

# SYNTHESIS AND CHARACTERIZATION OF BENZOXAZINE: URETHANE COPOLYMER FROM VANILLIN WITH ADAMANTANE SIDE CHAIN AND ITS ANTI-CORROSIVE COATING ON MILD STEEL

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## ABSTRACT

Corrosion is a significant issue with metallic materials, notably in steel due to its extensive use in a variety of industries. Benzoxazine polymers have been used to produce anti-corrosive compounds that have a remarkable ability to limit corrosion. In the same ink line, we have explored a new approach with a very hydrophobic benzoxazine monomer which is co-polymerized with urethane, and its characterization was studied with IR, UV, and NMR techniques. The corrosion resistance of the same is investigated using Tafel polarization and EIS experiment methodologies. The DFT and MEP studies explain the reactivity towards the anti-corrosive properties of the monomer.

**Keywords:** Hydrophobic Monomer, Polyurethane Co-Polymer, Corrosion, DFT Studies.

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## INTRODUCTION

Mild steel is a distinctive material among other metallic components that are related to a wide range of applications due to its importance in household, services, construction, maritime, industrial, and technical purposes.<sup>1-2</sup> But this distinctive metal is also susceptible to corrosion very easily. To address this issue, chemical inhibitors that are adsorbed on metal surfaces are utilized, for regulating or preventing, or limiting the corrosion reaction rate.<sup>3</sup> As a result, the necessity of steel protection in numerous fields of application is vital, and various corrosion scientists have a significant research interest in developing new chemicals for corrosion prevention.<sup>4-5</sup> Polymeric materials have concerned a lot of consideration recently, due to their potential uses in a variety of fields, including biomedicine<sup>6</sup>, sensors<sup>7</sup>, rechargeable batteries<sup>8</sup>, catalysis<sup>9</sup>, etc., Polybenzoxazine (PBz), a new kind of phenolic resin, has recently generated a lot of interest due to its distinctive qualities, including low water absorption<sup>11-12</sup>, flexible molecular design<sup>13-14</sup>, low surface energy<sup>15-17</sup>, and low dielectric constant.<sup>18-20</sup> Moreover, PBz can be produced by thermally activating ring-opening polymerization of the appropriate benzoxazine monomers without any external initiator, and it doesn't show any volatiles or by-product formation. Additionally, it was established that these polymers have great electrical insulating qualities in addition to strong thermal and chemical durability. However, there are certain drawbacks to PBz, the chief among which are the brittleness of the crosslinked resins and the very high temperature (nearly 493 K) required for the ring-opening polymerization of benzoxazines. As a result, it was noted that numerous attempts were made to solve these issues.<sup>21-24</sup> On the other hand, polyurethanes (PUs) are also the subject of intensive research in academic and commercial labs due to their significance.<sup>25-26</sup> The primary drivers behind PUs' wide range of applications are their diverse chemistry and adaptability to structural changes to meet ensemble-specific demands. Numerous approaches to study aimed at increasing the thermal stability of PUs have been explored. Among them, chemical alternation of their structure is the most accepted method to develop the thermal stability of PUs by introducing highly thermally stable heterocyclic groups in a cross-linked manner.<sup>27-34</sup>

To overcome less hydrophobicity of the benzoxazine monomers, a few polymers are used to produce a moderate outcome.<sup>35</sup>

As a result, we consider that increasing the benzoxazine monomer's hydrophobicity could inhibit the adsorption of water. Meanwhile, polyurethanes can reduce the brittleness of benzoxazine polymers, and benzoxazine may help increase the thermostability of polyurethanes. Finally, we decided to focus on developing a new co-polymer with improved thermostability, poor water absorption, and hardness. We have developed a more hydrophobic benzoxazine/polyurethane co-polymer that serves as an anti-corrosive substance in response to this. To study the corrosion inhibition characteristics, three distinct Bz: PU ratios were synthesized. Additionally, a thorough investigation of the monomer's electronic behavior using molecular elemental mapping and DFT analysis was conducted; the results demonstrate the monomer's surface's molecular electronic status. All three co-polymers were subjected to potentiometry and electrochemical investigation, and the results are thoroughly described.

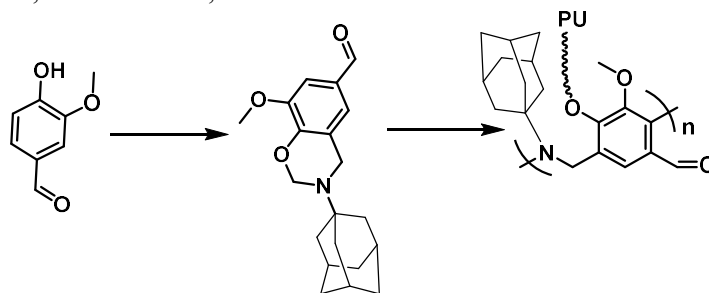
## EXPERIMENTAL

### General Methods

The IR and UV spectrum recording was done with Thermo Scientific Nicolet iS50 FT-IR Spectrometer and Labman LMSP UV-1200 UV-Vis spectrometer respectively.  $^1\text{H}$  NMR was recorded on Bruker 500 MHz with  $\text{DMSO-D}_6$  solvent similarly  $^{13}\text{C}$  NMR spectra were recorded on a 125 MHz instrument for carbon spectra. TLC was also carried out to confirm the completion of the reaction in the usual method. Conventional Biologic SP 300 model, a three-electrode cell, in which  $\text{Ag}/\text{AgCl}$  was the reference electrode and Pt was the counter electrode, was used for the Polarization studies.

### Synthesis of Monomer (3-((1S,3s)-adamantan-1-yl)-8-methoxy-3,4-dihydro-2H-benzo[e][1,3]oxazine-6-carbaldehyde) and Co-Polymerise with Urethane

The mixture of paraformaldehyde (0.395 g, 13.157 mmol) and adamantane-1-amine (0.993 g, 6.578 mmol) was charged in a 100 ml RB flask containing 10 mL of the chloroform. Then, allowed to reflux at  $50^\circ\text{C}$  for 30 minutes, this chloroform solution (20 mL) of vanillin (1.0g, 6.578 mmol) was added. The reaction was allowed to continue for 16 hr at  $70^\circ\text{C}$  meantime, the reaction was monitored by the TLC. After the completion of the reaction, it was diluted with 100 mL of chloroform and filtered the reaction mixture. The collected filtrate was washed with 1N sodium hydroxide solution, consequently, brine solution and water were used for the washing. The organic layer was separated and dried over anhydrous sodium sulphate then evaporated under reduced pressure, the obtained monomer product yielded a white-colored solid. The obtained crude monomer was used for the further synthesis of polymeric materials with isocyanate. This synthesized monomer was re-dissolved in a 1,4-dioxane mixed with a solution having a particular ratio of isocyanate hardener in toluene. Finally, three different benzoxazine and isocyanate compositions were prepared by varying the amount of isocyanate like 60, 80, and 100 concerning monomer quantity, which is denoted as Bz-PU100:60, Bz-PU100:80, and Bz-PU100:100.



Scheme-1: Synthesis of (3-((1S,3s)-adamantan-1-yl)-8-methoxy-3,4-dihydro-2H-benzo[e][1,3]oxazine-6-carbaldehyde) Co-Polymer with Polyurethane

### Coating and Curing (Polymerization on Mild Steel)

Before the coating, the mild steel plate was cleaned with several solvents such as water, hexane, and acetone to remove the impurities. Further, it was refined by emery paper to improve adhesion. Here, the mild steel plate is dip coated, and the thermal curing method was followed for the coating of the polymer.<sup>36-37</sup> To prepare the coating liquid, the monomer was dissolved in a mixture of solvents (7: 3 1,4-dioxime/toluene), and then significant amounts of the isocyanate hardener were added and three different solutions were made by changing the amount of hardener. The MS plate was dipped into the respective polymeric solution for a

minute and taken it out at a speed of 100 mm per minute. After that, thermal curing was performed at 200°C in the furnace for the 3 hours. The obtained specimens are used for the electrochemical analysis for their corrosive performance.

### Water Absorption Studies

As per ASTM D570, water absorption content in the coated, cured samples were carried out. The cured samples were immersed in the water at room temperature for 24 hours. After 24 hours, before weighing, the water particles are removed and also strained with a paper towel. The water absorption percentage was calculated by

$$\text{Water absorption \%} = [(W_a - W_b)/W_b] \times 100$$

Where  $W_a$  and  $W_b$  are the weight of the cured sample after immersion into the water and the weight of the cured sample before immersion into the water respectively.

### Gel Content Studies

The total gel content of the coated, cured sample was determined by the weighing method. The coated plates were weighed before and after being extracted from xylene, post 24 hours of immersion at room temperature. Then immersed coated samples were dried in the oven under a vacuum. The gel content of coated samples was calculated by,

$$\text{Gel content \%} = (W_a/W_b) \times 100$$

Where,  $W_a$  and  $W_b$  are the weight of coated, cured samples after and before the extraction respectively.

### Computational Calculations

Density Functional Theory (DFT) was applied to find out the electronic structure of the monomer in the ground and excited states molecular orbital, simply called frontier molecular orbital (FMO). This study was performed in the Gaussian 09W program software in which B3LYP/6.311 G basis set was used.<sup>38</sup> The Gauss view software was used to process the output data file to visualization of the three-dimensional structure, electron cloud identification on the compound, molecular electrostatic potential (MEP), and Mullikan charge distribution representations.

### Tafel Polarization Experiment

With the aid of these values, the corrosion efficacy was calculated using the following formulae,

$$\text{Corrosion rate} = (I_{\text{corr}} \times K \times EW)/\rho A \text{ mmpy}$$

Where,  $K = 3272 \text{ mm year}^{-1}$  (rate constant), the equivalent weight of the mild steel (EW) (27.9 g), mild steel density ( $\rho = 7.85 \text{ g cm}^{-3}$ ), and area of the sample ( $A = 1 \text{ cm}^2$ ).

$$\text{C.E (\%)} = [(I_{\text{corr(b)}} - I_{\text{corr(c)}})/(I_{\text{corr(b)}})] \times 100$$

Where,  $I_{\text{corr(b)}}$  is the corrosion current for the uncoated MS plate,  $I_{\text{corr(c)}}$  is the corrosion current for the material-coated MS plates.

The free energy of adsorption ( $\Delta G_{\text{ads}}$ ) was calculated from,

$$\Delta G_{\text{(ads)}} = -RT \ln (55.5K)$$

In which,  $K$  (Equilibrium Constant) =  $\theta / (C (1-\theta))$

Here,  $\theta$  is surface coverage, and  $C$  is the concentration of inhibitor (benzoxazine + urethane).

### EIS Experiments

The inhibition efficacy of all blank and coated samples was calculated by using the below formulae and data are exhibited in Table-2.

$$\text{Corrosion Efficiency (\%)} = [(R_{\text{ct(c)}} - R_{\text{ct(b)}})/(R_{\text{ct(c)}})] \times 100$$

Where  $R_{\text{ct(c)}}$  and  $R_{\text{ct(b)}}$  are the charge transfer resistances for the uncoated and coated MS samples respectively.

## RESULTS AND DISCUSSION

### NMR Spectrum of the Monomer

Nuclear magnetic resonance spectrophotometer analysis was used to confirm the structure of the monomer. For the confirmation of monomer structure, both spectroscopic techniques ( $^1\text{H}$  and  $^{13}\text{C}$ -NMR) were employed. Two peaks at 9.8 ppm and 3.1 ppm are corresponding to the carbonyl and methoxy protons,

<sup>13</sup>C NMR spectrum of compound 1. The x-axis represents the chemical shift in ppm, ranging from 0 to 200. The spectrum shows several peaks, with the most prominent one at approximately 77 ppm, which is the solvent peak (CDCl<sub>3</sub>). Other labeled peaks include: 151.122, 149.919, 148.943, 134.014, 133.607, 133.300, 127.725, 79.744, 77.465, 77.162, 76.962, 58.105, 55.058, 43.791, 43.542, 41.280, and -27.616.

### The IR spectrum of VaBz and VaBz-PU Blends

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attributed to the -C-N- bond stretching in the amide functional group. Finally, this study concludes the structural characterization of both monomer and polymeric composites.

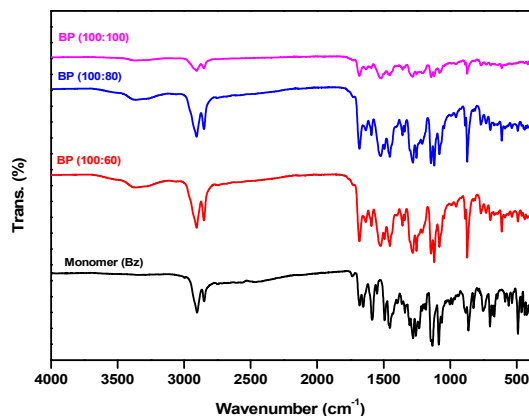


Fig-2: FT-IR Spectra of the Monomer and its Co-polymer in a Solid State at Room Temperature

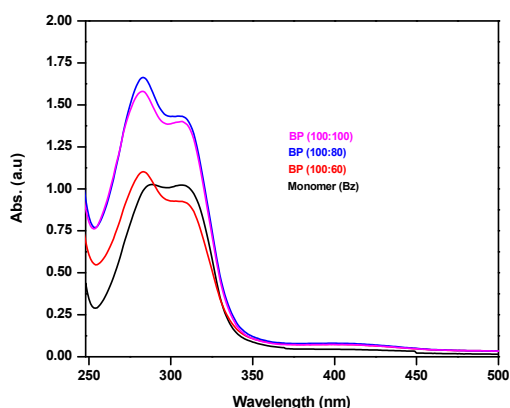


Fig-3: UV-Visible Spectra of the Monomer and Its Co-Polymer in Water at Room Temperature

### UV-Vis Spectrum of VaBz Monomer and VaBz-PU Blends

The electronic transition of the organic molecules is used to analyze, by electronic spectroscopy which is also known as UV-visible spectroscopy. Figure-3 shows the UV-visible spectra of the monomer and polymer composites recorded in the water at room temperature. Monomer exhibits a couple of soft-edged bands at 288 and 306 nm which are attributed to the  $\pi$ - $\pi^*$  electronic transitions; also, an additional band obtained with very poor absorbance at 405 nm is due to poor  $n$ - $\pi^*$  electronic transition. An alteration was observed in the  $\pi$ - $\pi^*$  band while the polymerization of urethane. Thus, the lower wavelength band gets improved whereas the band at a higher wavelength (306 nm) gets demised. Moreover, the band corresponding to the  $n$ - $\pi^*$  transition also enhanced its absorbance which indicates that polyurethane has induced the electronic transition of the monomer remarkably, thereby it could expect that synthesized copolymers may display better activity against corrosion.

### Corrosion Studies

#### Potentiostatic Polarization Measurements

Figure-4 displays the Tafel polarization curves for monomer and polymeric materials  $I_{\text{corr}}$  and  $E_{\text{corr}}$  were determined. By superimposing a straight line along the linear component of the cathodic or anodic curve, the current density was calculated, and projecting it via corrosion potential is calculated. These calculated parameters are exposing an anti-corrosive property of the material. In general, more corrosion current ( $I_{\text{corr}}$ ) indicates that the material offers more electron movement thus leading to a higher corrosion rate. Besides, more positive corrosion potential corresponds to a less corrosion rate. On the other hand, more negative potential and a higher current value of corrosion represent poor anti-corrosive activity which means materials possess higher corrosion rates.<sup>45</sup>

The collective data for the Tafel experiment for all materials including blank was given in Table-1. We can see from the Table, the blank itself shows that a high corrosion rate. Here, urethane-loaded compounds get improved in both  $E_{\text{corr}}$  and  $I_{\text{corr}}$  values. The 60 % loaded material attained  $I_{\text{corr}}$  and  $E_{\text{corr}}$  values of  $3.2 \times 10^{-4} \mu\text{A}$  and 174.01 mV respectively which is enhanced by loading 80 % urethane.

Table-1: Parameter Calculated from the Tafel Experiment

| Sample<br>(BZ: PU) | $I_{\text{corr}}$ ( $\mu\text{A}$ ) | $E_{\text{corr}}$<br>(mV) | Corrosion<br>Rate (mmpy) | Surface<br>Coverage<br>( $\theta$ ) | Corrosion<br>inhibition<br>Efficiency (%) | Tafel Constant<br>(mV/dec) |           | $\Delta G$ (ads)<br>KJ/mol |
|--------------------|-------------------------------------|---------------------------|--------------------------|-------------------------------------|-------------------------------------------|----------------------------|-----------|----------------------------|
|                    |                                     |                           |                          |                                     |                                           | $\beta_a$                  | $\beta_c$ |                            |
| Blank<br>(100: 0)  | $4.0 \times 10^{-3}$                | 109.60                    | 46.51                    | ----                                | ---                                       | 235.3                      | 190.6     | ----                       |
| 100: 60            | $3.2 \times 10^{-4}$                | 174.01                    | 3.72                     | 0.9211                              | 92.00                                     | 181.1                      | 239.8     | -12.75                     |
| 100: 80            | $5.2 \times 10^{-5}$                | 236.38                    | 0.60                     | 0.9870                              | 98.70                                     | 206.5                      | 237.4     | -20.97                     |
| 100: 100           | $2.5 \times 10^{-5}$                | 224.55                    | 0.29                     | 0.9937                              | 99.37                                     | 276.7                      | 497.1     | -22.52                     |

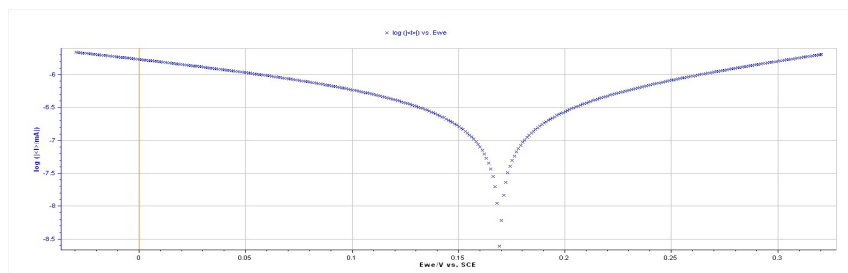


Fig.-4a: Blank

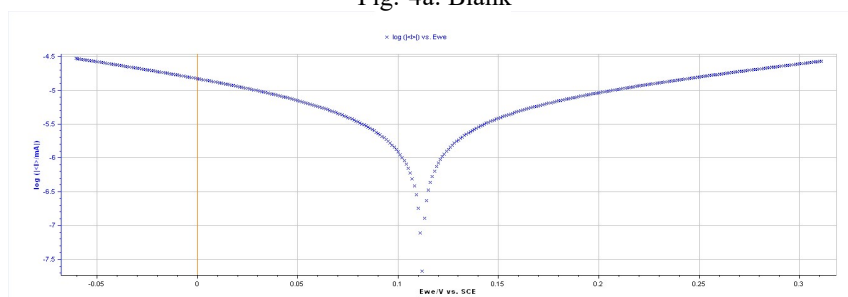


Fig.-4b: 100: 60

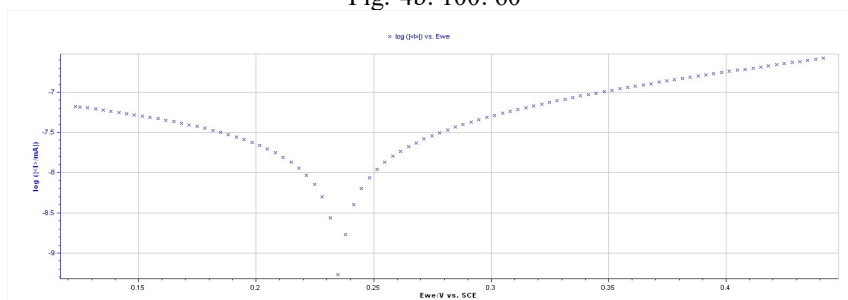


Fig.-4c: 100: 80

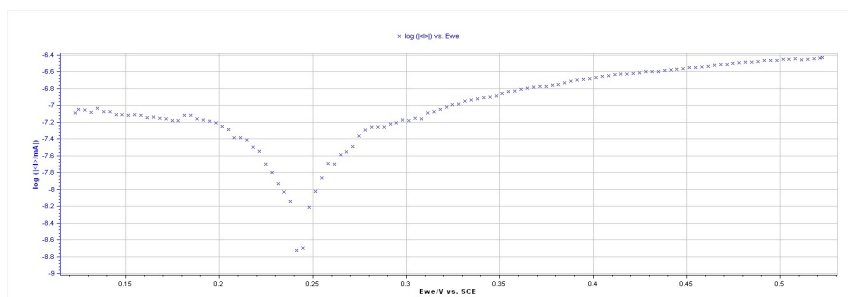


Fig.-4d: 100:100

Fig.-4: Tafel Polarization of the Blank (4a) and all Synthesised Co-Polymers (4b- 4d) Coated Samples

A usual observation has been obtained for the last two high-loaded urethane, that is maximum loaded material shows two times higher  $I_{\text{corr}}$  value thus leading to corrosion efficiency. Apart from this, 100 % urethane-loaded material having almost 100 % corrosion inhibition efficiency and lower content of urethane has attained 92 % corrosion inhibition efficiency. Additionally, the speed of the corrosion was also calculated, results indicate that blank having a higher corrosion rate that could be manipulated by loading the urethane, leads to a reduced corrosion reaction speed significantly. Finally, a compound having 100 % urethane displays better corrosion inhibition activity with a poor corrosion rate i.e., 0.29 mmpy.

### Electrochemical Behaviours of the BZPU Coatings

EIS technique is one of the finest methods to find out the resistivity of the materials, hence, this method was employed in the present synthesized materials (bare MS and coated MS) at room temperature. The EIS

spectra were recorded for all samples which are immersed in a 3.5% sodium chloride solution. Figure-5 displays a Nyquist plot, a depressed capacitive semicircle observed at a higher frequency range and an inductive loop obtained in the lesser frequency region are two-time constants. The earliest one is corresponding to the charge transfer of the corrosion, whereas the later one, is attributed to the tracing out of an intermediate product, formed during the corrosion reaction. Here also, corrosion inhibition efficiency has been calculated by using obtained charge transfer resistance value of uncoated and coated MS. This resistance value can be derived from the diameter of the semicircle obtained in the Nyquist plot. A further factor called the capacitance of the double layer (Cdl), can forecast how well the electrochemical properties of materials will perform. To mimic the impedance behavior of the electrical double layer, the constant phase element (CPE) in the model is used as a simulation in place of the ideal electrical capacitance. It can be explained by the exponential co-efficient and frequency-independent constants denoted by  $n$  and  $Y$  respectively in the CPE's expression. The capacitance of the double layer values is shown in Table-2, thus showing that blank gives less value and it could be increased for all other samples. The increasing value of Cdl for all samples is attributed to the increase in local dielectric constant and/or a decrease in electrical double-layer thickness.<sup>46</sup> Even though samples are reducing, the electrical double-layer, resistance has become a key factor in determining the material's corrosive properties.

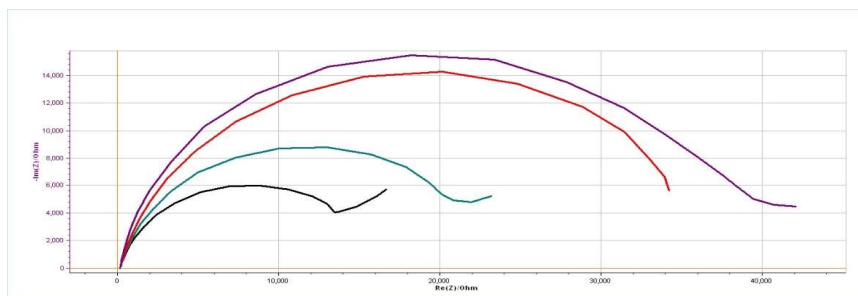


Fig.-5: EIS Studies of the Monomer and Its Co-Polymer Using Three Electrode System in 35% NaCl Solution

Table-2: Data Obtained from the EIS Studies

| Sample (BZ: PU) | Rct $\Omega\text{cm}^2$ | Cdl F/cm <sup>2</sup> | Inhibition Efficiency (%) |
|-----------------|-------------------------|-----------------------|---------------------------|
| Blank (100:0)   | 370.00                  | $0.21 \times 10^{-6}$ | -----                     |
| 100:60          | 1160.00                 | $0.24 \times 10^{-6}$ | 68.10                     |
| 100:80          | 1980.00                 | $0.27 \times 10^{-6}$ | 81.31                     |
| 100:100         | 6800.00                 | $0.81 \times 10^{-6}$ | 94.55                     |

The obtained results show, that blank having poor resistance thus leads to more corrosion rate observed in the EIS experiment. Whereas, urethane addition makes more resistance as compared to blank and the quantity of urethane also improves anti-corrosive behavior. The increasing number of urethanes from 60 to 100 % leads to a parallel increment of resistance from 1160 to 6800  $\Omega\text{cm}^2$ . The calculated inhibition efficiency shows that the significant amount of urethane in the materials improved from 68.1% to 94.55 % for 100:100 Bz-PU. This whole experiment strongly suggests that the synthesized polymeric compound could able to protect the mild steel effectively.

### Scanning Microscopic Analysis

The corrosion efficiency of the synthesized polymeric materials is examined and studied clearly with blank mild steel. The results are sightseen in Fig.-6, it seems clear that plain mild steel gets affected by the corrosion and thus shows a highly rough surface area while a smooth surface was visualized for the before corrosion experiment.

This corrosion has been reduced by the coating of the developed polymeric materials. In particular, the corrosion was significantly reduced by increasing the amount of polyurethane. For instance, sample 100-60 shows a polished surface compared to the blank after corrosion and this can be further improved by the sample which is coated with 80 percent polyurethane-containing material (100-80). Furthermore, almost nil rough surface of the mild steel was obtained for the 100 percent polyurethane coated sample which is reflected nearly as before corrosion material. This could conclude that more polyurethane contains material

exhibits better anti-corrosive properties on mild steel. In addition, SEM-EDAX analysis for all studied samples also proved that the presence of iron materials and data are shown in Fig.-7.

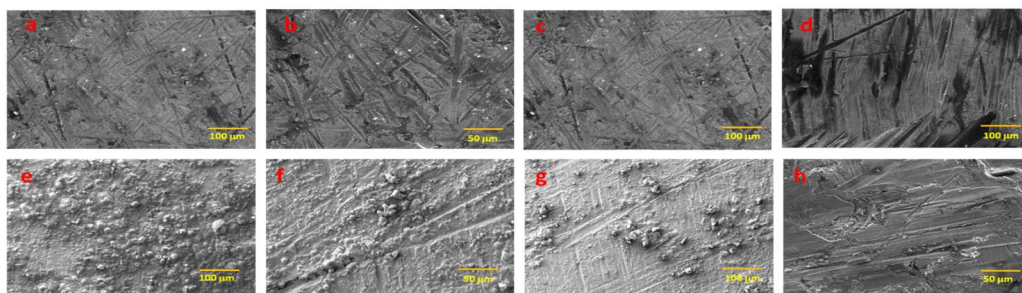


Fig.-6: SEM Images of the Before (a-d) and After (e-h) Corrosion of Samples of Blank (a & e), Sample 100-60 (b & f), Sample 100-80 (c & g) and Sample 100-100 (d & h)

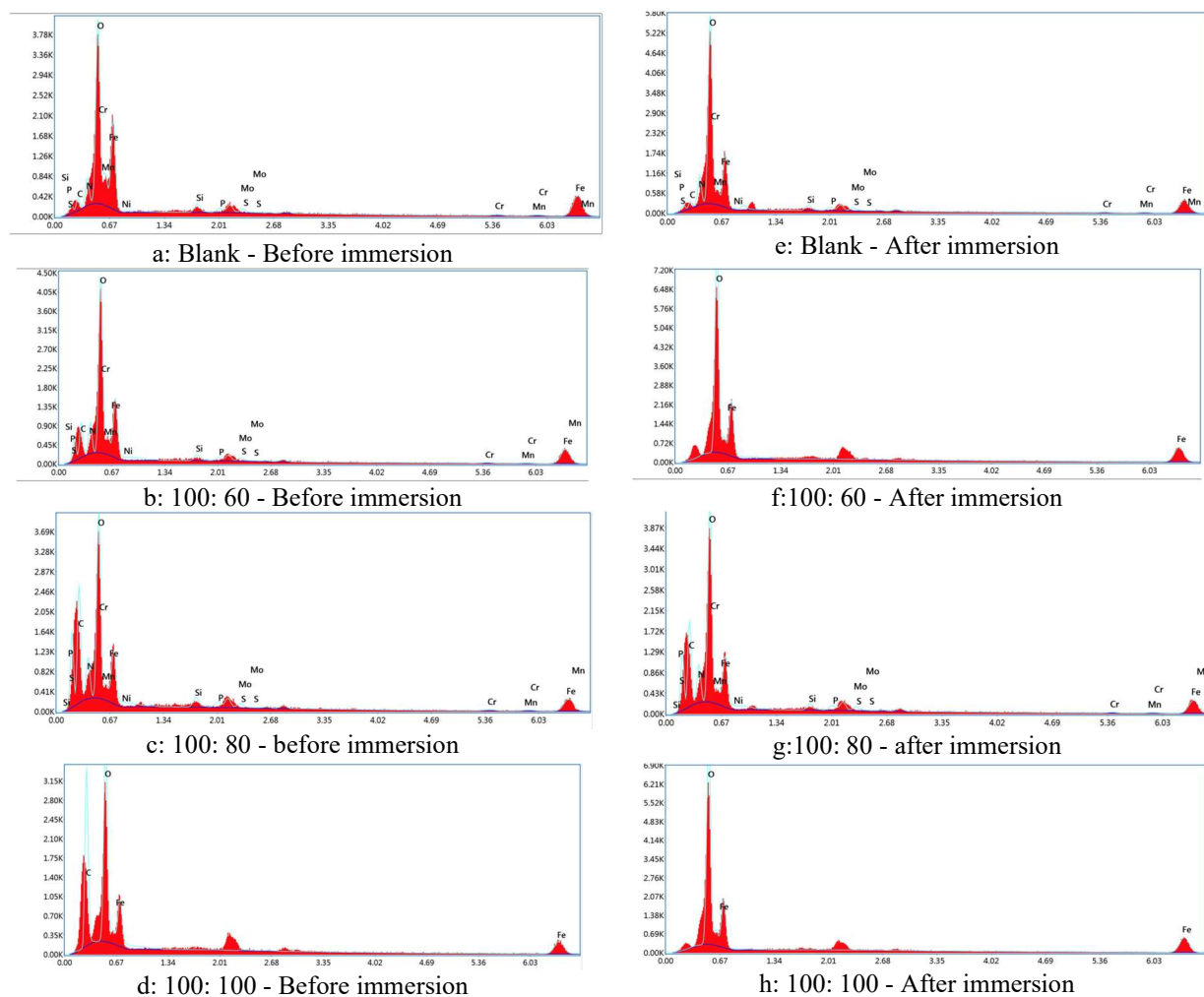


Fig.-7: EDAX Images of the before (a-d) and after (e-h) Corrosion of Samples of Blank (a & e), Sample 100-60 (b & f), Sample 100-80 (c & g) and Sample 100-100 (d & h)

### Water Adsorption Studies

A key factor in the development of polymeric materials for anti-steel corrosion is their hydrophobic character. The branching and cross-linkage density of polymeric materials may influence their hydrophobic properties. This characteristic was also influenced by the coating's binder activity, which led to the formation of materials with a higher cross-density-polymer content and a greater capacity for hydrogen bonding. As a result, urethane content may enhance the polymer's hydrophobic properties, raising the

possibility that more urethane-containing polymers may have lower water adsorption than the competitors. Figure-8 displays the water diffusion of all polymeric compounds as well as monomers. The amount of water diffusion in that monomer alone (1.12%) is smaller than previously reported. This fantastic outcome can be due to the adamantane ring, which increases the hydrophobicity of the entire molecule. The percentage of water diffusion decreases with the amount of urethane used in the polymeric material, reaching a maximum of 0.72% for BZ: PU 100. This study shows that the physical properties of the urethane and adamantane ring significantly contribute to the improvement of water diffusion restriction.

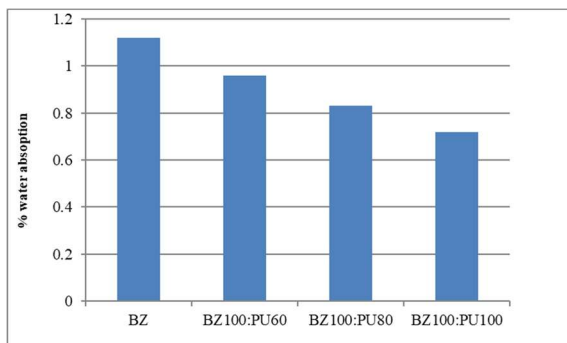


Fig.-8: Water Diffusion Experiment with all Polymeric Material and Monomer BZ.

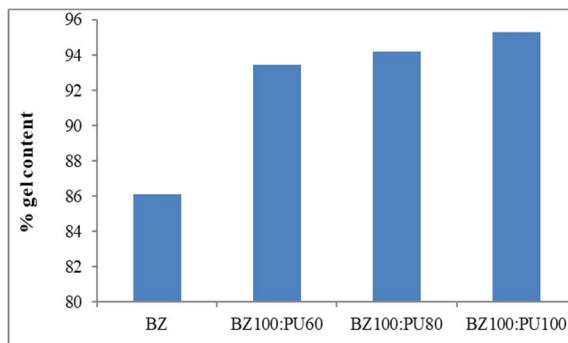


Fig.-9: Gel Formation Experiment with all Polymeric Material and Monomer BZ.

### Gel Formation Studies

Like water diffusion studies, gel formation is also an important study that could be directly correlated with each other. Materials having the capacity to make more strong intra-linkages between them that can also reduce the porosity of the molecule lead to more gel formation and reduce water diffusion. Henceforth, all the polymeric and monomer materials were examined, and the results are presented in Fig.-9. Monomer BZ has almost 87 % ability to form a gel which is greatly improved by urethane quantity. The 60 % urethane shows 93 % gel formation and it's upgraded to 2 points hike with 100 % urethane material. The better gel formation of all compounds except monomer thus, indicates that all polymeric materials could explore its anti-corrosive property.

### Quantum Chemical Calculations

#### DFT analysis

Density functional theory (DFT) analysis is a mathematical computing method this can be effectively used in various disciplines such as synthetic chemistry, reaction coordinates, and bio-analytical applications.<sup>47</sup> The excited state and ground state molecular orbitals are contributed significantly thus called frontier molecular orbitals (FMO). These orbitals could provide details of the electronic structure of the molecule and the electron cloud location on the molecule. Simply, the highest occupied molecular orbital is called HOMO and the lowest unoccupied molecular orbital is called as LUMO.<sup>48</sup> In the present studies, HOMO and LUMO were identified in the same part of the molecule, i.e., that is benzoxazine ring whereas adamantane doesn't show any electron density itself (Fig.-10). This is due to the aliphatic ring thereby having no chance for the presence of pi-electrons leading to poor electron density. The significance of this energy level could be useful for finding out several parameters which are relevant to the electronic property of monomer. The calculated parameters are tabulated in Table-3, wherein, the band gap obtained is 4.2654eV, and other parameters such as chemical potential, global hardness, global softness, and electrophilicity are calculated using the following formulae.

Table-3: Parameters Calculated from DFT Studies

| S. No | Compound name | HOMO    | LUMO    | Band gap(ΔE) | Chemical potential | Global hardness | Global softness | Electrophilicity index |
|-------|---------------|---------|---------|--------------|--------------------|-----------------|-----------------|------------------------|
| 1.    | VaBz(A)       | -5.9899 | -1.7244 | 4.2654       | -3.8571            | 2.1327          | 0.2344          | 3.4879                 |

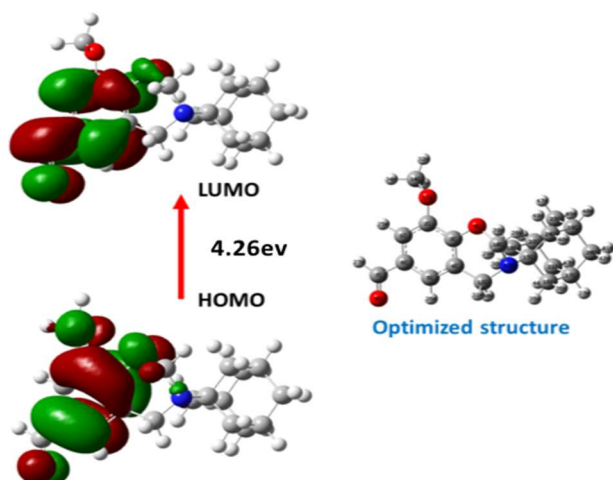


Fig.-10: FMO Analysis of The Synthesised Monomer with Its Optimized Structure using the DFT method.

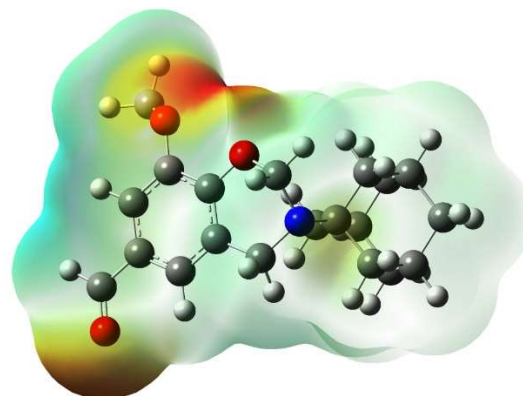


Fig.-11: Molecular Electrostatic Potential Mapping of the Synthesised Monomer Compound.

The positive electrophilicity indicates the more electronegative character of the molecule likewise, chemical potential value also strengthens the same through its observed more negative value. Similarly, other parameters such as global hardness and global softness also suggest better activity of a compound that might be involved in rigid interaction with steel plates after polymer synthesis.

### Molecular Electrostatic Potential (MEP)

The reliable quantum chemical method used for generating the data for this study and results could be more significant to realize and estimate the chemical reactivity of the molecules.<sup>49</sup> The optimized structure of the compound which used from the previous method and here a positive, negative, and neutral electrostatic potential was identified by the color. In this way, instantly, the probability of the electron distribution on the molecule surface has been visualized. The more negative potential could be donated by the red color, oppositely, the green color is used to suggest more positive potential. The blue color is representing no electron potential or neutral potential of the molecule.<sup>50</sup> In the present scenario, red color was obtained where oxygen atoms are present in the molecule which is spotted in the benzoxazine part of the molecule. Meantime, adamantane's attached nitrogen atom also shows yellowish color which indicates the moderate negative potential of the compound. On the other hand, the whole aromatic ring suggests that neutral potential is represented by green color. The more aliphatic adamantane shows a green shadow thus due to absence of the any moments of the electrons and suggested that no charge on the ring (Fig.-11).

### CONCLUSION

In this work, we report a successful synthesis of a benzoxazine-centered monomer with an extremely hydrophobic adamantane scaffold. Additionally, this is used to develop a co-polymeric material with polyurethane for anti-corrosion purposes. Various concentration of polyurethane containing co-polymer with monomer was synthesized and comprehensively assessed using FT-IR, NMR, and UV-visible spectroscopy. Additionally, some of the physio characterizations were also performed which gave a better idea about water diffusion capacity and gel formation of co-polymers. These results imply that co-polymers are more effective than monomers in the studies of corrosion. Of all three, 100 % loaded polyurethane contains co-polymer and could act as an excellent anti-corrosive agent having almost 100 % corrosion inhibition ability with a dead slow corrosion rate. Thus, could be attributed to the development of a synergic effect between polyurethane and the hydrophobic nature of monomer leads to better results. SEM- EDAX studies also conclude that more polyurethane contains material exhibits better anti-corrosive properties on mild steel.

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## CONFLICT OF INTERESTS

The author declares no conflict of interest.

## AUTHOR CONTRIBUTIONS

All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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