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ASSESSMENT OF NEWLY SYNTHESIZED SALICYLALDEHYDE-BASED SCHIFF BASES AS CORROSION INHIBITORS FOR CARBON STEEL IN AQUEOUS ENVIRONMENT

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ABSTRACT

A novel and eco-friendly approach for synthesizing two salicylaldehyde-based Schiff bases (2HPP and BHBD) in aqueous environments has been successfully conducted. These synthesized Schiff bases were subjected to a range of physicochemical analyses, including CHNS elemental analyses, molar conductivity measurements, and spectroscopic techniques like IR, electronic, 1HNMR, and mass spectra, to ascertain their properties. The research also involved investigating the inhibitory properties of these Schiff bases against mild steel corrosion in hydrochloric acid solutions at a temperature of 30°C. The results obtained from this study revealed the remarkable inhibitory potential of 2HPP and BHBD on mild steel corrosion in HCl solution. The inhibition efficiency was found to increase with increasing concentration, ultimately reaching an impressive maximum inhibition efficiency of 91.50% and 94.54 % for 2HPP and BHBD, respectively. The adsorption behavior of 2HPP and BHBD followed the Langmuir isotherm, indicating a favorable interaction with the metal surface. Moreover, the investigations included the use of quantum chemical parameters, which were computed utilizing the Density Functional Theory (DFT) method. These calculations included energy gap assessments, which lent support to the excellent inhibiting performance of both Schiff basses. However, BHBD appeared to be a more efficient inhibitor than 2APP.

Keywords: Salicylaldehyde, corrosion inhibitors, Schiff base, mild steel, inhibition efficiency

INTRODUCTION

Corrosion of carbon steel in aqueous environments poses significant challenges to various industrial sectors, including oil and gas, water treatment, and infrastructure.

The continuous deterioration of metallic surfaces due to corrosion results in substantial economic losses and safety concerns [1-4], To mitigate such adverse effects, the development of effective corrosion inhibitors has garnered substantial attention in recent years. These inhibitors can be inorganic or organic substances introduced into the corrosive environment [5, 6]. Organic inhibitors with specific molecular structures, containing heteroatoms (oxygen, nitrogen, sulfur, or phosphorus), multiple bonds, and aromatic rings capable of donating lone pairs of electrons, have demonstrated promise in preventing corrosion. Despite being very effective inhibitors, their usage was restricted because of recent environmental and health risks associated

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with them [7]. As a result, a shift in trend towards development of environmentally-friendly corrosion inhibitors is inevitable. Again, if the cost of corrosion inhibitors can be reduced, the application value of corrosion inhibitors will be greatly improved

Schiff bases derived from the condensation of primary amines and carbonyl compounds, have demonstrated excellent corrosion inhibitive properties for various metals, including carbon steel [8-11]. These compounds possess a unique chemical structure consisting of an imine (C=N) functional group, which plays a vital role in their inhibitive properties.

The imine functional group (C=N) facilitates electron transfer and charge transfer processes between the inhibitor and the metal surface. The metal surface provides a platform for the Schiff base molecules to adsorb, allowing them to form coordination bonds with metal atoms [12-15].

Once adsorbed onto the metal surface, the Schiff base molecules organize and self-assemble to form a protective film or barrier. This film acts as a physical barrier that shields the metal surface from corrosive species, such as oxygen, water, and ions. The film's thickness and stability are crucial factors influencing the overall inhibition efficiency.

Different parameters, including the inhibitor’s molecular size, the type of substituent, the nature of the metal and the electrolyte, influence the rate of adsorption on the surface [16].

Over the years, researchers have sought to understand the mechanism by which organic corrosion inhibitor molecules adsorb onto different metal surfaces, employing various electrochemical adsorptions-desorption models [17-20]. Some others used quantum chemical computations, and molecular dynamics simulation techniques to gain insight into the geometry, structure, and electronic properties of inhibitor molecules [21-24], and to visualize inhibitor molecule adsorption on metal surfaces [25-31]. These investigations provide valuable information about inhibitor properties, chemical reactivity, and conditions for the inhibition process at the molecular level.

This study presents a comprehensive assessment of newly synthesized salicylaldehyde-based Schiff bases as corrosion inhibitors for carbon steel in aqueous environments. The investigation takes a multidisciplinary approach, combining both experimental and theoretical methods to gain a deeper understanding of the inhibitive mechanisms and evaluate the inhibitors' performance. In parallel, theoretical studies utilizing density functional theory (DFT) were employed to elucidate the electronic structure and electronic properties of the Schiff bases. These calculations shed light on the molecular interactions between the inhibitors and carbon steel surfaces, offering a theoretical basis for the observed experimental results.

MATERIALS AND METHODS

Materials

Chemicals used included salicylaldehyde, aniline, *o*-phenylenediamine, 2-aminophenol, ethanol and hydrochloric acid were of BDH grade and were used as supplied. The electrolyte used in the corrosion test is 1 M HCl solution prepared by diluting from the stock using the appropriate information on the label.

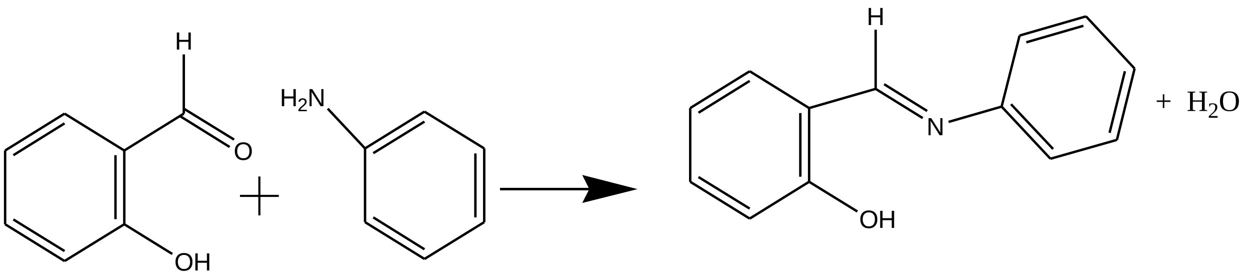
Methods

Preparation of 2HPPSchiff base:

This green approach was adopted from literature according to Srivasyva et al. [29]

The condensation reaction is given thus:

The preparation of 2HPP was accomplished by the condensation reaction of salicylaldehyde (0.05 mol, 2.03 g) and aniline (0.05mol, 1.55 g) in 60 ml ethanol. The mixture was kept under stirring at room temperature for 30 minutes, thereafter concentrated to half of original volume using the rotary evaporator. The final products were collected by filtration, washed with ethanol and purified by recrystallizing from EtOH dried in air and stored in a desiccator prior to use. The Percentage yield of the yellow compound (2HPP) is 85%.

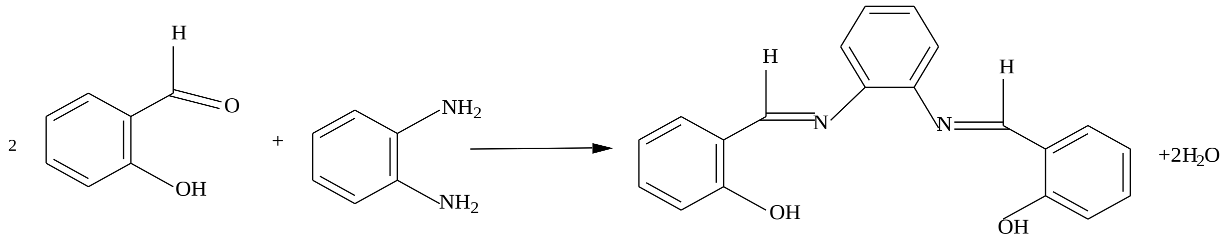


salicylaldehyde Aniline 2-hydroxyphenyl-phenylimine

Scheme 1: Synthesis of 2-hydroxyphenyl-Phenylimine (2HPP)

Preparation of BHBD Schiff base

The BHBD was prepared under similar condition by the condensation of salicylaldehyde (2 mmol, 2.94 g) and o- phenylenediamine (1mmol, 1.32 g) in 60 ml ethanol, giving a yellow product with percentage yield of 74%.



Salicylaldehyde *o*-phenylenediamine Bis(2-hydroxyphenyl)-1,2benzenediamine

Scheme 2: Synthesis of Bis (2-hydroxyphenyl)–1, 2-benzenediimine (BHBD)

Corrosion Inhibition Test

The weight loss of steel sample in 1.0 M HCl was determined following similar approach by Akalezi *et al*. [32]. Carbon steel (CS) (with the composition of 0.32% carbon, 0.75% manganese, 0.2 Cr & Si respectively, and balance iron) obtained from Engineering workshop of the Federal University of Technology Owerri was chosen as the working electrode (specimen) The specimens were cut to sizes with dimensions (40 x 40 x 10) mm, with a hole at the middle of top edge for hanging The surface of each specimen was prepared by wet grinding with 400 and 600 grit silicon carbide papers using deionized water, being degreased with high purity ethanol, rinsed with deionized water, and then dried before being introduced into the electrolyte solutions for testing. Gravimetric tests were performed by weighing cleaned and dried CS specimens before and after immersion in test solution of 1 M HCl for 24 hours at different concentrations ($1x10^{-5}$ M to $5x10^{-4}$ M) of the studied Schiff bases at 36°C. The experiments were carried out in duplicate and average values were obtained. The degree of surface coverage (θ) and the inhibition efficiency IE (%) were calculated at different concentrations [33] using the following equations:

$$\theta = \frac{w_o - w_i}{w_o} \qquad (1)$$

$$IE\% = \frac{w_o - w_i}{w_o} x100 \qquad (2)$$

where w_i and w_o are the weight loss values in the presence and absence of inhibitor respectively.

Theoretical Methods and Technical Details

Quantum chemical method was performed to explore the correlation between molecular properties of the studied inhibitors in line with its corresponding inhibition efficiency**.**

In this present study DFT calculations were performed using the Material Studio 7.0 from Accelrys. Complete geometry optimization of the molecules was carried out in the Dmol3 module using the DND basis set [5-7, 34]. and the generalized gradient approximation (GGA) of Perdew Burke-Ernzerhof (PBE). This approach is widely used in the analysis of the characteristics of the corrosion processes and allows obtaining favorable geometries for a wide variety of systems. Some molecular descriptors were evaluated from the obtained optimized molecular structure: HOMO and LUMO energy values, the energy band gap (ΔE), molecular dipole moment (µ), global hardness (η), softness (σ), the absolute electronegativity (χ), and the number of transferred electrons (ΔN), were calculated using DFT and correlated with inhibition efficiencies.

The molecule-metal interactions were modelled by the Forcite tool using the COMPASS forcefield. The Fe (110) was modelled by periodic slabs consisting of two (110) layers. The in-plane lattice spacing was fixed

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at the calculated equilibrium bulk lattice parameter of 3.31 A° [30] with the top layer of the slab kept frozen to the bulk positions, while all other degrees of freedom were relaxed. The adsorption of molecules onto the surface was modelled at 1/16 ML coverage by a (5 x 5) supercell.

RESULTS AND DISCUSSIONS

Characterization of the Schiff Base

Ligands were prepared by condensation of salicylaldehyde with anilines 1,2-phenylenediamine under reflux for specified time interval and solvent, as shown in the equations of scheme-1 and scheme-2. They were characterized by the available analytical techniques viz. ^{1}H NMR and ^{13}C NMR nuclear magnetic resonance 1H and 13C nuclear magnetic resonance (NMR), Infrared (IR), and UV- visible spectrometry. The electronic spectra of the Schiff base 2HPP (Figure1a) presented two bands at wavelengths 215 nm and 203 nm assigned to π-π attributed to the movement of lone pair of electrons from a bonding pi (π) orbital of the azomethine nitrogen atom

to anti–bonding pi (π^*) orbital of the azomethine group, while UV spectrum of BHBD (Figure 1b) showed absorption band at 349 nm due to n-π transition resulting from transition of non - bonding electrons of the nitrogen atom of the azomethine to the anti–bonding pi (π^*) orbital of the azomethine group.

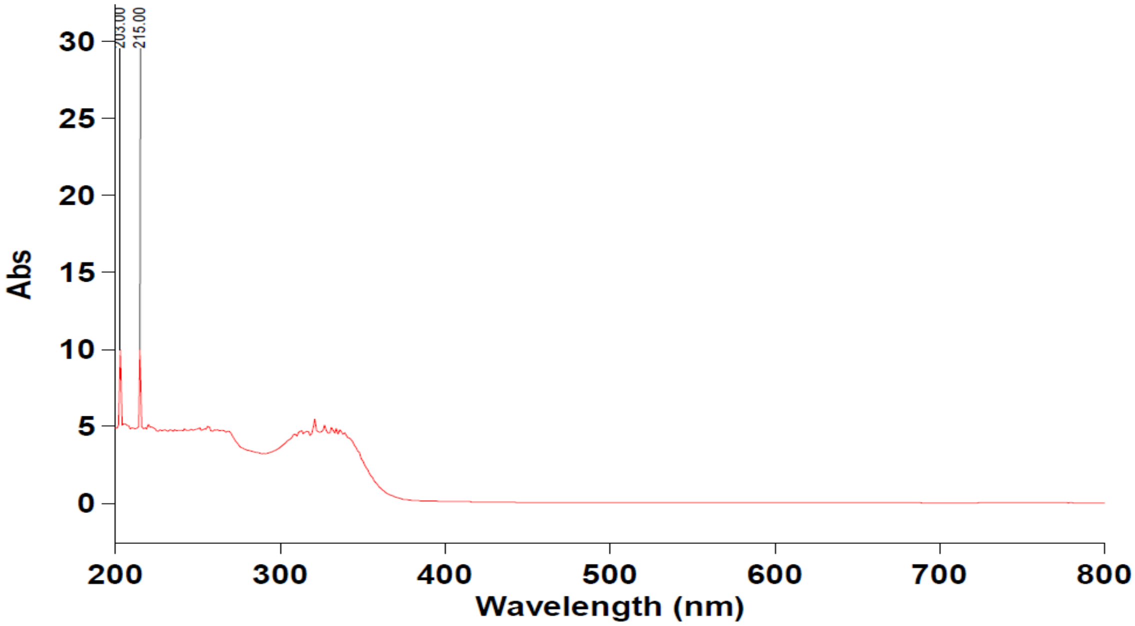

Figure. 1(a) UV SPECTRUM OF 2HPP

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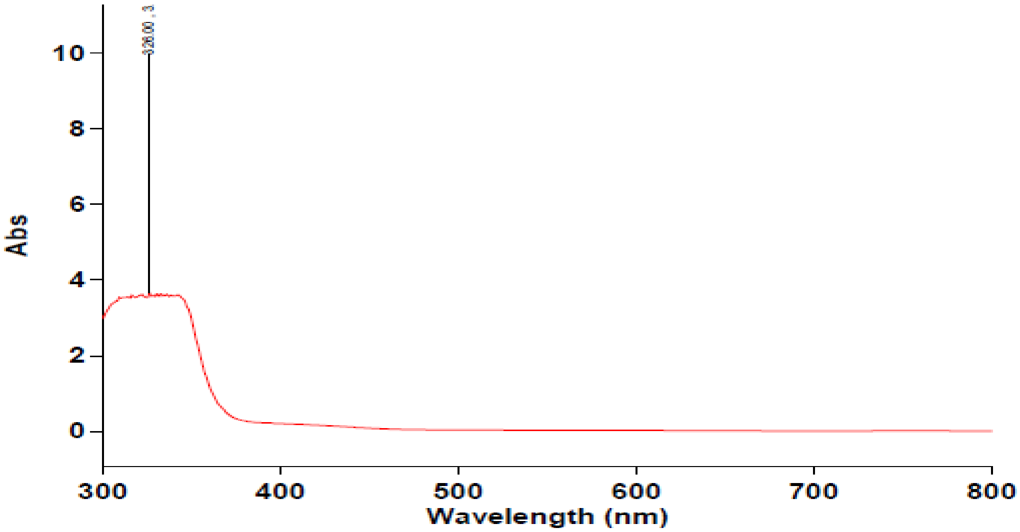

Figure 1(b). UV SPECTRUM OF BHBD

Figure 2a shows the vibration frequencies of certain peaks for 2HPP. They are: v(HC=N), v(C-H), v(C-O) and v(O-H) at 1689 cm^{-1}, 3016 cm^{-1}, 1273 cm^{-1} and 3479 cm^{-1} respectively, while BHBD (Figure 2b), exhibited same vibrations at 1697 cm^{-1}, 3070 cm^{-1}, 1273 cm^{-1}, and 3487 cm^{-1} respectively. This further confirms the formation of the Schiff bases [35].

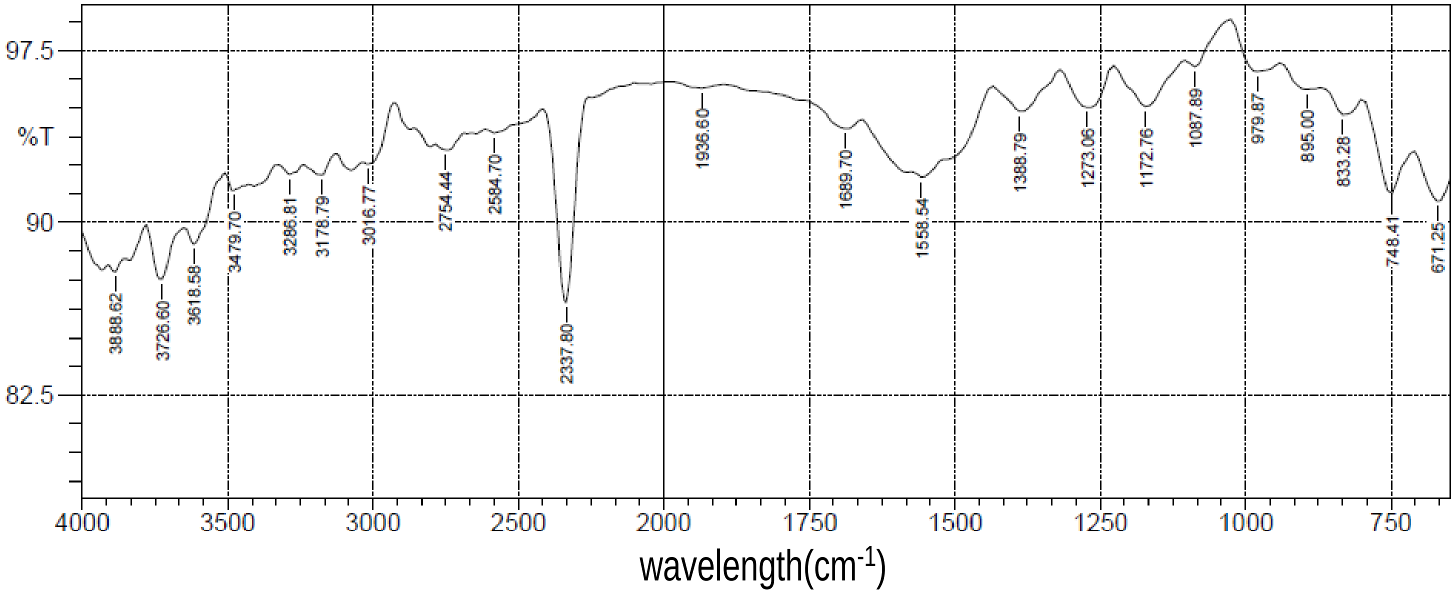

Figure.2(a) Infrared spectrum of 2HPP

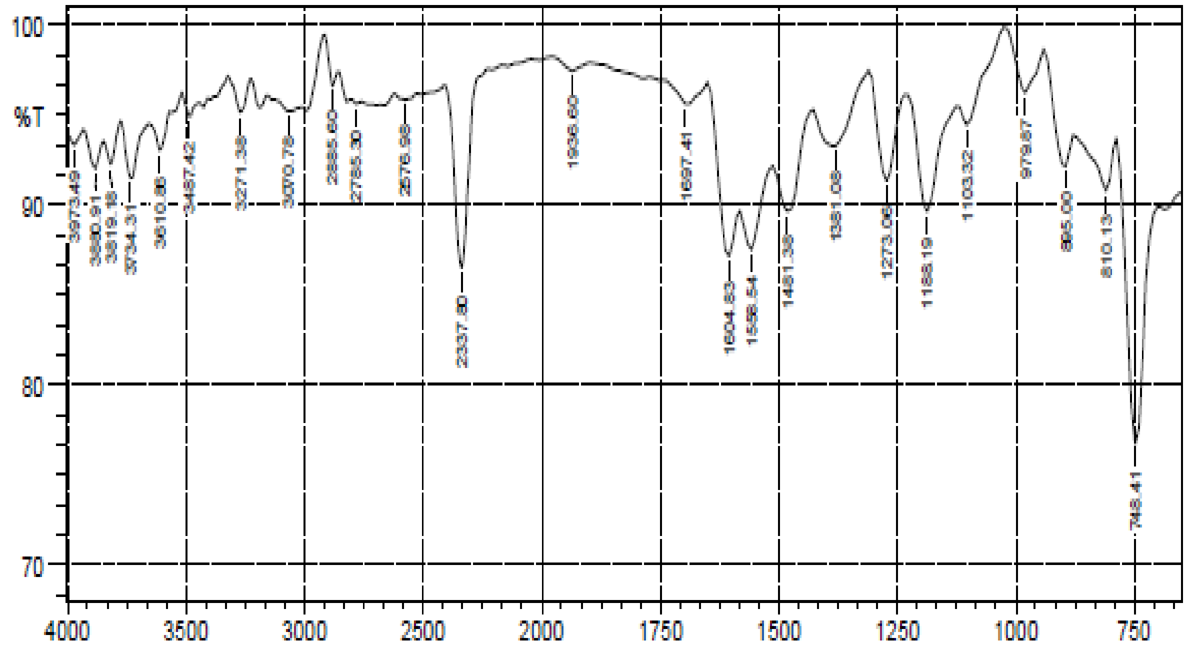

Figure 2(b) Infrared spectrum ff BHBD.

The 1-H NMR of the 2HPP (Figure 3a) reveals formation of the Schiff base with azomethine (HC=N) proton signal, (s, 1H, HC=N) δ = 8.96 ppm, and proton signal due to OH group, (s, 1H, OH), δ = 13.11ppm. The 13 -CNMR of 2HPP (Figure 3b) reveals the presence of the azomethine carbon at signal, δ=163.99 ppm. Formation of BHBD (Figure 4a) Schiff base was confirmed at frequency due to azomethine proton signal, (s, 1H, HC=N) δ = 8.94 ppm, and signal due to two protons of OH group of the Schiff base, (s, 2H, OH) δ =12.95 ppm. The 13-C NMR of BHBD (Figure 4b) confirms the presence of the azomethine carbon at signal, δ= 164.50 ppm.

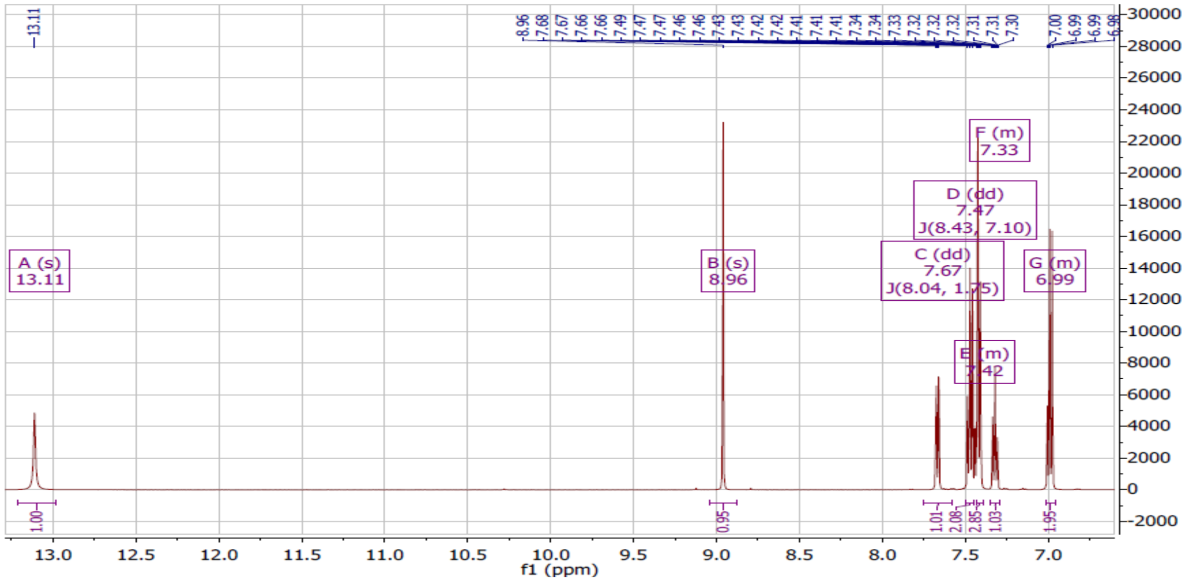

Figure 3(a): ^{1} H-NMR OF 2HPP

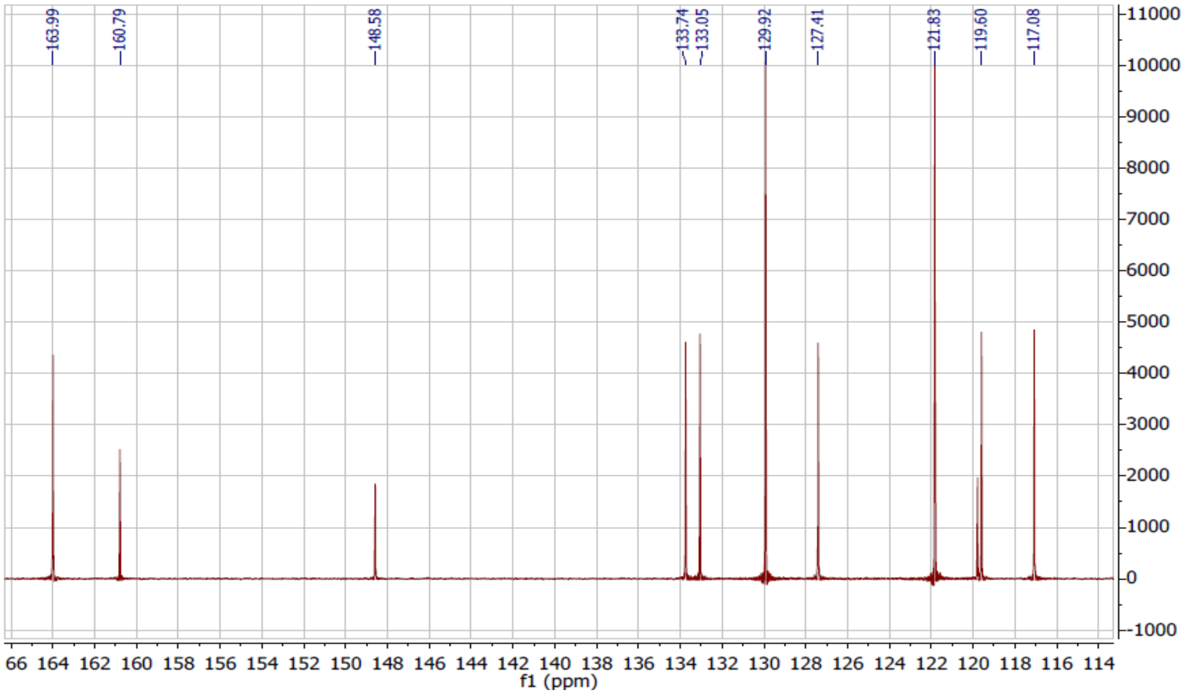

Figure 3(b): ^{13}C-NMR of 2HPP.

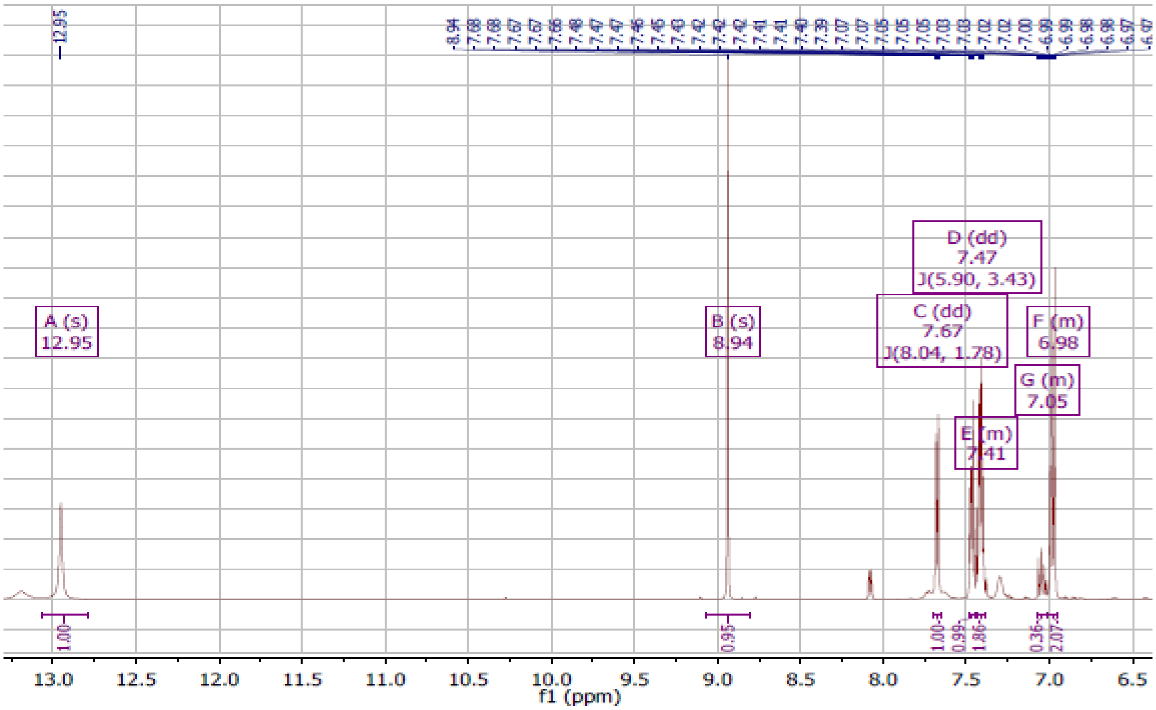

Figure 4(a): ^{1}H -NMR OF BHBD.

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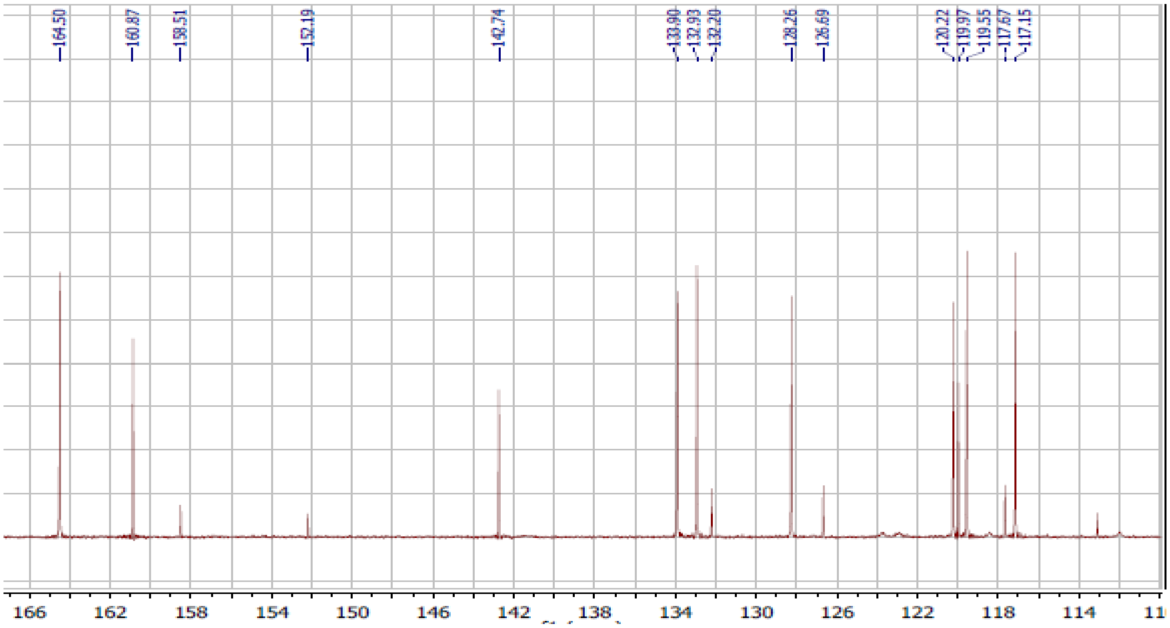

Figure 4(b): ^{13}C- NMR OF BHBD.

Corrosion Inhibition Test

The corrosion inhibition potential of the Schiff base was determined chemically by gravimetric method. Table 1 gives the weight loss and inhibitor efficiency for mild steel in 1.0 M HCl, and 10% DMF in the absence and presence of different concentrations of the Schiff bases at 303 K. The data obtained shows that the metal weight loss was reduced in the presence of the inhibitor and so much more as the concentration was increasing. Figure 5 represents the trend of inhibition efficiency with concentration and confirms that the effectiveness is concentration dependent. The increase in efficiency can be ascribed to the increase in surface coverage due to the adsorption of the inhibitors on the mild steel surface [36]. The adsorption film may then be destined to block the active sites and isolate the metal surface from the aggressive solution and further degradation. The corrosion inhibition efficiency of the two compounds was found to follow the order: BHBD > 2HPP. That BHBD exhibited better corrosion inhibition behavior can be related to the steric hindrance effect and the number of heteroatoms in the structure.

Table 1: Corrosion inhibition data for 2HPP **&** BHBD **Schiff bases in I M HCl**

Inhibitor ➡	2-hydroxyphenyl-Phenylimine (2HPP).				Bis (2-hydroxyphenyl) – 1, 2-benzenediimine. (BHBD)			
System [conc]	W L (mg/cm^2)	(*IE*%)	θ	C/θ	WL (mg/cm^2)	(*IE*%)	θ	C/θ
Blank	0.3676	-			0.3676	-		
1x10^{-4}	0.1442	60.77	0.61	1.6x10^{-4}	0.0646	82.43	0.82	1.2x10^{-4}
3x10^{-4}	0.0991	73.10	0.73	4.1x10^{-4}	0.0320	91.30	0.91	3.3x10^{-4}
5x 10^{-4}	0.0474	87.10	0.87	5.8x10^{-4}	0.0285	92.25	0.92	5.4x10^{-4}
7x10^{-4}	0.0421	88.55	0.89	7.9x10^{-4}	0.0241	93.44	0.93	7.5x10^{-4}
9x10^{-4}	0.0314	91.50	0.92	9.8x10^{-4}	0.0221	94.54	0.95	9.5x10^{-4}

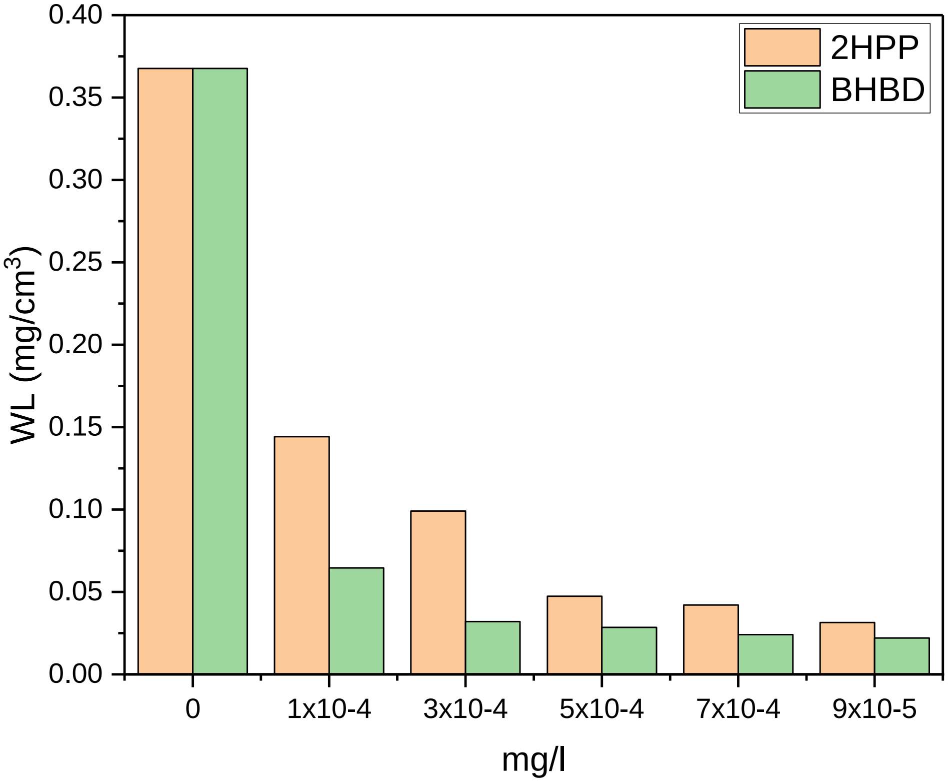

Figure (5): Variation of weight loss (WL) with the concentration of the Schiff bases at 30 ^{0}C

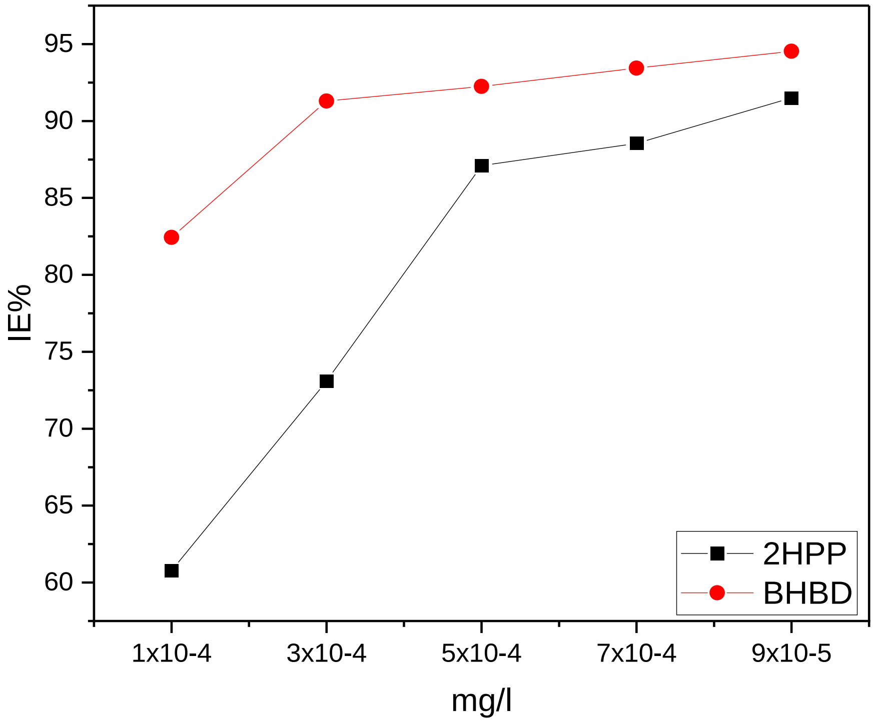

Figure (5b): Variation of the inhibition efficiency with the concentration of the Schiff bases at 30 ^{0}C

Adsorption Isotherm

Basic information on the interaction between inhibitor and the metal surface can be provided by the adsorption isotherm. For this purpose, the values of the surface coverage (θ) at the different concentrations of the Schiff base were used to test for the best fit isotherm including Frumkin, Langmuir, and Temkin. However, the best fit was obtained with the Langmuir isotherm. According to the Langmuir, θ is related to the inhibitor concentration, C

$$\frac{C}{\theta} = \frac{1}{K_{ads}} + C \qquad (3)$$

where K_{ads} is the equilibrium constant of the adsorption process.

Figure 6 shows the dependence of the fraction of the surface coverage $\frac{C}{\theta}$ as a function of inhibitor concentration, and the expected linear relationship is observed with a strong correlation coefficient (R^2 = 0.99998) for 2HPP and BHBD, respectively. The value of the regression coefficient R^2 established the validity of this approach. The almost unity slope for both inhibitor suggests that the adsorbed inhibitor molecules formed a monolayer on the steel surface and there is no interaction among the adsorbed Schiff base molecules.

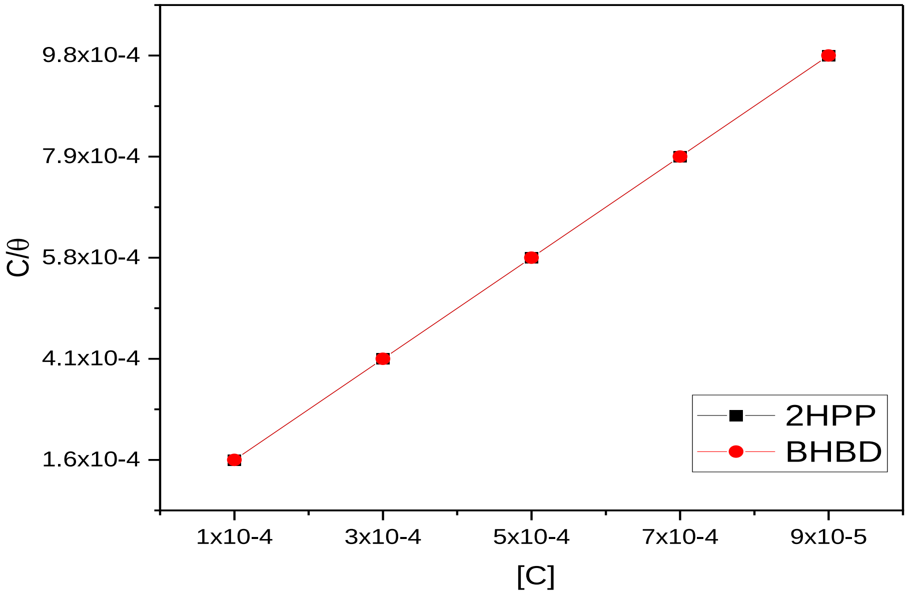

Figure 6: The Langmuir adsorption isotherm of the two Schiff bases

COMPUTATIONAL CHARACTERIZATION OF THE SCHIFF BASES

Molecular orbitals plots

Corrosion inhibitors can prevent metal corrosion by adsorbing on the surface of the substrate. This process is related to the interaction of electrons between frontier orbitals of organic molecules and vacant d-orbital of metal atoms [37]. To predict the corrosion inhibition performance of our Schiff bases, the frontier orbital of the molecules and their energy was calculated. The optimized structure and orbital distribution of the two Schiff bases calculated by software are shown in Figure 7. It has been frequently proposed that Schiff bases bind to the surface via lone-pair electrons of the azomethine-type N atoms or the π-electrons of the aromatic ring [1, 8, 35]. The molecular orbital plot obtained in the present case shows an even energy distribution over the three principal atoms, C, N, and O and over the aromatic ring as well. This format will no doubt facilitate exchange of electrons between the organic molecules and the metal atoms so that the corrosion inhibitor can exhibit ideal adsorption.

The Mulliken charge distributions of the inhibitors are presented in Table 2. The use of Mulliken population analysis to probe adsorption center of inhibitors has earlier been reported [38].

The areas of highest electron density are generally the potential sites for the electrophiles attacked [39, 40]. Based on the calculations, the highest electron densities were located on O, N, and C atoms implies that the O, N and C atoms were the active centers, which have the strongest ability of bonding to the metal surface.

Table 2: The Mulliken charge distributions of the inhibitors

BHBD	2HPP
Mulliken atomic charges:	
charge spin	Mulliken atomic charges:
C (1) -0.188 0.000	charge spin
C (2) -0.175 0.000	C (1) -0.240 0.000
C (3) -0.239 0.000	C (2) -0.175 0.000
C (4) 0.305 0.000	C (3) -0.186 0.000
C (5) 0.102 0.000	C (4) -0.236 0.000
C (6) -0.234 0.000	C (5) 0.101 0.000
C (7) -0.137 0.000	C (6) 0.306 0.000
N (8) -0.329 0.000	O (7) -0.645 0.000
O (9) -0.640 0.000	N (8) -0.332 0.000
C (10) 0.181 0.000	C (9) -0.132 0.000
H (11) 0.187 0.000	C (10) -0.241 0.000
H (12) 0.187 0.000	C (11) 0.230 0.000
H (13) 0.194 0.000	C (12) -0.229 0.000
H (14) 0.202 0.000	C (13) -0.177 0.000
H (15) 0.187 0.000	C (14) -0.181 0.000
H (16) 0.450 0.000	C (15) -0.186 0.000
C (17) 0.180 0.000	H (16) 0.200 0.000
N (18) -0.329 0.000	H (17) 0.193 0.000
C (19) -0.237 0.000	H (18) 0.187 0.000
C (20) -0.190 0.000	H (19) 0.187 0.000
C (21) -0.189 0.000	H (20) 0.440 0.000
C (22) -0.238 0.000	H (21) 0.184 0.000
C (23) -0.136 0.000	H (22) 0.184 0.000
C (24) 0.103 0.000	H (23) 0.192 0.000
H (25) 0.187 0.000	H (24) 0.187 0.000
C (26) 0.304 0.000	H (25) 0.184 0.000
C (27) -0.239 0.000	H (26) 0.184 0.000
C (28) -0.175 0.000	
C (29) -0.188 0.000	
C (30) -0.234 0.000	
O (31) -0.640 0.000	
H (32) 0.189 0.000	
H (33) 0.185 0.000	
H (34) 0.185 0.000	
H (35) 0.190 0.000	
H (36) 0.202 0.000	
H (37) 0.194 0.000	

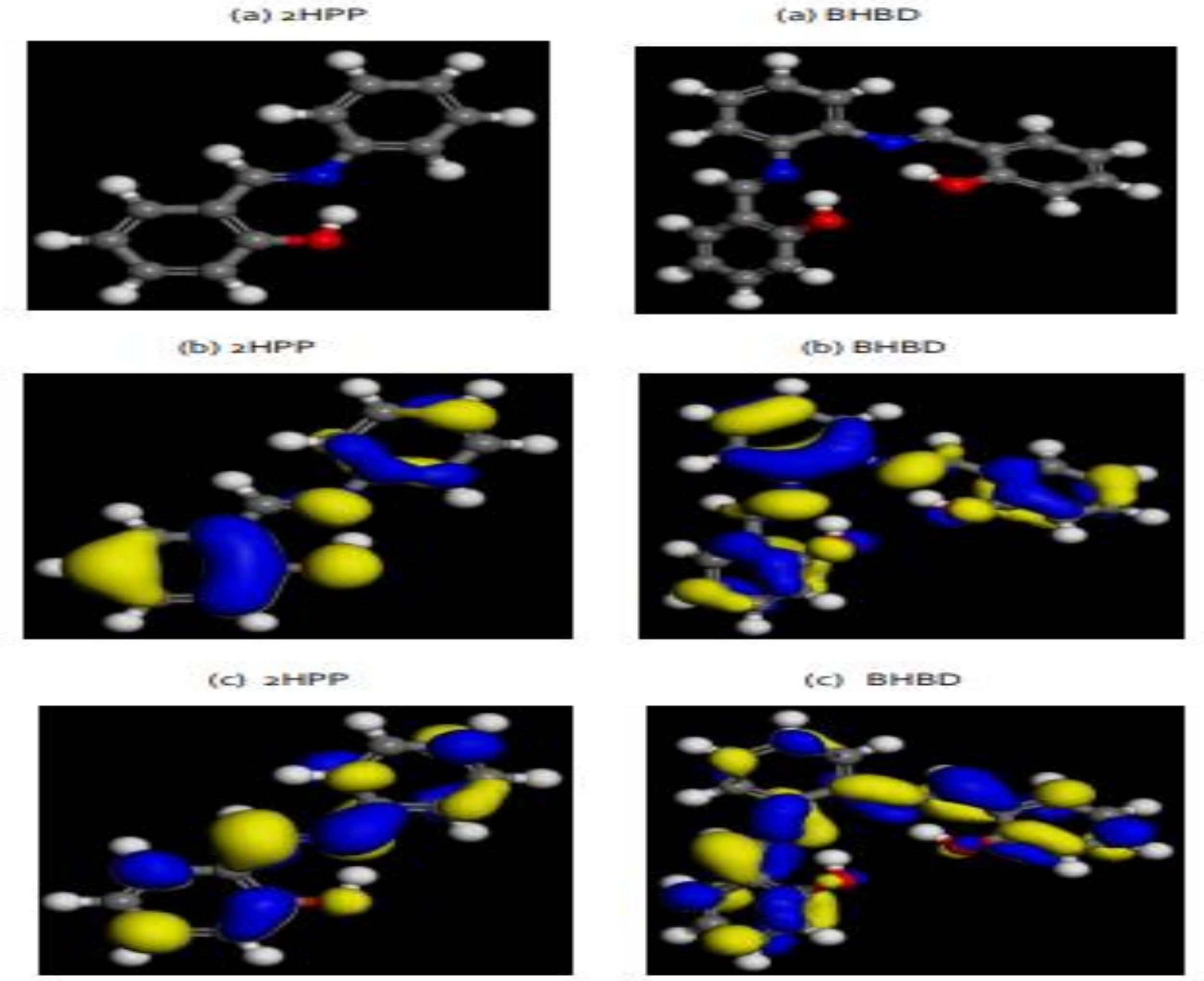

Figure 7: The optimized structure and orbital distribution of the two Schiff bases calculated by software

HSAB-type analysis

Quantum chemical parameters obtained from the calculations which are responsible for inhibitor efficiency such as the energy of highest occupied molecular orbital (E_{HOMO}), energy of lowest unoccupied molecular orbital (E_{LUMO}), the separation energy (E_{LUMO}-E_{HOMO}), ΔE, representing the function of reactivity, dipole moment (μ), the electronegativity χ, the global hardness (η), and softness (σ), are collected in Tables 3. Out of the whole lot, only the E_{HOMO}, E_{LUMO}, and the dipole moment were obtained directly from the software. Following the Koopman's HSAB principle **[41]**, the eigenvalues of HOMO and LUMO were related to ionization potential (I) and electron affinity (A) as:

$-E_{HOMO}$ and, $-E_{LUMO}$ respectively.

(4)

Absolute electronegativity, X, and absolute hardness, η of the inhibitor molecules are given by Pearson [42] as:

$$:\chi = \frac{1}{2}(I + A) \text{ and } \eta = \frac{1}{2}(I - A) \qquad (5)$$

Chemical softness (σ) is the measure of the capacity of an atom or group of atoms to receive electrons [41], it is estimated by using the equation: $\sigma = 1/\eta$.

The obtained values of X and η were used to calculate the fraction of electron transferred, ΔN, from the inhibitor to metallic surface as follow [43-45]:

$$\Delta N = \frac{1}{2}\left(\frac{X_{Fe} - X_{inh}}{\eta_{Fe} + \eta_{inh}}\right) \qquad (6)$$

In the equations above, for iron as bulk metal, a theoretical electronegativity value of 7.0 was used, and absolute hardness is considered to be zero [43-46].

Table 3.0 Quantum chemical parameters

Inhibitor/ Property	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE(ev)	I(ev)	A(ev)	μ(D)	X(ev)	η(ev)	σ(eV)	ΔN
BHBD	-5.284	-3.391	1.993	5.284	3.391	3.8803	4.338	0.947	1.056	0.307
2HPP	-5.246	-2.729	2.477	5.246	2.729	2.4947	3.988	1.258	0.795	0.378

Hardness and softness are the basic chemical concepts, called global reactivity descriptors have been theoretically justified within the framework of density functional theory [47]. These are the important properties to measure the molecular stability and reactivity. Chemical hardness fundamentally signifies the resistance towards the deformation or polarization of the electron cloud of the atoms, ions or molecules under small perturbation of chemical reaction. A hard molecule has a large energy gap and a soft molecule has a small energy gap [48]. In the present study 2HPP presents a higher energy gap value (2.477 eV), and lower global hardness compared with BHBD (1.993).

Normally, the inhibitor with the least value of global hardness (hence the highest value of global softness) is expected to have the higher inhibition efficiency [49].

The dipole moment is another crucial molecular property that comes into play during the assessment of an additive as a potential corrosion inhibitor [50-54]. Molecules with larger dipole moments exhibit greater polarity, enabling stronger electrostatic interactions with charged metal surfaces, which enhances the adsorption of the inhibitor onto the metal.

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BHBD again, showed the higher value of dipole moment (μ), which will favour accumulation of the inhibitor, and will translate to higher inhibition efficiency.

The ΔN values calculated are listed in Table 3. The sign of ΔN can be used to determine the tendency of electrons to transfer between iron atoms and organic molecules [55]. If ΔN is greater than zero, electrons tend to move from molecules to the metal surface [56]. Conversely, electrons are more easily transferred from iron atoms to organic molecules. If for a molecule, the value of ΔN with an iron atom falls in the range of 0−3.6, then this molecule may have good inhibition performance [57]. Within the same range, the larger the ΔN value is, the better the inhibition efficiency the molecule may have. The values obtained in this study show the two compounds are good inhibitors.

***Inhibitor Adsorption Simulation*.**

To simulate the interaction between the corrosion inhibitor and the steel surface, an adsorption module is carried out to obtain the adsorption structure and energy for 2HPP, and BHBD on a Fe(110) surface. The simulated spatial structures and their binding energy values are shown in Figure 8. Both binding energies of 2HPP and BHBD are negative, which means that these structures can be formed spontaneously and have strong interactions [3]. Comparing the binding energy of 2HPP and BHBD, the binding energy of BHBD (−172.88 kcal/mol) is stronger than 2HPP (−110.02 kcal/mol). Stronger adsorption often indicates better corrosion inhibition. Therefore, the corrosion inhibition potential of BHBD is better than that of 2HPP, which is similar to the conclusions obtained from actual experiments.

By careful examination of Figure 8, it could be observed that all the inhibitors adsorbed nearly parallel to the iron surface where a chemical bond could occur through donation of pi electrons of the aromatic ring and the lone pair of the hetero-atoms to the metal. In order to investigate the interaction between the inhibitor molecules and the surface, we calculated the adsorption energy (E_{ads}) from the relation:

$$E_{ads} = E_{complex-(E_{inh}+E_{Fe})} \qquad (7)$$

where E_{Fe} is the total energy of the iron surface and E_{inh}. is the total energy of the inhibitor compound. When the adsorption occurs between the compound and the iron, the energy of the new system is expressed as $E_{complex}$ [58]. It could be observed from Table 6 that all values of E_{ads} are negative, which means that the adsorption could occur spontaneously. The high values of E_{ads} for BHBD reflect the higher stability of the formed complex and accordingly increase their inhibition efficiencies. The lower E_{ads} and lower inhibition efficiency of 2HPP agrees well with the experimentally determined results. The binding energy E_{bind} is, the negative of the adsorption energy, E_{bind} = -E_{ads} [59. 60]. The higher the negative value of binding energy, the easier the inhibitor adsorbs on the metal surface and the higher the inhibition efficiency.

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Estimation of inhibition constant (KI)

The inhibition constant (KI) represents the affinity of an inhibitor for a substrate and is a measure of how effectively the inhibitor binds to the substrate's active site. The inhibition constant (KI) can be related to the adsorption energy using the following equation: KI = exp(ΔG/RT)

where

ΔG is the change in Gibbs free energy associated with the binding of the inhibitor to the metal (negative of the adsorption energy)

R is the gas constant (8.314 J/K-mole)

T is the temperature in Kelvin (350 K)

A lower KI value for BHBD (0.94232) indicates a stronger binding affinity of the inhibitor for the substrate meaning it is a more potent inhibitor. Conversely, a higher KI value for 2HPP (0.96290) suggests weaker binding.

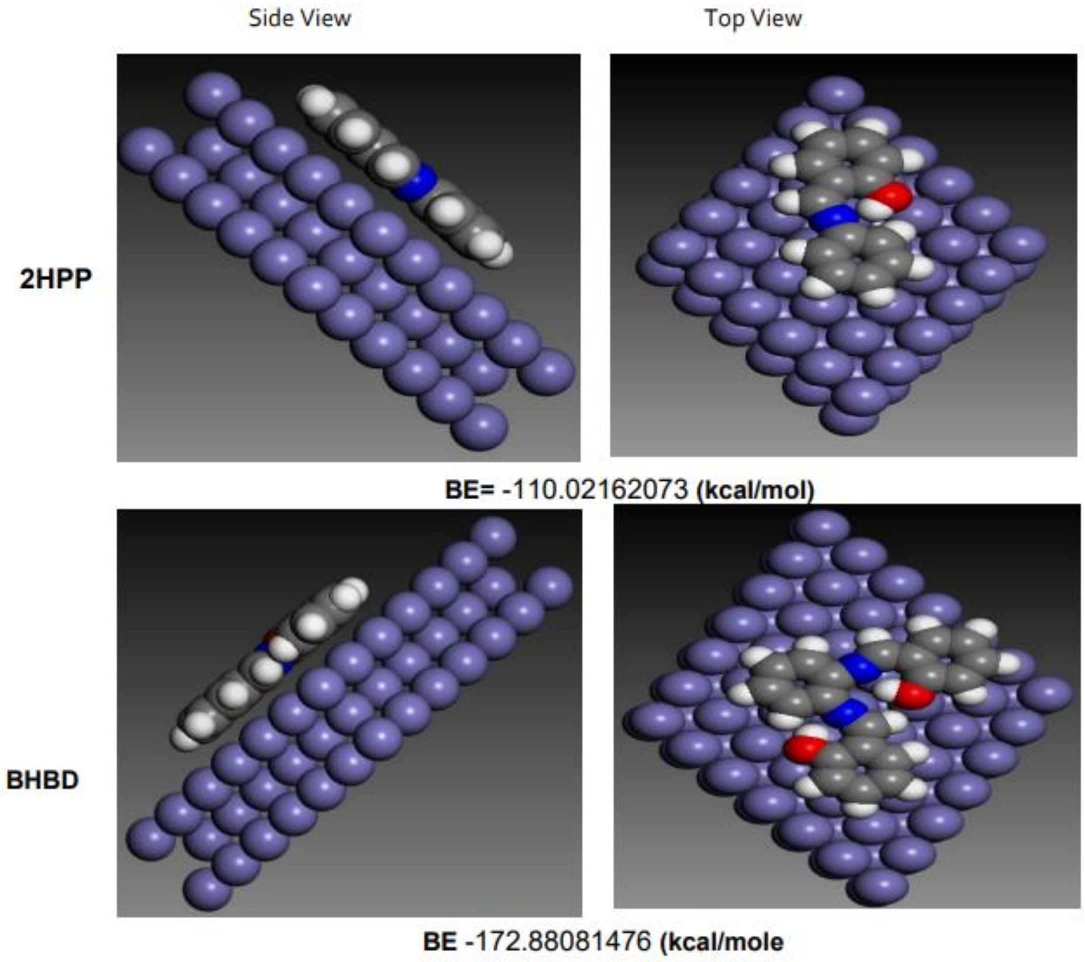

Figure 8. Simulated structures of 2HPP, and BHBD on the Fe(110) surface.

CONCLUSION

Two new Salicylaldehyde Schiff base inhibitors, 2HPP and BHBD, were synthesized and studied for their corrosion inhibition performance on mild steel in 1.0 M HCl. From the obtained experimental and theoretical results, the following conclusions were drawn:

1. Both 2HPP and BHBD show good inhibition properties for mild steel in 1.0 M HCl solution and the observed inhibition efficiency of the two inhibitors increased with increasing concentrations following the order: BHBD > 2HPP at same concentrations and conditions.

2. The adsorption model of 2HPP and BHBD obeyed the Langmuir adsorption model.
3. Molecular dynamics simulation results reveal that 2HPP and BHBD adsorb nearly parallel to the Fe (110) surface.
4. The inhibition ability of the two novel Salicylaldehyde Schiff base inhibitors follows the order, 2HPP < BHBD, which has been confirmed by the experimental measurements and theoretical calculation measurements.

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