Electronic Structure and Properties of Benzene and Hydroxylbenzene Molecule Group in Gas Phase: A Density Functional Theory (DFT) Study

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Abstract

In this paper, theoretical study of Optimized geometry and Electronic properties for Hydroxybenzene molecule group by using Density Functional Theory (DFT) at Becke3Lee Yang Parr (B3LYP) level of theory with basis set 6-31G(d,p) in a gas space have been studied. Benzene Molecule is the original Molecule before replacing Hydrogen by Hydroxyl (OH) radical, This replacement of hydrogen by Hydroxyl (OH) radical on Benzene molecule at different positions led/resulted in the study of Eleven molecules. The parameters studied for these molecules are Frontier orbital energies, ionization energy, electron affinity, Chemical potential, Absolute Hardness, Absolute softness, electrophilic index, Dipole moment, Quadrupole moment and Electric dipole polarazibility. The results have shown that the average polarizability increases with the increase of the number of hydroxyl (OH) radical and The predicted dipole moment for Benzene is zero, Thus, the molecule is non polar and the charge distribution is fairly symmetrical in gas phase. The predicted dipole moment for the Hydroquinol, Phloroglucinol, 1,2,4,5-TTHB and 1,2,3,4,5,6-HHB is very close to zero which also reveals that the molecules are non polar in gas phase. These Calculations/Investigations have been performed using Gaussian 03 package.

Keywords: DFT, Frontier orbital energies, Benzene, Dipole moment, Total energy

1.0   Introduction

The Benzene ring is an important example of conjugated molecule, and also an important building block of many organic semiconductors (OSC). However a single benzene ring is not yet large enough to bring the band-gaps Eg into the OSC regime. Nevertheless, many benzene rings are fused at their edges, π electrons can delocalize over a larger area. Since, the band gaps size depends on the delocalization of π electrons and, in turn, the band-gaps size decreases in few eV [1].

The study of organic ring systems is an attractive research field that allows work on the solution of fundamental questions in chemistry and physics. This leads to the development of materials with interesting properties on a molecule. The typical questions associated with the nature compounds of chemistry are: (i) different ring sizes, (ii) the magnitude of ring strain, (iii) the nature of the bonding and (iv), the chain lengths [2]. With advent of modern physics, new fundamental types of materials have been created. Various types of forces operating in different classes of solids are exploited in design of molecular materials. A variety of fabrication techniques have been developed with desired properties. The Quest for more efficient and cheaper materials for use in the industry has led to the discovery of molecular materials.

Benzene and its derivatives have attracted considerable interest since they have interesting applications. Therefore the purpose of this work is to examine the effect of hydroxyl OH radical added to the ring on benzene molecule. The Moleculecs that have been studied are Benzene, Phenol, isomers of Dihydroxybenzene(DHB) like catechol (1,2-dihydroxybenzene), resorcinol (1,3-dihydroxybenzene) and hydroquinol (1,4-dihydroxybenzene), Isomers of trihydroxybenzene(THB) are 1,2,3-trihydroxybenzene, 1,3,5-trihydroxybenzene and 1,2,4- trihydroxybenzene, Isomers of tetrahydroxybenzene (TTHB) are 1,2,3,4-tetrahydroxybenzene and 1,2,4,5- tetrahydroxybenzene, Pentahydroxybenzene(PHB) and hexahydroxybenzene(HHB) have been investigated and predicted

2.0   Computational Methodology
2.1   Geometry optimization

Geometry optimization is done by locating both the minima and transition states on the potential surface of the molecular

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orbital. It can be optimized in Cartesian coordinates that are generated automatically from the input Cartesian coordinates. It also handles fixed constraints on distances, bond angles and dihedral angles in Cartesian or (where appropriate) internal coordinates. The process is iterative, with repeated calculations of energies and gradients and calculations or estimations of Hessian in every optimization cycle until convergence is attained One of the most computationally demanding aspects of calculating free energy using electronic structure theory is the calculation of vibrational energy and entropy contributions. The computational expense is incurred by thecalculation of the matrix of second energy derivatives (i.e., the Hessian or force constant matrix), which yields harmonic vibrational frequencies upon diagonalization [3].

2.2   Computation of Molecular Properties

The molecular structures and geometries of the Benzene and Hydroxybenzene molecule groups are completely optimized using ab initio quantum mechanical calculations at the Density functional Theory (DFT) level of theory without using any symmetry constraints. Geometry optimizations are performed using the ab initio at DFT at Becke3LYP(B3LYP) method with 6-31G(d,p) basis set. The Density Functional Theory, is a cost effective method for inclusion of electron correlations with the three-parameter density functional generally known as Becke3LYP(B3LYP)

2.3   Gaussian Package

The Gaussian package is a computational physics and chemistry program. The name comes from the fact that it uses Gaussian type basis functions. It is used for electronic and geometric structure optimization (single point calculation, geometry optimization, transition states, and reaction path modeling), and molecular properties and vibrational analysis (IR, Raman, NMR vibrational frequencies and normal modes, electrostatic potential, electron density, multi-pole moments, population analysis, natural orbital analysis, magnetic shielding induced current densities, static and frequency-dependent polarizabilities, and hyperpolarizabilities) using both DFT and ab initio methods.

2.4   Theoretical Background

Energies of HOMO and LUMO are popular quantum mechanical descriptors. It has been shown [4] that these orbitals play a major role in governing many chemical reactions, and are also responsible for charge transfer complexes [5]. The treatment of the frontier molecular orbitals separately from the other orbitals is based on the general principles governing the nature of chemical reactions [6]. The energy of the HOMO is directly related to the ionization potential and characterizes the susceptibility of the molecule towards attack of elecrophiles. The energy of LUMO is directly related to the electron affinity and characterizes the susceptibility of the molecule towards attack of nucleophiles. The concept of hard and soft nucleophiles and electrophiles has been also directly related to the relative energies of the HOMO and LUMO orbitals. Hard nucleophiles have a low energy HOMO, soft nucleopphiles have a high energy HOMO, hard electrophiles have a high energy LUMO and soft electrophiles have a low energy LUMO [7]. HOMO-LUMO gap is an important stability index [8].

Koopman's theorem states that if the single particle energies are not affected by adding or removing a single electron, then the ionization energy is energy of the highest occupied single particle orbital (the HOMO) and the electron affinity is the energy of the lowest unoccupied orbital (the LUMO) with the negative sign as the following`[9].

$$IP \; = \; - \; E_{HOMO}$$

(2.1)

$$EA = \; - \; E_{LUMO}$$

(2.2)

Where IP: ionization potential , EA: electronic affinity, E_{HOMO} : energy of the highest occupied orbital. E_{LUMO}:energy of the lowest   unoccupied   orbital.
Koopman's theorem is extremely useful in predicting ionization energies and spectra. Energy gap generally refers to energy difference between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) according to the Koopmans theorem [10].

$$E \; = \; E_{LUMO} \; - \; E_{HOMO}$$

(2.3)

Ionization energy (IP) defined as the minimum energy required to remove an electron from the atom in a gaseous phase. Ionization energy is expressed in units of electron volt (eV). Also, it can be defined as the energy difference between the positive chargosed energy E(+) and the neutral energy E(n) [11].

$$IP \; = \; E\left(+\right) \; - \; E\left(n\right)$$

(2.4)

Electron affinity can be defined as the energy released upon attachment of an electron to an atom or molecule resulting in the formation of the negative ion. Also, it can be define as the energy difference between the neutral energy E(n) and the negative charged energy E(–), as in the following relation

$$EA = E(n) - E(-)$$

(2.5)

within the frame work of DFT, one of the global quantities is chemical potential (μ), which measures the escaping tendency of an electronic cloud, and equal the slope of the energy versus N (number of electrons) curve at external potential V(r)

$$\mu = \left(\frac{\partial E}{\partial N}\right)_{V(r)}$$

(2.6)

finite difference approximation to Chemical potential gives

$$\mu \approx -\chi = -\frac{(IP + EA)}{2}$$

(2.7)

Chemical hardness is the resistance of a species to lose electrons, the theoretical definition of Chemical hardness has been provided by the density functional theory as the second derivative of electronic energy with respect to the number of electrons N, for constant external potential V(r)

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{V(r)} = \frac{1}{2}\left(\frac{\partial \mu}{\partial N}\right)_{V(r)}$$

(2.8)

And for insulator and semiconductor finite difference approximation, Chemical hardness gives

$$\eta = \frac{(IP - EA)}{2}$$

(2.9)

Also, Softness is defined as the inverse of Chemical hardness as shown below [12].

$$S = \frac{1}{2\eta} = \frac{1}{2}\left(\frac{\partial^2 N}{\partial E^2}\right)_{V(r)} = \frac{1}{2}\left(\frac{\partial N}{\partial \mu}\right)_{V(r)}$$

(2.10)

Electro negativity is defined as "the power of an atom in a molecule to attract electrons to itself" by Pauling [13]. R. Mulliken defined electronegativity as the average of the ionization energy and electron affinity as follows [14].

$$\chi = \frac{(IP + EA)}{2}$$

(2.11)

The Electrophilicity index is defined as a measures of the stabilization in energy when the system acquires an additional electronic charge from the environment. On the other word, it can be defined as a measure of energy lowering due to maximal electron flow between donor and acceptor.

$$\omega = \frac{\mu^2}{2\eta}$$

(2.12)

One of the important global properties is the electric dipole polarizability, which is a measure of the linear response of the electron density in the presence of an infinitesimal electric field (F) and represents a second order variation in energy.

$$\alpha = -\left(\frac{\partial^2 E}{\partial F_a \partial F_b}\right) a, b = x, y, z$$

(2.13)

If some of applied molecules are planar and some are not, it will be useful to report polarizability quantities that are invariant to the choice of coordinate system. One of them is the mean polarizability $< \alpha >$ is evaluated using the equation :

$$< \alpha >= \frac{1}{2}\left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right)$$

(2.14)

where $\alpha_{xx} \leq \alpha_{yy} \leq \alpha_{zz}$ are the eigenvalues of the polarizability tensor.

3.0   Results and Discussions
3.1   Optimized Molecular Structures
Geometry optimizations usually attempt to locate minima on the potential energy surface, thereby predicting equilibrium structures of molecular systems[3]. At the minima, the first derivative of the energy (gradient) is zero. Since the gradient is the negative of the forces, the forces are also zero at such a point (stationary point). In Gaussian, a geometry optimization begins at the molecular structure specified at the input and steps along the potential energy surface. It computes the energy and the gradient at that point and determines which direction to make the next step. The gradient indicates the direction along the surface in which the energy decreases most rapidly from the current point as well as the steepness of that slope. Atoms in the molecule are numbered according to their order in the molecule specification section of the input.
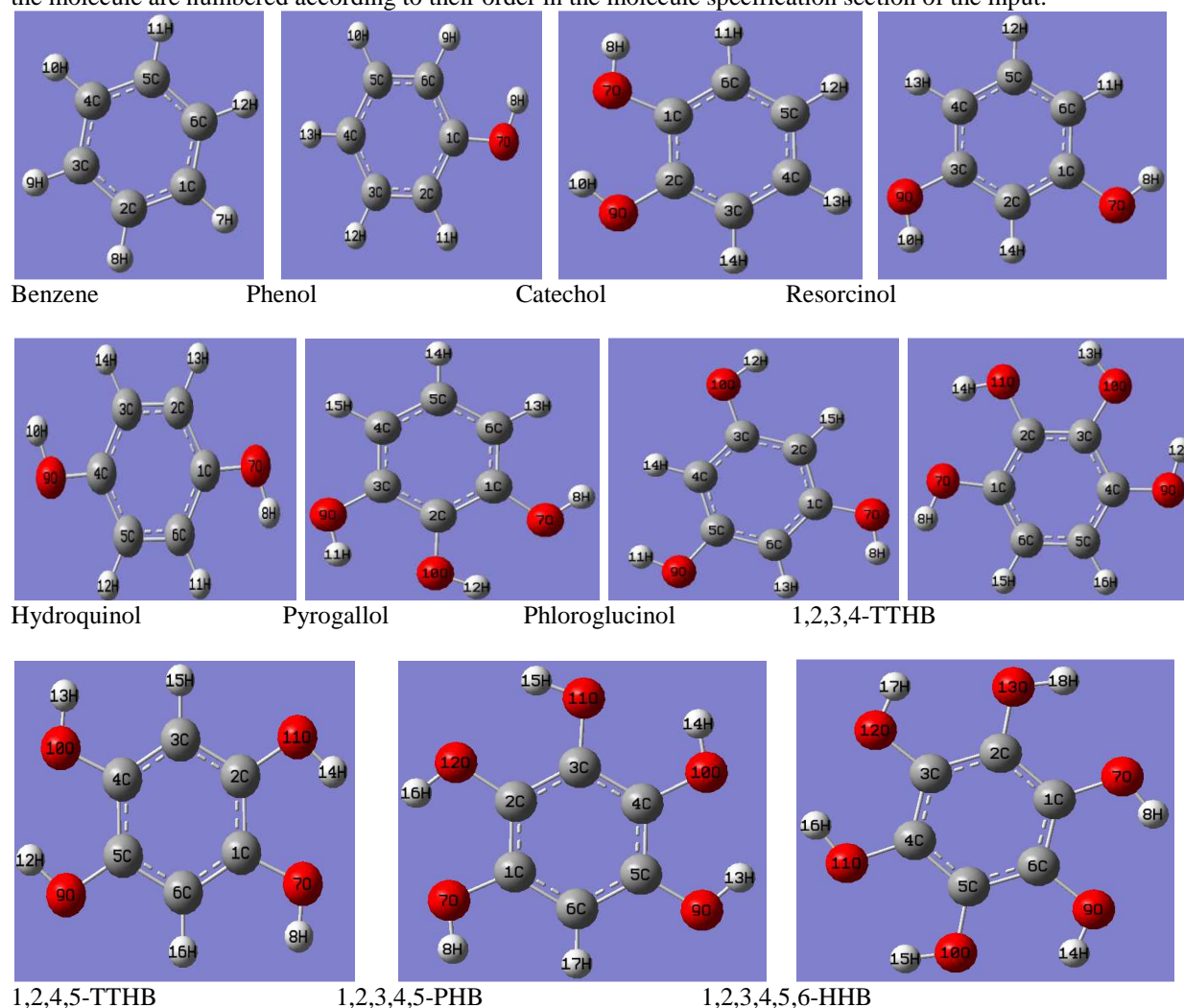

Benzene   Phenol   Catechol   Resorcinol

Hydroquinol   Pyrogallol   Phloroglucinol   1,2,3,4-TTHB

1,2,4,5-TTHB   1,2,3,4,5-PHB   1,2,3,4,5,6-HHB

Fig. 1: Optimized structures of the Studied Molecules

Table 3.1: Energy, Symmetry, Electronic state and Energy gap for the molecules

Molecule	Energy(au)	Symmetry	Electronic state (eV)		Energy gap(eV)
			Lumo	Homo	
Benzene	-232.3	C_{6h}	0.0727	-6.7186	6.7186
Phenol(1MHB)	-307.5	C_S	0.0147	-5.9676	5.9823
Catechol(12DHB)	-382.7	C_S	0.2041	-5.6296	5.8337
Rosorcinol(13DHB)	-382.7	C_S	0.1834	-5.7798	5.9632
Hydroquinol(14DHB)	-382.7	C_{2h}	-0.0773	-5.4152	5.4925
Pyrogallol(123THB)	-457.9	C_S	0.5012	-5.5967	6.0979
Phloroglucinol(135THB)	-457.9	C_{3h}	0.5905	-5.8424	6.4329
1234TTHB	-533.1	C_S	0.4591	-5.2903	5.7494
1,2,4,5-TTHB	-533.1	C_{2h}	0.2724	-4.9681	5.2405
12345PHB	-608.4	C_s	0.6310	-5.0522	5.6832
123456HHB	-683.6	C_{6h}	0.8047	-5.1406	5.9453

Table 3.1 shows that the total energy for all studied molecules as a linear function of OH side group number adding to the molecule. The final total energy of the product is the collection of total energy of all small molecules which build the product molecule, that means:

$E_{tot} \approx E_{tot}(benzene) + nE_{tot}(OH)$

Where n is the number of OH radicals.

It is clear that from Table 3.1, the total energy for all dihydroxybenzene molecules is approximately the same, also it is approximately the same for all trihydroxybenzene molecules which indicated that the total energy depends on the number of radical in the ring, The decrease of total en ergy with addition of OH radical gives the molecule more stability. The eigenvalues of HOMO and LUMO and their energy gap reflects the chemical activity of the molecule. LUMO as an electron acceptor represents the ability to obtain an electron, while HOMO as electron donor represents the ability to donate 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 [15]. It is observed that substitution of hydroxy group causes decreasing the HOMO and LUMO energies[16], and energy gap decreased. Therefore, the presence of substituent decreases the energy gaps improves the conductivities and also enhances the solubility of these molecules. The LUMO-HOMO energy gaps of hydroxybenzene molecule is less than that of the original molecule(Benzene), with decreasing the energy gap, electrons are excited from the ground state . This effect of the side group was the largest in 1,2,4,5-TTHB with energy gap of (5.2405eV).

Table 3.2: The electronic properties of hydroxybenzene molecules group

Molecule	IP(eV)	EA(eV)	μ(eV)	S(eV)	χ(eV)	ω(eV)
Benzene	6.7186	-0.0727	3.3593	0.1488	3.3230	1.6435
Phenol(1MHB)	5.9676	-0.0147	2.9912	0.1672	2.9765	1.4809
Catechol(12DHB)	5.6296	-0.2041	2.9169	0.1714	2.7123	1.2615
Rosorcinol(13DHB)	5.7798	-0.1834	2.9816	0.1677	2.7982	1.3130
Hydroquinol(14DHB)	5.4152	0.0773	2.7463	0.1821	2.6690	1.2969
Pyrogallol(123THB)	5.5967	-0.5012	3.0490	0.1640	2.5478	1.0645
Phloroglucinol(135THB)	5.8424	-0.5905	3.2165	0.1555	2.6260	1.0719
1234TTHB	5.2903	-0.4591	2.8747	0.1739	2.4156	1.0149
1245TTHB	4.9681	-0.2724	2.6203	0.1908	2.3479	1.0519
12345PHB	5.0522	-0.6310	2.8416	0.1760	2.2106	0.8599
123456HHB	5.1406	-0.8047	2.9727	0.1682	2.1680	0.7905

The calculated electronic properties for each studied molecules in Table 3.2 clearly revealed that these hydroxybenzene molecule group have tendency to donate electrons instead of accepting them. Soft molecules have a small energy gap and Low IP creates a better electron donor and large EA makes a better electron acceptor [15]. It is clear from the table that the ionization potential for hydroxybenzene molecule group is less than that of benzene, but the 1,2,4,5-tetrahydroxybenzene has the least, which means this molecule needs small energy to become cation comparing with other molecules. The hardness values for the new molecules were lowering as compared with Benzene, therefore all the newly studied molecules are softer than benzene, and this reduces the resistance of molecule to lose electrons[17].

Table 3.3: Total Dipole moment(μ) and Dipole polarizability (α)

Molecule	μ(D)	α_{xx}	α_{yy}	α_{zz}	$<\alpha>$
Benzene	0.0000	71.767	71.762	21.424	54.984
Phenol(1MHB)	1.3356	81.951	74.076	23.285	59.770
Catechol(12DHB)	2.4866	87.243	79.774	25.116	64.044
Rosorcinol(13DHB)	1.3347	88.455	79.459	25.146	64.350
Hydroquinol(14DHB)	0.0012	91.494	77.077	25.152	64.574
Pyrogallol(123THB)	2.9345	89.521	87.858	26.949	68.109
Phloroglucinol(135THB)	0.0005	89.622	89.619	27.014	68.752
1234TTHB	2.6261	98.052	90.230	28.781	72.354
1245TTHB	0.0028	103.304	87.261	28.812	73.126
12345PHB	1.5762	103.091	95.902	30.607	76.533
123456HHB	0.0010	104.132	104.137	32.386	80.218

The dipole moment is the first derivative of the energy with respect to an applied electric field. It is a measure of the asymmetry in the molecular charge distribution and is given as a vector in three dimensions. For Hartree-Fock calculations, this is equivalent to the expectation values of X, Y and Z, which are the quantities reported in the output. The predicted dipole moments (in Debye) at B3LYP level of theory are shown in Table 3.3 . The dipole moment of the molecules gives the strength of the polarity of the molecule. The predicted dipole moment for Benzene is zero at B3LYP/6-31G(d,p) level. Thus, the molecule is non polar and the charge distribution is fairly symmetrical in gas phase. The predicted dipole moment for the Hydroquinol, Phloroglucinol, 1,2,4,5-TTHB and 1,2,3,4,5,6-HHB is very close to zero which implies that the molecules are non polar in gas phase [18].

Polarizability refers to the way the electrons around an atom redistribute themselves in response to an electrical disturbance. The dipole moment of the molecules gives the strength of the polarity of the molecule. The result show that all substitution group leads to increase the average dipole moment and dipole polarizability and cause to more reactive than the original molecule. Also average dipole polarizability for all isomers of Dihydroxybenzenes is approximately the same, and also for the isomers of Trihydroxybenzene is the same, this indicated that average dipole polarizability depends on the number of the radicals in the ring as shown in Table 3.3.

Table 3.4: Quadrupole moments

Molecule	XX	YY	ZZ	XY	XZ	YZ
Benzene	-31.4718	-38.4736	-38.5312	0.0000	0.0000	0.0000
Phenol(1MHB)	-36.6280	-35.3850	-43.6612	4.3425	-0.0001	0.0001
Catechol(12DHB)	-41.3229	-39.7875	-48.7471	-4.0736	-0.0011	0.0016
Rosorcinol(13DHB)	-40.9462	-39.9424	-48.7962	5.4452	-0.0028	-0.0012
Hydroquinol(14DHB)	-42.0906	-39.2011	-48.7421	-9.9355	0.0005	-0.0001
Pyrogallol(123THB)	-44.7357	-45.3605	-53.8319	1.2620	-0.0013	-0.0016
Phloroglucinol(135THB)	-44.8292	-44.8328	-53.9382	-0.0008	0.0004	0.0010
1234TTHB	-50.3150	-49.0273	-58.8837	6.4553	0.0029	0.0055
1245TTHB	-51.3035	-48.1009	-58.8919	-11.5190	-0.0017	0.0004
12345PHB	-55.1481	-53.3668	-63.9412	6.2243	-0.0055	0.0051
123456HHB	-58.9468	-58.9468	-68.9553	-0.0121	0.0002	-0.0260

Quadrupole moments (Table 3.4) provide a second order approximation of the total electron distribution, providing at least a crude idea of its shape. One of the components being significantly larger than the others would represent an elongation of the sphere along that axis. If present, the off-axis components represent trans-axial distortion (stretching or compressing of the ellipsoid). The quadrupole moment for the molecule at B3LYP/6-31G(d,p) levels of theory is shown above. The molecules are predicted to be slightly elongated more along the ZZ axis in gas phase.

4.0   Conclusion

The practicability of our findings in this work is an encouraging factor. This work has exposed the molecular and electronic properties of Benzene and Hydroxybenzene molecule groups for use in our industry.

To compliment this research work, the experimental part of this study can be undertaken to ascertain the accuracy of this computational technique. Also, this work can be done using other computational physics softwares and results compared with our results in this work . The studied molecule can be studied in other environments to see the effect of these environments on their physical properties. Other solvents that can be considered include ethanol, hexane, hydronaphthalenes, Carbon disulfide, Chloroform, and other organic solvents.

5.0   Acknowledgments

6.0   References

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