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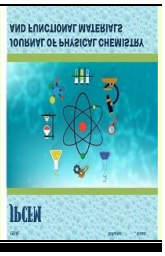

The Theoretical Investigation of the HOMO, LUMO energies and Chemical Reactivity of C_9H_{12} and $C_7F_3NH_5Cl$ Molecules

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ABSTRACT

In this study, the chemical reactivity, stability and electronic properties of Propylbenzene (C_9H_{12}) and 2-*chloro*-5-(trifluoromethyl) aniline ($C_7F_3NH_5Cl$) molecules have been investigated by using the Density Functional Theory (DFT) and Hartree Fock Theory (HFT) methods with difference basis sets like (B3LYP/3-21G, 6-31+G(dp), 6-31G,6-311G). The Lowest Unoccupied Molecular Orbitals (LUMO), and Highest Occupied Molecular Orbitals (HOMO) energies can be used to characterize the kinetic stability and chemical reactivity in chemical structure for these molecules.

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Hartree Fock Theory (HFT)

1. Introduction

The LUMO or acceptor orbitals and the HOMO or donor orbitals energies have been used to predict the electronic structure, bond orders and shapes of molecular orbitals and the properties of molecules. [1-3]. Consequently, many researchers in physics, chemistry, biology, and many other fields have been working in molecular orbital theory (MOs) for finding electronic structure and properties of molecules by using Hartree Fock Theory (HFT) [4]and Density Function Theory (DFT) [4,5]with the different basis sets by Gaussian 09W [6] package. This program is important for expecting many properties of atoms and molecules. In this study, quantum chemical theoretical calculations of Chloro-5-(trifluoromethyl) aniline ($C_7F_3NH_5Cl$) and Propylbenzene (C_9H_{12}) molecules were carried out by DFT and HFT methods with basis sets are (B3LYP/3-21G, 6-31+G(dp), 6-31G,6-311G). Then for these molecules, the structural and electronic properties like Highest Occupied Molecular Orbitals (HOMO) and Lowest Unoccupied Molecular Orbitals (LUMO), total energies, molecular structure, chemical potential (μ), electronegativity (χ), hardness of molecules (η), softness of molecules (S), dipole moment (D), and Electrophilic (ω) and energy gap(Eg) were theoretical investigated [7,8,9].

2. Theory

According to quantum mechanics, atomic orbitals could be expressed as wave functions that characterize the amplitude of electron waves. Their values can be studied from Schrödinger's wave equation solutions. Similarly, the wave equation of Schrödinger can be applied to molecules, but with some difficulty. In order to deal with the problem, an approximate method known as the linear combination of atomic orbitals is used [10] and the chemical reactivity of molecules can be determined using external orbitals known as Frontier Molecular Orbitals (FMOs) [11,12]. The Lowest Unoccupied Molecular Orbital (LUMO) and the highest occupied molecular orbital (HOMO) are named frontier molecular orbital because they are located at the outer boundary of the electrons of a molecule. HOMO as an electron donor is the capacity to give an electron, while LUMO as an electron acceptor denotes the aptitude to get an electron. This study is intended to study the electronic properties and structure of C_9H_{12} and $C_7F_3NH_5$ molecules by using Density Function and Hartree Fock theory with different basis sets.

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Table 1. HOMO, LUMO energies and chemical reactivity properties for ($C_7F_3NH_5Cl$) aniline by DFT and HFT with different basis sets.

($C_7F_3NH_5Cl$) aniline	**DFT**				**HFT**			
Basis set	3-21G	6-31G	6-31+Gdp	6-311G	3-21G	6-31G	6-31+Gdp	6-311G
HOMO (eV)	-7.6	-6.3	-6.5	-6.5	-8.7	-9.8	-9.8	-9.0
LUMO (eV)	-0.82	-1.12	-1.36	-1.44	2.72	1.58	1.55	2.29
Band gap (eV)	6.80	5.14	5.17	5.09	11.43	11.37	11.35	11.27
Total energy (a.u)	-1079	-1084	-1084	-1080	-1075	-1080	-1080	-1080
Dipole moment (Debye)	2.67	3.03	2.79	3.27	2.67	2.73	0.98	2.77
Electronegativity (χ) (eV)	4.2	3.7	3.9	4.0	3.0	4.1	4.1	3.3
Hardness (η) (eV)	3.4	2.6	2.6	2.5	5.7	5.7	5.7	5.6
Softness (S) $(eV)^{-1}$	0.15	0.19	0.19	0.20	0.09	0.09	0.09	0.09
Chemical potential (μ)(eV)	-4.2	-3.7	-3.9	-4.0	-3.0	-4.1	-4.1	-3.3
Electrophilicity (ω) (eV)	2.6	2.6	3.0	3.1	0.8	1.5	1.5	1.0

Table 2. HOMO, LUMO energies and chemical reactivity properties for Propylbenzene (C_9H_{12}) by DFT and HFT with different basis sets.

Propylbenzene (C_9H_{12})	**DFT**				**HFT**			
Basis set	3-21G	6-31G	6-31+Gdp	6-311G	3-21G	6-31G	6-31+Gdp	6-311G
HOMO (eV)	-8.87	-8.73	-6.6	-6.69	-8.87	-8.73	-6.67	-8.84
LUMO (eV)	4.09	4.00	-0.37	-0.19	4.08	4.00	1.86	3.65
Band gap (eV)	12.96	12.73	6.23	6.5	12.95	12.73	8.53	12.49
Total energy (a.u)	-345.9	-347.7	-350.2	-350.2	-345.9	-347.7	-347.8	-347.7
Dipole moment (Debye)	0.259	0280	0.408	0.317	0.259	0.280	0.401	0.345
Electronegativity (χ) (eV)	2.39	2.37	3.49	3.44	2.40	2.37	2.41	2.60
Hardness (η) (eV)	6.48	6.37	3.12	3.25	6.48	6.37	4.27	6.25
Softness (S) $(eV)^{-1}$	0.08	0.08	0.16	0.15	0.08	0.08	0.12	0.08
Chemical potential (μ)(eV)	-2.39	-2.37	-3.49	-3.44	-2.40	-2.37	-2.41	-2.60
Electrophilicity (ω) (eV)	0.44	0.44	1.95	1.82	0.44	0.44	0.68	0.54

3. Results

3.1. 2- Chloro-5-(trifluoromethyl) aniline ($C_7F_3NH_5Cl$)

2-chloro-5-(trifluoromethyl) aniline is a compound with the molecular formula ($C_7F_3NH_5Cl$) and by physical appearance, it is a colorless liquid, containing 17 atoms and 98 electrons. It is used in the production of the fluometuron and norflurazon herbicides as an intermediate. It is commonly used in a variety of commercial aim industrial, in manufacturing of pesticide, dyestuff, and pharmaceuticals. The optimized structures of structure Chloro-5-(trifluoromethyl) aniline (C7F3NH5Cl) compound have been shown in Figure 1.

At first, Density Function and Hartree Fock theory with different basis sets were used to compute the HOMO and the LUMO energy as shown Table 1. The energy gap between the HOMO and LUMO orbitals is enough to investigate the stability and the chemical reactivity of ($C_7F_3NH_5Cl$) molecule. The value of the energy gap is large, indicating greater stability of this compound. ($C_7F_3NH_5Cl$) is harder molecule and directly proportional to the energy gap ($\eta \propto E_g$). Other calculation by HF are ignored, because of is not similar the precise result.

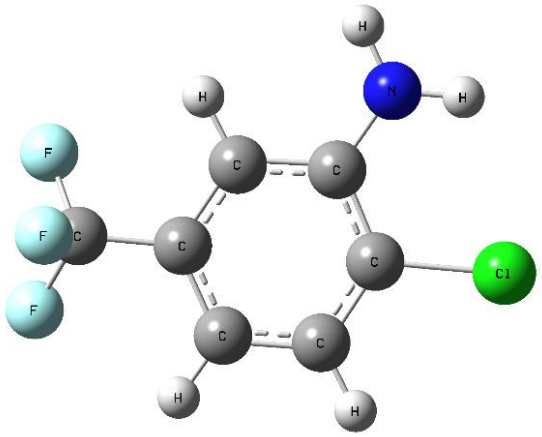

Figure 1. Optimized structure of 2-chloro-5-(trifluoromethyl) aniline ($C_7F_3NH_5Cl$)

3.2. Propylbenzene (C_9H_{12})

The optimized structures of Propylbenzene (C_9H_{12}) compound as shown in Figure 2. It is an organic compound with the C_9H_{12} chemical structure. Propylbenzene is an organic compound with an aliphatic substitution based on the aromatic hydrocarbon, and this compound consists of 21 atoms and 66 electrons. It is stable, colorless liquid and combustible. Other Propylbenzene synonyms include (n-Propylbenzene, Propylbenzene,Benzene, n-propyl

Isocumene, 1-Phenylpropane, Phenyl propane, and 1-Propylbenzene). Before purifying or heating system, Propylbenzene is significant for testing peroxide existence.

The obtained HOMO and LUMO energies, and the chemical reactivity properties of Propylbenzene (C9H12) have been shown Table 2. The value of energy gap is big and is indicate the more stability of this compound. Propylbenzene is harder molecule and depends on the energy gap value ($\eta \propto E_g$). Other calculation can be neglected, because of is not near the exact result.

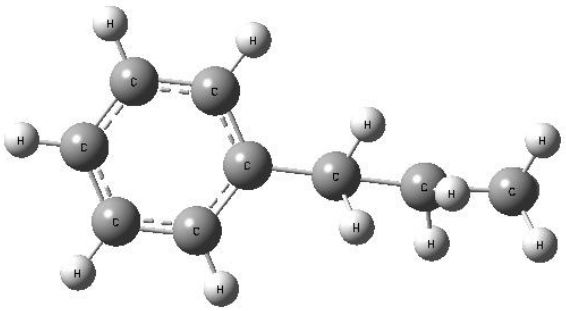

Figure 2. Optimization of Propylbenzene (C_9H_{12})

5. Conclusion

In this work, The Density Functional Theory (DFT) and Hartree Fock Theory (HFT) were used to investigate the structural and electronic properties of Chloro-5-(trifluoromethyl) aniline ($C_7F_3NH_5Cl$) and Propylbenzene (C_9H_{12}) molecules for the different basis sets. In the results, the higher frontier orbital gaps indicate that the molecule has more kinetic stability and can be describe as low reactive molecule. The most of our calculation by the Density Function Theory (DFT) are more consistent than Hartree Fock Theory (HFT), and by increasing the size of basis sets the rate of accuracy is increased.

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