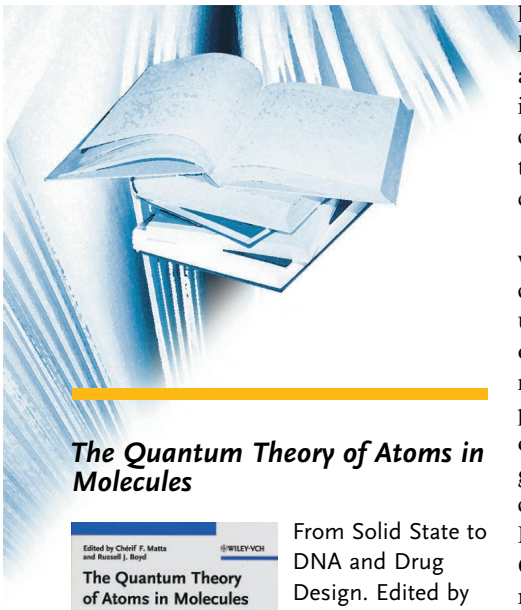
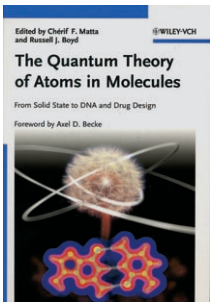


The Quantum Theory of Atoms in Molecules



From Solid State to DNA and Drug Design. Edited by *Chérif F. Matta* and *Russell J. Boyd*. Wiley-VCH, Weinheim 2007. 529 pp., hardcover € 159.00.—ISBN 978-3-527-30748-7

The quantum theory of atoms in molecules (QTAIM) developed by Richard Bader and co-workers is now having enormous impact across many areas of chemistry, physics, and biology, and this volume of collected works is dedicated to him on the occasion of his 75th birthday. It is a timely publication, since Bader's influential 1990 monograph, *Atoms in Molecules—A Quantum Theory* (Oxford University Press, **1990**), published nearly two decades ago, has received over 3000 citations, more than half of them in the last five years (2002–2006).

In the opening chapter, the editors provide a concise introduction to QTAIM. This is perhaps one of the most useful such introductions to the subject, defining and briefly describing the key concepts that underlie the applications discussed at length in subsequent chapters. Following this introduction, the book is divided into five parts comprising 19 chapters by 49 contributing authors. The division and order of the parts and chapters is "purely and exclusively based on what we think is their logical order", according to the editors, and, despite the unavoidable overlap between many of the parts, this lends order to what might otherwise have seemed chaotic. This is further assisted by the frequent cross-referencing between chapters, which provides a coherence across the different contributions, something that is often lacking in edited research works.

Part I, "Advances in Theory", opens with a chapter by Bader, "written by a chemist for other chemists", in particular for younger chemists. Despite this objective, and Bader's evident effort to make the material as accessible as possible, very few chemists—young or otherwise—will have the necessary grasp of the mathematics to do this chapter justice. Subsequent chapters in Part I focus on the applications of QTAIM to an atomic description of response properties such as polarizability and magnetizability, on a detailed analysis of Raman scattering intensities, on partitioning of the molecular exchange energy, and on the topology of the electron localization function (ELF) and its relationship with VSEPR theory. Reading these chapters highlights a conundrum: precisely what is conventionally collected under the banner of QTAIM, and what is not? What is quantum chemical topology (QCT), and how is it related to QTAIM? For example, the ELF is not an outcome of QTAIM, but its topological analysis has many parallels with the analysis of the electron density and its Laplacian. In Chapter 5, QCT is treated as being synonymous with QTAIM, while in Chapter 6, QCT is broadened to incorporate the topology of the ELF. This is not just a matter of semantics, because the very useful list of abbreviations provided on pages xxvii–xxxi includes not only QCT and QTAIM but also—confusingly—AIM (atoms in molecules) and QTAMC (quantum theory of atoms in molecules and crystals).

Part II, "Solid State and Surfaces", comprises three chapters that describe applications of QTAIM to a molecular solid (urea), silicon surfaces, inorganic clathrates, inorganic solids (with a focus on binary solids), and the active sites of surfaces, with special attention to the MoS_2 hydrodesulfurization catalysts; a very nice introduction to the source function is also included. These chapters are beautifully illustrated, with high-quality reproduction of figures, including color figures that are integrated into the text rather than being separated from the discussion; this is one of the many strengths of the volume.

QTAIM methods have been embraced enthusiastically by researchers who are working in the field of charge density analysis based on modeling of highly accurate low-temperature single-crystal X-ray diffraction data. Part III, "Experimental Electron Densities and Biological Molecules", summarizes recent applications from three of the groups active in this area. Chapter 10 describes the use of ideas derived from both QTAIM and DFT to obtain approximate energy densities from experimental electron densities. Unfortunately, in this chapter QTAIM is referred to as QTAMC, as though the two were distinctly different theories; they are, of course, one and the same. Chapter 11 describes recent work aimed at deriving experimental electron densities for proteins using the experimental multipolar database, and discusses in detail the topological and electrostatic properties based on the electron density distribution of human aldose reductase. In a complementary fashion, the following chapter focuses on transferability of fragments obtained from a theoretical database of multipole parameters, with particular application to amino acids and peptides. It also contains a concise summary of experimental electron density studies.

Part IV, "Chemical Bonding and Reactivity", includes contributions that describe recent applications of the techniques of QTAIM to study bonding to metals (dative bonds, metal carbonyls, metal–metal bonds, three-center bonding, and more exotic categories), electron delocalization, conformational analysis, aromaticity, and topological properties of hydrogen bonds, and to compare different types of bonding to hydrogen by separating the components of the interaction energy. As with other sections of this volume, these chapters provide excellent overviews of the authors' work in particular areas, and are extremely well referenced, providing the reader with essential links to the authors' original publications and to related work by others.

This excellent volume concludes with Part V, "Application to Biological Sciences and Drug Design", which comprises one chapter that introduces QSAR and drug discovery and the novel use of QTAIM-based descriptors, and a final chapter on volume-rendering of the Laplacian of the electron density, which has potential applications in many areas, including pharmacophore recognition.

This is a beautifully produced book on a topic of major relevance across many of the sciences, and it represents a substantial and impressive contribution to the literature on the subject. Although the publisher claims that "this volume may equally be used as a textbook without compromising its research-oriented character", there is little doubt that this is very much a research work. It will be highly sought after by researchers in the field, and should be the first resort by those who are curious about the subject and seek a concise introduction, backed up by summaries of state-of-the-art applications, all in a single package. It is a fitting tribute to Richard Bader on his 75th birthday.

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