Antimicrobial and corrosion inhibition activity of Schiff base in mild steel of HCl and H_2SO_4 acidic solutions

K. Senthil Murugan[a], T. Mohanapriya [b,*]
[a]*Research scholar, PG and Research Department of Chemistry, Erode Arts and Science College (Autonomous), Erode, Tamilnadu, India-638 009*
[b]*Associate Professor, PG and Research Department of Chemistry, Erode Arts and Science College (Autonomous), Erode, Tamilnadu, India-638 009*

The purpose of synthesizing two different types of Schiff base compounds, such as 2-[(4-Nitrophenyl)Imino]MethylPhenol (2, 4- NMP) and 2-[4-MethoxyPhenyl)Imino] Methyl}Phenol (2,4-MMP), are to improve the corrosion inhibition efficiency of Mild steel (MS) using acidic solutions of 1M HCl and 0.5M H_2SO_4 and investigated antimicrobial activity against bacteria gram positive *Staphylococcus aureus* and gram negative *Escherichia coli.* The – NO_2 and – OCH_3 substituent groups effects in the Schiff base azomethine system [– CH=N] have been investigated. The Fourier transform infrared (FTIR) spectral analysis confirms a range of 1728 –1760 cm^{-1}, the formation of the azomethine system [-CH=N] in synthesized compounds. Besides, the potential of corrosion was investigated studied by electrochemical impedance studies (EIS), which indicated a high semicircle formed because of the high resistance of allowing the moving of electrons through the metal-electrolyte solution, besides acting as a mixed kind of inhibitor. 2,4-MMP has better inhibition behavior than 2,4-NMP. The morphology of mild steel surface was revealed by the scanning electron microscope (SEM). Thermodynamic investigation showed that two synthesized Schiff bases have Langmuir adsorption isotherms with physisorption and chemisorptions mechanisms. Quantum chemical calculations have been investigated by density functional theory (DFT). These studies concludes that 2,4-MMP has a better corrosion efficiency found as 86.1 % compared with the 2,4-NMP found as 84.2% since the electron donating ability of the substituents – OCH_3 to the electron rich azomethine system [-CH=N] group. Further synthesized compounds exhibits high activity against *Staphylococcus aureus* and *Escherichia coli* due to substituted groups.

(Received September 4, 2023; Accepted January 5, 2024)

Keywords: Schiff base, Mild steel, DFT, Impedance studies, Tafel plot, Antimicrobial activities

1. Introduction

The protection of iron materials against corrosion is receiving much attention, and mainly steel is sustainably used in neutral and alkaline media and acidic environments. The steel equipment is used for various purposes; hence, it can be recreated (or cleaned) using procedures such as descaling, pickling, etc., for this purpose using acidic solutions in the range of pH < 1. Sulfuric acid and hydrochloric acid are commonly used for steel surface treatment because of their lower cost, limited fumes, and non-corrosive natures [1]. When the process of recreation (or cleaning) of steel can be affected by using an acidic solution because corrosion happens, this corrosion process can be inhibited using some synthetic organic compounds. The inhibition efficiencies are mainly inherent in the structural and chemical properties of organic compounds. Nitrogenous compound inhibition efficiency against acidic media depends on the functional group array in the aromatic ring besides electronic structure also determines the inhibition efficiency of organic molecules [2].

* Corresponding author: mohanapriyachem@gmail.com
https://doi.org/10.15251/JOBM.2024.161.1

Recently, focused on the major corrosion inhibitor, Schiff base, because it contains an electron-rich azomethine (-C=N-) group. The corrosion inhibition efficacy was improved by recent researchers through Schiff bases with ligands containing N, S, O, and P atoms. Moreover, the azomethine group has the ability to attract mild steel surface and also favors the metal/solution interface effect hence causes extensive adverse corrosion properties. Hulya Keles et al. [3]. reported the synthesis of an imine group-containing 2-[(4-phenoxy-phenylimino) methyl]phenol Schiff base and their corrosion inhibition against mild steel in presence of 1.0 M HCl solution, then suggested electronegative groups and pi-electrons in conjugated double bonds and triple bonds act as excellent inhibitors, and hetero atoms such as N, O, and S influence attraction with metal surfaces, increasing inhibition efficiency. Chandrabhan verma et al. reported electron rich centre of azomethine system [–CH=N] inhibition efficiency with various substituents –OH, –OCH_3, –NH_2 and suggested the electron donating –OCH_3 group has good corrosion inhibition efficiency since their electron donating ability mean while halogen atom present electron withdrawing group favors the inhibition efficiency [4]. The Schiff base with two different ligands such as 4-((4-ethylphenyl)imino)methyl)phenol (4EMP) and (E)-4-(naphthalen-2-ylimino)methyl)phenol (4NMP) has been prepared which concludes 4EMP has higher efficiency of corrosion on mild steel in 1 M HCl due to the existence of donor atoms (N and O), many π bonds and an alkyl group that facilitate adsorption on mild steel, as reported by Elias E. Elemike et al [5]. Fahimeh et al. investigated that Schiff bases use corrosion inhibition in HCl/H_2SO_4 medium for mild steel and focused on the effect of functional groups and hetero atoms affecting corrosion protection performance and found the azomethine system [-CH=N] group in the structure of organic compound Schiff bases favors corrosion inhibition efficiency in an acidic medium using the potential anti-corrosive activity [6]. Abdellah Elyoussfi et al. reported that imidazopyridine derivatives exposed the groups such as -OH, -OCH_3 and -NO_2 substituents efficiency in Imidazo pyridines for corrosion efficiency in mild steel against 1 M HCl media and found this group forms a protecting film on the mild steel surface cause increases corrosion efficiency [7]. Walid Daoudi et al. investigates corrosion inhibition efficiency effect of substituents -NO_2 and -OH groups in the structure of imidazo pyridines Schiff compound presence of mild steel in acidic medium [8]. Sheheryar et al. reported that synthesize Schiff base and investigated antibacterial effect investigated. The (E)-2-(4-aminobut-1-enyl) 5-methyl benzamine and (E)-2-(((2-amino ethyl) imino)methyl) phenol Schiff base synthesized and effect of –OH and –NH_2 group on antibacterial activity in gram positive and gram negative bacteria [9]. Mohd Hussain et al. synthesized benzylidene derivative benzylidene-N^1-(2-bromo-3-phenylallylidene)-2-chlorobenzene-1,4-diamine.The synthesized compound under antimicrobial activity against gram positive and negative bacterial and fungal strains. It concludes electron withdrawing group present in aromatic ring show antimicrobial activity besides amino group shows significant corrosion activity [10].

In this research article, two Schiff base compounds synthesized with substituent – NO_2 and – OCH_3 are presented in 2-[(4-Nitrophenyl) Imino] Methyl Phenol (2,4 NMP) and 2-[4-MethoxyPhenyl) Imino] Methyl Phenol (2,4 MMP), respectively. Specifically, we introduced these substituents in the functional groups R-OH and -CH=N containing the above Schiff base compounds and investigated the corrosion inhibition potential of mild steel against acidic mediums of 1M HCl and 1M H_2SO_4. The 2,4-NMP and 2,4-MMP anti bacterial efficiency studied against gram positive *Staphylococcus aureus* and gram negative *Escherichia coli* respectively. Further structural parameter and corrosion inhibition potential were investigated with impedance studies (EIS), Quantum chemical calculations for HOMO and LUMO interactions, density functional theory (DFT), thermodynamic adsorption behavior on mild steel, and morphology.

2. Experimental

2.1. Chemicals and materials

p-nitroaniline [$C_6H_6N_2O_2$ (Assay 98%)], Salicylaldehyde [$C_7H_6O_2$ (98%)] p-anisidine $CH_3OC_6H_4NH_2$ [99%], HCl (37%), and H_2SO_4 (97%) chemicals obtained from Merck.Further distilled water used for prepare 1M HCl and 0.5 H_2SO_4 acidic solutions.

1.5 x 1.5.0 x 0.1 cm size of mild steel was used.

2.2. Characterization methods

FT-IR (Shimadzu-Prestige-21), Electrochemical measurements (CH1660C-electrochemical analyzer) and Surface morphology (Joel-JSM-6390). Quantum chemical parameter study was done using density functional theory using the Gaussian 09W operating system.

2.3. Synthesis procedure of 2-{[(4-Nitrophenyl)Imino]Methyl}Phenol

The p- nitroaniline and salicylaldehyde taken in 1:1 molar ratio followed refluxed 45° C for 6 hrs. Finally, poured into ice cold water grey colour crystal formed.

2.4. Synthesis procedure of 2-{[4-MethoxyPhenyl)Imino]Methyl}Phenol

The p-anisidine and Salicylaldehyde taken in 1:1 molar ratio furtehe refluxed 45° C for 6 hrs then poured into ice cold water grey color crystal separated.

The synthesized schiff base 2-{[(4-Nitrophenyl)Imino]Methyl}Phenol and 2-{[4-MethoxyPhenyl)Imino]Methyl}Phenol expressed name as 2,4-NMP and 2,4-MMP respectively [11].

3. Results and discussion

3.1. FT- IR analysis

2,4-NMP formation is confirmed by the FT-IR peak >C=N- at 1753 cm^{-1} since the carbonyl group of salicylaldehyde has disappeared, as well as the 2,4-MMP peak at 1728 cm^{-1}. These peaks confirmed the formation of the Schiff base group (CH=N). The FT-IR peak pattern and figures are given in Table 1 and Figure 1 respectively [12].

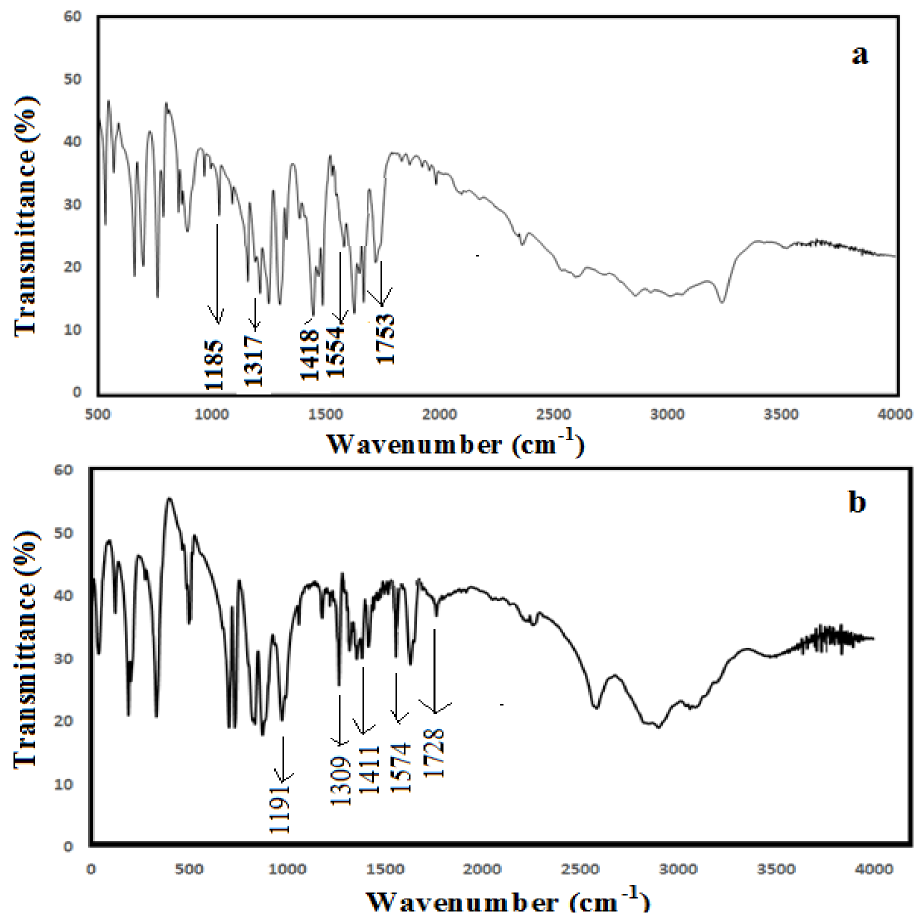


Fig. 1. FT-IR spectrum of (a) 2,4-NMP (b) 2,4 MMP schiff base compounds.

Table 1. FT-IR peak pattern of synthesized schiff base.

2,4-NMP		2,4 - MMP	
Peaks (cm^{-1})	**Assignments**	**Peaks (cm^{-1})**	**Assignments**
1753 cm^{-1}	>C=N-	1728 cm^{-1}	>C=N-
1295 and 1185	C-O symmetric stretching	1284 and 1191	C-O symmetric stretching
1317	OH deformation	1309	OH deformation
1418	C-H bending	1411	C-H plane bending
1554, 1520	C = C stretching	1574, 1511	C=C stretching

3.2. Crystal structure

The compound 2, 4-NMP has imino - phenolic ring and nitro-benzene ring with monoclinic structure shown in Figure 1. The non-planar with phenol ring contains a dihedral angle of 45.00° among a nitrobenzene ring. Besides, the nitro group makes an angle 35.27° with a nitro benzene ring. The C1-N1 bond length is 1.507 Å, which is resembled with usual C-N bond (1.47 Å). There is absence of small π….π ring attractions, however two extended C—H…π ring attractions through hydrogen to centroid length of 2.38 Å and 2.87 Å by way of the phenol and nitrobenzene ring respectively.

Meanwhile, structure of 2, 4-MMP is monoclinic with a dihedral angle of phenol 45.00° with the plane by anisole ring shown in Figure 2. The bond length of C=N is 1.507 Å. The bond torsion angle seems to be C1-C11-C12-C13 and C1-N1- C21- C26 showing 179.98 and 176.61 respectively the, the largest valve due to the steric effect of OCH3 group. There is absence of shortest π-π ring attractions. The phenol group interaction with a C-H--- π interaction distance is 2.39 and the anisole group shows 2.91 Å. The particulars of molecular arrangement are given in Figure 2 and 3 and structural refinements given in table 2 and 3 for synthesized Schiff bases [13, 14].

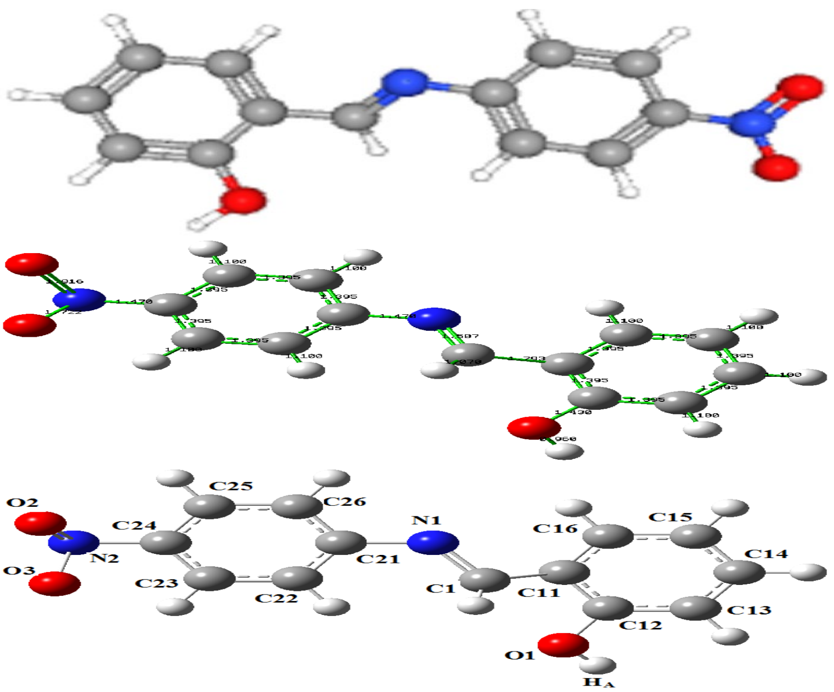


Fig. 2. The molecular structure of 2-[(4-Nitrophenyl)Imino]MethylPhenol (2,4-NMP).

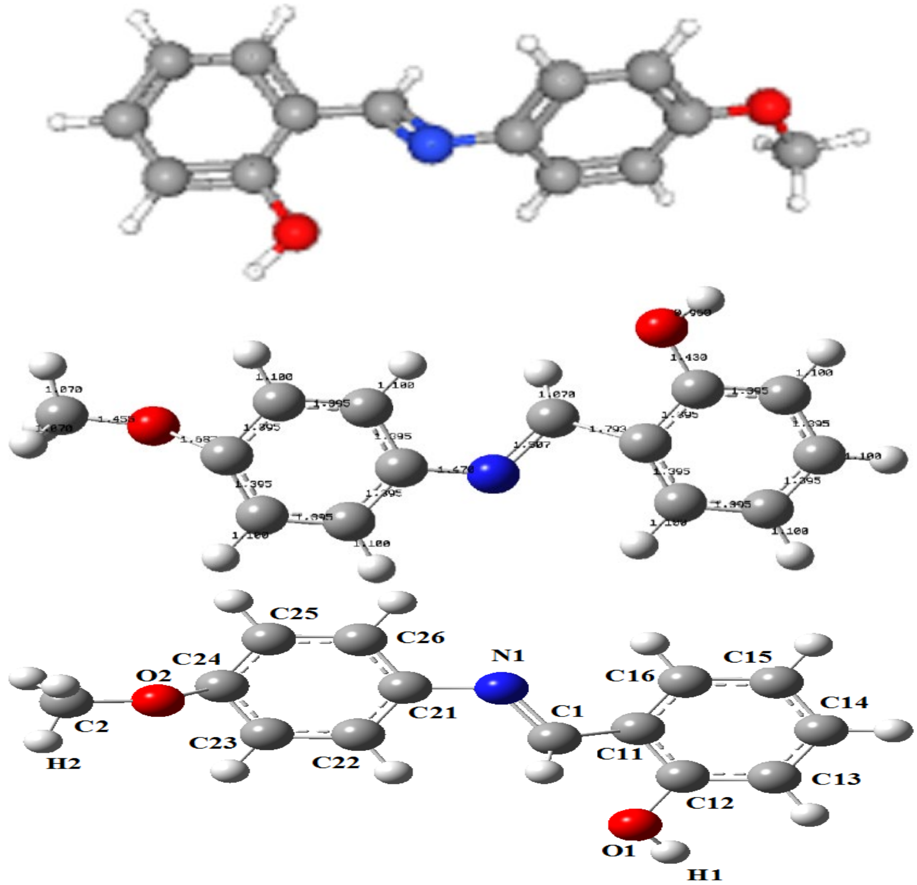


Fig. 3. The crystal structure 2-[4-MethoxyPhenyl)Imino] Methyl}Phenol.

Table 2. Crystal structural parameters of synthesized schiff base.

Compound	**2,4-NMP**	**2,4-MMP**
Formula	$C_{13}H_{10}N_2O_3$	$C_{14}H_{13}NO_2$
a (A°)	12.413	14.3587
b (A°)	5.744	6.8765
c (A°)	15.597	15.0779
α	90	90
β	97.69	97
γ	90	90
Cell volume (A^3)	1102	1268
Space group	P121/c1	P21/c
Crystal structure	Monoclinic	Monoclinic

Table 3. The significant bond length and bond angles of synthesized schiff base.

2,4- NMP				2,4- MMP			
Bond length		Dihedral angle		Bond length		Dihedral angle	
O1-C12	1.430	N1-C21-C26	119.99	C1-C11	1.793	N1-C1-C11	104.09
N2-C24	1.470	N1-C1-C11	104.09	C12-O1	1.430	C12-O1-H1	120.00
N1-C21	1.470	O1-C12-C13	120.00	C24-O2	1.687	C24-O2-C2	141.34
N1-C1	1.793	C23-C24-N2	119.99	C2-H2	1.070	O2-C2-H2	109.47
N2-O2	1.916	C24-N2-O3	100.11	O2-C2	1.450	O2-C24-C23	95.20
N2-O3	1.722	C24-N2-O2	106.00	N1-C1	1.507	N1-C21-C26	119.99
				N1-C21	1.400	N1-C1-C11	123.04

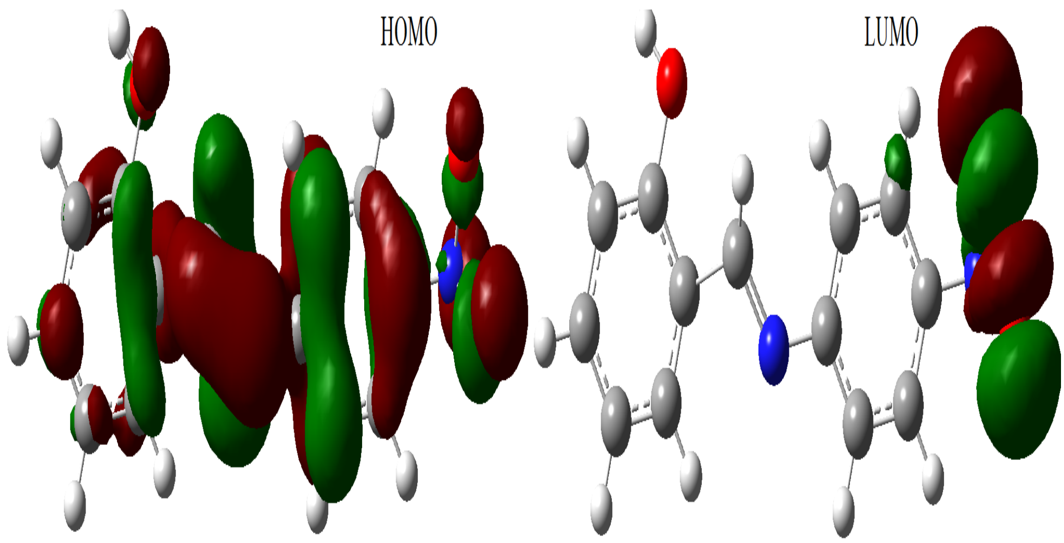
3.3. Quantum chemical analysis

Quantum chemical studies explained the attractions of compounds with mild steel surfaces through the orbital system. The electron movements and distribution within the molecules have been established by quantum chemical parameters. The DFT theory based on molecular orientation, structural properties, HOMO and LUMO which have been investigated DFT-B3LYP/6-31G+ level of theory. The properties depend on the existence of electronegative atoms, N and O atoms in the presence of π-electrons in the molecules as sources of adsorption by means of active centers. Figures 4 and 5 show HOMO and LUMO of 2,4-NMP and 2,4- MMP, respectively.

The synthesized Schiff bases 2, 4, NMP, and 2, 4, MMP have more corrosion resistance behavior due to,

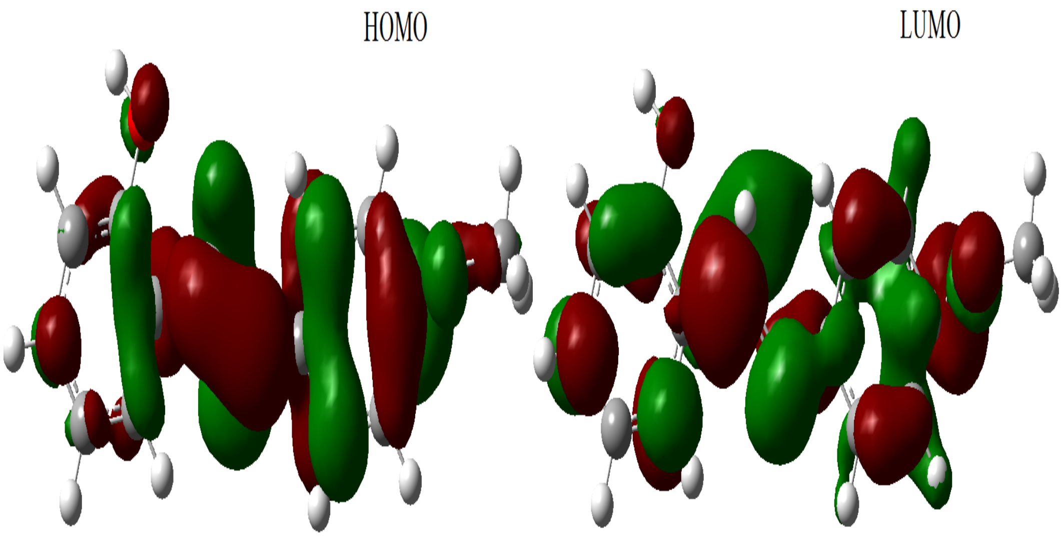
- The non bonding electrons in the nitrogen and oxygen atoms bonded with 3d-unoccupied orbital of the iron metal, forming a defending layer on the surface of the metal.
- The molecule's active site has the significant role that is making co-ordinate bond with unfilled‘d’ orbital of the iron.
- The metal atoms to the LUMO back donation of inhibitor compounds form a barrier that able to protect metal surfaces from corrosion.

Elias E. Elemike et al. reported Schiff bases of 4-((4-ethylphenyl) imino) methyl) phenol and (E)-4-((naphthalen-2-ylimino) methyl) phenol exposed quantum parameter energy gap found 3.767–4.178 eV and electron transfer of 0.763–0.864. These results are similar to the parameters we obtained. The other quantum parameter shows other parameters of hard molecules include a huge energy gap, while soft molecules shows small energy gap hence it facilitates electron transfer. The absolute softness (σ) of SB2 has a lower value compared to SB1; therefore, it has a more reactive compound. The inhibition efficiency was found to be 86.1% and 83.2% for 1.0M HCl and 0.5M H_2SO_4, correspondingly. This is because chemisorptions, as the distribution of a non bonding electrons between an electronegative atom and mild steel. The physisorption occurs because the electrons of aromatic systems absorb electrons from metal surfaces, creates hyper conjugation [15]. The quantum chemical assignments listed in Table 4.



(a) *(b)*

Fig. 4. (a) HOMO (b) LUMO of Schiff base 2,4 – NMP.



(a) *(b)*

Fig. 5. (a) HOMO (b) LUMO of Schiff base 2,4 –MMP.

Table 4. Quantum chemical assignments of synthesized Schiff base compounds.

S. No.	QC Parameters	2,4- NMP	2,4-MMP
1	E_{HOMO} (eV)	-9.522	-8.6
2	E_{LUMO}(eV)	-1.832	-0.847
3	ΔE (eV)	7.69	7.753
4	Ionization potential (I/eV)	9.522	8.6
5	Electron affinity (A/eV)	1.832	0.847
6	Hardness (η/ev)	3.845	3.8765
7	Softness (S/eV)	0.1300	0.1289
8	Electro negativity (χ)	5.677	4.7235
9	Electrophilicity (ω)	4.1909	2.8777
10	Fraction of electrons transferred (Δ N)	0.1720	0.2936
11	Dipole moment	5.3455	2.5918

3.4. Electrochemical impedance studies:

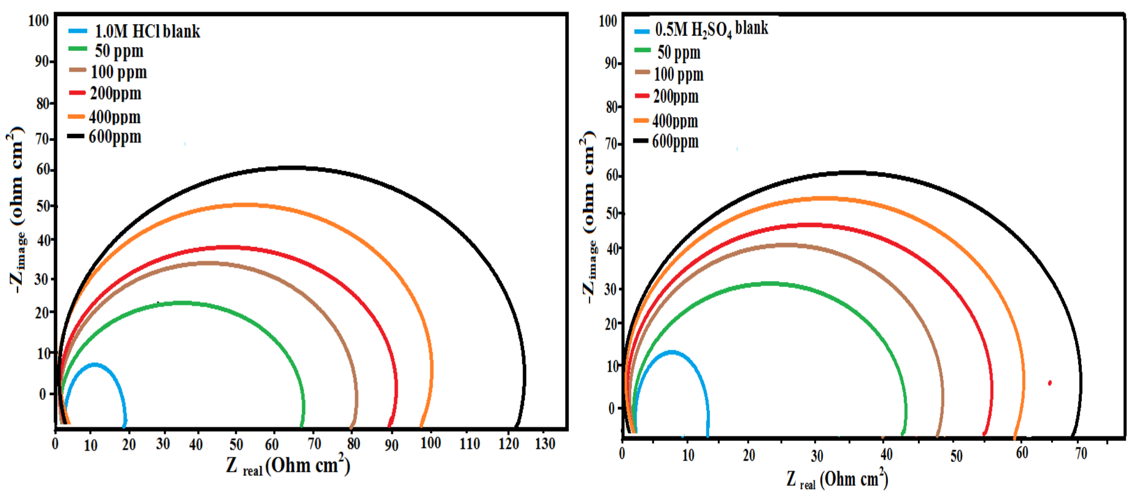
Electrochemical behavior of metal solution interface has been analyzed through impedance studies. Nyquist plot of MS immersed with 1M HCl and 1M H_2SO4 shown in figures 6 and 7 for 2,4-NMP and 2,4-MMP, respectively, then found impedance parameters such as charge transfer resistance (Rct), Phase shift (n) and inhibition effectiveness (%) attributed in tables 5 and 6 which was revealed that *resistance* values enlarged considerably at inhibitors concentrations high range. At 600 ppm concentrations of Schiff base 2,4 NMP and 2,4 MMP shows higher inhibition efficiency, which reflects defensive layer formation on mild steel surface[16]. Among, 2,4 MMP shows better corrosion inhibition efficiency, with 86.3% and 83.7% for 1M HCl and 0.5M H_2SO_4 respectively.

Table 5. Impedance parameter of MS in 2, 4 – NMP.

Medium	Schiff base concentration (ppm)	R_{ct} (Ohm cm^2)	n	C_{dl} (µF cm^{-2})	Efficiency of inhibitor (I.E%)
	Blank	19.10	0.9120	173	-
	50	68.70	0.9380	101	72.2
	100	79.90	0.9410	89	76.1
1.0 M HCl	200	90.10	0.9720	63	78.8
	400	96.40	0.9780	41	80.2
	600	120.90	0.9810	29	84.2
	Blank	12.5	0.909	207	-
	50	42.1	0.924	132	70.3
0.5 M H_2SO_4	100	48.3	0.965	104	74.1
	200	55.3	0.947	87	77.4
	400	58.9	0.951	69	78.8
	600	67.9	0.949	43	81.6

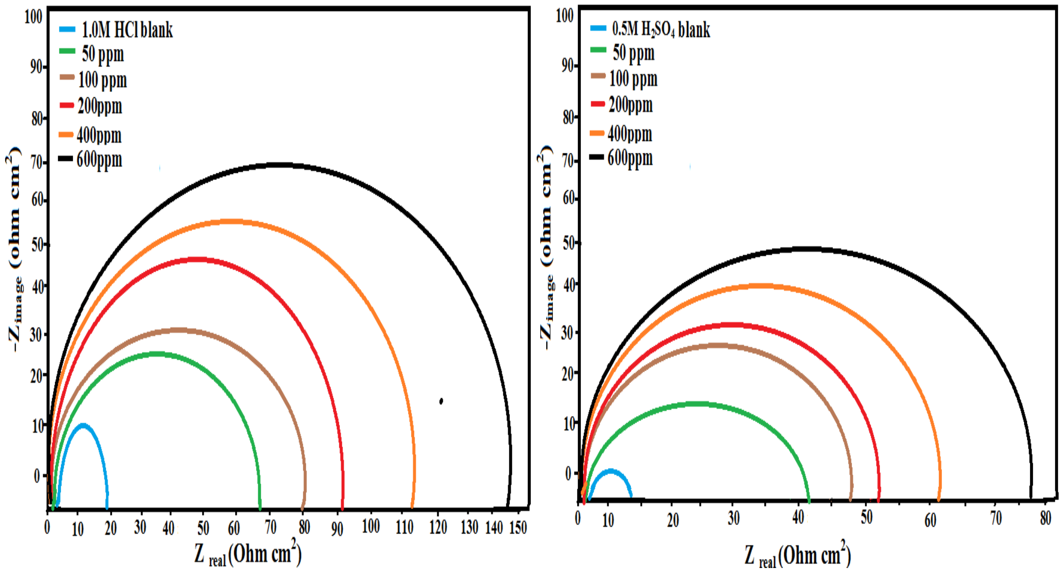
Table 6. Impedance parameter of MS in 2, 4 – MMP.

Medium	Concentration of the Schiff base (ppm)	R_{ct} (Ohm cm^2)	n	C_{dl} (µF cm^{-2})	Efficiency of inhibitor (I.E%)
	Blank	19.10	0.9120	173	-
	50	66.0	0.941	122	71.1
	100	79.9	0.933	94	75.6
1.0 M HCl	200	90.3	0.941	72	78.4
	400	111.4	0.962	51	82.5
	600	146.6	0.947	39	86.7
	Blank	12.5	0.909	207	-
	50	41.2	0.932	154	69.7
0.5 M H_2SO_4	100	47.5	0.939	116	73.7
	200	51.6	0.937	97	75.8
	400	61.3	0.955	75	79.6
	600	76.7	0.972	51	83.7



(a) *(b)*

Fig. 6. (a) Nyquist plot of 2, 4 NMP Schiff base - Mild steel immersed in (a) 1M HCl (b)H_2SO_4.



(a) *(b)*

Fig. 7. (a) Nyquist plot of 2,4 –MMP Schiff base - Mild steel immersed in (a)1M HCl (b)1M H_2SO_4.

3.5. Tafel plot

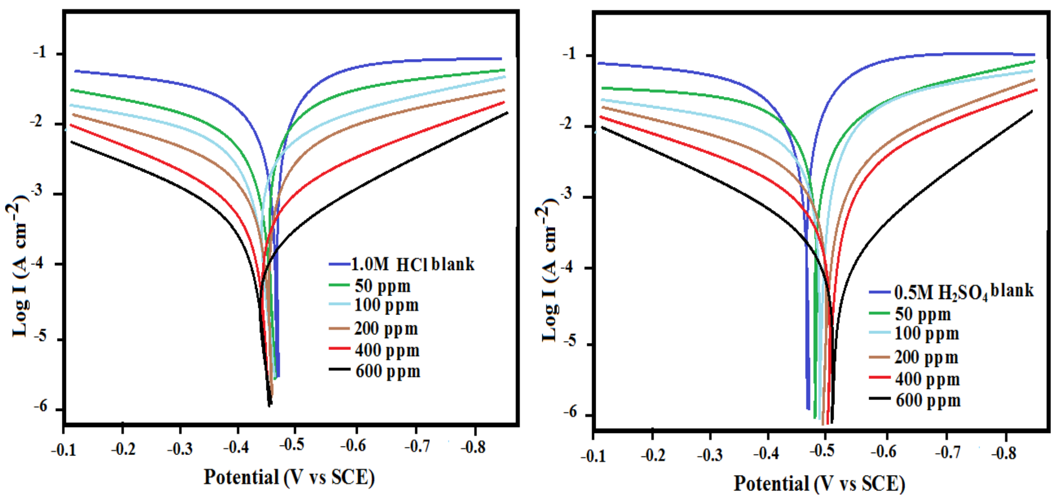
The anodic and cathodic polarization characteristics of mild steel in 1M HCl and 0.5M H_2SO_4 with a range of concentrations of inhibitor have been found using Tafel plot polarization measurements. The reaction of metal dissolution in the anode and hydrogen evolution in the cathode was considerably inhibited due to a mixed-type inhibitor. The increasing concentration of inhibitor corrosion current density (I_{corr}) decreased significantly for 2,4-NMP compared to 2,4-MMP. The significant decrease in I_{corr} and insignificant changes in E_{corr} values since protective film formed on mild steel surfaces without necessarily altering the reaction mechanism because corrosion efficiency increased for 2,4-MMP besides the mixed type of inhibitor [17]. The Tafel plots for 2,4-NMP and 2,4-MMP are shown in figures 8 and 9 for 2,4-NMP and 2,4-MMP, respectively, along with the polarization parameters given in tables 7 for 2,4-NMP and 8 for 2,4-MMP.

Table 7. Polarization parameter of MS in 2,4 NMP in acidic solutions.

Medium	Concentration of inhibitor (ppm)	E_{corr} (mV)	I_{corr} (mA cm^{-2})	β_c	β_a	Surface Coverage θ	Efficiency of inhibitor (I.E%)
1.0 M HCl	Blank	-450	1.17	257	110	-	-
	50	-432	0.333	251	111	0.7061	71.5
	100	-448	0.289	249	118	0.8375	75.3
	200	-460	0.256	397	156	0.8764	78.1
	400	-459	0.237	235	105	0.8819	79.7
	600	-466	0.193	176	71.2	0.9464	83.5
0.5 M H_2SO_4	Blank	-455	2.930	245	143.9	-	-
	50	-451	0.876	124	81.9	0.7598	70.1
	100	-448	0.771	138	69.3	0.8205	73.7
	200	-442	0.668	122	69.5	0.8743	77.2
	400	-453	0.630	130	75.9	0.8837	78.5
	600	-450	0.551	124	77.7	0.90	81.2

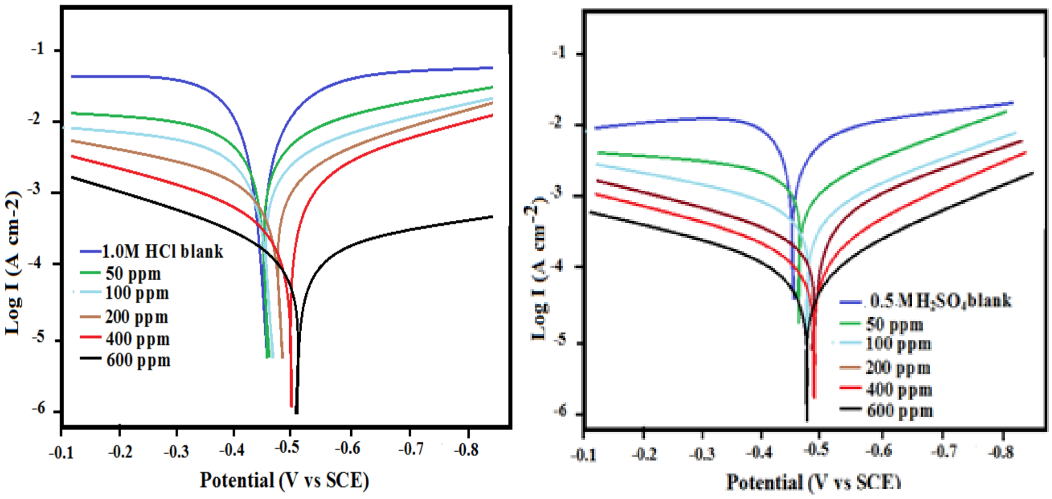
Table 8. Polarization parameter of MS in 2,4 – MMP in acidic solutions.

Medium	Concentration of inhibitor (ppm)	E_{corr} (mV)	I_{corr} (mA cm^{-2})	β_c	β_a	Surface Coverage (θ)	Efficiency of inhibitor (I.E%)
1.0 M HCl	Blank	-450	1.17	257	110	-	-
	50	-432	0.427	251	111	0.7061	70.8
	100	-448	0.373	249	118	0.8375	75.1
	200	-460	0.334	397	156	0.8764	77.9
	400	-459	0.306	235	105	0.8819	81.8
	600	-466	0.289	176	71.2	0.9464	86.1
0.5 M H_2SO_4	Blank	-455	2.930	245	143.9	-	-
	50	-451	1.163	124	81.9	0.7598	69.1
	100	-448	1.005	138	69.3	0.8205	73.2
	200	-442	0.888	122	69.5	0.8743	75.4
	400	-453	0.809	130	75.9	0.8837	78.8
	600	-450	0.768	124	77.7	0.90	83.2



(a) *(b)*

Fig. 8. (a) Tafel plot of 2,4 –NMP (a)1M HCl (b)1M H_2SO_4.



(a) *(b)*

Fig. 9. (a) Tafel plot of 2,4 –MMP in (a)1M HCl (b)1M H_2SO4.

3.6. Adsorption studies

The interface of metal/solution of both water and inhibitor molecules interaction information is established by the adsorption isotherm. It shows the reliable mechanism by synthesized organic compounds inhibit metal dissolution through adsorption on the surface of metal.

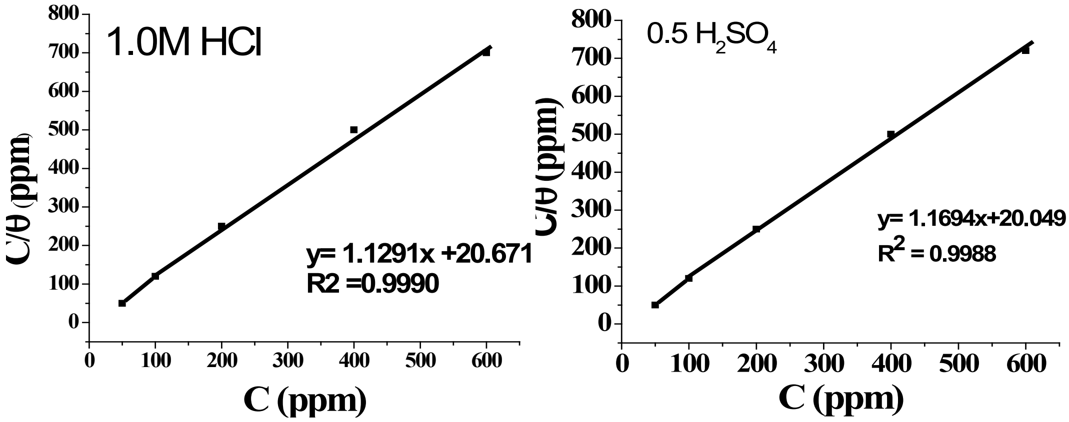
The Langmuir isotherm,

$$C_{inh}/\theta = C_{inh} + 1/K_{ads}$$

where,
θ = degree of surface coverage; K_{ads} equilibrium constant of the adsorption/desorption process; and C_{inh} *concentration* of the inhibitor. The plot C_{inh} vs. C_{inh}/θ was used to found K_{ads}. It is applied for found the standard free energy denoted:

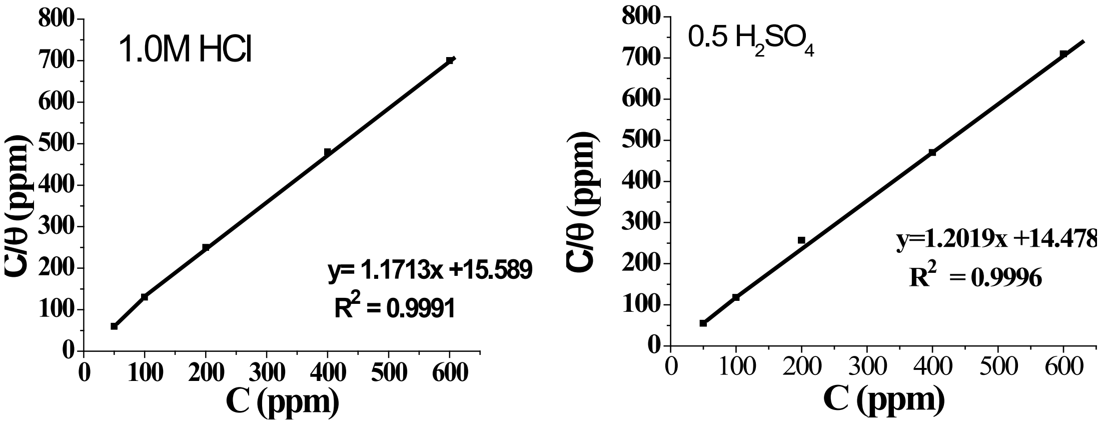
$$K_{ads} = 1/55.5 \exp\left(-\mathbf{\Delta G^0_{ads}}/RT\right)$$

where, ΔG_{ads} – standard free energy of adsorption, *R*- Gas constant, and *T -Absolute* temperature besides 55.5 is the concentration of water (mol L^{-1}). The Langmuir's adsorption isotherm plots are shown in figures 10 and 11 for 2,4-NMP and 2,4-MMP, respectively. The values of 2, 4-NMP in 1M HCl and 0.5M H_2SO_4 was -27.89 and -28.08, respectively. The G_{ads} values for 2,4-NMP lie between -20 $kJmol^{-1}$ and -40 $kJmol^{-1}$. It indicates that 2,4-NMP and 2,4-MMP molecules attract on surfaces of the mild steel in acidic solutions by means of physical and chemical adsorption means. Besides 2, 4-MMP Schiff base, the values of 1M HCl and H_2SO_4 were found -27.18 $kJmol^{-1}$ and -27.25 $kJmol^{-1}$ respectively, since physical-chemical absorption [18, 19].



(a) *(b)*

Fig. 10. Langmuir's isotherm of (a)1M HCl (b)0.5M H_2SO4 for 2,4 –MMP



(a) *(b)*

Fig. 11. (a) Langmuir's isotherm of (a) 1M HCl (b) 0.5M H_2SO4 for 2,4 –NMP.

3.7. SEM analysis

The surface investigation studied by SEM morphology of mild steel with Schiff base and without Schiff base were shown in Figures 12 and 13 for 2, 4 NMP and 2, 4 MMP respectively. The MS present in the 1M HCl and 0.5 H_2SO_4 solution shows a highly damaged and rough surface. After being immersed in the inhibitor solutions, a passive film with layers appeared the mild steel surface [20].

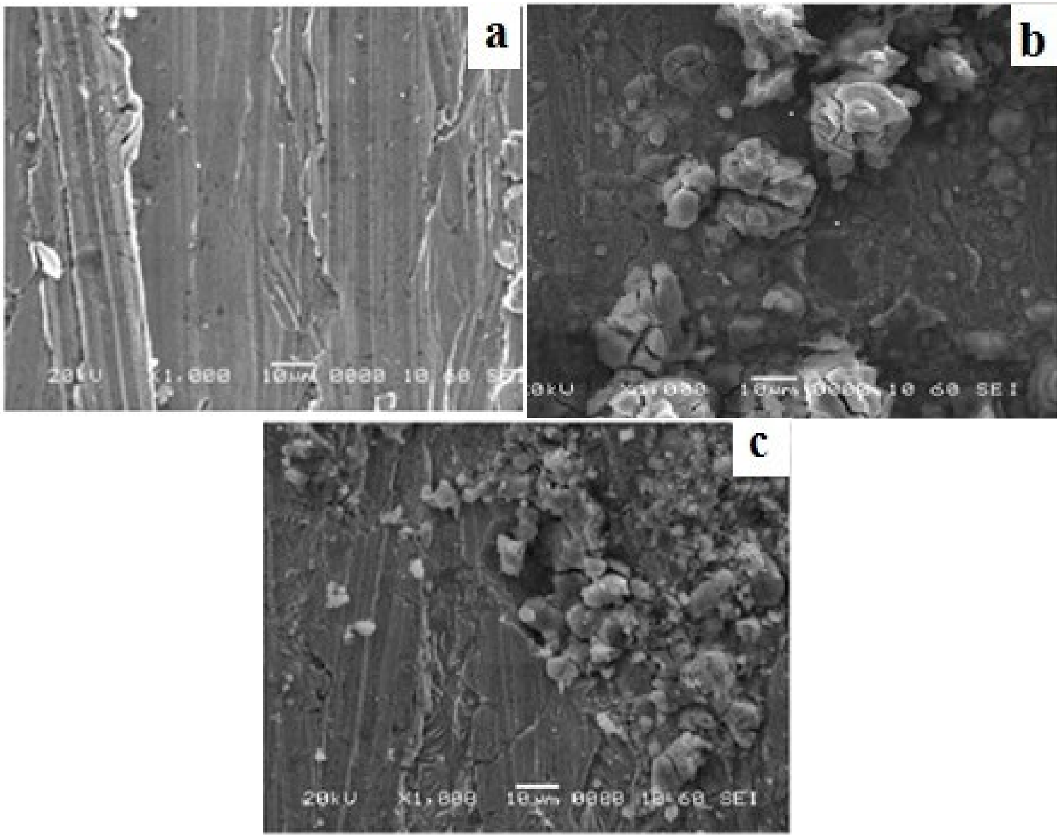


Fig. 12. (a) SEM morphology of mild steel in (a) 0.1M HCl (b) 2,4 –NMP (c) 2,4-MMP

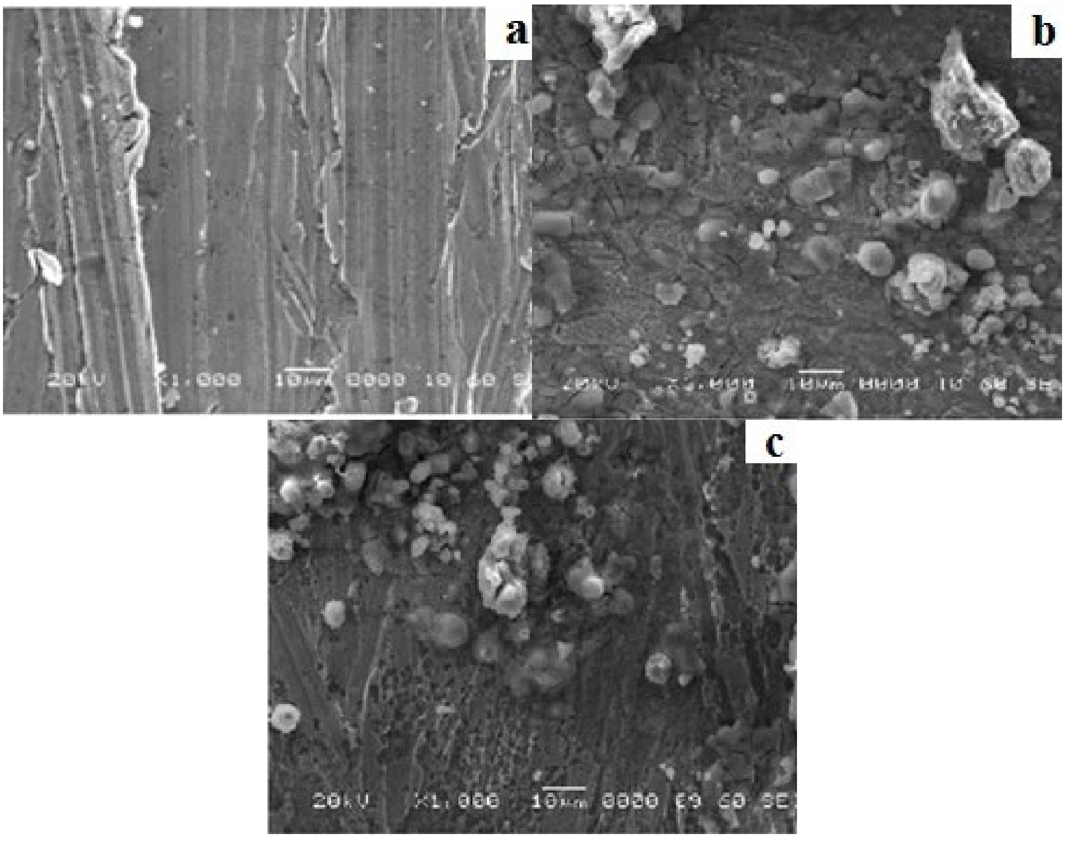


Fig. 13. (a) SEM morphology of MS in (a) 0.5M H_2SO_4 (b) 2, 4 –NMP (c) 2, 4 –MMP

3.8. Antimicrobial activity

The Schiff base 2,4-NMP and 2,4-MMP were used to investigate microbial activity of gram positive Staphylococcus aureus and gram negative Escherichia coli bacteria respectively, which has been shown in Figure 14. The synthesized Schiff base has aromatic rings, hetero atoms N, O atom act as the reason for enhanced antimicrobial activity of Schiff base. The occurrence of nitro group ($-NO_2$) and methoxy ($-OCH_3$) groups prolonged the antimicrobial activity of the synthesized Schiff base [21]. It can be established through the data of biological studies of synthesized Schiff bases 2,4-NMP and 2,4-MMP. The microbial activities are shown in Table 9.

Table 9. Zone of inhibition synthesized 2,4 NMP and 2,4-MMP.

Schiff base	Test Organism	Zone inhibition (mm)				
		Blank	25µL	50µL	75µL	100µL
2,4 - NMP	*Staphylococcus aureus*	5	10	12	13	15
2,4 - MMP	*E. coli*	1	8	12	15	18

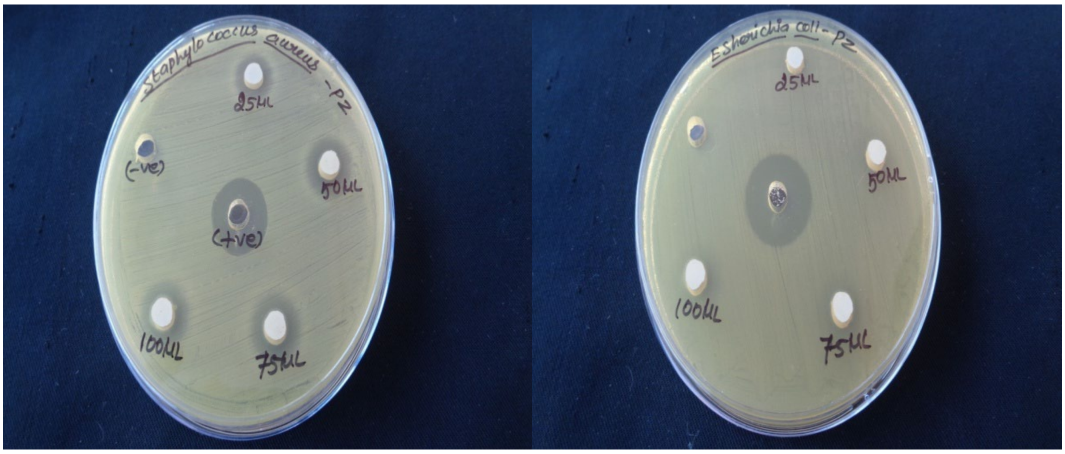


Fig. 14. Antimicrobial activity of synthesized Schiff bases.

4. Conclusion

The Schiff base compounds 2, 4 -NMP and 2, 4 -MMP were synthesized and investigated through several spectroscopic techniques. The theoretical calculation investigated B3LYP/6-31G+ (d, p) theory. It concludes that 2, 4 -MMP attributed to better corrosion inhibition efficiency than 2, 4 -NMP because of HOMO and LUMO interaction efficiency. The investigation is summarized as:

Polarization EIS investigations determine that mixed-type inhibitors with the high concentration of 1M HCl and 0.5 H_2SO_4 in mild steel. Besides, the semicircle increased for high concentrations of Schiff base since it increased charge transfer resistance. Tafel plots show anodic and cathodic mixed-type inhibitors of polarization behavior.

Schiff bases 2,4-NMP and 2,4-MMP obey Langmuir's isotherm with both physisorption and chemisorption mechanisms.

The excellent corrosion inhibition performance studies of 2,4-MMP on mild steel showed that N and O atoms with few π bonds in the aromatic system facilitated adsorption and increased the electron clouds in the azomethine system [-CH=N].The significant antimicrobial activity observed that the zone of inhibition obtained 15mm and 18mm for Schiff base 2,4-NMP and 2,4-MMP respectively at higher concentration of dosage 100μL.

These results were predicts these synthesized simple compounds useful for better inhibitor and antimicrobial activity than higher structural molecules.

Acknowledgements

The authors are grateful to the Principal, Erode Arts and Science College (Autonomous), and Head PG and Research Department of Chemistry, Erode Arts and Science College (Autonomous), Erode, Tamil Nadu, India. Provision of research facilities and the laboratory's experimental work contribution Also, the first author thanks his guide for his moral support in completing this work.

References

[1] K. P. Bryliakov, E. P. Talsi, Journal of molecular catalyst A, Vol. **264**, no.1-2, pp. 280-287, 2007; https://doi.org/10.1016/j.molcata.2006.09.038

[2] J. D. Talati, M. N. Desai, N. K. Shah, Material Chemistry and Physics vol. **93**, no.1, pp.54-64, 2005; https://doi.org/10.1016/j.matchemphys.2005.02.004

[3] Hulya Keles, Materials Chemistry and Physics, vol. **130**, no.3, pp. 1317-1324, 2011; https://doi.org/10.1016/j.matchemphys.2011.09.022

[4] Chandrabhan Verma, M. A. Quraishi, Coordination Chemistry Reviews vol. 446, no.214105, 1-22, 2021; https://doi.org/10.1016/j.ccr.2021.214105

[5] Elias E. Elemike, Henry U. Nwankwo, Damian C. Onwudiwe, Eric C. Hosten, Journal of Molecular Structure vol. 1136, pp.253-262, 2017; https://doi.org/10.1016/j.molstruc.2017.01.085

[6] Fahimeh Afshari, Erfan Rezvani Ghomi, Mohammad Dinari, Seeram Ramakrishna, Chemistry Select, vol.8, no.9, pp.1-31, 2003; https://doi.org/10.1002/slct.202203231.

[7] Abdellah Elyoussfi, Issam Azghay, Said Dadou, Walid Daoudi, M'hamed Ahari, Hassan Amhamdi, Nourededine Benchat, Abdelmalik El Aatiaoui, Amin Salhi, Ali Dafali, Journal of Molecular Structure vol. 1291, 2023; https://doi.org/10.1016/j.molstruc.2023.136025.

[8] Abdellah Elyoussfi, Walid Daoudi, Amin Salhi, Issam Azghay, M'hamed Ahari, Hassan Amhamdi, Noureddine Benchat, Ali Dafali, Elaatiaoui Abdelmalik, Journal of Applied Electro Chemistry vol.**53**, 2023; https://doi.org/10.1007/s10800-023-01917-9

[9] Sheheryar, Mohib Ullah Shah, International Journal of Drug Development and Research, vol.14,no.10, pp.1-4, 2022; https://doi.org/10.36648/0975-9344.22.14.1001

[10] Mohd Hussain, Suchitra Yadav, Shweta Yadav, Anuradha Sharma, Azaz Khan, Rani Mansuri, Mahesh Kumar, Journal of Pharmaceutical Negative Results, vol.13,no.10, pp.6019-6028, 2022

[11] Tuncay Tunc¸ Musa Sarı, Murat Sadıkoglu, Orhan Buyukgungor, Journal of Chemical Crystallography, vol. **39**, no.9, pp.672-676, 2009; https://doi.org/10.1007/s10870-009-9556-6

[12] Y. Stiadi, Rahmayeni, L. Rahmawati, M. Efdi, H. Aziz, Emriadi. Rasayan Journal of Chemistry, vol.**13**, no.1, pp.230-239, 2020; http://dx.doi.org/10.31788/RJC.2020.1315325

[13] T. Doleck, J. Attard, F. R. Fronczek, A. Moskun, R. Isovitsch, Inorganica Chimica Acta,, vol. **362**, no.10, pp.3872-3876, 2009; https://doi.org/10.1016/j.ica.2009.04.034

[14] M. S. Alam, D. Lee, Spectrochimca Acta A: Molecular and biomolecular spectroscopy, vol. **145**, pp.563-574, 2015; https://doi.org/10.1016/j.saa.2015.03.071

[15] K. F. Khaled, Electrochimica Acta, vol.**53**, no.9, pp. 3484-3492, 2008; https://doi.org/10.1016/j.electacta.2007.12.030
[16] P. M. Dasami, K. Parameswari, S. Chitra, Measurement, vol.69,no.195, pp.195 -201, 2015; https://doi.org/10.1016/j.measurement.2015.03.025
[17] C. Verma, M. A. Quraishi, L.O. Olasunkanmi, E. E. Ebenso, RSC Advances, vol. 5, no.104, pp. 85417-85430, 2015; https://doi.org/10.1039/C5RA16982H
[18] T. Mohanapriya, P. E. Kumar, International Journal of Innovative Research in Science, Engineering and Technology, vol. 5, no.10, pp.18706-18721, 2016; https://doi.org/10.15680/IJIRSET.2016.0510124
[19] Tarik Attar, Abbes Benchadli, Tayeb Mellal, Boumediene Dali Youcef, Esma Choukchou-Braham, Malaysian Journal of Chemistry, vol. 23, no.1, pp.60-69, 2021.
[20] Amit Kumar Nunach, Gita Rani, Rachna Ahlawat, Asian Journal of Chemistry, vol 35, no.8, pp.1810-1818, (2023); https://doi.org/10.14233/ajchem.2023.27966
[21] M. A. Ashraf, M. J. Maah, I. Yusoff, International Journal of Environmental Science & Technology, vol.8, no. 2, pp.401-416, 2011; https://doi.org/10.1007/BF03326227