J.Thi-Qar Sci. Vol.3 (1) July/2011

ISSN 1991- 8690 **الترقيم الدولي ٨٦٩٠ - ١٩٩١**

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Theoretical study of the Structural and Electronic Properties of the Phenol, Phenoxy

Phenol-water complex and Phenoxy-water complex

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Abstract

The theortical calculations of phenol, phenoxy, phenol-water complex, phenoxy-water complex (I, II, III, IV) were studied by quantum chemical calculations. The optimized structures of the compounds were obtained by the Density functional theory (DFT) in gas phase at B3LYP / 6-311G (d, p) & MP2 / 6-311G (d, p) level of theory. The study shown that the value of total energy for compound (II) has much more energy and accordingly less stability in comparison with the compound (I), the compound III (phenol-complex) and compound IV (pheoxy-complex), have more stable structure than compounds (I, II). In addition we calculated the HOMO-LUMO, energy gap and system properties such as ionization potential (I), hardness (η), electronegetivity(X), electrophilicity (ω). The calculation interaction energies show that the compound (IV) showed larger energy than compound (III). All calculations was carried out for (I, II, III, IV) and shows the favorable state for stabilities (more stable) (I>II, III>IV).

KeyWord**:** Phenol, Phenoxy, Intermolecular Hydrogen Bonding (IHB), DFT, MP2.

Introducation

Phenols are widely used as synthetic organic materials and also as antioxidants in living organisms, also are known as important intermediates in many biological and industrial applications. Phenols are of special interest in organic chemistry and in the production of bonded-wood products. Phenolic antioxidants have been extensively used in chemical industry, food industry, and pharmaceutical industry(1-2) .Specific interactions of type X-H···Y between proximate moieties can be important to determine conformational structures as well as stabilization energies in molecules, especially biomolecules, in intramolecular complexes or molecular solids. Therefore, the study of intramolcular hydrogen bonding is very important because, as known to all, the boiling and melting points ,vapour pressure, solubility, density , viscosity, heat conductivity, heat expansion, dielectric constant, dipole moment, electro conductivity, ionization, and another optical properties, depends on the presence of intramolecular hydrogen bond (IHB). Hydrogen bonds are frequently separated into two categories: weak or normal hydrogen bonds and strong or very strong hydrogen bonds (3). The normal hydrogen bonds are regarded as those with strengths of about 3-5 kcal/mol and of generally less than 12 kcal/mol. Strong hydrogen bonds may have energies in excess of 12 kcal/mol. Such strong hydrogen bonding always involves features such as a short bond distance (4-5).

Computational chemistry has played an important role in identifying and quantifying hydrogen bonding geometries and energies of pertinent model systems. There have been a lot of attempts to explain the nature of bonding and reactivity of molecular systems based on some intuitive ideas and empirical rules that are essentially derived from several experimental observations and many chemical facts. During the development of the quantum chemical methods, many of the empirical chemical concepts were derived rigorously and it has provided a method for the calculation of the properties of chemical systems, molecular orbital density, charge on atoms and the bonding that is involved in the molecular systems (5-8). .

In this work we attempt to study the intramolecular hydrogen bonding, electronic properties, and relative stabilities by performing Density functional theory (DFT) at B3LYP / 6-311G(d, p) & MP2 / 6-311G(d, p) level of theory .

Computational method

All calculations have been carried out using PCGAMESS program for phenol----water complex and phenoxy----water complex. The geometries of these two complexes, phenol and phenoxy have been optimized at B3LYP method of DFT theory and MP2 method at 6-311G (d, p) level of theory (9). All calculations were performed on the Pentium (R) 4/IPM-PC- CPU 3.00GHz, 2.00GB

Results and Discussion

The geometry optimized structures phenol, phenoxy, phenol-water complex and phenoxy-water complex (I, II, III, IV) are visualized in (Figs 1)

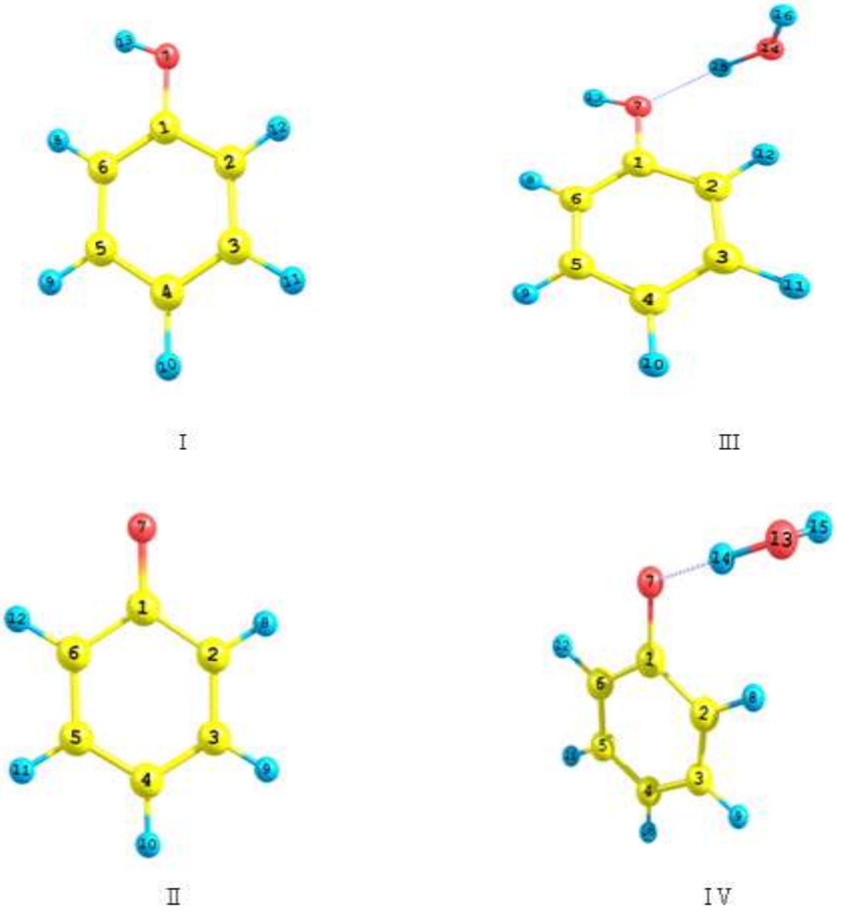


Figure (1): DFT-calculated optimized structures of the Phenol, Phenoxy, Phenol-water and Phenoxy-water in gas phase at B3LYP / 6-311G (d, p) & MP2 / 6-311G (d, p) level of theory.

It can be seen from Table 1 that, the total energy of the phenol, phenoxy, phenol-water complex and phenoxy-water complex (I, II, III, IV sequence) have almost similar energies and thus comparable stabilities, The phenoxy ion (II) has much more energy and accordingly less stability in comparison with the compound (I) (decrease energy and high stability). The calculated energies show that the compound III (phenol-complex) and compound IV (pheoxy-complex), have more stable structure than compounds (I,II), because of the complexes have intermoluclare hydrogen bonding(IHB). As well as the compounds (I&III) have less energy potential compare with compounds (II&IV) In addition the ionization potential for compounds (III, IV) are larger than compounds (I, III). (10-11)

Table 1: Energy (Kcal/mol) of the Phenol, Phenoxy, Phenol-water and Phenoxy-water in gas phase at B3LYP / 6-311G (d, p) & MP2 / 6-311G (d, p) level of theory

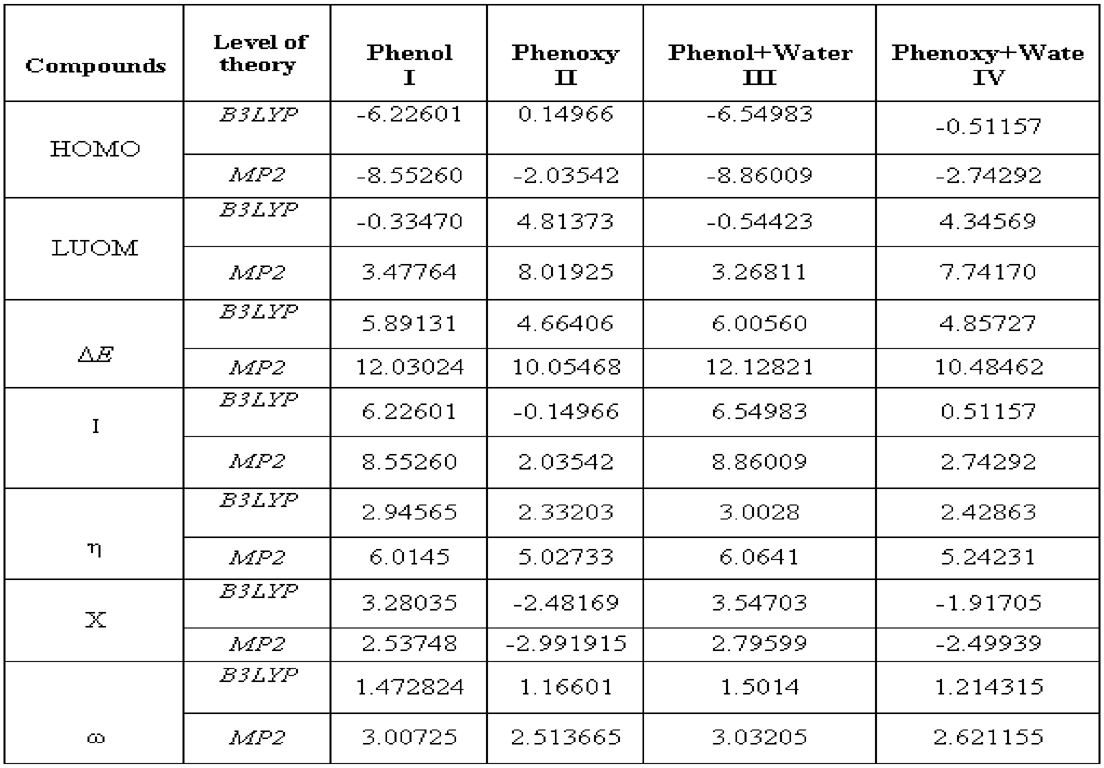
Compound	**Level of theory**	***Total Energy In Hartree**	***Total Potential Energy in Hartree**
Phenol I	*B3LYP*	-307.5552	-613.5490
	MP2	-306.6676	-613.2492
Phenoxy II	*B3LYP*	-306.9799	-612.5471
	MP2	-306.0875	-612.2656
Phenol+Water III	*B3LYP*	-384.0134	-766.2557
	MP2	-382.9454	-765.8940
Phenoxy+Water IV	*B3LYP*	-383.4588	-765.8077
	MP2	-382.3858	-764.9246

*: Minus sign denotes lower energy (stabilization)for the total energies calculated.

Table 2; 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, IV) calculated at 6-311G basis set. The eivgenvalues 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. The energy gap of the compound I is larger than that of the compound II. While the energy gap of compound III larger than that of the compound IV. So from the energies band gaps results that the stabilities of compounds are ((I >II & III>IV). A compound (II&IV) with a small HOMO-LUMO gap can be associated with a high chemical reactivity that the complexes (III, IV) with water more ability to react with the bases compare with and low kinetic stability (12-14).

In addaition the calculated energy gap by (MP2) method is larger than the calculated energy gap by (B3LYP) method this may in agreement with the calculated the total energy data for compounds (Table 1). The calculated the total energy by (MP2) method is larger than the calculated total energy by (B3LYP) method). As well as from Table 3; the molecule reactivity is related to the system properties, such as ionization potential(I),hardness(η),lectronegetivity(X), electrophilicity(ω).The compounds (II&V) have high electron affinity(A) compare with the compounds (I&III). While the increase of the data of ionization potential (I), when transfer from the compounds (I, II) to compounds (III, IV), this referred to the difficult of ionization of this compounds (III, IV). The Compounds (I, II) have less of electronegetivity(X) compare with the compounds (III, IV) which referred to that this compounds (III, IV) it is hard bases which agreement with data of $\boldsymbol{\eta}$ in table(2). Also the data of $\boldsymbol{\omega}$ referred to the reflects it compare with the data of (X), η, It is appear compounds (I, II). From these results the compound has more stable, its have larger of the HOMO-LUMO energy gap and hardness. So that the stabilities of the compounds are (I >II & III>IV), this agree with the energy data (Table 1) (15).

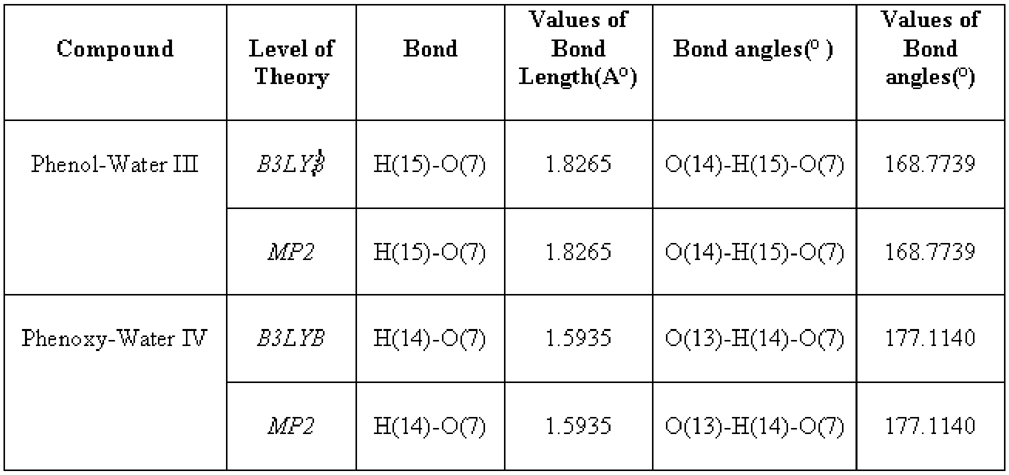
Table 2: Electronic properties of the studied molecules, The MO energy of HOMO, LUMO levels, Δ*E* (in eV), Electron affinity (A), Ionization potential (I), Global hardness (η), Electronegetivity(X), Electrophilicity (ω) (in eV). At B3LYP / 6-311G (d, p) & MP2 /6- 311G (d, p) level of theory.



Compounds	**Level of theory**	**Phenol I**	**Phenoxy II**	**Phenol+Water III**	**Phenoxy+Wate IV**
HOMO	*B3LYP*	-6.22601	0.14966	-6.54983	-0.51157
	MP2	-8.55260	-2.03542	-8.86009	-2.74292
LUOM	*B3LYP*	-0.33470	4.81373	-0.54423	4.34569
	MP2	3.47764	8.01925	3.26811	7.74170
Δ*E*	*B3LYP*	5.89131	4.66406	6.00560	4.85727
	MP2	12.03024	10.05468	12.12821	10.48462
I	*B3LYP*	6.22601	-0.14966	6.54983	0.51157
	MP2	8.55260	2.03542	8.86009	2.74292
η	*B3LYP*	2.94565	2.33203	3.0028	2.42863
	MP2	6.0145	5.02733	6.0641	5.24231
X	*B3LYP*	3.28035	-2.48169	3.54703	-1.91705
	MP2	2.53748	-2.991915	2.79599	-2.49939
ω	*B3LYP*	1.472824	1.16601	1.5014	1.214315
	MP2	3.00725	2.513665	3.03205	2.621155

From table 3, we can see that important optimized bond lengths and bond angles which participate in forming HB in the compounds (III, IV). The bond length H (14)-O (7) in compound (IV) founded 1.5935(A) and is shorter than bond length H (15)-O (7) in compound III. Also the bond angle O(13)-H(14)-O(7) in compound IV largest than bond angle O(14)-H(15)-O(7) in compound III, The changes of the bond lengths and bond angles in the compounds (III, IV) indicate the presence of π-conjugation which participates in forming the HB. As a result, a shortening of [H (14)-O (7) =1.5935] distances in compound (IV) compared with the compound III [H (15)-O (7) = 1.8265], this showed and reflects the strong to be electrostatic attraction in compound IV. (16-18).

Table 3: Selected structural parameters of the optimized compounds, bond distance (A°) X1—H- - - - X2 and bond angles (°) X1—H-----X2. At B3LYP / 6-311G (d, p) & MP2 / 6- 311G (d, p) level of theory.



Compound	Level of Theory	Bond	Values of Bond Length(A°)	Bond angles(°)	Values of Bond angles(°)
Phenol-Water III	*B3LYB*	H(15)-O(7)	1.8265	O(14)-H(15)-O(7)	168.7739
	MP2	H(15)-O(7)	1.8265	O(14)-H(15)-O(7)	168.7739
Phenoxy-Water IV	*B3LYB*	H(14)-O(7)	1.5935	O(13)-H(14)-O(7)	177.1140
	MP2	H(14)-O(7)	1.5935	O(13)-H(14)-O(7)	177.1140

On other hand the Interaction energy were calculated according to the equations shown below [19-20]

*__Interaction energy of compound III =__ $E_{\text{Phenol-complex}} — [E_{H_2O} + E_{\text{Phenol}}]$

*__Interaction energy of compound V=__ $E_{\text{Phenoxy-complex}} — [E_{H_2O} + E_{\text{Phenoxy}}]$

The value of the interaction energy in compound (III) was at B3LYP/6-311G(d,p) level of theory [-6.198788 kcal/mol] and at MP2/6-311G(d,p) level of theory [-6.23054 kcal/mol], while in the compound (IV) the interaction energy was at B3LYP/6-311G(d,p) level of theory [-19.25362 kcal/mol] and at MP2/6-311G(d,p) level of theory [-19.09881 kJ/mol] . The interaction energy in Minus sign denotes exothermic energy [21] .

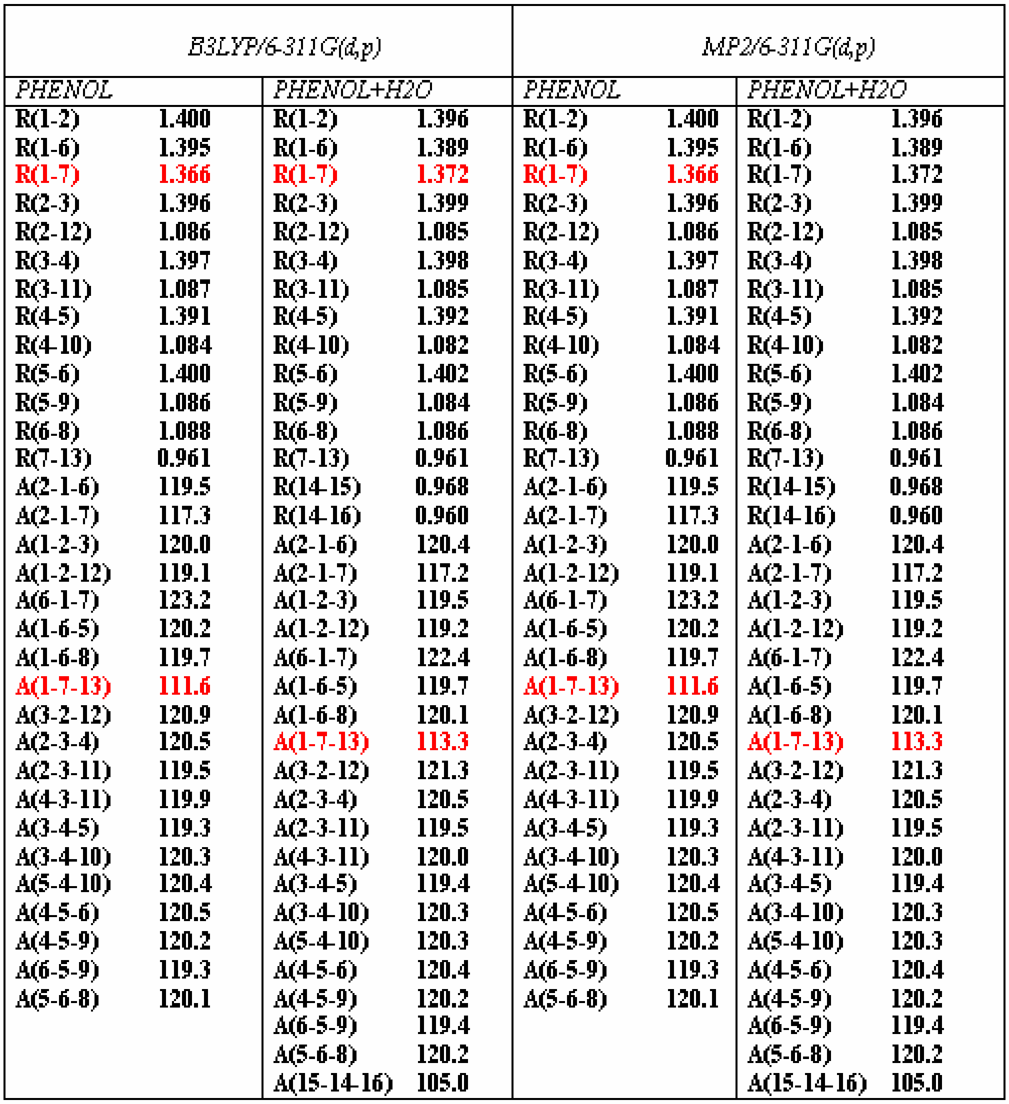
The calculation interaction energies showed that the water molecule binds stronger in compound (IV) compare with the compound (III), so that the bond H(14)-O(7) in compound (IV) is smaller than the bond H(15)-O(7) in compound (III) [22]. The bond lengths and angles of compounds (I, II, III, V) are listed in Table 4, 5: As shown there are slight changes in the bond lengths and angles of compounds. The changes of the bond length and angles affected considerably with the formation hydrogen bonding. When the water binds with O7 atom of compound (I, II), and participates in forming complexes (III, IV). The bond length C1-O7, and bond angle H13-O7-C1 are slightly increased in compounds (III, IV) comparison with the compound (I, II) due to cancel the forming partial double bond because of the partial double bond its disappear in compounds (I,II) when forming the complexes (III,IV) and as result of the effect of hydrogen bonding on the ring of phenol or phenoxy which leads to redistribution of electron cloud in the ring of compounds which causes changes on the bond lengths and angles[23]

*__Interaction energy of compound = Energy of hydrogen bonding__

Table 4: Selected structural parameters of the optimized compounds (I, III), bond distance (A°) and bond angles (°) at B3LYP / 6-311G (d, p) & MP2 / 6- 311G (d, p) level of theory

B3LYP/6-311G(d,p)				MP2/6-311G(d,p)			
PHENOXY		PHENOXY+H2O		PHENOXY		PHENOXY+H2O	
R(1-2)	1.447	R(1-2)	1.440	R(1-2)	1.447	R(1-2)	1.440
R(1-6)	1.448	R(1-6)	1.436	R(1-6)	1.448	R(1-6)	1.436
R(1-7)	1.262	R(1-7)	1.285	R(1-7)	1.262	R(1-7)	1.285
R(2-3)	1.387	R(2-3)	1.388	R(2-3)	1.387	R(2-3)	1.388
R(2-8)	1.089	R(2-8)	1.082	R(2-8)	1.089	R(2-8)	1.082
R(3-4)	1.405	R(3-4)	1.397	R(3-4)	1.405	R(3-4)	1.397
R(3-9)	1.089	R(3-9)	1.090	R(3-9)	1.089	R(3-9)	1.090
R(4-5)	1.405	R(4-5)	1.397	R(4-5)	1.405	R(4-5)	1.397
R(4-10)	1.086	R(4-10)	1.088	R(4-10)	1.086	R(4-10)	1.088
R(5-6)	1.386	R(5-6)	1.388	R(5-6)	1.386	R(5-6)	1.388
R(5-11)	1.089	R(5-11)	1.089	R(5-11)	1.089	R(5-11)	1.089
R(6-12)	1.089	R(6-12)	1.083	R(6-12)	1.089	R(6-12)	1.083
A(2-1-6)	113.6	R(13-14)	1.013	A(2-1-6)	113.6	R(13-14)	1.013
A(2-1-7)	123.2	R(13-15)	0.960	A(2-1-7)	123.2	R(13-15)	0.960
A(1-2-3)	122.8	A(2-1-6)	115.3	A(1-2-3)	122.8	A(2-1-6)	115.3
A(1-2-8)	116.7	A(2-1-7)	123.4	A(1-2-8)	116.7	A(2-1-7)	123.4
A(6-1-7)	123.2	A(1-2-3)	121.5	A(6-1-7)	123.2	A(1-2-3)	121.5
A(1-6-5)	122.9	A(1-2-8)	116.9	A(1-6-5)	122.9	A(1-2-8)	116.9
A(1-6-12)	116.7	A(6-1-7)	121.4	A(1-6-12)	116.7	A(6-1-7)	121.4
A(3-2-8)	120.5	A(1-6-5)	121.9	A(3-2-8)	120.5	A(1-6-5)	121.9
A(2-3-4)	121.5	A(1-6-12)	116.3	A(2-3-4)	121.5	A(1-6-12)	116.3
A(2-3-9)	119.5	A(3-2-8)	121.6	A(2-3-9)	119.5	A(3-2-8)	121.6
A(4-3-9)	119.0	A(2-3-4)	121.7	A(4-3-9)	119.0	A(2-3-4)	121.7
A(3-4-5)	117.8	A(2-3-9)	118.7	A(3-4-5)	117.8	A(2-3-9)	118.7
A(3-4-10)	121.1	A(4-3-9)	119.6	A(3-4-10)	121.1	A(4-3-9)	119.6
A(5-4-10)	121.1	A(3-4-5)	118.1	A(5-4-10)	121.1	A(3-4-5)	118.1
A(4-5-6)	121.4	A(3-4-10)	121.0	A(4-5-6)	121.4	A(3-4-10)	121.0
A(4-5-11)	119.0	A(5-4-10)	120.9	A(4-5-11)	119.0	A(5-4-10)	120.9
A(6-5-11)	119.6	A(4-5-6)	121.5	A(6-5-11)	119.6	A(4-5-6)	121.5
A(5-6-12)	120.5	A(4-5-11)	119.7	A(5-6-12)	120.5	A(4-5-11)	119.7
		A(6-5-11)	118.8			A(6-5-11)	118.8
		A(5-6-12)	121.8			A(5-6-12)	121.8
		A(14-13-15)	103.2			A(14-13-15)	103.2

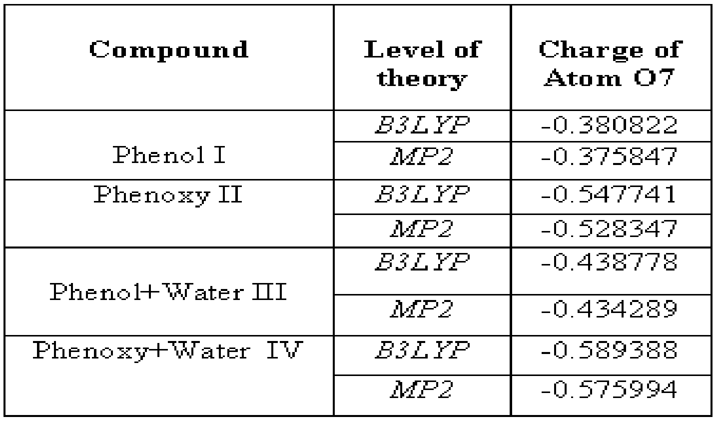
Table 5: Selected structural parameters of the optimized compounds (II, IV), bond distance (A°) and bond angles (°) at B3LYP / 6-311G (d, p) & MP2 / 6- 311G (d, p) level of



B3LYP/6-311G(d,p)				MP2/6-311G(d,p)			
PHENOL		PHENOL+H2O		PHENOL		PHENOL+H2O	
R(1-2)	1.400	R(1-2)	1.396	R(1-2)	1.400	R(1-2)	1.396
R(1-6)	1.395	R(1-6)	1.389	R(1-6)	1.395	R(1-6)	1.389
R(1-7)	1.366	R(1-7)	1.372	R(1-7)	1.366	R(1-7)	1.372
R(2-3)	1.396	R(2-3)	1.399	R(2-3)	1.396	R(2-3)	1.399
R(2-12)	1.086	R(2-12)	1.085	R(2-12)	1.086	R(2-12)	1.085
R(3-4)	1.397	R(3-4)	1.398	R(3-4)	1.397	R(3-4)	1.398
R(3-11)	1.087	R(3-11)	1.085	R(3-11)	1.087	R(3-11)	1.085
R(4-5)	1.391	R(4-5)	1.392	R(4-5)	1.391	R(4-5)	1.392
R(4-10)	1.084	R(4-10)	1.082	R(4-10)	1.084	R(4-10)	1.082
R(5-6)	1.400	R(5-6)	1.402	R(5-6)	1.400	R(5-6)	1.402
R(5-9)	1.086	R(5-9)	1.084	R(5-9)	1.086	R(5-9)	1.084
R(6-8)	1.088	R(6-8)	1.086	R(6-8)	1.088	R(6-8)	1.086
R(7-13)	0.961	R(7-13)	0.961	R(7-13)	0.961	R(7-13)	0.961
A(2-1-6)	119.5	R(14-15)	0.968	A(2-1-6)	119.5	R(14-15)	0.968
A(2-1-7)	117.3	R(14-16)	0.960	A(2-1-7)	117.3	R(14-16)	0.960
A(1-2-3)	120.0	A(2-1-6)	120.4	A(1-2-3)	120.0	A(2-1-6)	120.4
A(1-2-12)	119.1	A(2-1-7)	117.2	A(1-2-12)	119.1	A(2-1-7)	117.2
A(6-1-7)	123.2	A(1-2-3)	119.5	A(6-1-7)	123.2	A(1-2-3)	119.5
A(1-6-5)	120.2	A(1-2-12)	119.2	A(1-6-5)	120.2	A(1-2-12)	119.2
A(1-6-8)	119.7	A(6-1-7)	122.4	A(1-6-8)	119.7	A(6-1-7)	122.4
A(1-7-13)	111.6	A(1-6-5)	119.7	A(1-7-13)	111.6	A(1-6-5)	119.7
A(3-2-12)	120.9	A(1-6-8)	120.1	A(3-2-12)	120.9	A(1-6-8)	120.1
A(2-3-4)	120.5	A(1-7-13)	113.3	A(2-3-4)	120.5	A(1-7-13)	113.3
A(2-3-11)	119.5	A(3-2-12)	121.3	A(2-3-11)	119.5	A(3-2-12)	121.3
A(4-3-11)	119.9	A(2-3-4)	120.5	A(4-3-11)	119.9	A(2-3-4)	120.5
A(3-4-5)	119.3	A(2-3-11)	119.5	A(3-4-5)	119.3	A(2-3-11)	119.5
A(3-4-10)	120.3	A(4-3-11)	120.0	A(3-4-10)	120.3	A(4-3-11)	120.0
A(5-4-10)	120.4	A(3-4-5)	119.4	A(5-4-10)	120.4	A(3-4-5)	119.4
A(4-5-6)	120.5	A(3-4-10)	120.3	A(4-5-6)	120.5	A(3-4-10)	120.3
A(4-5-9)	120.2	A(5-4-10)	120.3	A(4-5-9)	120.2	A(5-4-10)	120.3
A(6-5-9)	119.3	A(4-5-6)	120.4	A(6-5-9)	119.3	A(4-5-6)	120.4
A(5-6-8)	120.1	A(4-5-9)	120.2	A(5-6-8)	120.1	A(4-5-9)	120.2
		A(6-5-9)	119.4			A(6-5-9)	119.4
		A(5-6-8)	120.2			A(5-6-8)	120.2
		A(15-14-16)	105.0			A(15-14-16)	105.0

Mulliken charge on the oxygen atoms in the compounds were calculated for the optimized structures at B3LYP / 6- 311G (d, p) & MP2 / 6- 311G (d, p) level of theory. The results are shown in Table 6, it can be seen from this table that the charge on O7 atom in compound (I, II) increase when participates in forming (HB) complex with water molecule, so the complexes (III, IV) are more bases compared with compounds (I,II),which mean that complexes (III, IV) react more quickly with acids from (I, II), this amount of energy will increase the energy gap (Table 2) due to electronic effect for water molecule$^{(24)}$.

Table 6: Calculated Charge Density Distribution (Mulliken Charge) of compounds at B3LYP / 6-311G (d, p) & MP2 / 6- 311G (d, p) level of theory.



Compound	Level of theory	Charge of Atom O7
Phenol I	*B3LYP*	-0.380822
	MP2	-0.375847
Phenoxy II	*B3LYP*	-0.547741
	MP2	-0.528347
Phenol+Water III	*B3LYP*	-0.438778
	MP2	-0.434289
Phenoxy+Water IV	*B3LYP*	-0.589388
	MP2	-0.575994

Conclusions:

The quantum chemical calculations can be successfully used for the prediction of intramolecular hydrogen bonding, electronic properties, and relative stabilities in phenol, phenoxy, phenol-water complex, phenoxy-water complex.

The methods adopted here for calculation density functional theory (DFT) at B3LYP / 6-311G(d, p) & MP2 / 6- 311G(d, p) level of theory is proved to be good to give the optimized geometry and minimized energy for the compounds under study. There are multiple of concluding remarks of calculations in study, include as: The calculated energies show also that within the compound (III) (phenol-complex) and compound (IV) (pheoxy-complex), are most stable structure than compound (I, II). The energy gap of the compound I is larger than that of the compound II. While the energy gap of compound III larger than that of the compound (IV). So from the energies band gaps results that the stabilities of compounds are ((I >II & III>IV). Compounds (II&IV) with a small HOMO-LUMO gap can be associated with a high chemical reactivity and low kinetic stability. The bond length H (14)-O (7) in compound (V) founded 1.522(A) which is shorter than bond length H (15)-O (7) in compound (III). Also, the bond angle O (13)-H (14)-O (7) in compound (IV) was found largest than bond angle O (14)-H (15)-O (7) in compound (III). The calculation interaction energies showed that compound (IV) has higher energy than compound (III), this behavior reflects the strong electrostatic attraction in compound (IV). The calculation of Density functional theory (DFT) at B3LYP / 6-311G(d, p) & MP2 / 6- 311G(d, p) level of theory, showed the calculations gave good results for the analysis of structural properties through closely data of the bond length which is calculated theoretically[C1-O7] togather with the bond length which is calculated experimentally.

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دراسة نظرية للخواص التركيبية والالكترونية للفينول والفينوكسي والمعقد الفينول – الماء , والمعقد الفينوكسي – الماء

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المستخلص

تم في هدا البحث دراسة نظرية للخصائص والصفات التركيبية والالكترونية للفينول , الفينوكسي , والمعقد فينول – ماء, والمعقد فينوكسي - ماء(I,II,III,IV) بوجود التاصر الهيدروجيني البيني بواسطة كيمياء الكم. انجزت الموائمة الهندسية للتراكيب بطريقة DFT وMP2 وعند المستوى النظري MP2/B3LYP وعند مستوى المجموعة الاساسية-6 .311 (d, p)

اظهرت الدراسة أن الطاقة الكلية للجزيئة II أعلى من الطاقة الكلية للجزيئة Iوهدا يؤكد الاستقرارية العالية للجزيئة II بينما الطاقة الكلية للجزيئات(III,IV) أقل من الطاقة الكلية للجزيئات(I,II) . كدلك تم حساب , طاقة الاوربيتال الجزيئية HOMO, LUMOوقيمة ΔE , I , η, X, ω . واظهرت حسابات طاقات التداخل أن المركب IV يمتلك طاقة تداخل أعلى من المركب III. كل الحسابات التي أنجزت للمركبات (I,II,III, IV) أظهرت أن تسلسل الحالة المفضلة للاستقرارية للمركبات هي .(I>II, III>IV)