



Analytical Study of Some Properties Biomaterial Original: Phenazines

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Abstract

This study has focused on just synthesized materials that were produced from bacteriological practice. So, the density functional theory calculations with hybrid B3LYP at 6-31G sets of basis retain lived utilized to examine the properties of structural and electronic properties of biomaterial original. The determinations include been displayed thereof that is a lowering in the energy of total beyond merging the OH and CH₃ with Phenazine. HOMO and LUMO levels of energy investigations exhibit that the estimation HOMO energy was boosted slightly at 1-Hydroxyphenazine and 2-Hydroxyphenazine but increasing more in 5-Methylphenazin-1(5H)-one, while the value for the LUMO level energy lowered greatly in these strategies of adding the OH at Phenazine. In addition, the lowering of the gap of energy between HOMO and LUMO ensures a bond of strongly between the hydroxyl group and Phenazine. Ultimately, the Biomaterial stability was investigated by estimating the reaction of chemical factors such as the potential of Ionization (I), Affinity (A), global hardness, and Electronegativity χ . As a result, the hydroxyl group and a methyl group can be considered as factors of important changes within biological systems in many chemical and physical properties.

Key Words: Biomaterial, Phenazines, Density Functional Theory, Optical, Electrical, and Thermal Properties.

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Introduction

Focus newly on pigment synthesized from biophysical and chemists who were concerned with the bacteriological method. Historically, recorded secondary metabolites' as a wide set of molecules affected at delayed phases of microbial growth in cultures of a laboratory (Soliev *et al.*, 2011) (Solano, 2014) (Stankovic *et al.*, 2014) (Wadday *et al.*, 2019) (Numan *et al.*, 2018). Phenazines are derivatives including heterogeneous nitrogen-containing antibiotic action (Karuppiah *et al.*, 2016) (Pierson and Pierson, 2010), and antimicrobial activity. It synthesizes a set of bacterial species include *Pseudomonas* and *Streptomyces* and additional types of bacteria (Ray *et al.*, 2015) ("Phenazine derivatives cause proteotoxicity and stress in *C.*

elegans", n.d.). Among the compounds that occur naturally are Phenazines as 1-Hydroxyphenazine, 2-Hydroxyphenazine, and 5-Methylphenazin-1(5H)-one which choice focus on in our analysis.

Phenazines dyes are regularly water-dissolvable, are emitted into the medium. Therefore, derivatives of Phenazines diffuses quickly within agar-solidified media which converts to colored blue. It is sparingly water-soluble and precipitates (Parsons *et al.*, 2007) (Reszka *et al.*, 2010). (5-Methylphenazin-1(5H)-one) its name from the blue phoenix color produced by *Pseudomonas aeruginosa* and also As well as for the rest of the compounds of phenazines derivatives by the same bacteria and bacteria of other types (Dong *et al.*, 2015) (Numan *et al.*, 2018) (Usman *et al.*, 2017).

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Its alchemical conversion to a colorless dye and also other colors support it; via oxidation and reduction transformations (Price-Whelan *et al.*, 2007) (Elbargisy, 2021) (Reszka *et al.*, 2004) (Xia *et al.*,

2013) (Ray *et al.*, 2015). It has also been found that the growth requirements change the relative amounts of various metabolites so it has various applications as shown in fig (1).

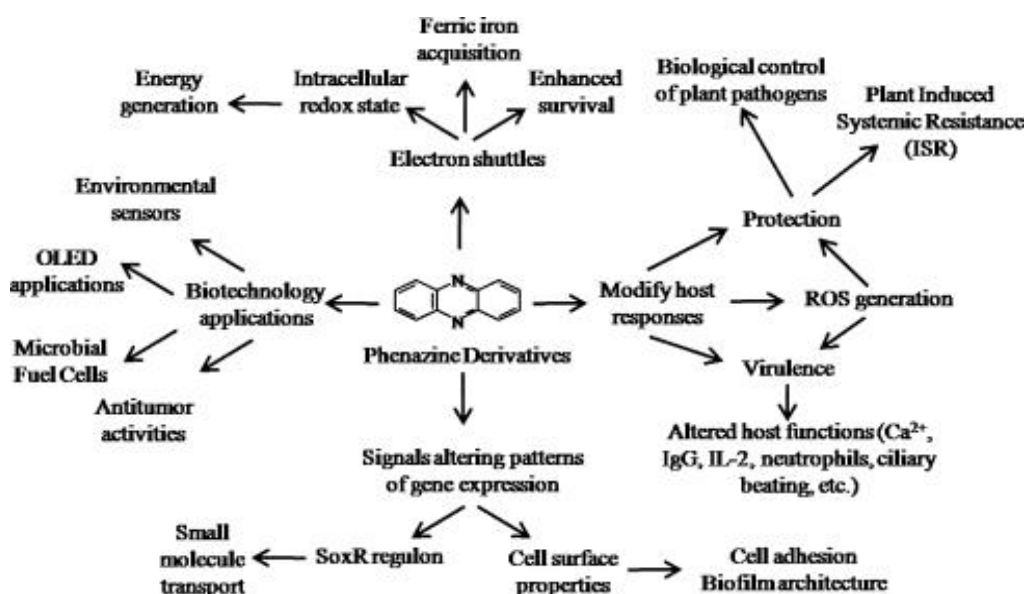


Figure 1. The various applications for phenazines of bacterial origin (Pierson and Pierson, 2010).

The vibrational spectra analysis of phenazine owns tempted numerous Interests over the years (Fu *et al.*, 2003a) (Mattioda *et al.*, 2005). The determined X-ray structure of phenazine by Shouting Wu *et al.* (Wu *et al.*, 2021). Polubotko reported enhanced of surface hyper Raman in phenazine; showed that formation of strong lines are supported with symmetric totally of vibrations (Polubotko, 2011). Olasunkanmi studied many properties via theoretical geometry of molecular, electronic, and thermodynamic characteristics of some phenazines compounds. However, the Computations inform all molecules that exist basically planar (Olasunkanmi *et al.*, 2013).

Newly, the theory of density functional possesses stood accepted from the community of quantum chemistry as a famous procedure for the analysis of molecular structures, frequencies of vibrational, and significances of chemical responses (Fu *et al.*, 2003a) (Zendaoui and Zouchoune, 2013) (De La Cruz *et al.*, 2020) (Merzoug *et al.*, 2018). The vibrational frequencies computation operating DFT strategies is largely promoted by the availability of analytical second-derivative methods, therefore; DFT delivers a favorable cost-effective process for large molecules computing for its vibrational spectra. Multiple analyses of facts displayed that DFT approaches are successful surprisingly in forecasting vibrational frequencies; also,

investigations existed established on molecules of small. To additionally evaluate the dependability of DFT vibrational frequencies used to heterocycles of aromatic molecules, in the present investigation, computed the geometries and the vibrational frequencies of phenazine compounds using B3LYP methods. To the best of our understanding, there are no DFT computations of all these on chosen molecules in the literature computational details.

Computational Details

All the analyses were obtained operating the Gaussian 09 program [46]. The optimizations of geometrical were achieved at the status of DFT; the B3LYP/6-31G base set to attain the numerous stable compounds. The B3LYP is an exceedingly operated DFT that includes frequently existed paired with a 6-31G basis for analyzing the structure of electronic and researching the diverse properties of Biomaterial [47–54]. Phenazine is composed of 22atoms (C 12, H 8, and 2 N). Phenazine can be configured utilizing a vital Anthracene installation but replace that C atoms in N atoms reciprocally in a two-ring, such that alternate to the overhead atoms is equivalent to alternating C atoms at themselves in the exact format a number of some atoms refer in Table 1.



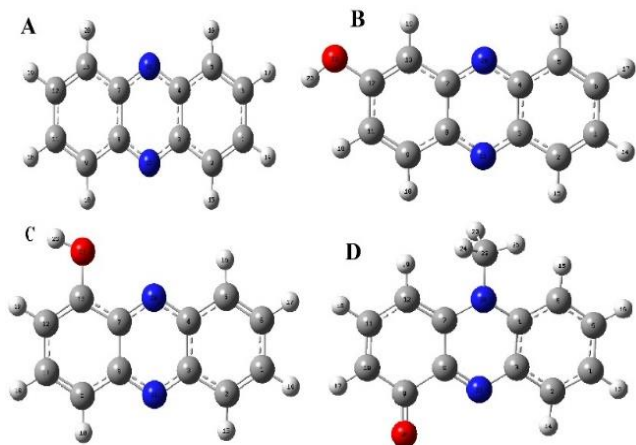


Figure 2. Optimized structure of Phenazines compound: (A) Phenazine. (B) 2-Hydroxyphenazine. (C) 1-Hydroxyphenazine. (D) 5-Methylphenazin-1(5H)-one

Where the Biomaterial arrangement was formulated in excellent measurements structure without deformation. Gauss View existed operated to simulate the Phenazine compounds as illustrated in Fig. 1. The computations have geometrical optimizations; length of the bond, energy of total, also electronic characteristic such as HOMO and LUMO energy levels, energy gaps. Hardness also Softness are important visions for analyzing the reaction and behavior of chemical combinations. The soft material includes a miniature energy gap while the material of hard encloses a comprehensive energy band-gap is largest from above; In addition, It is slightly more reactive than soft ones for the reason that these molecules can facilely submit electrons to the acceptor (Miar *et al.*, 2020; Radhi *et al.*, 2020) So, the hard material is less polarizable than the soft material.

The analyses contain optimizations of geometrical, length of the bond also; the total energy, and electronic characteristic such as the HOMO LUMO of energy levels, energy gap. The energy of electronic is computed by (Engelberts *et al.*, 2005):

$$E = E_T + E_V + E_I + E_{XC} \quad (1)$$

The electronic kinetic energy rewrites are E_T , E_V , and E_I , in equation (1) of the electron on nuclear as interest, and the electron from electron revulsion spans, respectively. The correlation of electrons is obtained into interpretation in DFT theory through the exchange-correlation term (E_{XC}) (Taouali *et al.*, 2018). Energy gap (E_g) is delivered as (Bouzzine *et al.*, 2015):

$$E_g = E_{LUMO} + E_{HOMO} \quad (2)$$

The ionization potential (I_P), also the electron affinity (E_A) are computed according to a theorem of Koopmans' as the below mathematical equations (Zhan *et al.*, 2003):

$$I_P = -E_{HOMO} ; E_A = -E_{LUMO} \quad (3)$$

Electronegativity (η) offers is the capacity of an atom in a molecule to entice a charge to itself, defined as (Namitha and Vidya, 2021):

$$\eta = -(E_{HOMO} + E_{LUMO})/2 \quad (4)$$

Electronegativity, denoted as χ , known as the atom movement for a shared chemical element to attract shared electrons when creating a bond rewrite as equation below (Muhsen *et al.*, 2021):

$$\chi = -(I_P + E_A)/2 \quad (5)$$

Results and Discussion

1. The Optimized Geometries

It was found that the results of studies regarding the length of bonds for compounds in the published literature are identical and close in some of them (Kabanda *et al.*, 2012) (Fu *et al.*, 2003b)(Robins *et al.*, 2010). The geometries optimized on the studied compounds are shown in Fig. 2. Table 1 shows the bond length for all studied molecules. In 2-Hydroxyphenazine, the bonds of longest exist in the C-O is equal (1.388) single bonds and the shortest bonds are the O-H and N=C bonds of double; structures 2-Hydroxyphenazine, 1-Hydroxyphenazine, 5-Methylphenazin-1(5H)-one, Phenazine all these; it's symmetric roughly a plane via the hetero-atoms in the heterocyclic ring. In 1-Hydroxyphenazine, the bonds of longest exist in the C-O which denotes that this is the bond of weakest also may contain an anti-bonding nature and less than from 2-Hydroxyphenazine. In structure 1-Hydroxyphenazine, the weakest bonds represent bonds of longest are the C-O also C=N bonds in two locations. Moreover, the fact that the all above of bond suggests that there is charge delocalization, the C-N bond in R(7,20) is the shortest also shows charge delocalization.



Table 1. Bound length (A) of (C=C & C-C, N-C & N=C, C-O & O-H) calculated geometric parameters of Phenazine compounds

2-Hydroxyphenazine			1-Hydroxyphenazine		5-Methylphenazin-1(5H)-one		Phenazine	
R	Definition	Bound length (A)	Definition	Bound length (A)	Definition	Bound length (A)	Definition	Bound length (A)
R1	R(1,2) C=C	1.3743	R(1,2) C=C	1.3745	R(1,2) C=C	1.3871	R(1,2) C=C	1.3741
R2	R(1,6) C=C	1.4312	R(1,6) C=C	1.4313	R(1,6) C=C	1.4079	R(1,6) C=C	1.4314
R4	R(2,3) C=C	1.4276	R(2,3) C=C	1.4278	R(2,3) C=C	1.4093	R(2,3) C=C	1.4281
R6	R(3,4) C=C	1.4465	R(3,4) C=C	1.4445	R(3,4) C=C	1.4264	R(3,4) C=C	1.4466
R7	R(3,21) C=N	1.3558	R(3,21) C=N	1.3548	R(3,21) C-N	1.3845	R(3,22) C=N	1.3552
R8	R(4,5) C=C	1.4282	R(4,5) C=C	1.4275	R(4,5) C=C	1.4117	R(4,5) C=C	1.4281
R9	R(4,20) C=N	1.355	R(4,20) C=N	1.3551	R(4,20) C-N	1.3953	R(4,21) C-N	1.3552
R10	R(5,6) C=C	1.3744	R(5,6) C=C	1.3745	R(5,6) C=C	1.3927	R(5,6) C=C	1.3741
R13	R(7,8) C-C	1.4484	R(7,8) C-C	1.4486	R(7,8) C-C	1.4684	R(7,8) C=C	1.4466
R14	R(7,13) C=C	1.4215	R(7,13) C=C	1.4386	R(7,12) C=C	1.3778	R(7,13) C=C	1.4281
R15	R(7,20) C=N	1.3572	R(7,20) C=N	1.3481	R(7,20) C-N	1.4063	R(7,21) C=N	1.3552
R16	R(8,9) C=C	1.4279	R(8,9) C=C	1.4265	R(8,9) C-C	1.509	R(8,9) C=C	1.4281
R17	R(8,21) C=N	1.3526	R(8,21) C=N	1.3555	R(8,21) C=N	1.3123	R(8,22) C=N	1.3552
R18					R(9,10) C-C	1.4486		
R19	R(9,11) C=C	1.3716	R(9,11) C=C	1.3736	R(9,26) C=O	1.257	R(9,11) C=C	1.3741
R20	R(11,12) C=C	1.4322	R(11,12) C=C	1.426	R(10,11) C=C	1.367	R(11,12) C=C	1.4314
R22	R(12,13) C=C	1.3752	R(12,13) C=C	1.3776	R(11,12) C=C	1.4338	R(12,13) C=C	1.3741
R23	R(12,22) C-O	1.388						
R24	R(13,19) C-H	1.0819	R(13,22) C-O	1.3811				
R25	R(22,23) O-H	0.9762	R(22,23) O-H	0.9773	R(20,22) N-CH3	1.4679	-	-

2. Parameters of Compounds

Shows table 2 the computed parameters for the goal of investigating the activity of the molecules. The characteristics controlling the state or power of

being reactive of the molecule enclose HOMO level and LUMO level also the energy difference between the HOMO and the LUMO; add to global hardness; global softness and the dipole moment etc.



Table 2. The computed total energy and electronic properties of the Phenazine compounds using hybrid B3LYP/6-31G(d,p) basis sets

Property	Energy (Hartrees)	Enthalpy	Gibbs Free Energy	Dipole Moment (Debye)	E(HOMO) (Hartrees)	E(LUMO) (Hartrees)	
Phenazine	-571.4384894	0.182107	0.137761	0.0009	-0.22521	-0.09138	
1-Hydroxyphenazine	-646.6209062	0.186968	0.140082	1.3679	-0.21363	-0.08772	
2-Hydroxyphenazine	-646.6217564	0.186658	0.139574	1.9267	-0.21803	-0.09004	
5-Methylphenazine-1(5H)-one (Pyocyanin)	-685.875053	0.217687	0.167	8.282	-0.19254	-0.09997	
Property	Electronegativity (χ)	Hardness (η)	Chemical softness (σ)	Global electrophilicity index (ω)	Electron affinity (EA)	Ionization Potential (I)	Energy gap (e.V)
Phenazine	0.158295	0.066915	14.94433	0.187232362	0.0913	0.22521	3.6417
1-Hydroxyphenazine	0.150675	0.062955	15.88436	0.180310981	0.0877	0.21363	3.4261
2-Hydroxyphenazine	0.154035	0.063995	15.62622	0.185379961	0.0900	0.21803	3.4827
5-Methylphenazine-1(5H)-one (Pyocyanin)	0.146255	0.046285	21.60527	0.231074052	0.0999	0.19254	2.5189

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The symmetry and also building the HOMO level energy and LUMO level energy are necessary for indicating the molecule reactivity's as well as signifying suggestions on the chemical responses (Santos *et al.*, 2014). The investigation of the (HOMO)energy level shows molecule areas that retain an inclination to contribute electrons as species of electrophilic while the study of the (LUMO)energy level indicates part of the molecules with an increased preference to receive electrons via nucleophiles species. The developments exhibit that (HOMO)energy level and (LUMO)energy level is

delocalized throughout the molecules chosen. (HOMO)the energy level and (LUMO)energy level density, was conveyed Fig. 3 is deliver indicated an analysis of better for the molecules on which (HOMO)energy level and (LUMO) energy level have the most increased localization; the green color of the (HOMO)energy level and the (LUMO)energy level densities displays the provinces that have the most increased allocation of the (HOMO) energy level, the (LUMO) energy level respectively; while the red color of HOMO and LUMO levels shows densities quite the opposite.



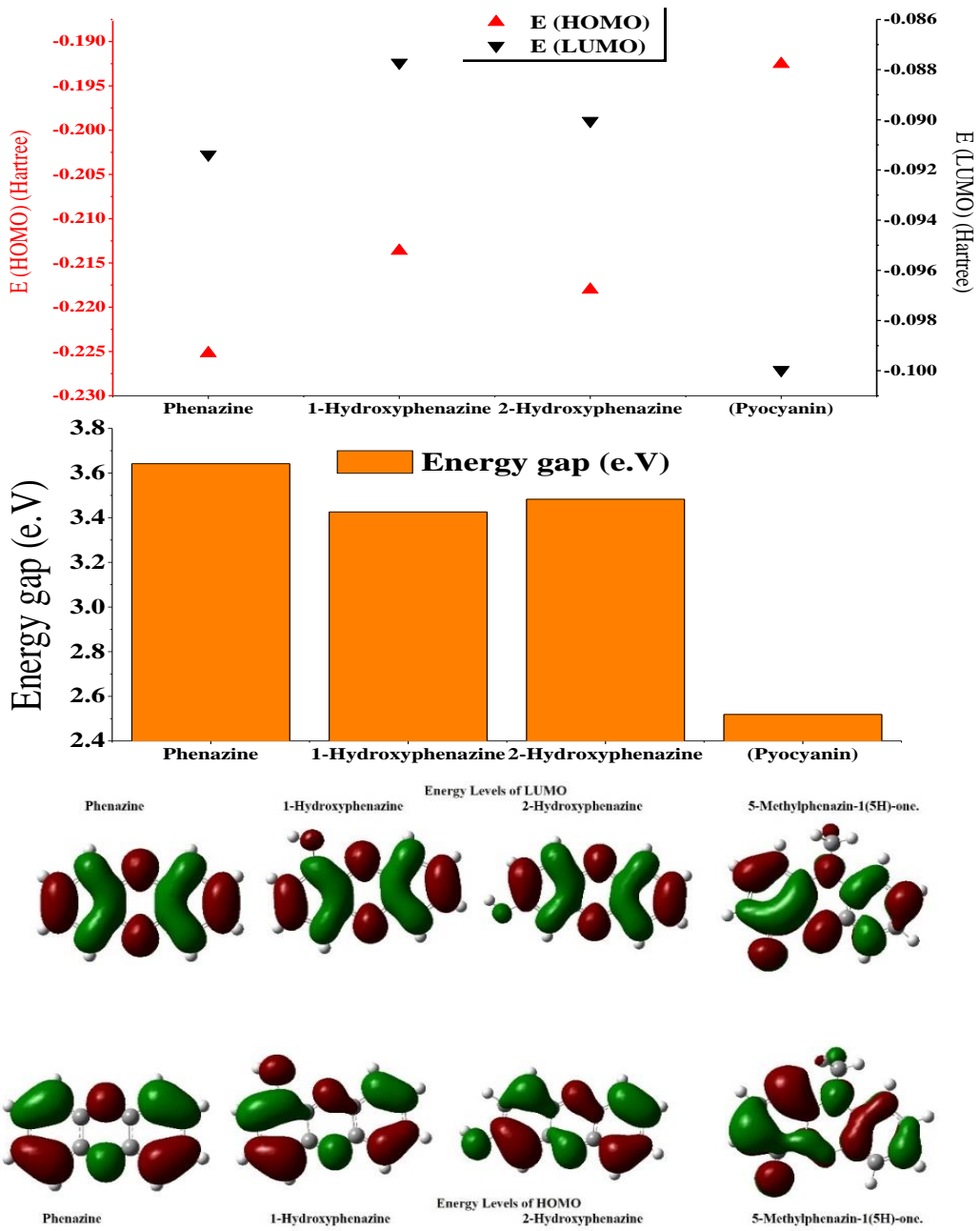


Figure 3. Phenazines compounds of Energy Level of (HOMO and LUMO) & energy gap: (1) Phenazine. (2) 1-Hydroxyphenazine. (3) 2-Hydroxyphenazine. (4) 5-Methylphenazin-1(5H)-one

The (HOMO) energy level denotes the molecule ability to grant electrons (Miar *et al.*, 2020). The molecule with the most elevated (HOMO) energy level contains electrons that have the most heightened energy and thus, have the most increased propensity to donate electrons. In the studied molecules, the order of the (HOMO) energy level is such that 5-Methylphenazin-1(5H)-one > 1-Hydroxyphenazine > 2-Hydroxyphenazine > Phenazine. The energy of the (LUMO) energy level shows the propensity of the compounds to take electrons from molecules of electron-rich. The

lowest energy of the (LUMO) energy level of the molecule, it has the highest propensity to accept electrons. The trend in the (LUMO) energy level for the calculated combinations is such that 5-Methylphenazin-1(5H)-one < Phenazine < 2-Hydroxyphenazine < 1-Hydroxyphenazine, which implies that 5-Methylphenazin-1(5H)-one would preferentially accept electrons from the compound's surfaces, so this material has a redox activity (Sismaet HJ *et al.*, 2017) (Wadday *et al.*, 2019). In Phenazine compound, the HOMO level is applied on C5, C2, C9, and C13 also N21 & N22 atoms while



the (LUMO)energy level is distributed of molecule throughout. While 5-Methylphenazin-1(5H)-one has the (HOMO)energy level contains the most elevated allocation on the C12=C7 and C10=C11 bonds of double, this means that these exist the parts from the molecule with the most increased bias to contribute electrons; the (LUMO) energy level is fully localized on the C2 atom. In 1-Hydroxyphenazine, the (HOMO)energy level is distributed in the area between the heteroatoms C13-O22 single bond and C11=C9 bond of double. The lone pair of on C and O atoms supervise to outstretch their density of electron in the section between C and O atoms also between C and C, may account for the statement that this area exists of high (HOMO) level for density; the (LUMO)energy level is laid out basically on all the aromatic rings atoms linked to the O-H bond. In 2-Hydroxyphenazine, the (HOMO)energy level was intensely localized on N20 and C9=C11, C2=C1; the LUMO is distributed throughout the molecule (Engelberts *et al.*, 2005). Highest in hardness directs to growths in the activity of the system towards a better stable arrangement.

Handling this in senses, and the results offered in Table 2, the chemical hardness the most stable compounds are Phenazine> 2-Hydroxyphenazine> 1-Hydroxyphenazine> 5-Methylphenazin-1(5H)-one (Pyocyanin)as shown in fig 4. Increased significances of softness would solve into raised reactivity of chemical. It is associated with component stability in relation to bonding in the molecule also reactivity of chemicals also the molecule's solubility. The softness significances computed for the investigation molecules revolve about 21.6, suggesting reactivities of high (Talmaciu *et al.*, 2016).

The dipole moment reports concerning the molecule polarity, many investigators in the corrosion scope science include shown that the efficiency of inhibition is connected to the increase in the dipole moment (Al-Baghdadi *et al.*, 2021). The dipole of moment ranking for the investigated compounds exists such as 5-Methylphenazin-1(5H)-one > 2-Hydroxyphenazine > 1-Hydroxyphenazine> Phenazine (Xu *et al.*, 2019).

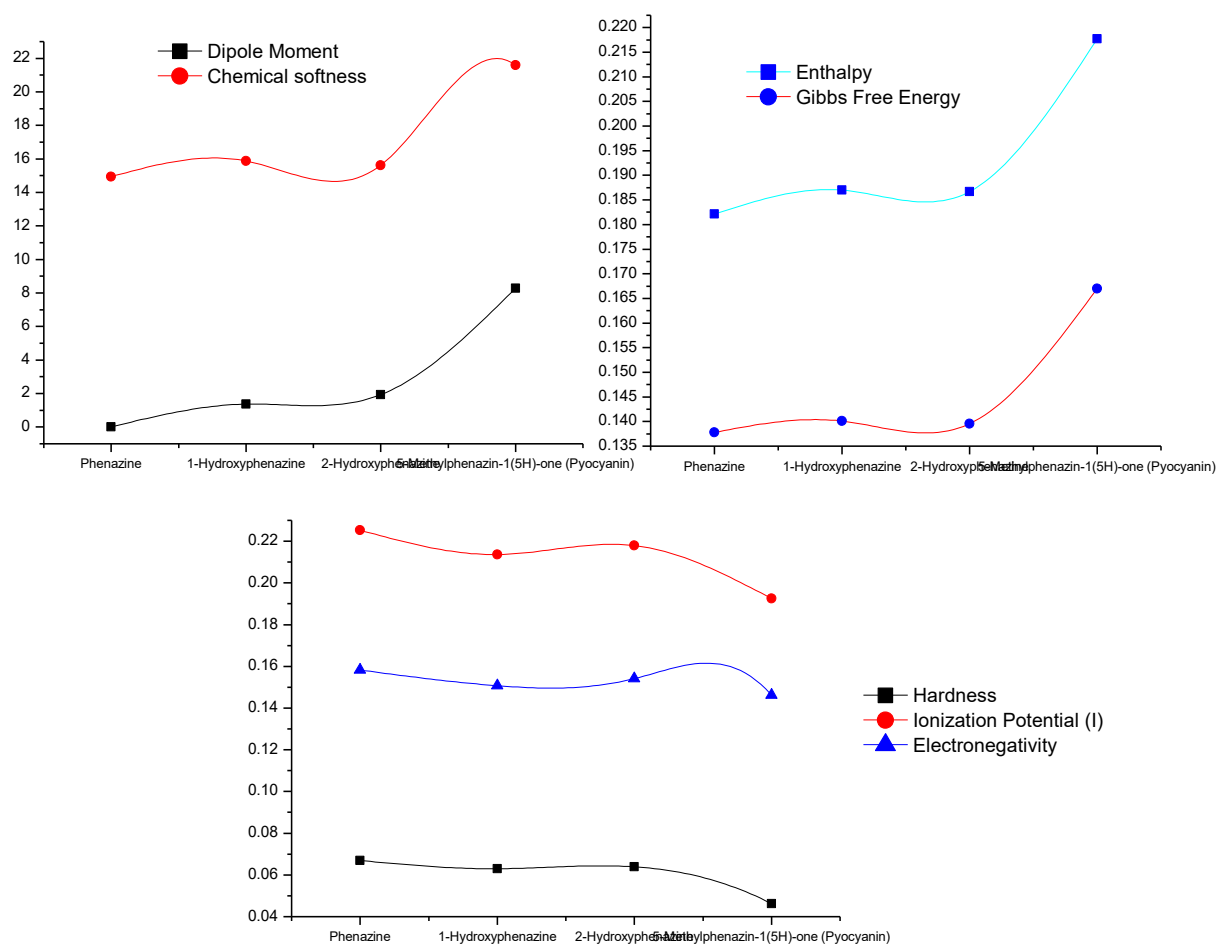


Figure 4. Phenazines compounds of Parameters



3. Vibrational Spectra

In the B3LYP methods, the performance of ranking exists tested in the heterocycles of aromatic in the analysis of Vibrational. This is in good agreement phenazine with the previous studies of the dependability of the B3LYP strategy in producing the frequencies of vibrational fundamental [18], [22]. totally symmetric vibrations, In this case, overall the phenazine fundamentals; it's associated very well. This is absolutely equivalent to the quinoline and isoquinoline correlation with the naphthalene molecule for the complete modes of symmetric vibrational. The divergences in the frequencies compared to the other societies could be described established on the transformation due to the existence of nitrogen in the ring of middle (Brewer *et al.*, 2013).

The IR spectra of molecules under study are provided in fig. (4). The harmonic vibration frequencies are estimated for it's at the B3LYP level using the 6-31(d, p) basis set. The (C - H) stretching vibrations of aromatic molecules in the region (3010- 3150) cm^{-1} which is a characteristic region

for ready identification of (C - H) stretching vibrations and particularly the region (3250 - 3100) cm^{-1} for asymmetric stretching and (3100 - 2900) cm^{-1} for symmetric stretching modes of vibration (Litvinov and Shestopalov, 2011). The out-of-plane (C - H) deformation vibrations were calculated at 628.407 cm^{-1} and 758.48 cm^{-1} . It is clear from fig. (4) that the IR spectrum for phenazine molecules by multiplying the vibration mode due to existing of (N = C), (C - N) bonds, (C = C) stretching, and (C - O) stretching, for (1 - 4) molecules the stretching of (C - N) bond has been observed at (1277 - 1264) cm^{-1} , the (C - H) stretching stay in the region (3100 - 3265) cm^{-1} , the stretching of (N = C) bond has been observed at (1661- 1693) cm^{-1} and the stretching of (C = C) bond at the range (1400 - 1500) cm^{-1} (Muhsen *et al.*, 2021). The electron density on the aromatic ring was delocalized by the presence of the -N2 and OH, which reduced the strength of the (C = C) bond and depended on the position of the nitrogen molecule. The torsion vibrations appear at a very low frequency for (1- 4) molecules at below 500 cm^{-1} .

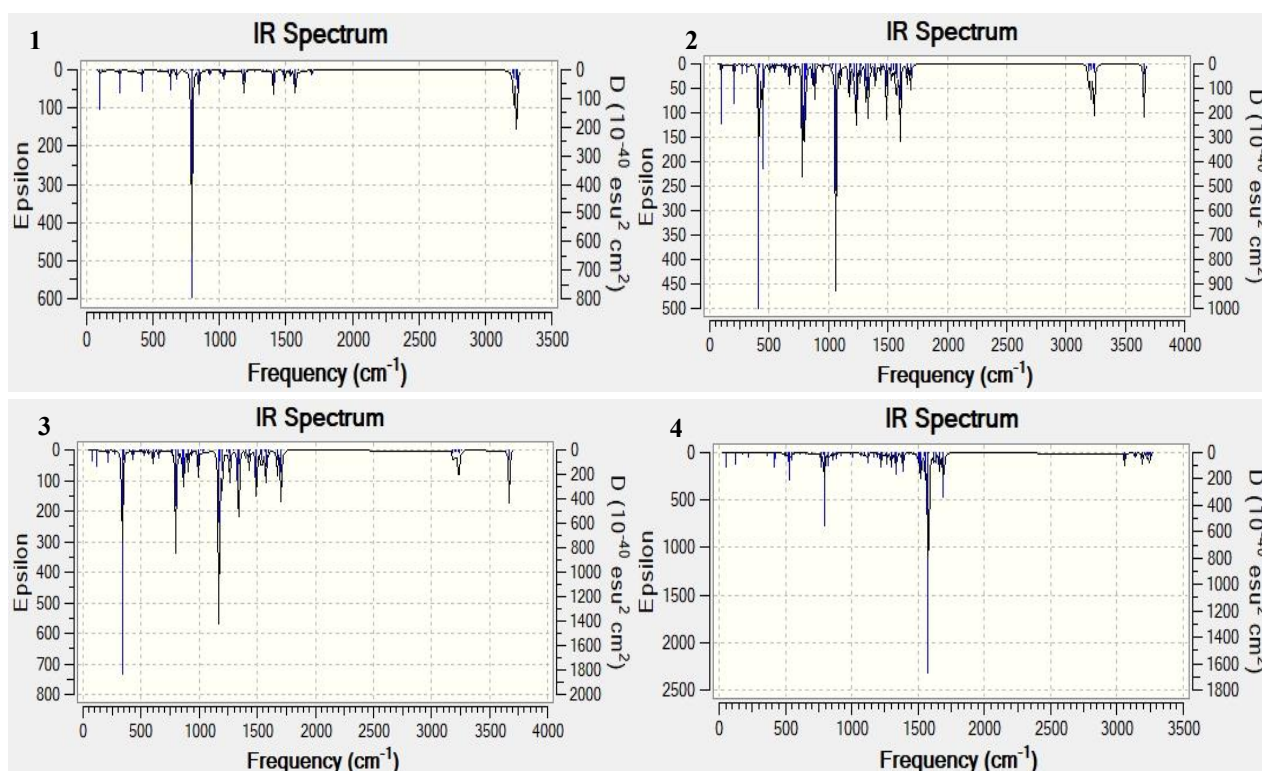


Figure 4. Illustrates the detailed IR spectral frequencies of molecules: (1) Phenazine. (2) 1-Hydroxyphenazine. (3) 2-Hydroxyphenazine. (4) 5-Methylphenazin-1(5H)-one.

Conclusions

The structural and electronic Parameters of phenazine compounds, 2-Hydroxyphenazine, 1-

Hydroxyphenazine, 5-Methylphenazin-1(5H)-one, Phenazine were analyzed utilizing DFT computations. The geometry optimization for structures of phenazine compounds is in agreement



with the previous studies. It was found from results that 5-Methylphenazin-1(5H)-one includes an energy gap, its value 2.52eV. The structure resulting from it is reactive of extremely due to the raised value of Electron affinity. Also, the (HOMO) energy levels analyses show that the values of (HOMO) energy levels have been raised little. Similarly, it existed caught that the total of energy is lowered after combining the hydroxyl group and a methyl group with phenazine, while the value of LUMO energy decreased significantly in 5-Methylphenazin-1(5H)-one. Finally, a result, the hydroxyl group and a methyl group can be considered as factors of changes within biomaterial systems in many chemical and physical properties.

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