Theoretical Study of the Structural, Electronic Properties and GIAO ^{1}H-NMR, ^{13}C-NMR and the Effect of Substitutes on the Succinimide

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الخلاصة

تم في هدا البحث دراسة نظرية للخصائص والصفات التركيبية والالكترونية للسكسنمايد المعوض (I, II, III). بواسطة كيمياء الكم. الموائمة الهندسية للتراكيب انجزت بطريقة DFT وعند مستوى الحساب B3LYP وعند مستوى المجموعة الاساسية .(6-311++G(3d,3p. الدراسة اظهرت أن الموائمة الهندسية لتراكيب المركبات (I, II, III) تمتلك اقل طاقة. كذلك اظهرت الدراسة القيمة العالية لعزم ثنائي القطب للجزيئة (II) مقارنة مع الجزيئات (I, III). وتم حساب الخواص الالكترونية والتركيبية للدوال التالية طاقة االمدار الجزيئية HOMO , LUMO. وقيمةΔE , A, I, η, X, ω . والتي أظهرت ان المركب (I) أكثر استقرارا من المركبات الاخرى وبهذا يكون ترتيب استقرارية المركبات I>II>III. وكذلك تم أجراء الحسابات النظرية لطيف ^{1}H-NMR و^{13}C-NMR للمركب (I) ومقارنتها مع القيم العملية وتنبأ لطيف ^{1}H-NMR و^{13}C-NMR وتوزيع الكثافة الالكترونية للمركبات(II, III). كذلك بينت أن تأثير المعوضات على الحلقة والذي يؤدي الى تغيرات في أطوال الأواصر والزوايا .

Abstract

The calculations of Substituted Succinimide (I, II, III) were carried out by using quantum chemical calculations. The optimized structures of the Compounds(I, II, III) were obtained by the Density functional theory DFT/B3LYP level of theory using the basis set 6-311++G(3d,3p). The study shown, the optimized structures of compounds (I, II, III) have the global minimum energy. Also the dipole moment of compound (II) found to have high values compared with the Compounds (I, III). Global descriptors such as the MO energies of HOMO, LUMO levels, Δ*E*, electron affinity(A),ionization potential(I), hardness(η), electronegetivity(X), electrophilicity(ω) were determined and used to identify the differences in the stability and reactivity of compounds. In general calculated values lead to the conclusion that the stability of the compounds are I>II>III . On the other hand theoretical calculations for ^{1}H-NMR and ^{13}C-NMR for compound(I) were carried out and compare with experimental data for compound (I) and predicate the ^{1}H-NMR and ^{13}C-NMR, Charge Density Distribution for compounds (II, III). As well as the calculations show the effect of substitution on the ring leads to change of the bond length and angles.

Key Words: *Substituted Succinimide, ^{1}H-NMR and ^{13}C-NMR spectra, DFT/B3LYP(6-311++G(3d,3p)).*

Introduction

Succinimide its derivatives are biologically and industrially useful compounds. Pharmaceutically they are used as analgesics, nephrotoxic, anticonvulsant, antiepileptic, fungicidal, ionic inhibitors of human leukocyte, etc. They are also used in industries as antifoaming agent, and biodegradable polymer, lubricating oil, lubricating tackifiers, emulsion explosives and also corrosion inhibitors, Some new succinimide and sulfonated derivatives were confirmed to have analgesic activity through abdominal constriction tests in mice. It has been reported that sulfonated derivatives of succinimide are more effective than aspirin and paracetamol. Consideration of these factors lead to undertake the detailed spectral investigation of succinimide [1-6]. Theoretical foundation for modern chemistry was laid more than 70 years ago at this time it becomes possible, in principle, to use this for

predication and understanding how electrons, atoms, and molecules interact. Theoretical calculation methods are helpful tools for elucidating structure and behavior of molecules , atoms and electrons. Computational chemistry (also known as molecular modeling) is the application of computer-based models to the simulation of chemical processes and the computation of chemical properties. One major method of computational chemistry ; Density Functional Theory (DFT) has been accepted by the ab initio quantum chemistry community as a cost effective general procedure for studying physical properties of the molecules, because it is based on total electron density rather than wave functions[7-11]. In this work we attempt to study the predication of structure and electronic properties, relative stabilities for the succinimide is substituted by sulfur atom, by performing Density functional theory (DFT)/B3LYB level of theory using the basis set 6-311++G(3d,3p).

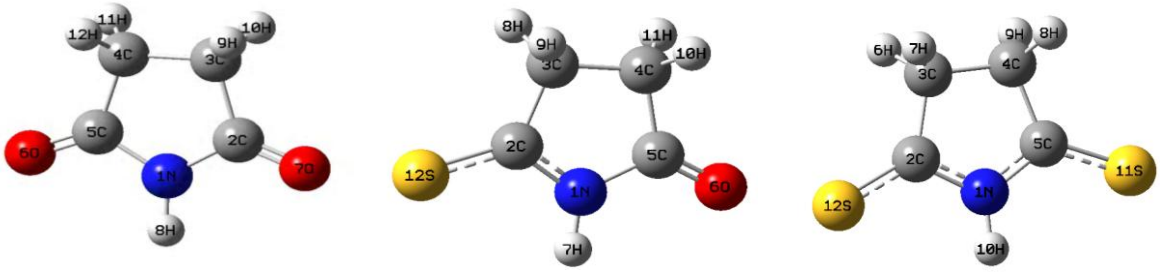
Computational Method

A full quantum mechanical geometry optimization was performed using Gaussian 03 computational program for calculation[12-13].The calculations were done at the DFT/B3LYP level of theory using the basis set 6-311++G(3d,3p) and the resulting Hessian Matrix showed no negative frequencies. The ^{1}H-NMR and ^{13}C-NMR spectra have been investigated for all compounds. HOMO, LUMO and energy band gap (ΔE) calculation have been done using Chemcraft program[14]. The Mulliken method was employed to derive the partial charges on the atoms of the compounds[15]. Three types of succinimide substitutes(I, II, III) species were optimized and used for the calculation of the ^{1}H-NMR and ^{13}C-NMR. All calculations were performed on the Pentium (R)4/IPM-PC- CPU 3.00GHz, 2.00GB.

Results and Discussion

The geometry optimized structures (I, II, III) are visualized in **Figure 1** and selected parameters of their structural data are summarized in **Table 1**.

Chemical Structures



Predication of I **Predication of II** **Predication of III**

Fig. 1: DFT/B3LYP -6-311++G(3d,3p) Calculated Optimized Structures of The Possible Predication for The Compounds in Gas Phase

Table 1: Electronic properties of the studied molecules, Total Energy(in a.u), Dipole Moment (In Debyes), The MO energy of HOMO, LUMO levels, Δ*E*, ,Global hardness(η), Electronaffinity(A),Ionizationpotential(I),Electronegetivity(X),Electrophilicity(ω)(in eV), at B3LYP / 6-311G(d, p) level of theory. Minus sign denotes lower energy (stabilization)for the total energies calculated*

Compounds	**I**	**II**	**III**
*Total Energy In a.u	-360.7940	-683.7483	-1006.7030
Dipole Moment In Debyes	2.1551	2.2327	2.1822
HOMO In eV	-7.565369	-6.485340	-6.505656
LUOM In eV	-1.037034	-2.116790	-2.726330
Δ*E* In e.V	6.528334	4.368550	3.780235
I In eV	7.565369	6.485340	6.505656
A In eV	1.037034	2.116790	2.726330
η In eV	3.26416	2.184275	1.889663
X In eV	4.3012015	4.301065	4.615993
ω In eV	1.6320799	1.0921358	0.9448313

The global minimum energy obtained by the DFT structure optimization obtained by the large basis set calculation (the global minimum energy) in this study for the compounds (I, II, III) are presented in **Table 1** It can be seen from **Table 1** that, the dipole moment has maximum values for compound (II) compared with compounds(I, III). This high dipole moment may

make the compound (II) attractive for the interaction with other systems and to form complexes[16-19].

HOMO-LUMO, **Table 1**; summarizes the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and HOMO and LUMO energy gaps (ΔE) for compounds (I, II, III) calculated at 3d-3p level in the 6-311++G basis set. The eigenvalues of LUMO and HOMO and their energy gap reflect the chemical activity of the molecule. LUMO as an electron acceptor represents the ability to obtain an electron, while HOMO as an electron donor represents the ability to donate an electron. The smaller the LUMO and HOMO energy gaps, the easier it is for the HOMO electrons to be excited; the higher the HOMO energies, the easier it is for HOMO to donate electrons; the lower the LUMO energies, the easier it is for LUMO to accept electrons. From the resulting data shown in **Table 1**, it is obvious that the LUMO energies of III are lower than those of (II and I) and the energy gap of (III)is smaller than that of (I, II) Consequently, the electrons transfer from HOMO to LUMO in(III) is relatively easier than that in (II and I). With the decrease of the LUMO energies, LUMO in (III) accepts electrons easily. The band gaps values of the (III) are less than that of the (II and I). This means that in any excitation process, the forms(II and I) need less(ca. 3.242, 0.567, 4.318 eV respectively) energy than that the (III). A compound (III) with a small HOMO-LUMO gap can be associated with a high chemical reactivity and low kinetic stability, so we expect the compound (III) have high biological activity compare with other compounds (I and II) [20-23]. There is relationship between hardness and stability, the principle of maximum hardness (PMH) represents that the system would be more stable if the global hardness related to HOMO-LUMO gap, is a maximum. As well as based on the principle it has been suggested after extensive study that a system of maximum chemical hardness value would have minimum energy, so from the **Table 1** the compound (I) more s**Table** than compounds (II, III) because of have high energy gap ΔE and hardness η, in addition according to this principle the minimum energy system has maximum chemical hardness value. Hence, PMH is a qualitative tool to study the stability of the system. So that from **Table 1**, it is obvious that the compound (I) have minimum total energy and maximum hardness. There for the compound (I) more stable than compounds (II, III). The stabilities for compounds are I>II>III according to the values of hardness, energy gap and total energy system. Also we note from **Table 1** the electronegative for compounds are III>II>I. The calculated values of global reactivity index ω show the nucleophility power of compounds. We obtained lower ω value for compound (III) compare with compounds (I, II) that explain better propensity of compound (III) to be involved in the reactions with electrophiles than for compounds (I, II) [24-28].

^{1}H-NMR and ^{13}C-NMR ; The optimized structure of compounds (fig.1) was used to calculate ^{1}H-NMR and ^{13}C-NMR chemical shifts by using the GIAO method at level B3LYP/6-311++G(3d,3p), and examination if the theory level suitable for studying ^{1}H-NMR and ^{13}C-NMR and agreement with experiment value. So the values of correlation coefficients of the

proton and carbon chemical shifts for compound (I) are found to be R=1 for proton and R=1 for carbon **Figure 2**. From the theoretical calculation it found that the theory level B3LYP/6-311++G(3d,3p) excellent and agreement with experimental value figure(3). Depend on this theory level to calculation theoretical for ^{1}H-NMR and ^{13}C-NMR for compound(I) and compare with experimental data and predicate the ^{1}H-NMR and ^{13}C-NMR for compounds (II,III) [29-30].

Table 2: Calculated ^{1}H- NMR Chemical Shifts (Ppm) of Compounds(GIAO, B3LYP/6-311++G(3d,3p)

Compounds	H-NMR		
	No. Of Atom	**Chemical Schift**	***Experimental Chemical Schift**
I	H8	6.840	7.250
	H9,H10,H11,H12	2.438	2.850
	H10,H11	2.532	
	H9,H8	3.056	----------
II	H7	8.218	
	H10	9.318	
III	H9,H8,H7,H6	3.187	----------

References ; 29, 30

^{1}H -NMR, Concerning the compound (I and III) have two different chemical environments, but the compound (II) have three different chemical environments. In compounds (I and III) two signals attributed to the protons (N-H, CH_2 and CH_2), but the compound (III) shift to down field compare with compound (I) because of the different electronegativities of oxygen and sulfur atoms. On the other hand compound (II) have three signal attributed to the protons (N-H, CH_2, CH_2),but because different substitutes causes different chemical environments. Also observed that the chemical shift to the protons closely to sulfur atom is shifted down field compare with the protons closely to oxygen atom. The theoretical and experimental values for this compounds are given in **Table 2** [31-33].

^{13}C-NMR; As can be seen in **Table 3**, the values of ^{13}C-NMR agreed with values of ^{1}H-NMR for compounds under study. Compounds (I and III) have two different chemical environments while compound (II) have three different chemical environments. In the compound (I) the carbonyl carbon atoms C_2 and C_5 are more deshielded (down field) as a consequence of binding to the oxygen atoms, compare with carbon atoms C_3 and C_4 that attached to the two hydrogen atoms(high field). On the other hand in the compound (III) the carbon atoms C_2 and C_5 connected to the sulfur atoms are more deshielded (down field) as a

consequence of binding to the sulfur atoms, compare with carbon atoms C_3 and C_4 that attached to the two hydrogen atoms(high field). Also in compound (II) similar effect was also observed for carbon atom C_2 connected to the sulfur atom and carbon atom C_5 connected to the oxygen atom with different electronegativities of oxygen and sulfur atoms which causes charge in chemical schifts to(down field) [34-35].

Charge Density Distribution; The trend of the charge density distribution is qualitatively in agreement with the ^{13}C-NMR results; In the compound (I), the electron density is less at C_5 and C_2, because of xist of two oxygen atoms decrease electron density and deshielding on the $C_5$and C_2(down filed- high chemical shift), whereas the electron density it is much greater at C_4 and C_3 this indicate shielding on the C_5 and C_2 (high filed- less chemical shift). Similar effect was also observed in compound (III). In the compound (II) there are four different charge because of existed the oxygen atom from side and another side existed the sulfur atom which causes different inductive effect with different electronegativities of oxygen and sulfur atoms. It can be seen that C_5 and C_2 atoms indicate significant charge change as a function of substituent. At last the calculation theoretical of charge density distribution agreement with the theoretical calculation of ^{13}C-NMR. The theoretical values of charge density distribution for this compounds are given in **Table 3** [36-37].

Table 3: Calculated ^{13}C-NMR chemical shifts (ppm) and Charge Density Distribution

Compounds	C^{13}-NMR			Charges	
	No. of atom	**Chemical Schiff**	***Experimental Chemical Schiff**	**No. of atom**	**Mulliken Charge**
I	C_4,C_3	32.967	30.2	C_3,C4	-0.229
	C_5,C_2	180.769	179.0	C_2,C5	1.004
II	C_4	33.736		C_4	-0353
	C_3	43.626	----------	C_3	-0.387
	C_5	183.407		C_5	1.149
	C_2	221.648		C_2	0.645
III	C_4,C_3	46.263		C_3,C_4	-0.099
	C_5,C_2	223.626	----------	C_2,C_5	0.382

(Mulliken Charge) of compounds(GIAO, B3LYP/6-311++G(3d,3p). *References ; 29, 30

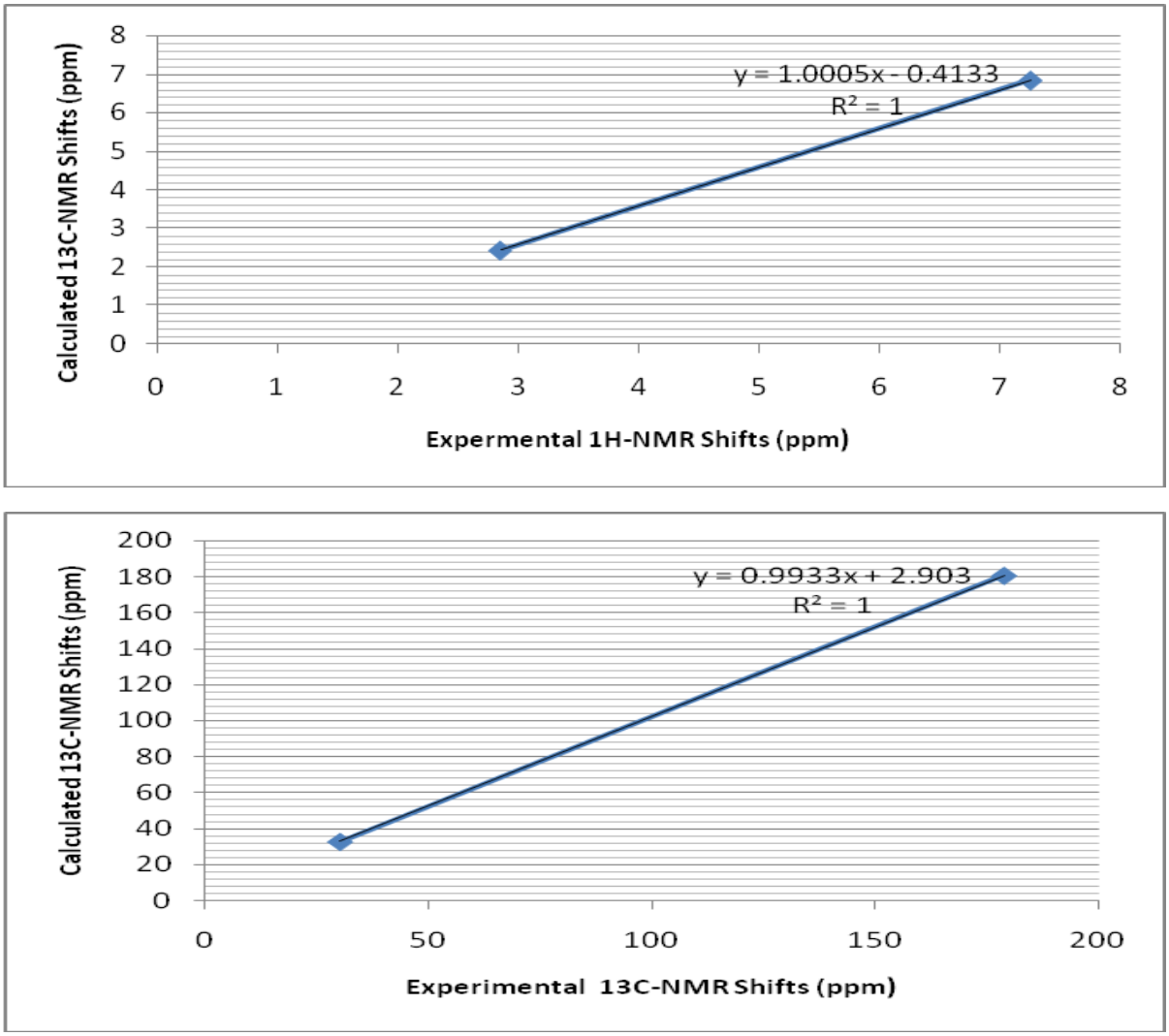
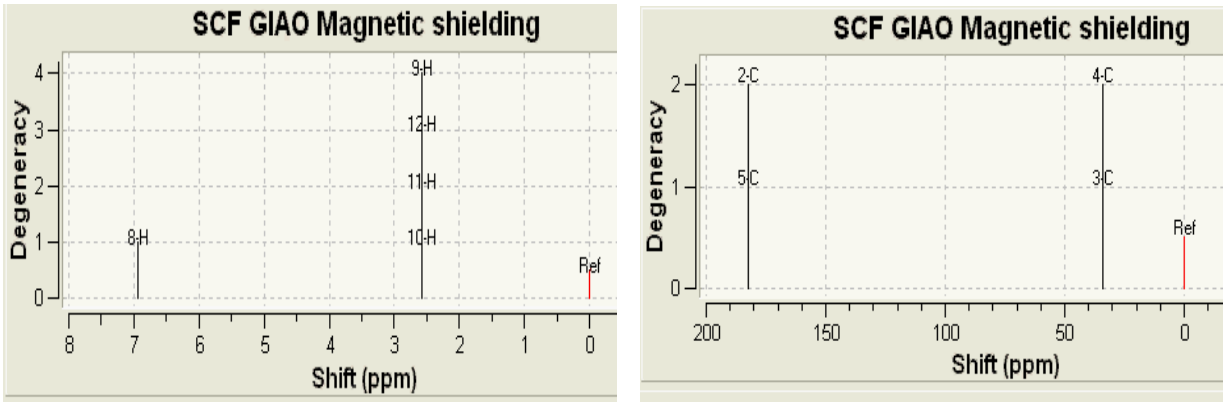


Fig. 2: Plot of The Calculated Vs. The Experimental ^{1}H-NMR And ^{13}C-NMR Chemical Shifts(ppm) for Compound I



^{13}C-NMR **^{1}H –NMR**

Fig. 3: ^{1}H -NMR &^{13}C-NMR spectrum fo compound (I) calculated by(GIAO, 3LYP/6-311++G(3d,3p)

The bond lengths and angles for compounds (I, II and III) are listed in **Table 4**; As shown from this table, there are slight changes in the bond lengths and angles of compounds, like . The changes of the bond length and angles in the ring indicate the presence of π-conjugation which causes of the electrostatic attraction between atoms. Also the effect of substitution on the ring leads to redistribution of electron cloud in the ring of the compounds (I, III and II) [38-40].

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Table 4: Selected Structural Parameters of The Optimized Compounds, Bond Distance(A°) and Bond Angles(°) Obtained By B3LYP/6-311++G(3d,3p) Method

Compounds					
Bonds / Angles	**I**	**Bonds / Angles**	**II**	**Bonds / Angles**	**III**
R(1-2)	1.391	R(1-2)	1.366	R(1-2)	1.373
R(1-5)	1.391	R(1-5)	1.400	R(1-5)	1.373
R(1-8)	1.010	R(1-7)	1.011	R(1-10)	1.011
R(2-3)	1.525	R(2-3)	1.522	R(2-3)	1.517
R(2-7)	1.204	R(2-12)	1.634	R(2-12)	1.633
R(3-4)	1.537	R(3-4)	1.539	R(3-4)	1.542
R(3-9)	1.089	R(3-8)	1.089	R(3-6)	1.089
R(3-10)	1.089	R(3-9)	1.089	R(3-7)	1.089
R(4-5)	1.525	R(4-5)	1.522	R(4-5)	1.517
R(4-11)	1.089	R(4-10)	1.089	R(4-8)	1.089
R(4-12)	1.089	R(4-11)	1.089	R(4-9)	1.089
R(5-6)	1.204	R(5-6)	1.202	R(5-11)	1.633
A(2-1-5)	115.1	A(2-1-5)	115.9	A(2-1-5)	116.7
A(2-1-8)	122.4	A(2-1-7)	122.2	A(2-1-10)	121.6
A(1-2-3)	107.0	A(1-2-3)	106.9	A(1-2-3)	106.4
A(1-2-7)	125.1	A(1-2-12)	125.5	A(1-2-12)	124.9
A(5-1-8)	122.4	A(5-1-7)	121.9	A(5-1-10)	121.6
A(1-5-4)	107.0	A(1-5-4)	106.5	A(1-5-4)	106.4
A(1-5-6)	125.1	A(1-5-6)	124.5	A(1-5-11)	124.9
A(3-2-7)	127.9	A(3-2-12)	127.6	A(3-2-12)	128.6
A(2-3-4)	105.4	A(2-3-4)	105.7	A(2-3-4)	105.2
A(2-3-9)	108.5	A(2-3-8)	108.9	A(2-3-6)	109.1
A(2-3-10)	108.5	A(2-3-9)	108.9	A(2-3-7)	109.1
A(4-3-9)	113.5	A(4-3-8)	113.2	A(4-3-6)	113.2
A(4-3-10)	113.5	A(4-3-9)	113.2	A(4-3-7)	113.2
A(3-4-5)	105.4	A(3-4-5)	105.0	A(3-4-5)	105.2
A(3-4-11)	113.5	A(3-4-10)	113.6	A(3-4-8)	113.2
A(3-4-12)	113.5	A(3-4-11)	113.6	A(3-4-9)	113.2
A(9-3-10)	107.2	A(8-3-9)	106.8	A(6-3-7)	106.9
A(5-4-11)	108.5	A(5-4-10)	108.7	A(5-4-8)	109.1
A(5-4-12)	108.5	A(5-4-11)	108.7	A(5-4-9)	109.1
A(4-5-6)	127.9	A(4-5-6)	129.0	A(4-5-11)	128.6
A(11-4-12)	107.2	A(10-4-11)	107.2	A(8-4-9)	106.9

Conclusions

The quantum chemical calculations can be successfully used for the prediction of geometry optimization (minimized energy), relative stabilities, electronic properties. (HOMO & LUMO) and ^{1}H-NMR and ^{13}C-NMR, charge density distribution, bond distance and bond angles.

The method adopted here for calculation Density functional theory DFT/ B3LYP level of theory using the basis set 6-311++G(3d,3p) proved to be good to give the optimized geometry and minimized energy for the compounds under study. From the results it was shown that the dipole moment have maximum value for compound (II) compared with compounds(I,III) . This high dipole moment makes the compound (II) effective to interaction with other systems and to formation complexes. the Structural, Electronic Properties such as electron affinity(A), ionization potential(I), hardness(η), electronegetivity(X), electrophilicity(ω) of the compounds (I, II, III) shown the compound (I) more stable than compounds (II, III). The stabilities for compounds are I>II>III according to the values of the principle of maximum hardness (PMH), energy gap and total energy system[16&22-23]. Calculation density functional theory (DFT), its good to give the standard calculations for predication spectrum of ^{1}H-NMR and ^{13}C-NMR, charge density distribution and the theory level suitable for studying ^{1}H-NMR and ^{13}C-NMR and agreed with experiment value. The results shown that the substituents have significant influences on the structural properties of molecules studied, the significant effects of substituents appeared on the electronic properties, LUMO-HOHO, energy band gap, ^{1}H-NMR and ^{13}C-NMR, charge density distribution, bond length, angles. Gaussian 03 computational chemistry program and its calculations gave good results for the analysis of structural properties such as : bond length, angles, total energy , dipole moment, spectrum of ^{1}H-NMR and ^{13}C-NMR.

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