1. Record Nr. UNINA9910876772103321

Titolo	The quantum theory of atoms in molecules : from solid state to DNA and drug design / / edited by Cherif F. Matta and Russell J. Boyd
Pubbl/distr/stampa	Weinheim, : Wiley-VCH [Chichester, : John Wiley [distributor]], c2007
ISBN	1-280-92161-7 9786610921614 3-527-61070-7 3-527-61069-3
Descrizione fisica	1 online resource (569 p.)
Altri autori (Persone)	MattaCherif F BoydRussell J
Disciplina	530.12
Soggetti	Quantum theory Atomic structure Molecular structure Solid state physics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	The Quantum Theory of Atoms in Molecules; Foreword; Contents; Preface; List of Abbreviations Appearing in this Volume; List of Contributors; 1 An Introduction to the Quantum Theory of Atoms in Molecules; 1.1 Introduction; 1.2 The Topology of the Electron Density; 1.3 The Topology of the Electron Density Dictates the Form of Atoms in Molecules; 1.4 The Bond and Virial Paths, and the Molecular and Virial Graphs; 1.5 The Atomic Partitioning of Molecular Properties; 1.6 The Nodal Surface in the Laplacian as the Reactive Surface of a Molecule; 1.7 Bond Properties 1.7.1 The Electron Density at the BCP ((b))1.7.2 The Bonded Radius of an Atom (r(b)), and the Bond Path Length; 1.7.3 The Laplacian of the Electron Density at the BCP ((2)(b)); 1.7.4 The Bond Ellipticity (); 1.7.5 Energy Densities at the BCP; 1.7.6 Electron Delocalization between Bonded Atoms: A Direct Measure of Bond Order; 1.8 Atomic Properties; 1.8.1 Atomic Electron Population [N()] and Charge [q()]; 1.8.2 Atomic

Volume [Vol.()]; 1.8.3 Kinetic Energy [T()]; 1.8.4 Laplacian [L()]; 1.8.5 Total Atomic Energy [E(e)()]; 1.8.6 Atomic Dipolar Polarization [()]
1.8.7 Atomic Quadrupolar Polarization [Q()]1.9 ""Practical"" Uses and Utility of QTAIM Bond and Atomic Properties; 1.9.1 The Use of QTAIM Bond Critical Point Properties; 1.9.2 The Use of QTAIM Atomic Properties; 1.10 Steps of a Typical QTAIM Calculation; References; Part I Advances in Theory; 2 The Lagrangian Approach to Chemistry; 2.1 Introduction; 2.1.1 From Observation, to Physics, to QTAIM; 2.2 The Lagrangian Approach; 2.2.1 What is The Lagrangian Approach and What Does it Do?; 2.2.2 The Lagrangian and the Action Principle - A Return to the Beginnings; 2.2.3 Minimization of the Action
2.2.4 Steps in Minimizing the Action2.3 The Action Principle in Quantum Mechanics; 2.3.1 Schrodinger's Appeal to the Action; 2.3.2 Schrodinger's Minimization; 2.3.2.1 Two Ways of Expressing the Kinetic Energy; 2.3.3 Obtaining an Atom from Schrodinger's Variation; 2.3.3.1 The Role of Laplacian in the Definition of an Atom; 2.3.4 Getting Chemistry from G(,;); 2.4 From Schrodinger to Schwinger; 2.4.1 From Dirac to Feynman and Schwinger; 2.4.2 From Schwinger to an Atom in a Molecule; 2.5 Molecular Structure and Structural Stability; 2.5.1 Definition of Molecular Structure
2.5.2 Prediction of Structural Stability2.6 Reflections and the Future; 2.6.1 Reflections; 2.6.2 The Future; References and Notes; 3 Atomic Response Properties; 3.1 Introduction; 3.2 Apparent Origin-dependence of Some Atomic Response Properties; 3.3 Bond Contributions to ""Null"" Molecular Properties; 3.4 Bond Contributions to Atomic Charges in Neutral Molecules; 3.5 Atomic Contributions to Electric Dipole Moments of Neutral Molecules; 3.6 Atomic Contributions to Electric Polarizabilities; 3.7 Atomic Contributions to Vibrational Infrared Absorption Intensities
3.8 Atomic Nuclear Virial Energies

Sommario/riassunto

This book distills the knowledge gained from research into atoms in molecules over the last 10 years into a unique, handy reference. Throughout, the authors address a wide audience, such that this volume may equally be used as a textbook without compromising its research-oriented character. Clearly structured, the text begins with advances in theory before moving on to theoretical studies of chemical bonding and reactivity. There follow separate sections on solid state and surfaces as well as experimental electron densities, before finishing with applications in biological sciences and drug-de