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Corrosion Inhibition and Quantum Mechanical Studies of Galvanized Steel Sheets in Chloride Environment

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ABSTRACT---- ***The corrosion inhibition of galvanized steel (GI steel)sheets in 5% NaCl with Esomeprazole (EPZ) as green inhibitor has been reported by Mass loss, Potentiodynamic polarization, electrochemical impedance spectroscopy , hydrogen permeation and quantum mechanical studies. All these techniques reveal that the EPZinhibits the corrosion of galvanized steel in 5% NaCl medium.Polarization studies indicated that inhibitors are acted as mixed type inhibitor. The adsorption of the compounds on galvanized steel surface follows Langmuir adsorption isotherm.***

Keywords---- antibiotics, hydrogen permeation, corrosion inhibitors,green inhibition

1. INTRODUCTION

Galvanized steel is most commonlyused in the applications such as building, automotive metal parts and water pipeline systems owing to its good resistance to environmental corrosion [1-4]. The protections obtained by zinc coating are by barrier and galvanic double protective effect [5-6]. However, many cases of failure of galvanized pipes and tanks have been reported as being due to corrosion processes in aggressive environment, as evidently proved by the formation of rust in those systems that leads to severe damage to GI sheets[7].

Several methods were used to retard the dissolution of metals in acidic medium, but the use of inhibitors is most commonly used [8-10].

The usage of inhibitors is inexpensive and real method to reduce electrochemical corrosion. Numerous organic compounds which have π bonds and contains hetero atoms such as sulphur, nitrogen, oxygen and phosphorous which allows the adsorption of compounds on the metal surface were reported as corrosion inhibitors by several investigators [11-16] for dissolution of iron metal in acid medium. Research findings in recent times are stimulated towards emerging the cheap, non-toxic drugs as environment responsive corrosion inhibitors [17-24].

The literature review indicates that few antibiotics have been reported as corrosion inhibitors for the corrosion of steel and aluminium in acidic and alkaline media [25]. Very Recently, Hari Kumar et al [26] used ampicillin drug as inhibitor for the corrosion of mild steel in 1 M HCl. Nevertheless, no concrete results have been published for the corrosion inhibition of GI steel sheet in 5% NaCl with use of Esomeprazole (EPZ) as inhibitor and hence the present study.

The inhibition efficacies of the compound were calculated using mass loss, electrochemical techniques. Rarely, theusage of hydrogen permeation measurement studies for this green inhibitor established the prominent performance of the inhibitors. This inhibitor is big enough, amply planar and could be able to block more galvanized steel surface area.

2. EXPERIMENTAL SECTION

2.1 Materials

GI steel sheet specimens of size 1×4 cm^2 were used for mass loss and electrochemical studies. The aggressive solution of 5% NaCl [AR Grade] is used for all the studies. The antibiotic namely esomeprazole was procured from the medicine shop and used as such without further purification. The structure of the green inhibitor is given in the fig.1 which also includes 13 C-NMR shifts. Electrochemical experiments were performed with a three electrode cell assembly with GI samples as working electrode, platinum as counter electrode and saturated calomel [SCE] as the reference electrode by EG&G Princeton Applied Research Model 263A Potentiostat/Galvanostat, Germany.

2.2 Mass Loss and Hydrogen Permeation Studies

Mass loss and hydrogen permeation studies were done as described earlier [27]. The concentrations of inhibitor used for weight loss and electrochemical study were from 10 ppm to100 ppm.GI sheet specimens of size 1×4 cm^2 were abraded with different emery papers and then degreased with acetone. The cleaned surfaces were washed with double distilled water, air dried and preserved in the desiccator. The mass loss study was followed at room temperature for three hours in 5% NaCl. The inhibition efficiency (IE%) was calculated by the following equation ,

Inhibition Efficiency, $$IE\% = \left(\frac{W_a - W_p}{W_a}\right) \times 100 \qquad \text{……… (1)}$$

where W_a and W_p are the weight loss values in absence and presence of the green inhibitor respectively.

2.3 Potential-Current Measurements by Electrochemical Studies

Potentiodynamic polarization measurements were monitored in a conventional three electrode cylindrical glass cell, using CH electrochemical analyzer at a scan rate of 5 mVs^{-1}. Before carrying out the polarization measurements the solution was deaerated for 20 min. and the working electrode was maintained at its corrosion potential for 20 minutes until a steady state was obtained. The galvanized steel surface was put in to various concentrations of inhibitors in 100 ml of 5% NaCl at room temperature. The inhibition efficiency (IE%) was calculated using the equation:

Inhibition Efficiency, $$IE\% = \left(\frac{i_a - i_p}{i_a}\right) \times 100 \qquad \text{…………(2)}$$

where i_a and i_p are the corrosion current density in the absence and presence of the green inhibitor respectively.

The potentiodynamic current-potential curves were recorded by changing the electrode potential automatically from -950 mV to +100mV versus the open circuit potential. The corresponding corrosion current (i_{corr}) was recorded. Tafelplots were made by plotting E versus I. Corrosion Potential (E_{corr}), corrosion current density (i_{corr}) and cathodic and anodic slopes (β_c and β_a) were calculated according to the Tafel extrapolation method.

Impedance measurements were done in the frequency range from 0.1 to 10000 Hz by means of amplitude of 20 mV and 10 mV peak to peak with an AC signal at the open-circuit potential. Charge transfer resistance (R_{ct}) and double layer capacitance (C_{dl}) values were got from Nyquist plot [28-30]. The percentage inhibition efficiency was calculated from the equation.

Inhibition Efficiency, $$IE\% = \left(\frac{C_{dl_a} - C_{dl_p}}{C_{dl_a}}\right) \times 100 \qquad \text{……………(3)}$$

where C_{dl_a} and C_{dl_p} are the charge transfer resistance of GI sheets in the absence and presence of green inhibitor respectively.

3. RESULTS AND DISCUSSION

3.1 Mass Loss Studies

The values of inhibition efficiency (IE%) and surface coverage (θ) calculated for green inhibitor at different concentrations for the corrosion reaction of GI sheets in 5% NaCl from the mass loss data is summarized in the Table 1. It is established that inhibition efficiency increases with increase in the inhibitor concentration. It was also ostensible that corrosion rate decreases with increase in green inhibitor concentration. It was illustrious that inhibitor retard the galvanized steel corrosion at all the concentrations used in this study. Maximum inhibition efficiency is observed at 100 ppm concentrations of the esomeprazole.

3.2 Potential-Current Measurements by Electrochemical Studies

Polarization results such as the values of corrosion potential E_{corr}, corrosion current densities i_{corr}, anodic Tafel slope (β_a) ,cathodic Tafel slope (β_c), surface coverage (θ) and inhibition efficiency (IE%) were calculated from polarization curves for the corrosion of GI sheets in 5% NaCl are summarized in Table 2.

It can also be seen from the table that corrosion current (i_{corr}) value declines with increase in the concentration of the green inhibitor. The presence of inhibitor with three concentrations shift the Tafel slopes to lower values, and the anodic slopes were lower than the cathodic slopes, this infer that the rate of change of current with change of potential was smaller during anodic polarization than that during cathodic polarization.

Hence the inhibition of corrosion by this compound is under cathodic control, but chiefly under mixed type due to the random shifts in Tafel slopes. At 100 ppm of inhibitor, the maximum inhibition efficiency achieved was 98%. Beyond this concentration, the inhibition efficiency declined to 79% due to peel off of inhibitor could be the reason.

The inhibition efficiency (IE%) and surface coverage (θ) increases with increase in EPZ dosage in the experiment . The maximum inhibition efficiency was obtainable at 100 ppm concentration. A definite relationship exists between the results obtained from mass loss and potential-current studies for the above inhibitor.

3.3Electrochemical Impedance Studies

The Nyquist representations of impedance behavior of galvanized steel in 5% NaCl with and without addition of various concentrations of inhibitors are given in table 3. The table also contained the values of charge transfer resistance (R_{ct}) and double layer capacitance (C_{dl}) derived from Nyquist plots for the dissolution of GI steel in 5% NaCl. It can be visualized that the values of R_{ct} was seen to increase with increase in concentration of green compound in the acid. It was found that values of C_{dl} are brought down by enhancing concentrations of Esomeprazole in the acid medium. This can be accredited tothe increasing adsorption of the inhibitor on the metal surface with increase in its concentration [33].

3.4 Adsorption Isotherm

The degree of surface coverage (θ) for different concentrations of Esomeprazole in 5% NaCl has been calculated from weight loss, Polarization and Electrochemical Impedance studies. The obtained data was tested graphically for fitting suitable isotherm [34- 36].A straight line was observed by plotting log (C_{inh}/θ) vs log C_{inh} which ratifies that the adsorption of this green inhibitor obey Langmuir adsorption isotherm.

The Langmuir isotherm for the adsorbed layers is given by the equation [37]:

$$\frac{C_{inh}}{\theta} = \frac{1}{K_{ads}} + C_{inh} \qquad \text{……………} (4)$$

where C_{inh} is concentration of inhibitor and K_{ads} is the equilibrium constant of the adsorption/desorption process.

Adsorption equilibrium constant (K_{ads}) and free energy of adsorption (ΔG^o_{ads}) were calculated using the equation [38]

$$\Delta G^o_{ads} = -2.303RT\, log 55.5\, K_{ads}, \quad where\ K_{ads} = \frac{\theta}{C_{inh}(1-\theta)} \qquad \text{……..}(5)$$

where 55.5 is the molar concentration of water in solution [38-39]. R is the gas constant, T is the absolute temperature. The values of adsorption equilibrium constant (K_{ads}) and free energy of adsorption (ΔG^o_{ads}) are given in Table 4. The temperatures (298K, 313 K, 323K and 333K) were maintained constant by keeping the experimental setup in water bath of suitable temperatures required for calculating Gibbs free energy. The negative values of (ΔG^o_{ads}) showed that adsorption of esomeprazole on GI steel surface in chloride environment is an spontaneous process. It is well-known that values of (ΔG^o_{ads}) is of order 20 kJmol^{-1} or lower indicates a physical adsorption, those of order of -40 kJmol^{-1} or higher involve charge sharing or transfer from the inhibitors to the metal surface to form a co-ordinate bond, the process known as chemisorption . The values of free energy of adsorption (ΔG^o_{ads}) in this study lies in the range -28 to -32 kJmol^{-1}, demonstrating that the adsorption is not a simple but it may include some other interactions [40-43].

3.5 Mechanism of Inhibition

In Esomeprazole, the presence of lone pairs of electrons of nitrogen atoms of both dimethyl pyridine and benzo imidazole groups along with sulphur atom which favour the adsorption of esomeprazole on oxidized GI surfaces because of the existence of the positively charged Fe atoms by corrosion of GI surfaces when exposed to chloride environment.

3.6 Quantum Mechanical Studies

Quantum mechanical calculations were carried out to explore the adsorption and inhibition mechanism of the EPZ compound on the corrosion of galvanized steel surfaces in 5% NaCl. Figure 2&3 indicate HOMO and LUMO structure of esomeprazole inhibitor. The values of calculated quantum chemical parameters i.e. E_{HOMO} (highest occupied molecular orbital), E_{LUMO} (lowest unoccupied molecular orbital), ∆E (energy gap), μ (dipole moment) etc. are presented in table-5.E_{HOMO} is related to the electron-releasing capability of the inhibitor molecule while E_{LUMO} is explained for electron with drawing capacity of inhibitor molecule. In the present investigation, the adsorption of a EPZ on metal surface acquired on the basis of donor-acceptor interactions between the π-electrons of nitrogen and sulphur atoms of benzoimidazole and dimethyl pyridine groups which favors effective adsorption of EPZ on GI surfaces evidenced from the dense electrons cloud in HOMO and LUMO structure wherein the electroic cloud is similar in both orbitals. It is well understood that if both HOMO and LUMO structures are resemblingeach other, the resultant adsorption of inhibitor will be better on metal surface. The gap between HOMO–LUMO energy levels of molecules was another important factor that needs to be considered. Higher the value of ∆E of an inhibitor, higher is the inhibition efficiency of that inhibitor. It has been reported that, large values of the dipole moment will improve corrosion inhibition. Based on the values of ∆E and dipole moment, the compound EPZ has strongly been adsorbed on galvanized steel surface immersed in 5% NaCl.

4. CONCLUSIONS

The controlled dissolution of galvanized steel surfaces were monitored and controlled in 5% NaCl solutions without and with various concentrations of Esomeprazole as green inhibitor by adapting chemical and electrochemical methods. The main conclusions are:

(i) Esomeprazole drug exhibited inhibiting properties for galvanized steel corrosion in 5% NaCleffectively.
(ii) Tafel polarization plots indicated that tested inhibitor was showing mixed mode of inhibition.
(iii) Corrosion parameters obtained from the impedance measurements were in good agreement with those recorded using the potential-current plots. This confirms the validity of the corrosion rates measured by the potentiodynamic polarization.
(iv) Adsorption of the Esomeprazole on GI surfaces was found to follow Langmuir isotherm.
(v) Apparent activation energies in the presence of Esomeprazole drug for the corrosion of GI sheets in chloride medium lie in the range 28 to -32 kJmol^{-1}, indicating that the adsorption is not a simple physisorption.
(vi) Quantum mechanical results validate the impressive performance of EPZ inhibitor through its effective adsorption on GI surfaces exposed in 5% NaCl.

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Table 1: Values of Inhibition Efficiency and Surface coverage for the dissolution of GI SHEET in 5% NaCl in presence of different concentrations of Esomeprazole obtained from mass loss measurements

Inhibitor Concentration	**Inhibition efficiency (*IE*) (%)**	**Surface coverage (*θ*)**
ESOMEPRAZOLE		
Blank		
10 ppm	75.42	0.75
50 ppm	87.87	0.88
100 ppm	98.32	0.98

Table 2: Electrokinetic parameters and Inhibition Efficiency for corrosion of GI SHEET in 5% NaCl obtained by Polarization method in presence of Esomeprazole

Inhi. Con. (ppm)	**E_{corr} (mV vs. SCE)**	**i_{corr} (μA. cm^{-2})**	**βa (mV. dec^{-1})**	**βc (mV. dec^{-1})**	***IE* (%)**	***θ***
Blank	-857.78	647.47	100.9	150.2	-	-
ESOMEPRAZOLE						
10	-837.35	161.80	82.4	129.3	75.01	0.75
50	-801.63	77.89	99.7	138.6	87.97	0.88
100	-792.77	10.74	77.2	104.5	98.34	0.98

Table 3: Electrochemical impedance parameters for dissolution of GI SHEET rod in 5% NaCl with and without EPZ compound

Inhibitor Conc. (ppm)	**R_{ct} (Ω. cm^{2})**	**C_{dl} (F. cm^{-2})**	***IE* (%)**	**Surface coverage (*θ*)**
Blank	47.2	0.296	-	-
ESOMEPRAZOLE				
10	126.3	0.0739	75.02	0.75
50	177.4	0.0385	86.96	0.87
100	270.71	0.0049	98.32	0.98

Table 4: Gibbs free energy parameters and adsorption equilibrium constant (K_{ads}) of green inhibitor (EPZ) at different temperatures evaluated by mass loss method

Temperature [K]	**K_{ads} Green inhibitor**	**$-\Delta G^{o}_{ads}$[kJmol^{-1}] Green inhibitor**
298	865	26.41
313	931	28.33
323	1164	29.82
333	1341	31.17

Table 5: Quantum mechanical parameters for Esomeprazole for the corrosion of GI surfaces

Inhibitor	**LUMO (eV)**	**HOMO (eV)**	**ΔE (Cal.Mol^{-1})**	**Dipole moment (Debye)**
Esomeprazole (EPZ)	-0.6023	-8.1775	7.5752	3.8

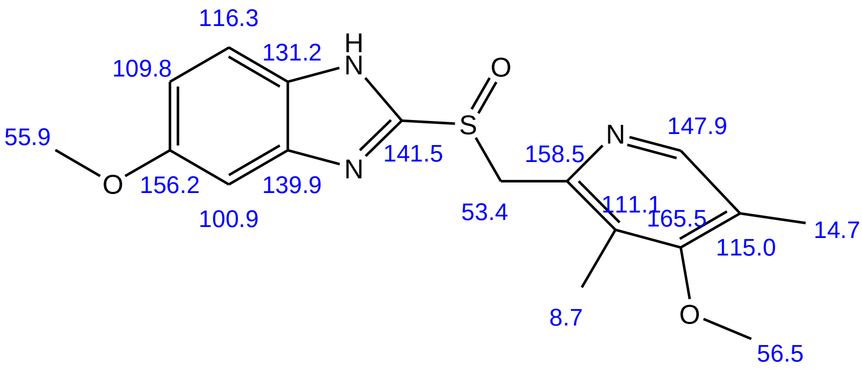

Figure 1: Structure of Esomeprazole OR
5-methoxy-2-((4-methoxy-3,5-dimethylpyridin-2-yl)methylsulfinyl)-1*H*-benzo[*d*]imidazole

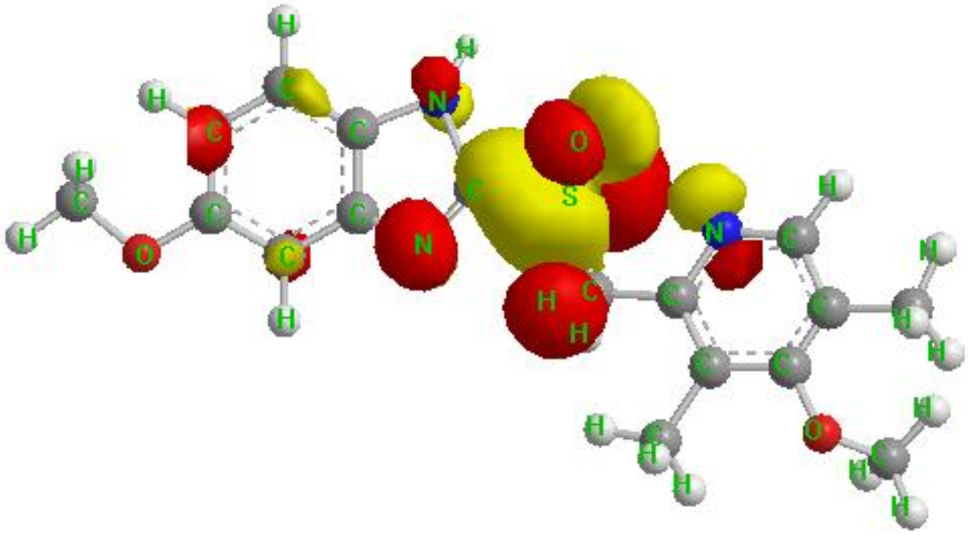

Figure 2: Highest Molecular Orbital of EPZ Molecules during the Adsorption on GI Surfaces

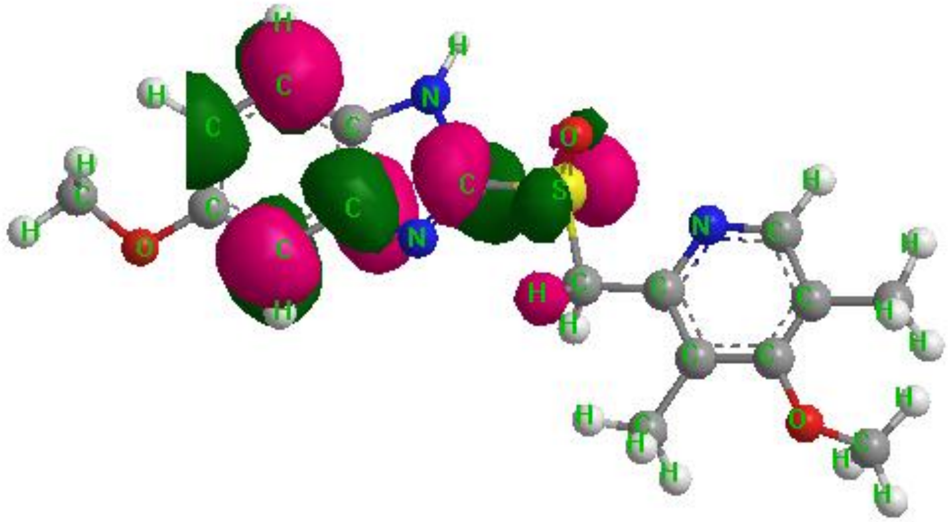

Figure 3: Lowest Unoccupied Molecular Orbital of EPZ Molecules during the Adsorption on GI Surfaces