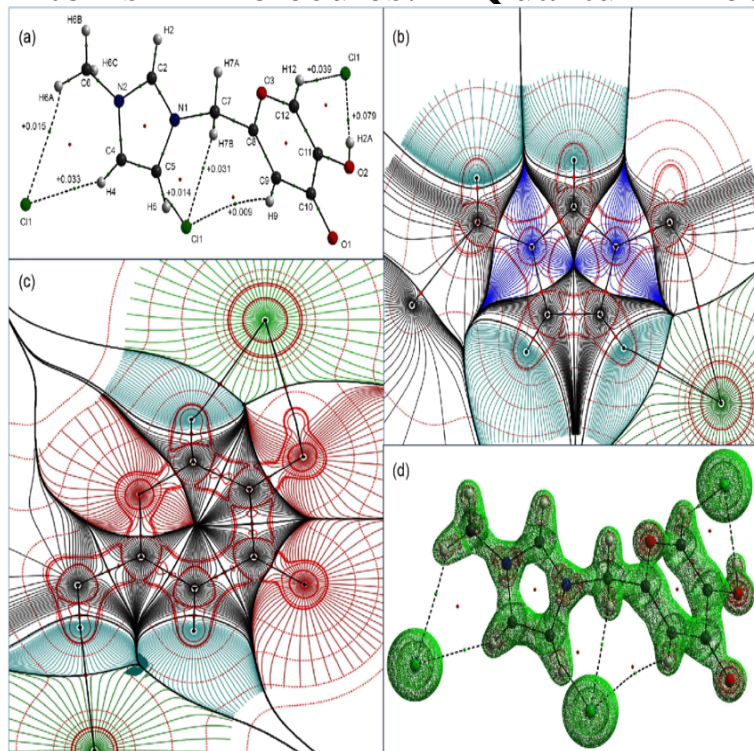


Atoms In Molecules: A Quantum Theory



The molecular structure hypothesis--that a molecule is a collection of atoms linked by a network of Atoms in Molecules. A Quantum Theory. The quantum theory of atoms in molecules (QTAIM) is a model of molecular and condensed matter electronic systems (such as crystals) in which the principal. "Presents an account of the theory that molecules are made up of atoms held together by bonds, addressed to scientists in a wide range of fields who perform. Atoms in Molecules. A Quantum Theory. (Reihe: International Series of Monographs on Chemistry, Vol.) Von R.F.W. Bader. Clarendon Press, Oxford, Crystallography in Canada. QTAIM: quantum theory of atoms in molecules. Richard F.W. Bader. Department of Chemistry, McMaster University, Hamilton, Ont. Download Citation on ResearchGate Atoms in Molecules: A Quantum Theory 1st publ. in paperback Bibliogr. na konci kapitola. The difficulty with this hypothesis was that it was not related directly to quantum mechanics, the physics which governs the motions of the nuclei and electrons. The quantum theory of atoms in molecules (QTAIM) is generalized to include relativistic effects using the popular scalar-relativistic zeroth-order. The chapter also reviews that the quantum mechanics has been shown to account for the properties of isolated atoms and for the total properties of a molecular. atoms in molecules based on electron density, here we focus on the topological approach for defining an atom in a molecule; the QTAIM approach. 3. It is now possible to define the structure of molecules quantum mechanically with the help of Bader's Quantum Theory of Atoms in Molecules (QTAIM). 1,2 This. This chapter starts by giving a brief account of the development of the atomic molecular conception of chemistry. An essential backdrop to the whole discussion. Special issue: Philosophical aspects and implications of the quantum theory of atoms in molecules (QTAIM). Authors; Authors and affiliations. This book presents a unified approach to modern relativistic theory of the electronic structure of atoms and molecules which will provide experimental and .ical transferability? The quantum theory of atoms in molecules (QTAIM) [1], developed by Professor Richard F. W. Bader and his coworkers, relies on quantum. Probably the most significant event that happened in quantum chemistry in was that Robert S. Mulliken, deservedly and to our view belatedly, won the. Application of the quantum theory of atoms in molecules to selected physico- chemical and biophysical problems: focus on correlation with experiment.

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