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Effect of structure on the anti-corrosive properties of starting organic compounds and the produced amine epoxy adducts on mild steel in 0.1M HCl: An experimental and theoretical study

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ABSTRACT: Studies were carried out to evaluate the structural effects of four inhibitors (Mono ethanolamine (MEA), phenyl glycidyl ether (PGE), N – (2- hydroxy – 3- phenoxy propyl) ethanolamine (NHPE) and N, N' – (-2 hydroxy – 3 – phenoxy propyl) ethanolamine (N N' HPE) in inhibiting the corrosion of mild steel in 0.1M HCl. Appropriate analytical procedures and instrumentation such as the use of Fourier transform infrared (FTIR) spectrophotometer were employed in the analysis of the structures of the inhibitors.

Quantum chemical modeling calculation was employed to better understand the variation in the inhibition efficiencies of the studied inhibitors.

After eight weeks of immersing the mild steel sheets in 0.1M HCl with each of the four studied inhibitors, the mean percentage weight loss of the mild steel were 17.74, 30.13, 5.39 and 1.08% for MEA, PGE, NHPE and NN^1HPE respectively. The FTIR analysis of the structure of the inhibitors shows that the presence of functional groups such as –OH, -NH, Ar—C = C – and $–OCH_3$ significantly helped to increase the inhibition efficiencies of NHPE and NN' HPE respectively.

From the weight loss experiment, it was observed that the inhibition efficiencies of the four studied inhibitors on the mild steel in the acidic media decreased in the following order: $N N^1HPE$ > NHPE > MEA > PGE which was further confirmed by the FTIR analysis.

The lower values of parameters such as E_{LUMO}, energy gap, ionization potential, global hardness and total energy and as well as the higher valves of parameters such as E_{HOMO}, dipole moment, electro affinity, electro negativity, chemical softness, total surface area and polarizability, obtained for NHPE and NN^1HPE respectively greatly increased the adsorption and donation of their electrons to the metal substrate surface thus were able to more efficiently inhibit the rapid corrosion of the mild steel in the acidic media than the two other studied inhibitors (MEA and PGE).

KEYWORDS: Corrosion, Inhibitors, Mild steel, Inhibition efficiency and Quantum chemical parameters.

1 INTRODUCTION

Mild steel is an important metal regarding its wide applications in various mechanical and structural purposes in the industry. It is the most common form of steel because its price is relatively low while it provides material properties that are acceptable for many applications [1]. It is widely used in engineering fabrications like building bridges, industrial complex, houses, steam engine parts and automobiles. According to [2] the challenge with mild steel is that it has low corrosion resistance especially in acidic environments. Hence, industrial processes such as acid-cleaning, pickling, descaling and drilling operations in oil and gas exploration which uses extensive acid solutions in these environments exposes the surfaces of metals such as iron and steel to corrosion. The life span of metallic materials is unfortunately cut short by corrosion as a result of chemical and electrochemical reaction with corrosive environments [3]. Metallic corrosion is a costly problem. According to [4], the annual worldwide cost of corrosion is over $2.5 trillion USD, which constitutes about 4.2% of the world's gross domestic product. In India for instance, the annual cost of corrosion is over 5, 000, 000 million Indian rupees (i.e. about $100 billion USD), while in Africa, the direct cost of corrosion is estimated to be around $61.9 billion USD [5]. Corrosion is defined as the deterioration of a substance or its properties due to the interaction between the substance and its environment [6]. The tendency of a metal to corrode depends on grain structure of the metal, its composition as formed during alloying, or the temperature for the deformation of a single metal surface developed during fabrication. Factors that cause corrosion includes reactivity of metal, presence of impurities, presence of air, moisture, gases like sulphur IV oxide and carbon IV oxide and presence of electrolytes [7]. Corrosion returns a metal to its combined state in chemical compounds that are similar or even identical to the minerals from which the metals were extracted. The protection of materials especially steel structures from corrosion is achieved by basically two methods namely; cathodic protection and the use of corrosion inhibitors. Amongst these methods, corrosion inhibition is the most economical, practical and convenient technique for controlling the corrosion of metal in aqueous environments [8]. Corrosion inhibitors control the metal dissolution as well as the acid consumption. Inhibitors are adsorbed on the metal surface, forming a protective barrier and interact with anodic or/and cathodic reaction sites to decrease the oxidation or/and reduction of corrosion reactions [9]. The use of many inorganic inhibitors particularly those containing phosphate, chromate and other heavy metals like lead, nickel, antimony and arsenic is now being gradually restricted or banned by various environmental regulations because of their toxicity and difficulties faced in their disposal especially in the marine industry, where aquatic life is threatened [10]. The use of organic compounds for corrosion inhibition of metals has assumed great significance due to their efficient ability to prevent corrosion in various corrosive environments [11]. The utilization of organic inhibitors is a foremost corrosion prevention technique and it is often considered as the first line of defense against the corrosion of metals in corrosive media. This is also reflected in the wise use of organic corrosion inhibitors in the formulation of cleaning solutions for industrial applications, as primary components in pretreatment compositions and oil-well acidification [4]. Literature reports revealed that many organic compounds used as corrosion inhibitors are heterocyclic compounds that contains polar functional groups such as –OH, $-OCH_3$, - Cl, $-NO_2$, - CN, - C ≡ N -, - CH_3 and – NH_2, as well as unsaturated (double and triple) bonds that can serve as adsorption centers using the lone pairs or л electrons [12]. These heterocyclic and unsaturated compounds adsorb on metallic surfaces through their active centers. The adsorbed inhibitor molecules shield the metal surface from direct attack by corrosive ions and the organic compound is said to inhibit metallic corrosion. Adsorption of most organic molecules, especially those that contain hetero atoms is usually chemisorptioned, which is often preceded by electrostatic interactions between the inhibitor molecules and metal substrate [4]. The adsorption tendency of inhibitor molecules depends on a number of molecular properties, including steric factors, electron density and donor atoms (or groups), planarity, aromaticity and л – orbital characters of the active adsorption sites. According to [13] adsorption of organic hetero molecules also depends on the possible interaction of p-orbital's of the donor atoms of the inhibitors with the d-orbital's of the metals. The inhibition efficiency and nature of adsorption also depends on the molecular size of the inhibitor molecules [14]. An inhibitor molecule with large molecular area usually provides wider protective coverage for the metallic substrate compared to similar molecule with smaller molecular size. Quantum chemical methods have undoubtedly played a significant part in the better understanding of these factors [14]. Several studies have reported the effectiveness of organic compounds such as amines, carboxylic acids and hetero cyclic compounds in inhibiting the corrosion of mild steel in corrosive aqueous media [15]. Amines have been extensively used as organic inhibitors because of their good water solubility, low molecular weight and its high nucleophilic and basic character [16]. According to [13] the inhibiting properties of amines are linked mainly to the capability of the amino groups to adsorb on metal surfaces by sharing their unshared electron pair on the nitrogen atom with the metal substrate thereby covering the surface. Also, amino groups are capable of displacing water molecules at the metal surface, and thus forming a hydrophilic film which protects against corrosion. Nitrogen containing compounds generally exhibit good inhibitive effect due to their high basicity as a result of lone pair of electrons on N – atoms [4]. Quantum chemical parameters such as highest occupied molecular orbital energy, lowest unoccupied molecular orbital energy, dipole moments, electronegativity, polarizability and surface area etc., among others have been used theoretically to understand the inhibition efficiencies of organic compounds such as amines in aqueous media. Aqueous solutions of acids are among the most corrosive media. Amongst the acid solutions, hydrochloric acid is one of the most widely used agents. Studies was therefore carried out to evaluate the effect of structure of mono ethanolamine, phenyl glycidyl ether, N – (- 2 hydroxy – 3 – phenoxy propyl) ethanolamine and N, N' Bis - (-2 hydroxyl – 3 – phenoxy propyl) ethanolamine on their anti corrosive properties on mild steel in 0.1M HCl.

2 MATERIALS AND METHODS

2.1 RAW MATERIALS

Mono ethanolamine (MEA), phenyl glycidyl ether (PGE) and ethanol were of analytical grade and obtained from Sigma Aldrich, UK.

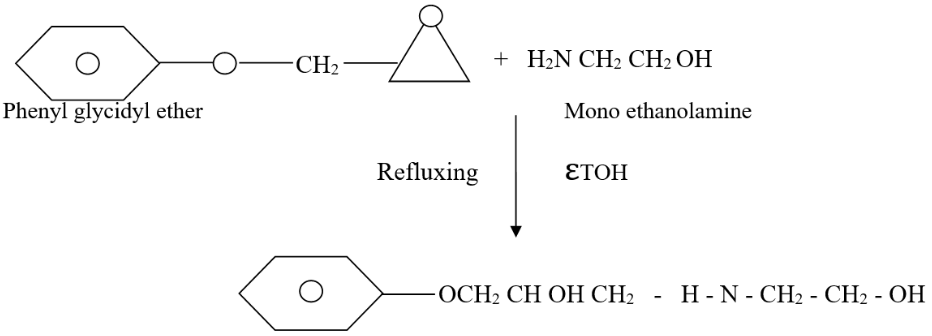
Mild steel was sourced locally while concentrated hydrochloric acid was obtained from Merck laboratories, India.

Preparation of N – (- 2 hydroxy – 3 – phenoxy propyl) ethanolamine (NHPE) and N, N' Bis- (-2 hydroxy – 3 – phenoxy propyl) ethanolamine (NN^{1}HPE)

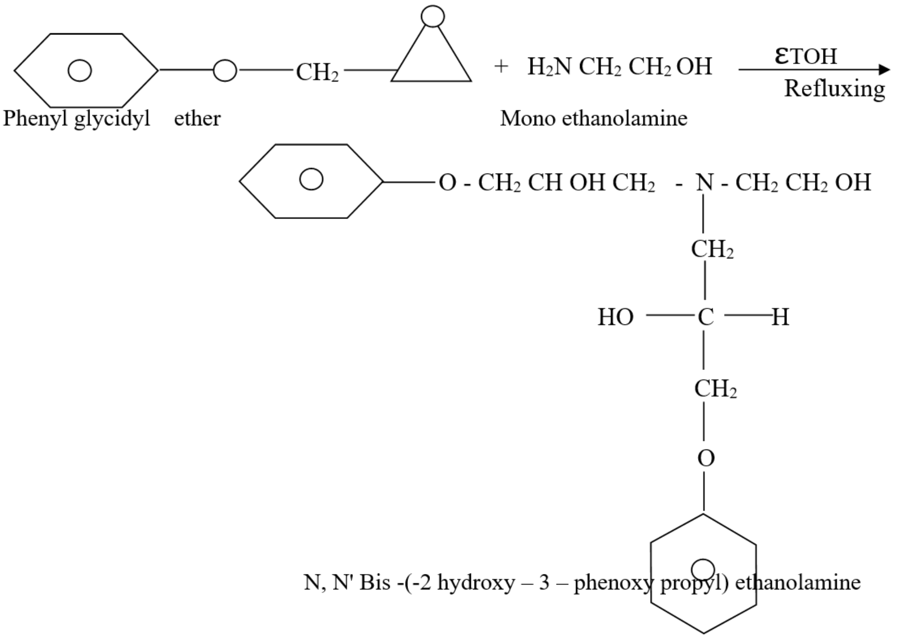
N – (- 2 hydroxy – 3 – phenoxy propyl) ethanolamine (NHPE) was prepared by mixing 50ml of 0.167 molar solutions of phenyl glycidyl ether and mono ethanolamine in a 500ml conical flask. About 100ml of ethanol was added into the mixture and heated to 100℃ under reflux for 12 hours. After cooling, the solid product was filtered and recrystallized to get the adduct.

The preparation of N, N' Bis- (-2 hydroxyl – 3 – phenoxy propyl) ethanolamine (NN'HPE) followed the procedure adopted in the preparation of NHPE, however this time around, 100ml of 0.334 molar solution of phenyl glycidyl ether and 0.167 molar solution of mono ethanolamine were used.

The equation of the synthesis is as follows:



N – (- 2 hydroxy – 3 – phenoxy propyl) ethanolamine



N, N' Bis -(-2 hydroxy – 3 – phenoxy propyl) ethanolamine

2.2 SOLUTIONS

M Solution Of Conc. Hcl Was Prepared With Distilled Water Following Standard Analytical Guide Lines. The Molar Concentration Of The Raw Materials, PGE And MGA And The Products (Adducts), NHPE And NN’HPE Used For The Corrosion Inhibition Was 0.8mol/Dm3.

2.3 CORROSION INHIBITION TESTING

The corrosion inhibition efficiencies of the raw material chemicals and the product amines on the mild steel in 0.1M HCl was carried out in accordance with the procedures of [17].

2.4 FTIR ANALYSIS

The chemical structures of phenyl glycidyl ether (PGE), mono ethanolamine (MEA), N – (- 2 hydroxy – 3 – phenoxy propyl) ethanolamine (NHPE) and N, N' Bis - (-2 hydroxy – 3 – phenoxy propyl) ethanolamine (NN’HPE) were identified using Fourier Transform Infra red (FTIR) Spectroscopy, Nicolet Avatar 380.The FTIR analysis of the cured Inhibitors were carried out by preparing the pellets with potassium bromide (KBr). The inhibitors concentrations were maintained in the KBr pellets. The spectra recorded on the Nicolet Avatar 380 spectrophotometer in the 700 – 4000cm^{-1} wavelength range.

2.5 QUANTUM CHEMICAL STUDY

The molecular structures of the raw material and product inhibitors were optimized using Austin Model 1 (AM 1) with hyper Chem quantum chemistry software as described by [14].

The quantum chemical parameters calculated include, energy of the highest occupied molecular orbital, energy of the lowest unoccupied molecular orbital, dipole moment, polarizability, electron affinity, ionization/potential, global hardness, chemical softness, total energy, total surface area, electronegativity and energy gap.

3 RESULTS AND DISCUSSION

Table 1. Mean percentage weight loss of mild steel after eight weeks of immersion in dilute HCl with the respectively studied inhibitors

Inhibitor in dilute HCl	Initial weight of mild steel	Final weight of mild steel	Percentage % weight loss
MEA	120	98.71	17.74
PGE	120	83.85	30.13
NHPE	120	113.53	5.39
NN^{1}HPE	120	118.71	1.08

Table 1 shows the inhibition efficiencies of the starting materials (MEA and PGE) and the products (NHPE and NN^{1}HPE) on mild steel immersed in 0.1M HCL for eight weeks.

Mono ethanolamine, phenyl glycidyl ether, N – (- 2 hydroxy – 3 – phenoxy propyl) ethanolamine and N, N' Bis - (-2 hydroxy – 3 – phenoxy propyl) ethanolamine gave mean percentage weight losses for mild steel after eight weeks in the acidic media to be 17.74, 30.13, 5.39 and 1.08% respectively.

Result of Table 1 indicates that the four studied inhibitors produced mean percentage weight loss for the mild steel in the acidic media in the following decreasing order: PGE > MEA > NHPE > NN'HPE. The table further shows that NN'HPE most inhibited the corrosion of mild steel in the acid solution (0.1M HCl) while PGE least inhibited it.

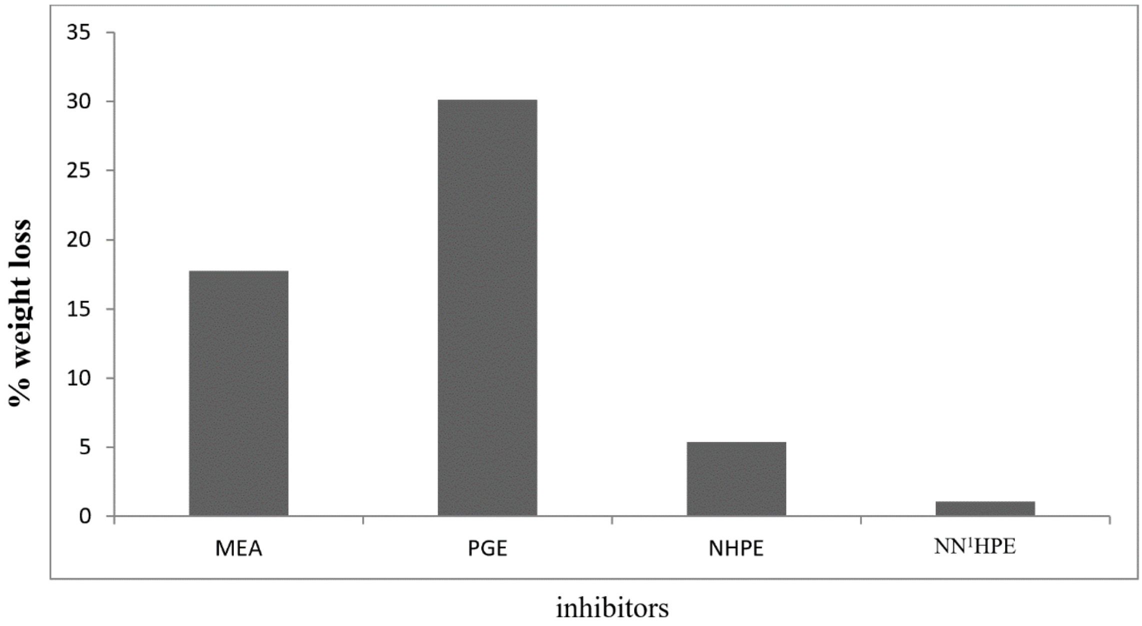


Fig. 1. Bar chart representation of the mean percentage weight loss for the mild steel in 0.1M HCl with the respectively studied inhibitors

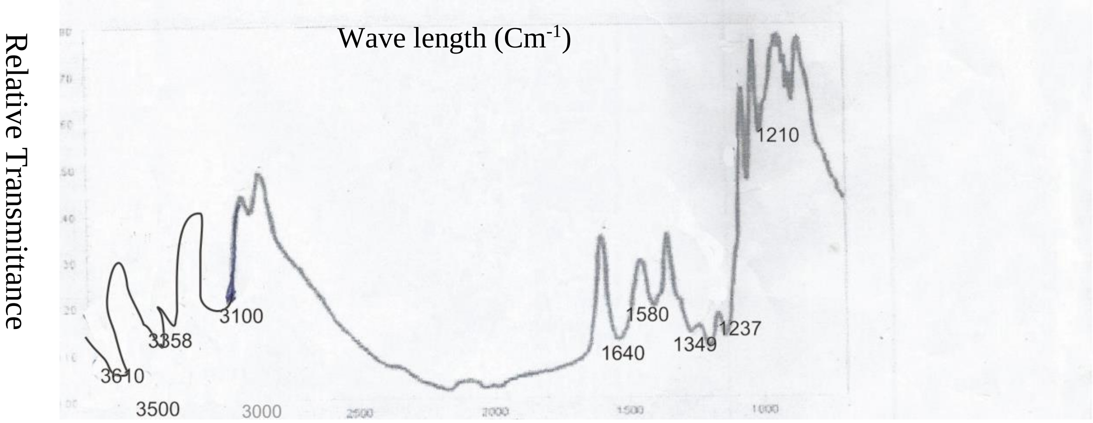


Fig. 2. IR Spectra of mono ethanolamine (MEA)

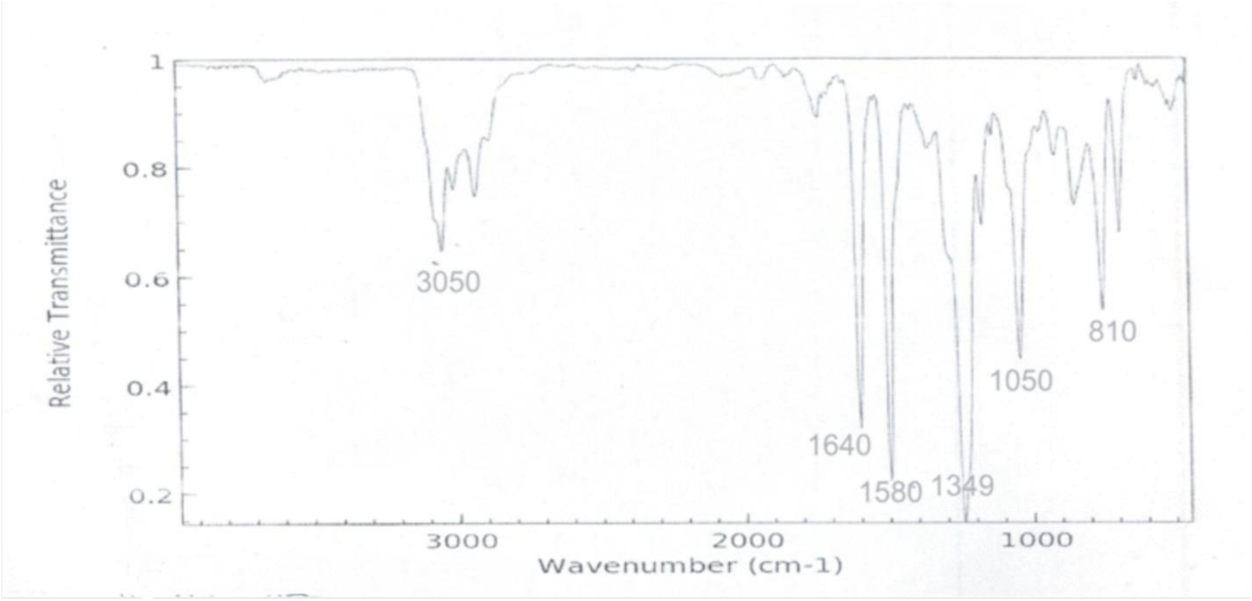


Fig. 3. IR Spectra of phenyl glycidyl ether (PGE)

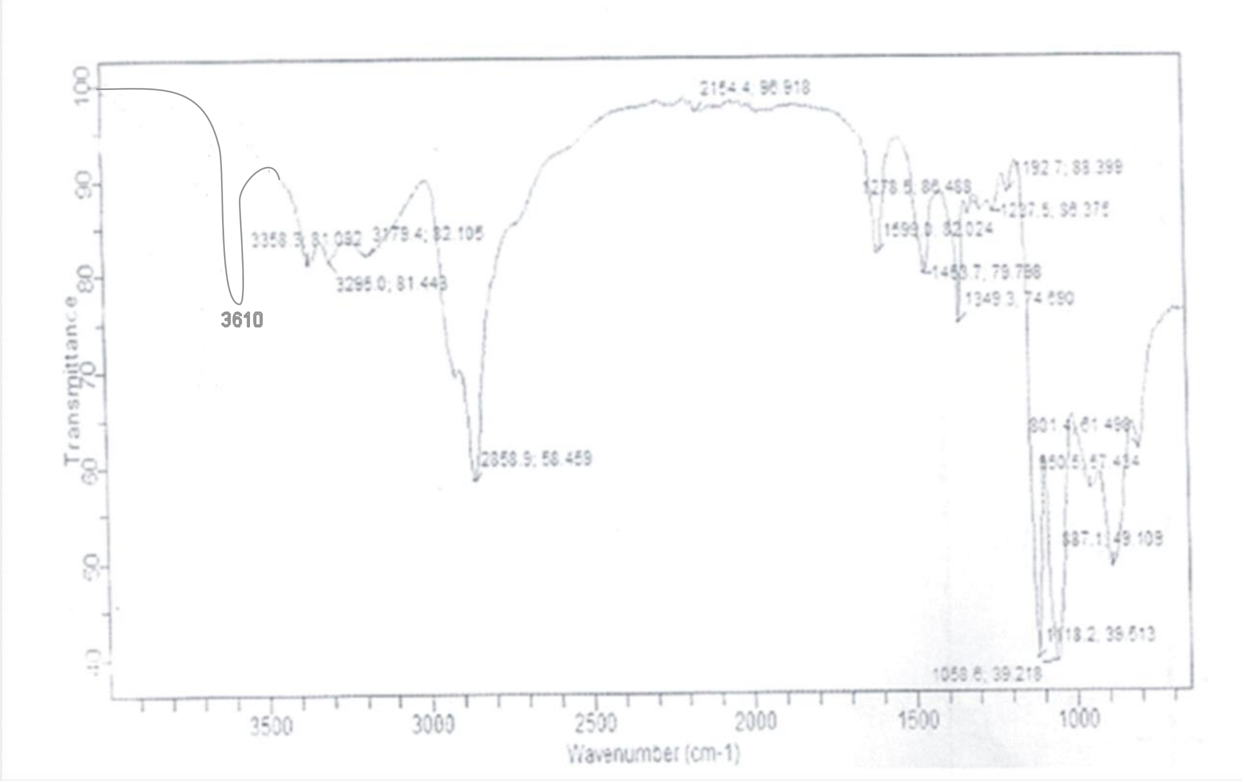


Fig. 4. IR Spectra of N – (- 2 hydroxy – 3 – phenoxy propyl) ethanolamine

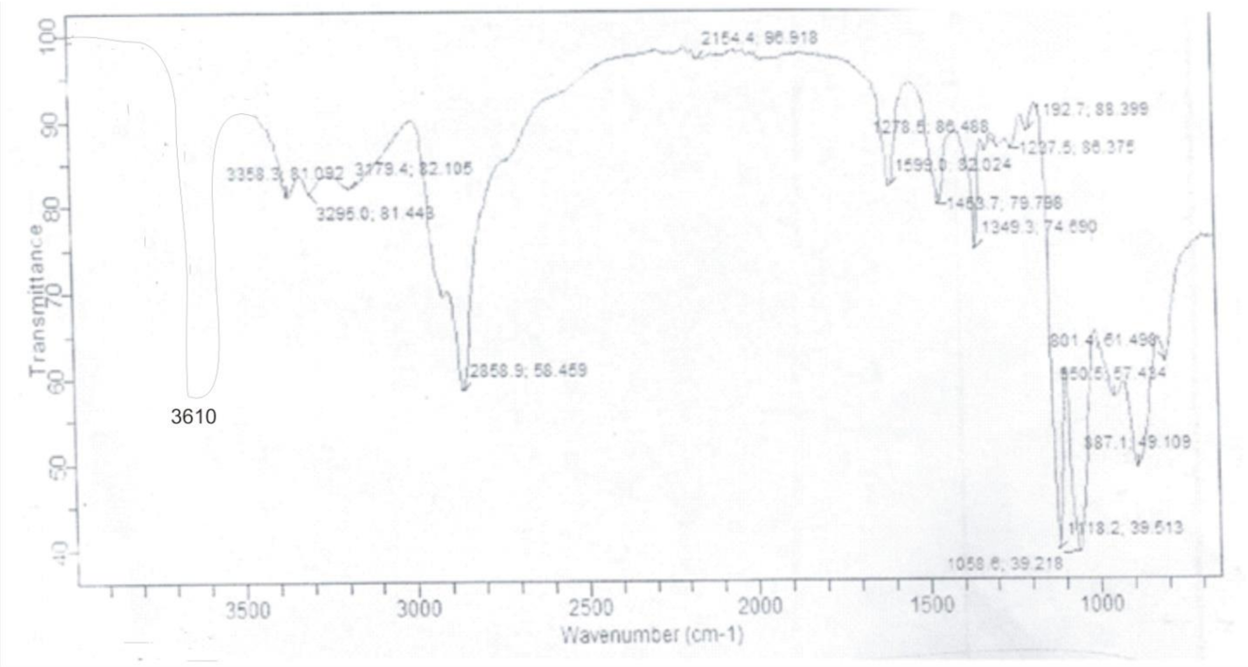


Fig. 5. IR Spectra of N, N' Bis - (-2 hydroxy – 3 – phenoxy propyl) ethanolamine

Table 2. IR absorption bands of the functional groups in MEA, PGE, NHPE and NN'HPE in the spectrophotometer.

IR frequency (cm^{-1})	Functional group	MGA	PGE	NHPE	NN'HPE
1237	OCH_3	Present	Absent	Present	Present
1349	CH_2, CH_3 bend	Present	Present	Present	Present
1580	Ar-C = C – H	Present	Present	Present	Present
1640	Ar – C – H	Present	Present	Present	Present
3358	N – H	Present	Absent	Present	Present
3610	OH broad	Present	Absent	Present	Present
1210	-C – N	Present	Absent	Present	Present

Table 2 makes a representation of the absorption bands of the main functional groups present in the studied inhibitors as captured in Figures 2 -5. The functional groups depicted in the IR spectra that could help the studied inhibitors in inhibiting the corrosion of mild steel in the HCl media were – OCH_3, - CH_2 – CH_2 – N – H and OH for MEA; -CH_2 and Ar—C=C—H for PGE; - OCH_3, - CH_2, -CH_3, Ar—C=C-H, - N – H, and – OH for NHPE and finally – OCH_3, - CH_2, - CH_3, Ar—C= C – H, –N–H and – OH for NN'HPE.

[4] observed that the presence of electron donating groups such as – OH, - NH, - CH_3 and – OCH_3 increases the inhibition performance of organic inhibitors in a corrosive environment. It is therefore safe and right to say that NN'HPE with extra – OH, - NH_2, - CH_3 and – OCH_3 occasioned by its size will more efficiently inhibit the corrosion of the mild steel in the HCl media than the other studied inhibitors. This was further substantiated by the mean percentage weight loss of the mild steel in the acidic media with the respective studied inhibitors as depicted in Table 1. NN'HPE and NHPE were very efficient inhibitors based on their functional group make-up and their molecular size.

[14] corroborated this result in their findings by stating that an inhibitor molecule with larger molecular size usually provides a wider protective coverage for the metallic substrate compared to a similar molecule with smaller molecular size. In addition to the presence of the functional groups (– OCH_3, - CH_3, - CH_2, - N – H and – OH) in NHPE and NN'HPE, another edge they have over MEA and PGE is the presence of Ar – C = C – H which confirm the planarity of the molecules and its configuration.

[12] observed that a planar molecule has the tendency of higher inhibition efficiency due to more effective adsorption onto the metallic surface since, generally planar molecules adsorb onto metallic surface in a flat orientation and cover larger surface area compared to non-planar inhibitor molecules.

Therefore, the order of corrosion inhibition efficiency of the studied inhibitors on mild steel as shown in their functional group absorption bands in the IR Spectra represented in Table 2 decreased as follows: NN'HPE > NHPE > MEA > PGE.

Table 3. Quantum Chemical Parameters of the Studied InhibitORS

Quantum Chemical Parameters	**MEA**	**PGE**	**NHPE**	**NN'HPE**
E_{HOMO} (eV)	-4.336	-4.581	-4.011	-3.695
E_{LUMO} (eV)	0.868	1.442	0.572	0.259
DIPOLE MOMENT (μ)	1.973	1.181	2.066	2.346
Energy gap ΔE (eV)	5.204	6.023	4.583	3.954
Electron affinity (A) (eV)	-1.873	-2.194	-1.016	-0.840
Electronegativity (x, eV mol^{-1})	2.351	1.960	3.088	3.604
Ionization potential (I) (eV)	3.360	4.211	2.624	2.171
Global hardness (ŋ) (eV mol $^{-1}$)	2.461	3.252	1.692	0.983
Chemical softness (σ)	0.696	0.331	0.844	1.205
Total energy E_T (eV)	-1238.110	-841.28	-1901.16	-2648.372
Total surface area (nm^2)	280.081	175.177	411.260	561.437
Polarizability, pol (Å^3)	35.036	23.694	48.116	66.437

Molecular orbital energies (E_{HOMO}, E_{LUMO}, $\Delta E_{LUMO-HOMO}$, eV): Table 3 shows that the E_{HOMO} values for MEA, PGE, NHPE and NN'HPE were -4.336, -4.581, -4.011 and -3.695 eV respectively.

The order of the decrease of E_{HOMO} values for the inhibitors were NN^{1}HPE > NHPE > MEA > PGE. Equally, the E_{LUMO} values for MEA, PGE, NHPE and NN'HPE from Table 3 were 0.868, 1.442, 0.572 and 0.259 eV respectively. The order of the decrease of E_{LUMO} values for the inhibitors were PGE > MGA > NHPE > NN'HPE. Research has shown that as the E_{HOMO} values of inhibitors increases and the E_{LUMO} value decreases, it indicates a very strong ability of the inhibitor molecules to donate their p-electrons to the unoccupied d-orbital's of the metal substrate. This is an indication that inhibition efficiency of inhibitor molecules increases with increase in their E_{HOMO} values and a decrease in their E_{LUMO} values. The energy gap ΔE for MEA, PGE, NHPE and NN'HPE were 5.204, 6.023, 4.583 and 3.954 eV. The result indicates that NN'HPE has the lowest ΔE value while PGE has the highest ΔE value. According to [18] low values of the energy gap, ΔE will result in good inhibition efficiencies for inhibitors because the energy required to remove an electron from occupied orbital's will be low. Also, the ΔE of a molecule is a measure of the hardness or softness of a molecule. Hard molecules are characterized by larger ΔE values while soft molecules are characterized by smaller ΔE values. Therefore the unoccupied electrons in the 3d orbital of the metal atom can accept electrons from the HOMO of the inhibitor molecule at a very reduced energy requirement. Inhibition efficiency increases if the compound (inhibitor) can donate electrons from its HOMO to the LUMO of the metal in which chelation on the metal surface occurs.

Dipole Moment: The dipole moment is a quantum parameter that represents the electron distribution in a molecule and is a measure of the polarity of a polar covalent bond. According to [19], dipole moment is related to the hydrophobic character of molecules. Organic compounds with amino and methoxy functional groups are usually associated with large dipole moments and this makes them to easily displace water molecules at metal surfaces, thus forming a hydrophobic film, which protects against corrosion. Results of Table 3 shows that the dipole moment values for MEA, PGE, NHPE and NN^{1}HPE were 1.873, 1.181, 2.066 and 2.346 μ respectively. The order of the decrease of the dipole moment values of the studied inhibitor molecules were NN'HPE > NHPE > MEA > PGE. The result of the study therefore shows that increase in the values of the dipole moments of inhibitors increases their corrosion inhibition efficiencies in corrosive environments. Hence increase in values of dipole moment of inhibitors increases their rate of adsorption on the surface of metal thus increasing the inhibition effectiveness.

Electron Affinity: Table 3 shows that the electron affinity A, values for MEA, PGE, NHPE and NN'HPE were -1.873, -2.194, -1.016 and -0.840 eV respectively. The result further indicates that among the studied inhibitors, the electron affinity values of NN^{1}HPE was the highest while that of PGE was the lowest. As electron affinity of inhibitor molecules increases, their eagerness to accept electrons from the metal (substrate) surface onto their anti-bonding orbital increases and their inhibition efficiency increases indicating more protection for the mild steel surface.

[14] made a similar observation as done in this study when they obtained electron affinity values of -6.92, -5.914 and -5.760 eV for 1, 8 – Diamino octane, Ethoxylated 1, 8 diamino octane and propxylated 1, 8 diamino octane as inhibitors respectively for mild steel in acidic media.

Electronegativity: Electronegativity is related to the ability of atoms to attract electrons towards themselves. Inhibitor molecules with high electronegativity values have greater ability to attract electrons from the metal surface unto their antibonding orbitals and thus easily forms a hydrophobic film on the metal surface which protects against corrosion. Therefore as the electronegativity values of inhibitor molecules increases, their corrosion inhibition efficiency equally increases. Table 3 shows that the electronegativity values for MEA, PGE, NHPE and NN'HPE wer, 2.351, 1.960, 3.088 and 3.604 eVmol^{-1} respectively.

The studied inhibitor molecules had electronegativity values in the following decreasing order; NN'HPE > NHPE > MEA > PGE.

Ionization Potential: According to [14] ionization potential is directly related to the energy of the HOMO. Table 3 indicates that as the ionization potential of the inhibitors decreases, an increase in their inhibition efficiency would result as evidenced in the result of Table 2. The result of Table 3 shows that the ionization potential values for MEA, PGE, NHPE and NN'HPE were 3.360, 4.211, 2. 624, 2.171 eV respectively. NN'HPE had the least ionization potential value while PGE had the highest ionization potential value of the four studied inhibitors.

[4] observed that a decrease in ionization potential results in a decrease in the minimum energy required for the adsorption of inhibitor molecules on metal surfaces because of the stability factor of the inhibitor molecules in the corrosive media.

Global Hardness: Global hardness provides information about the reactive behaviour of molecules. A high value of global hardness indicates low reactivity of a molecule and thus a high energy gap. This therefore means that inhibitor molecules with high values of global hardness will require a very high energy to remove electrons from their orbital's which then gives rise to low inhibition efficiency for such inhibitor molecules. Table 3 shows that the global hardness values for MEA, PGE, NHPE and NN'HPE were 2.461, 3.252, 1.692 and 0.983 eV mol^{-1} respectively. The studied inhibition molecules had global hardness values in the following decreasing order: PGE > MGA > NHPE > NN'HPE. The findings of [20] on the corrosion inhibition efficiency of selected natural inhibitors in which the global hardness values of the major components of the inhibitor were found to decrease with increase in inhibition effectiveness was in agreement with what this study reported.

Chemical Softness: A soft molecule is more reactive than a hard molecule because a softer molecule is associated with a lower energy gap. Hence, an inhibitor molecule with an increased chemical softness means a molecule that can transfer the highest number of electrons to the metal substrate surface. (14) reported that there is a positive correlation between chemical softness and inhibition efficiency. It therefore implies that as the chemical softness values of an inhibitor molecules increases, their inhibition efficiency equally increases. Results of Table 3 shows that the chemical softness values for MEA, PGE, NHPE and NN^{1}HPE were 0.696, 0.331, 0.844 and 1.205 eV^{-1} respectively. NN^{1}HPE was the inhibitor with the highest value of chemical softness of the four studied inhibitors while the lowest value was for PGE.

Total Energy: The total energy of a molecule including all forms of kinetic motion and all forms of potential energy and determines the reactivity and stability of the molecule.

According to [14], the higher the total energy (E_T), the higher the stability of the molecule and hence the lesser the tendency of it to donate electrons.

Results of Table 3 shows that the total energy values for MEA, PGE, NHPE and NN'HPE were -1.238.11, -841.281, -1901.16 and -2648.372 eV respectively.

The studied inhibitors had total energy values in the following decreasing order: PGE > MEA > NHPE > NN'HPE. The result clearly indicates that as the total energy of inhibitor molecules decreases, their corrosion inhibition efficiency increases.

Total Surface Area (Nm^2): As the total surface area of inhibitor molecule decreases which is relative to its size and presence of adsorption sites, the surface coverage it will have on the metal surface becomes low and minimal, thereby resulting in low inhibition efficiency for such a molecule.

The presence of - NH and -OH functional groups helps to increase the metal surface coverage.

Table 3 shows that the total surface area values for MEA, PGE, NHPE and NN'HPE were, 280.081, 175.177, 411.260 and 561.437nm^2 respectively. The surface area of NN'HPE, NHPE and MEA were much higher than that of PGE because of the presence of active adsorption sites (-NH, $-CH_3$, CH_2, $-OCH_3$ and OH) and which ultimately aided their molecular sizes. Hence, as the total surface area of inhibitor molecules increases, their inhibition efficiency equally increases occasioned by a better surface coverage of the metal substrate.

The findings of [14] on the total surface area values of 1, 8 – Diamino octane, Ethoxylated 1, 8 diamino octane and propxylated 1, 8 diamino octane as inhibitors for mild steel in acidic media was in agreement with the result on surface area values of the studied inhibitors in this research.

Polarizability (Å^3)

The tendency of an electron cloud to be distorted from its normal shape is referred to as its polarizability. The polarizability of a molecule or an atom depends largely on how it diffuses or spreads over its electron cloud.

According to [21] polarizability plays a crucial role in the corrosion inhibition process since the greater the polarizability the higher the inhibitor molecules leaves the solvent bulk to be adsorbed on the metal surface to form a protective film. So, increase in values of polarizability for inhibitor molecule signifies an increase in inhibition efficiency.

Results of Table 3 shows that the polarizability values for MEA, PGE, NHPE and NN'HPE were 35.036, 23.694, 48.116 and 66.312 Å^3 respectively. The studied inhibitors had polarizability values in the following decreasing order: NN'HPE > NHPE > MEA > PGE.

4 CONCLUSION

The study shows that the structure of an inhibitor molecule plays a significant role in the ability of that molecule to efficiently inhibit corrosion of mild steel in a corrosive environment. FTIR analysis of the structure of the two of the four studied inhibitors, N – (2- hydroxy – 3- phenoxy propyl) ethanolamine and N, N^1 – (-2 hydroxy – 3 – phenoxy propyl) ethanolamine shows that the presence of functional groups such as – NH, OCH_3, -OH and CH_3 and their increased planarity occasioned by the delocalized л electron on their aromatic ring system offers them the greater ability for adsorption and donation of electrons on the metal substrate surface, thereby increasing their inhibition efficiencies more than the other studied inhibitors (mono ethanolamine and phenyl glycidyl ether).

The four studied inhibitors produced mean percentage weight loss of mild steel in the acidic media in the following decreasing order: PGE > MEA > NHPE > NN'HPE, which thus corroborates the observations drawn from the FTIR analysis.

The quantum chemical analysis of the inhibitors shows that NN'HPE and NHPE were able to more efficiently inhibit the corrosion of the mild steel in the acidic media because of the decrease in the values of parameters such as E_{LUMO}, energy gap, ionization potential, global hardness and total energy and as well as increase in the values of other quantum parameters such as $E_{HOMO,}$ dipole moment, electron affinity, electronegativity, chemical softness, total surface area and polarizability.

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