

Using of QTAIM approach in the study of bonding in M-M clusters (Article review)

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Abstract

QTAIM is the appropriate framework for the quantum-theory of atoms in molecules, and Bader's-analysis is among a group of methods used to analyze the electron density in each system under study. This method provides an explanation of what is inside the molecules and the characteristics of the reactions that take place, because of its importance in enabling chemists to clarify and adequately explain the science of experimental chemistry. The continuous understanding and use of the topological data from the QTAIM approach is possible for obtaining of good physical / chemical answer to the question that arise, and this allows prediction and correct understand the structure of electrons in every atom and molecule. In this article, we explain the properties of QTAIM theory in our discussion and examine the interactions in atoms of electronic density, and apply QTAIM analysis to clearly understand the nature of bonding within a ruthenium cluster.

Keywords: Quantum-theory, QTAIM, nature of bonding

Introduction

In quantum chemistry, the quantum theory concerned with the study of atoms in molecules is referred to as (QTAIM). It is also sometimes known as atoms in molecules (A.I.M), and is the ideal model for electronic systems of matter at the molecular level and in condensed form as in crystals, where the principal modes of molecular and atomic structure are natural expressions of the electronic density distribution function that can be notes in order. Due to the atoms of QTAIM mostly confined to surface with (0 flux) of the carrier domain in the electronic density gradient, they've quantum mechanical properties that are unique compared to the definitions of the rest of the subsystems, especially the unique electronic kinetic energy that agrees with the theory of electron viruses. On this basis, QTAIM has gradually become the appropriate ways for addressed potential subjects relating to any systems of chemistry, within many locations not previously addressed by each model or theory in the chemical subject (1, 2). In chemical science, high proximity of each two non-bonding atoms leading to destabilized steric antagonism, but in QTAIM the monitored (hydrogen=hydrogen) interaction is in actual stabilized. Its famous that all kinking phenanthrene, and chrysene ranged about (6 kcal / mol, 25 k J / mol) extra stabilization than the linear-isomers anthracene, and tetracene. One traditions commentary given through Clar's-rule. The density of electrons at the crucial stage between the two hydrogen-atoms is lower, 0.012e for phenanthrene. Other appropriate of the bonded-path is its bending. Recently, a large number of studies of triosmium-groups in which electron deficiency is evident were conducted in order to model heterogeneously catalyzed hydrogen treatments (3, 4). QTAIM, by relying on the quantitative basis of atoms in a single molecule, restores all concepts associated with experimental chemistry. On this basis, in addition to the well-known definition of atoms and molecular structure, QTAIM provides a physical basis for the Lewis model and the rest of the chemical concepts associated with it. Through QTAIM, a new way is available for answers to many questions related to the structure and its relationship to the

measured properties that were considered topics of intense debate and controversy, and the definition of the structure itself. we used (QTAIM) to assess the topological-distributed of electron density, to found some key bonds (5).

1. Purpose of QTAIM

There are many purposes, some of which have been clarified in this article, so the quantum theory of atoms in molecules (QTAIM) is used in order to clarify and understand the physics of bonding between atoms, especially with regard to metal groups and their bonds. Considering the great importance of click chemistry, the reaction of copper (I) catalyzed azide loading (CuAAC) has received great interest (6). It's possible to estimate the electronegativity-built on QTAIM\based domains of the bond electron density-Ferro Costas, as shown in figure (1) below:

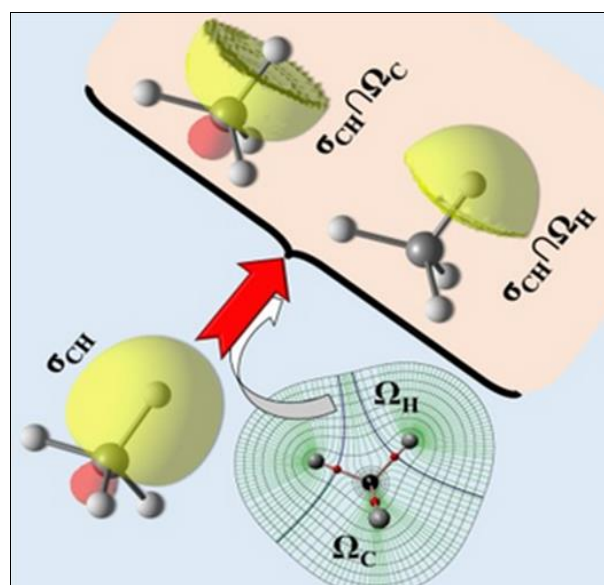


Fig 1: electronegativity estimator built on QTAIM- based of the bond electron density – ferro-Costas.

In the later period, the cycloaddition reaction of azides with di-alkynes will be highly realized for their application in the production of bis-triazoles. It is known that bis-triazoles have important applications in pharmaceutical, organometallic, supramolecular, and biological chemistry as well. There are a number of basic methods for the synthesis of di-triazoles, but the most popular method involves the reaction of azides with di-terminal alkynes (7). There are some techniques that help in understanding some theories related to QTAIM, as shown in the figure (2, and 3) below:

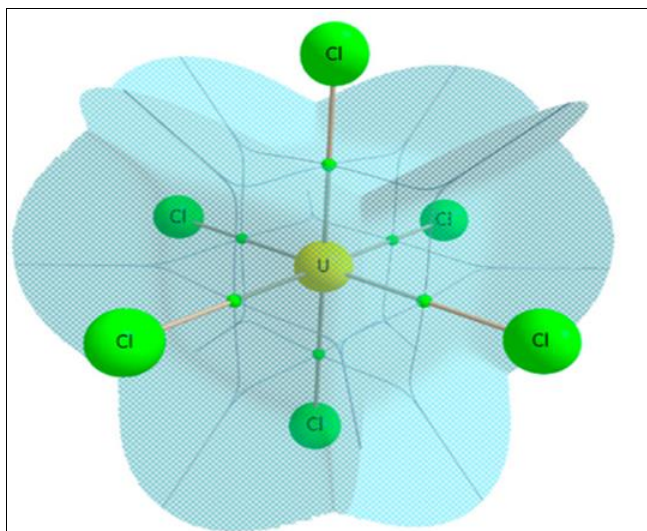


Fig 2: Inorganics! Free full text Decomposition of d- and Shell contributions to uranium bonding form the quantum theory of atoms in molecules: Application to uranium and uranyl Halides.

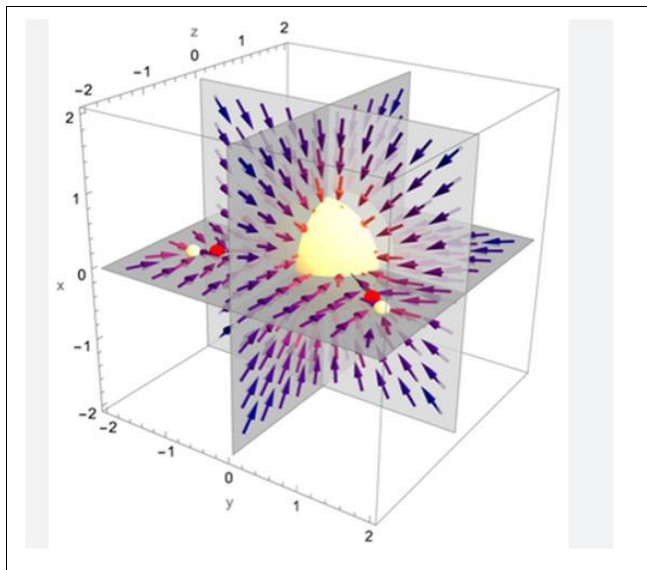


Fig 3: QTAIM: a package for quantum theory of atoms in molecules- online Technical discussion Group- Wolfram Community

2. QTAIM approach

In the recent period, QTAIM appeared as the analysis of the quantum theory of atoms in molecules, and gives a clear depiction of the topology of electronic density, and is considered a useful tool for the analysis and elucidation of chemical bonding. Recently, a study was carried out on (triosmium groups), in which electron deficiency is demonstrated at a broad level in order to model the heterogeneously catalyzed hydro-treating of heterogeneous

cycles (8). These groups have also been widely used for the activation of heterocyclic substrates, and this has led to the formation of new useful compounds that cannot be easily obtained by conventional organic methods. The analysis of the distribution of electron density by the theory (QTAIM/5-9) is a good tool for analyzing chemical bonds and comparing the properties of atoms as well as molecules (9,10). The topological analyzes of light atomic systems help us to devise a good and suitable way to combine topological properties and patterns of binding as an experimental and theoretical study of electron density. It is difficult for this pathway to convert easily into compounds that contain heavy (transition) metal atoms. Heavy (transition) metal atoms have a spectrum that differs from the topological properties and is narrower than it. There are many studies and researches that rely on the QTAIM approach of the (Diminishing Musharakah Bonds).. There are many approaches and fields related to QTAIM, as well as various related studies conducted by a number of researchers, As in the case of modeling the cyclic load (lazido-methyl-benzene) with (2,2-di-prop-2-yn-1-yl) propane-1,3-diol with the presence of a copper catalyst by electronic and thermodynamic methods using quantum chemistry methods. Where the transfer states were investigated related to two reaction catalytic pathways, and this led to the establishment of the synthesis of a statistical mixture of mono- and di-triazoles both structurally and biologically, as shown in Fig (4) below (11):

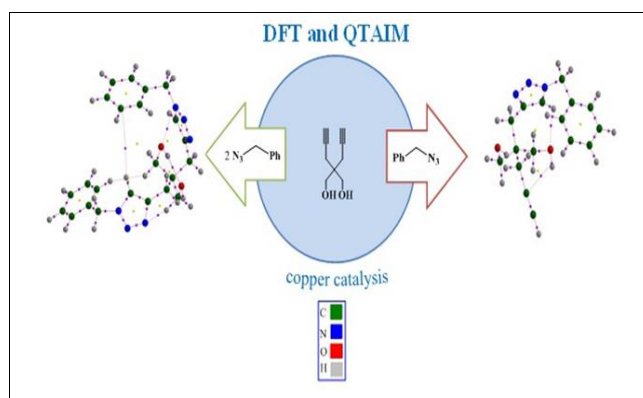


Fig 4: (copper Catalyzed Cycloaddition Reaction of Azidomethyl Benzene with 2, 2- Di (prop-2-yn-1-y1) propane 1, 3-diol: DFT and QTAIM investigation).

3. Application

One of the most important applications of QTAIM is evident in the full description of organic crystals that have short intermolecular distances that are adjacent to each other, and this is evident in the diffraction of X-rays. As we find in the molecular crystalline structure of chlorine, there is a clear empirical distance Cl....Cl between two molecules (327pcm), and this distance is less than the total Vander Waals radius distance of (350pcm). Considering that it starts with 12 bond pathways in each chlorine atom with other chlorine atoms even in a single molecule, this theory aimed for the explaining and clarify the metallic properties of hydrogen in the similar way as mentioned. We can also apply the same theory to hydrogen bonds together (12), in addition to molecules like phenanthrene and chrysin. Many previous scientific studies showed that the dispersions that occurs is an essential-components in the interactions

energy obtained which binds each monomer in binary complexes that are diverse (13, 14). There is a peculiarity in the application of (QTAIM), shown by the dispersion being highly strong, as the binary complexes in certain cases despite the small (Columbian) repulsion the positive sites are weak (or negative negative), as shown in Fig (5) below:

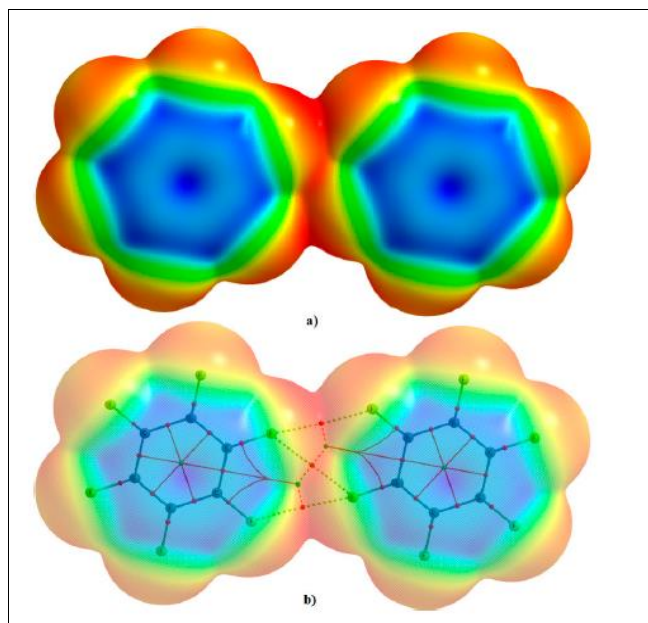


Fig 5: MP2/co-pVTZ00 demity mapped electrostatic potential of (a) solid flippederlaying the QTAIM molecular graph Rep-bp-connectivity is shown in (b where Rep wiring critical po

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