

Limits and developments in organic inhibitors for corrosion of mild steel: a critical review (Part two: 4-aminoantipyrine)

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Abstract

The control of mild steel corrosion is of technical, economic, environmental and aesthetic importance. One of the best options is to use inhibitors to protect mild steel from corrosion. Some organic corrosion inhibitors are toxic to the environment, as they are degradable but have the advantage of not containing heavy metals. The toxicity of some organic inhibitors has led to a search for green corrosion inhibitors or non-toxic organic compounds that may be derived from a natural product. Plant products are inexpensive, readily available, and renewable, in addition to being environmentally friendly and acceptable. Investigations into the corrosion inhibition capabilities of 4-aminoantipyrine and its derivatives are of interest as it is the basis for the manufacture of many drugs and pharmaceutical products. Recently, scientists have started using 4-aminoantipyrine as a promising inhibitor. Reports regarding the mechanisms of the 4-aminoantipyrine adsorption process and the mechanism of corrosion inhibition are still unclear, although substantial research has been devoted to preventing corrosion by 4-aminoantipyrine. The development of computational modeling which supported by experimental results will help fill this void and help to understand the mechanism of action of 4-aminoantipyrine absorption patterns on the mild steel surface. Thus, the use of theoretical studies will help to develop excellent corrosion inhibitors with an understanding of the mechanisms of inhibition. The present review article limits the use of 4-aminoantipyrine derivatives as anti-corrosive agents.

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1. Introduction

Corrosive environments, are generally utilized in manufacture processing such as cleaning, descaling, pickling, and acidizing, which require the usage of inhibitors for corrosion to inhibit their corrosion attack on mild steel surface [1–8]. Corrosion is characterized as the

gradual deterioration of the properties of metals induced by the chemical reaction and/or the electrochemical reaction with the atmosphere around it [9]. Galling, wear, and corrosion are categorized as physical metal decay. Instead, Fontana describes corrosion as a reverse extractive metallurgy process, which occurs because the basic metal types are less thermodynamically stable compared to their corresponding ores [10]. The natural consequence of their temporary subsistence in the metallic state may be the actuation that routes the metals undergo corrosion. The machine needs a necessary energy feed to achieve this metallic shape from its original state (ores), which has been reversed later by means of corrosion progression [11]. The exposure of materials to acidic environments is more common and frequent in the oil and gas industry than in neutral or alkaline environments [12, 13]. This requires exploring options and effective methods for mitigating and controlling the corrosion of the various steel types as they constitute a large fraction of the metallic materials exposed to acidic media. Mild steel is often used as construction material in industries, and when exposed to aggressive environments, it is vulnerable to corrosion attacks. Corrosion mitigation approaches adopted by some sectors include, among others, the selection of materials, coatings and linings, cathodic protection, and the use of corrosion inhibitors [14–17]. In combating corrosion, the use of corrosion inhibitors is the most practical and cost-effective method. Corrosion inhibitors retard corrosion by adsorbing and blocking one or more of the electrochemical reactions occurring at the solution/metal interface on the low carbon steel surface. Organic compounds, including imidazolines, amides, amines, and their derived salts, are well-known corrosion inhibitors [18]. In their structures, these organic compounds typically contain nitrogen, sulfur and oxygen, and hydrophobic chains of hydrocarbons. However, inhibitors are usually effective in a certain environment only for a specific material [19], but the corrosion environment is highly variable; therefore, an inhibitor working in one well may not work in another [20]. Therefore, new formulas for different environments need to be continually developed [21] and numerous compounds have been designed [22]. Organic compounds alone are also generally not sufficiently effective and a proper blend containing additional intensifiers, surfactants, and solvents is required [23]. In organic molecules, the functional groups impart corrosion inhibition [24]. 4-Aminoantipyrine is known for the variety of its clinical applications such as anti-inflammatory, analgesic, antipyretic [25, 26], and several chemotherapeutic agents [27]. It is evident from the reported literatures that compounds possessing pyrazole nuclei showed significant anthelmintic as well as antimicrobial activities [28–30]. The life of mechanical hardware is established by good corrosion control. Corrosion inhibitors have become more important nowadays due to their use in industries. Chemical inhibitors are considered much more natural than organic inhibitors. Organic inhibitors decrease the rate of corrosion by absorbing phosphorus, sulfur, oxygen, nitrogen atoms, or pi-bonds on the surface of the metal through the active sites [31]. Quantum chemical computations based on density function theory (DFT) have recently become a strong theoretical research method for researchers to examine the ability of organic molecules to inhibit corrosion. This tool provides a glimpse at physical insights into the mechanisms of corrosion inhibition [32–37].

Various natural compounds explored as natural corrosion inhibitors for mild steel in a hydrochloric acid environment. However, literature reviews about 4-aminoantipyrine and derivatives as corrosion inhibitors for mild steel, in a hydrochloric acid environment are discussed here. A comprehensive review of the usage of various types of 4-aminoantipyrine (Figure 1) as corrosion inhibitors for mild steel is reviewed. The available deficiency and the futurity domain of research in this direction have also been demonstrated in the current study.

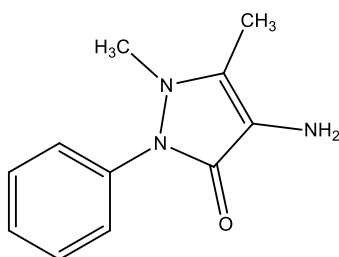


Figure 1. 4-Aminoantipyrine.

2. Corrosion inhibition of mild steel by natural or organic synthetic compounds

In the literature concerning the corrosion inhibition actions of natural or organic synthetic compounds for mild steel, there are a large number of reports available. In the literature concerning the corrosion inhibition action of natural or organic synthetic compounds for mild steel, there are a large number of reports available. Many organic compounds have been used as corrosion inhibitors for the corrosion of mild steel in various acid environments. The role of 4-aminoantipyrine derivatives as corrosion inhibitors on mild steel alloys and scientific advances are a major focus of the present work. The aim of this study is to review the literature centered on mild steel benign inhibitors and to review the possible inhibition mechanism of the inhibition property, *etc.*

2.1. Corrosion inhibition of mild steel by organic synthesized compounds

Corrosion inhibitors are of considerable practical significance because they are widely used to reduce metallic waste during manufacturing and to minimize the risk of material failure, both of which can lead to the sudden shutdown of industrial processes, resulting in additional costs [68]. To prevent metal dissolution and minimize acid consumption, it is also essential to use corrosion inhibitors [39–41]. Organic compounds that contain atoms of nitrogen, sulfur and oxygen are the majority of well-known acid inhibitors. The inhibitory effect of organic compounds on the dissolution of metallic species is usually associated with interactions of adsorption between inhibitors and the surface of the metal [42, 43]. 1,5-Dimethyl-4-((2-methylbenzylidene)amino)-2-phenyl-1*H*-pyrazol-3(2*H*)-one (DMPO) as in Figure 2, was synthesized to be considered as an inhibitor for corrosion of mild steel.

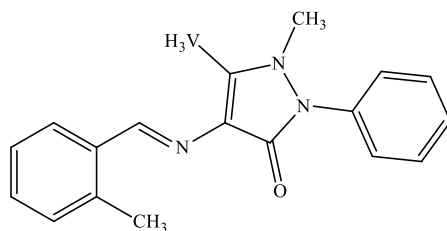


Figure 2. The chemical structure of DMPO.

Electrochemical impedance spectroscopy (EIS), potentiodynamic polarization, open circuit potential (OCP) and electrochemical frequency modulation were used to investigate the corrosion inhibitory effects of DMPO on mild steel at 1.0 M HCl (EFM). The results showed that DMPO prevented mild steel corrosion in the acid solution and suggested that with increasing inhibitor concentration, the inhibition efficiency improved. Impedance parameter changes meant that DMPO was adsorbed onto the mild steel surface, resulting in the creation of protective films. It measured and addressed electronic properties such as maximum occupied molecular orbital energy, lowest unoccupied molecular orbital energy (E_{HOMO} and E_{LUMO} , respectively) and dipole moment (μ). The results showed that the efficiency of corrosion inhibition increased with an increase in E_{HOMO} values and with a decrease in E_{LUMO} [44]. Two pyrazole carboxamides called 5-(4-(dimethylamino)phenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazole-1-carboxamide DPC-1 and (*E*)-5-(4-(dimethylamino)phenyl)-3-(4-(dimethylamino)styryl)-4,5-dihydro-1*H*-pyrazole-1-carboxamide DPC-2 shown in Figure 3 behaved as corrosion inhibition of mild steel in hydrochloride acid solution using weight loss measurements, Tafel polarization curves, and electrochemical impedance spectroscopy (EIS). The results obtained show that DPC-1 and DPC-2 are effective corrosion inhibitors in a solution of 1 mol·L⁻¹ HCl. As the concentration of inhibitors increases, the inhibition efficiency increases to 84.56% at 4·10⁻⁴ mol·L⁻¹ and 80% at 1.6·10⁻⁴ mol·L⁻¹ for DPC-1 and DPC-2 at 303 K, respectively.

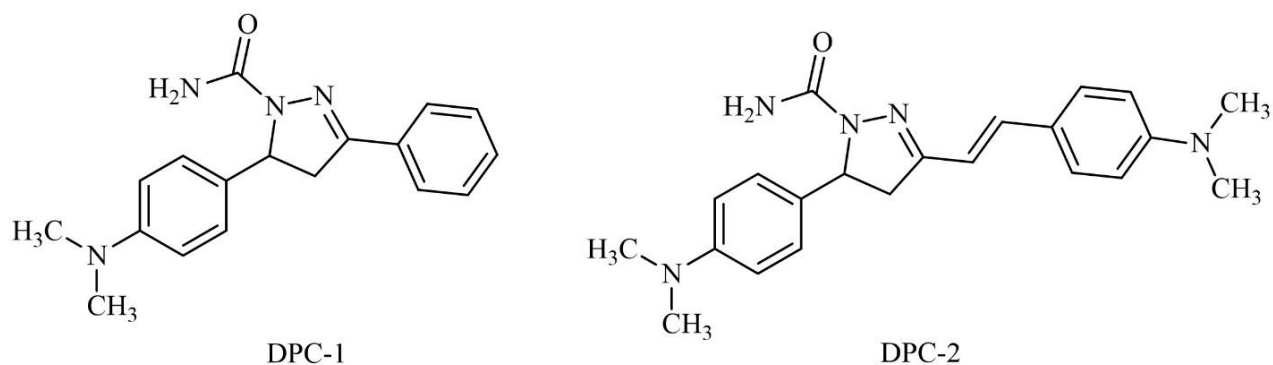


Figure 3. The chemical structures of DPC-1 and DPC-2.

Using DFT calculations [45], the relationship between the inhibition efficiency of the pyrazol parameters was investigated. For the first time, the synthesis and characterization of

a novel organic corrosion inhibitor (4-(3-mercapto-5,6,7,8-tetrahydro-[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazin-6-yl)phenol) has been successfully documented as shown in Figure 4 for mild steel in 1 M hydrochloric acid (HCl).

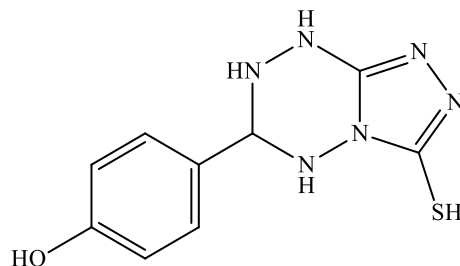


Figure 4. The chemical structure of 4-(3-mercapto-5,6,7,8-tetrahydro-[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazin-6-yl)phenol.

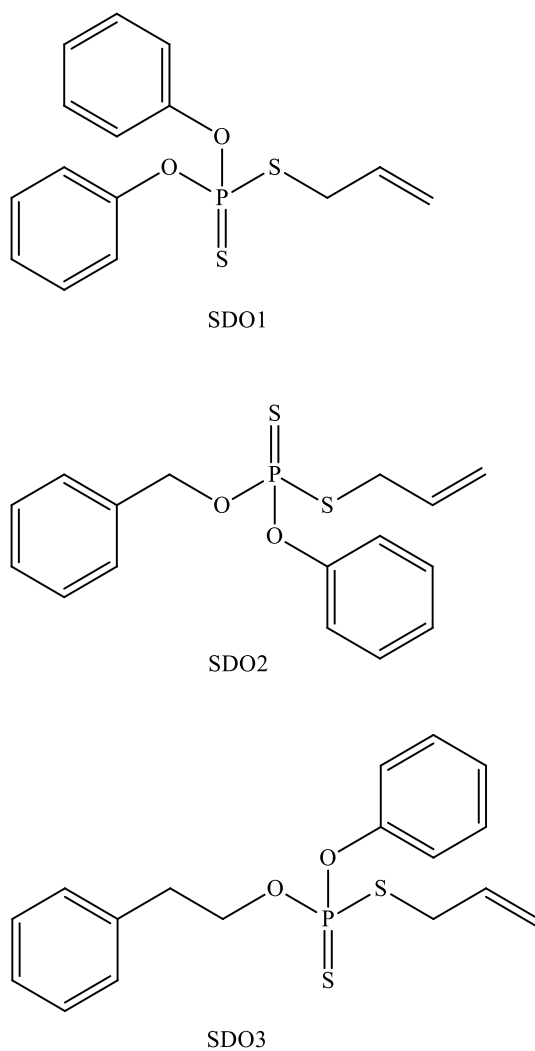


Figure 5. The chemical structures of SOD1, SOD2, and SOD3.

The inhibitor was tested in 1 M of hydrochloric acid solution using electrochemical impedance spectroscopy (EIS) and electrochemical frequency modulation (EFM) measurement techniques as a corrosion inhibitor for mild steel. The results show that the efficacy of inhibitions increased with increasing inhibitor concentrations and decreased with the temperature. Up to 67% maximum inhibition efficiency at a maximum concentration of 0.5 mM was reached. This demonstrates that these inhibitors are effective in helping to minimize and slow down the corrosion process of mild steel with a solution of hydrochloric acid by supplying mild steel with an organic inhibitor that can be weakened by increasing the temperature [46]. *S*-allyl-*O,O'*-diphenyldithiophosphate (SOD1), *S*-allyl-*O,O'*-dibenzylthiophosphate (SOD2) and *S*-allyl-*O,O'*-di(2-phenylethyl)dithiophosphate (SOD3), as shown in Figure 5, was successfully synthesized and characterized by electrochemical measurements, weight loss calculation and scanning electron microscopy, acting as novel corrosion inhibitors for mild steel in hydrochloric acid (HCl) solution.

Measurement of potentiodynamic polarization suggests that the synthesized inhibitors are effective inhibitors of mixed forms. As inhibitor concentration increases, the inhibition efficiency increases, HCl concentration decreases, and temperature increases. The mild steel surface adsorption of SOD1 and SOD3 is a mixed adsorption involving both physisorption and chemisorption, and the mild steel surface adsorption of SOD2 belongs to chemical adsorption [47]. Using weight loss measurements, corrosion inhibition of mild steel in 0.5 M hydrochloric acid by six synthesized heterocyclic compounds was tested. The efficiency of inhibition exceeded 95%. The excellent performance of the inhibitor was due to the formation on the steel surface of defense adsorption films. To explain the inhibition process, quantum chemical calculations were also adopted [48]. Using electrochemical impedance spectroscopy (EIS), potentiodynamic polarization, open circuit potential (OCP) and electrochemical frequency modulation, the acid corrosion inhibition process of mild steel in 1 M HCl by azelaic acid dihydrazide was investigated (EFM). Studies of potentiodynamic polarization suggest that dihydrazide azelaic acid (Figure 6) is a mixed-type inhibitor. With increased inhibitor concentration, the inhibition efficiency increases and reaches its maximum of 93 percent at $5 \cdot 10^{-3}$ M.

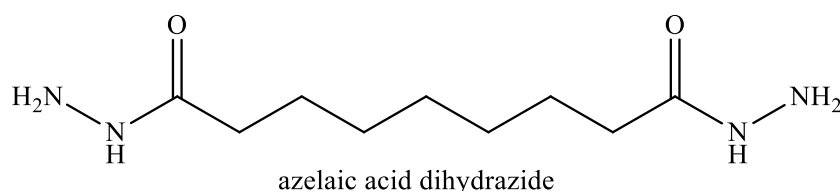


Figure 6. The chemical structure of azelaic acid dihydrazide.

Langmuir's adsorption isotherm describes the adsorption of the inhibitor on a mild steel surface. The effect of temperature on corrosion behavior in the presence of an inhibitor of $5 \cdot 10^{-3}$ M was studied in the 30–60°C temperature range. The results showed that the efficiency of inhibitions increased with an increase in inhibitor concentration and decreased

with an increase in temperature [49]. New research was reported in which two novel corrosion inhibitors BP-1 and BP-2 were synthesized (Figure 7) and their corrosion inhibition properties on mild steel (MS) in acid solution were evaluated by weight loss and electrochemical corrosion techniques.

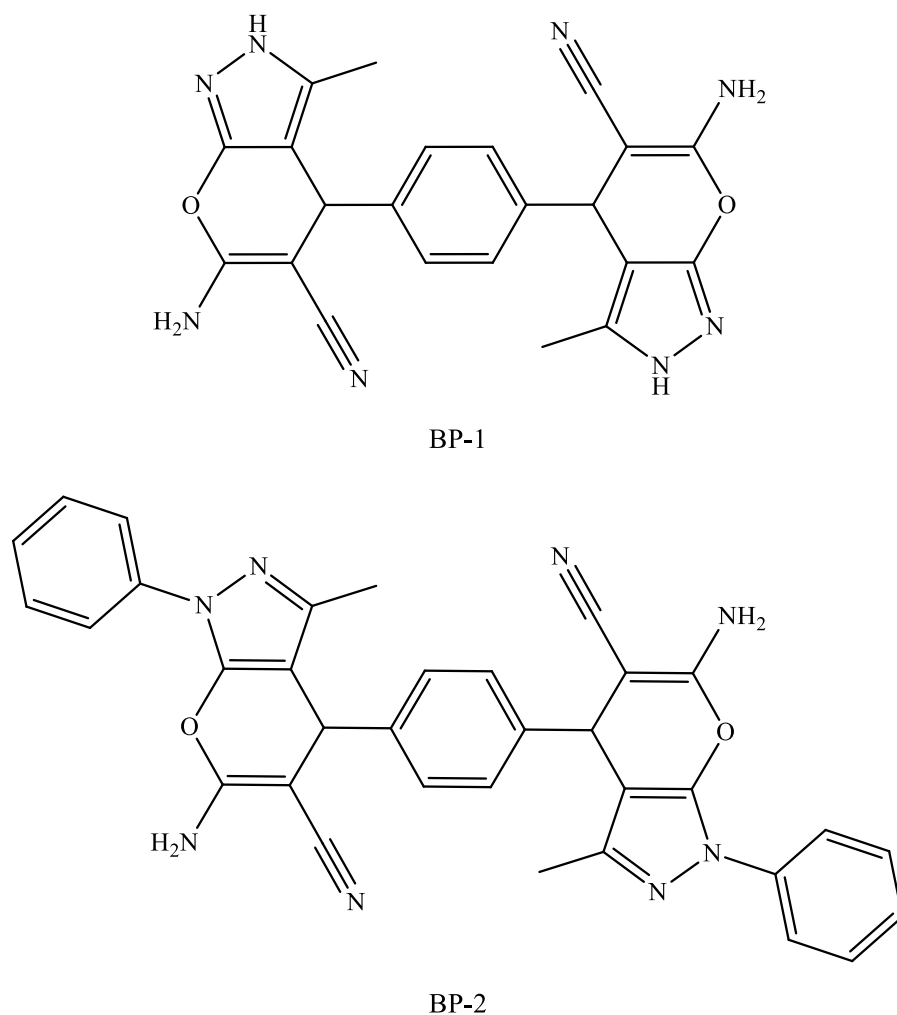


Figure 7. The chemical structures of BP-1 and BP-2.

The corrosion test results show that both compounds inhibit corrosion through an adsorption mechanism and demonstrate more than 95 percent inhibition efficiency at a low concentration of $1.72 \cdot 10^{-4}$ M. Simulated evidence from density functional theory helps link the experimental pattern with the theoretical analysis [50].

2.2. Corrosion inhibition of mild steel by 4-aminoantipyrine derivatives

Researchers from a wide variety of industrial sectors have drawn attention to studies on the prevention of steel corrosion in acidic environments and the problematic chemical processes that arise [51]. For steel, corrosion is a common problem and directly affects its cost and protection. Mild steel corrosion can cause structural damage and alter the mechanical and

chemical properties of plants, vessels, tubes, and other processing equipment. These results indicate that if an appropriate remedy from its analysis and testing is not found, corrosion will generate considerable costs. In different industries, the prevention of steel corrosion has played an important role, especially in the chemical and petrochemical processing industries that use steel. The inhibiting action of 4-aminoantipyrine (Figure 8) and its Schiff bases 4-[(benzylidene)-amino]-antipyrine (Figure 8a), 4-[(4-hydroxy benzylidene)-amino]-antipyrine (Figure 8b) and 4-[(4-methoxy benzylidene)-amino]-antipyrine (Figure 8c) which are derived from 4-aminoantipyrine with benzaldehyde, salicylaldehyde and anisaldehyde, toward the corrosion behavior of mild steel in 1 M HCl solution was studied using weight loss, potentiodynamic polarization, electrochemical impedance and FT-IR spectroscopic techniques. Although AAP was found to retard the corrosion rate of mild steel, the synthesized Schiff base compounds were seen to retard the corrosion rate very effectively. The inhibitor efficiencies calculated from all the applied methods were in good agreement and were found to be in the order: **a** > **b** > **c** > 4-aminoantipyrine [52].

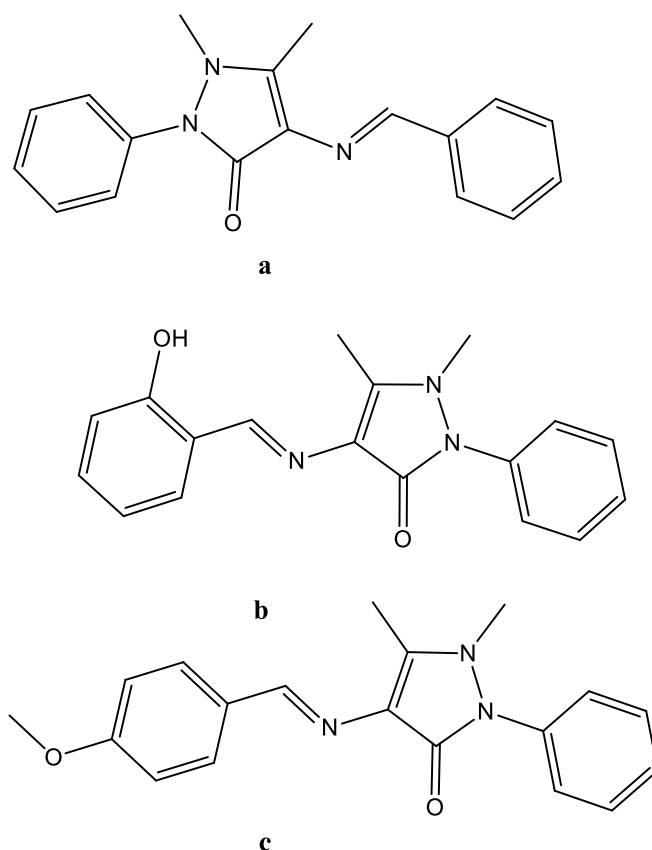


Figure 8. The chemical structures of 4-aminoantipyrine derivatives (a–c).

The inhibitive effect of newly synthesized 4-aminoantipyrine Schiff base derivative (**d**) (Figure 9) against steel and its adsorption behavior were investigated in 2 M HCl solution using weight-loss method, potentiodynamic polarization, electrochemical impedance spectroscopy (EIS) and electrochemical frequency modulation (EFM) techniques. The

results showed that the inhibition efficiency increased with the increase of the inhibitor concentration. The derivative (**d**) is a mixed-type inhibitor whose adsorption behavior onto steel can be well fitted by Temkin isotherm equation. The quantum chemistry was used to gain some insight, about structural and electronic effects in relation to the inhibiting efficiency. EIS spectra exhibit one capacitive loop and confirm the inhibitive ability.

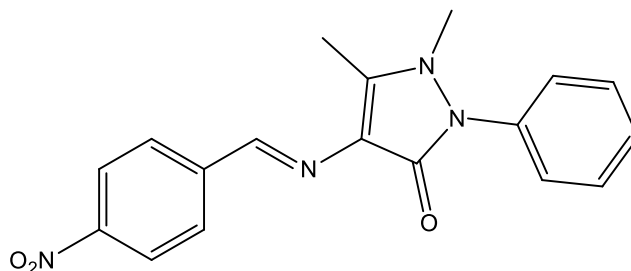


Figure 9. The chemical structure of 4-nitroantipyrine derivative (**d**).

The corrosion of zinc in phosphoric acid containing 4-aminoantipyrine has been studied at different acid concentrations, inhibitor concentration and temperatures. Corrosion increases with the concentration of acid and the temperature. Inhibition efficiency (*I.E.*) of 4-aminoantipyrine increases with the concentration of inhibitor and decreases with the increase in concentration of acid. As temperature increases, percentage of inhibition decreases. The plot of $\log(\theta/1-\theta)$ versus $\log C$ results in a straight line suggest that the inhibitors cover both the anodic and cathodic regions through general adsorption following Langmuir isotherm. Galvanostatic polarization curves show polarization of both anode as well as cathode [54].

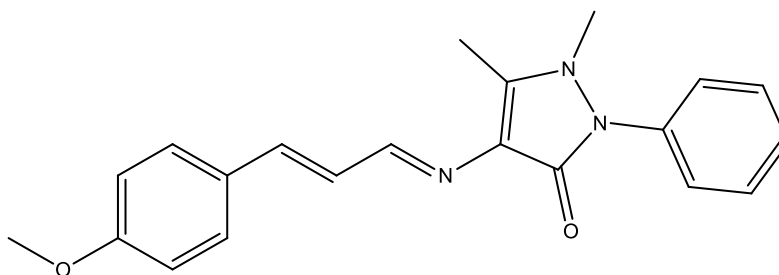


Figure 10. The chemical structure of TMCATP.

The corrosion inhibition of steel in 1 M HCl in the presence of the synthesized Schiff base, 4-[3-(4-Methoxy-phenyl)-allylideneamino]-1,5-dimethyl-2-phenyl-1,2-dihydropyrazol-3-one (TMCATP), was studied by potentiodynamic polarization (PDP), electrochemical impedance spectroscopy (EIS), surface analyses and computational studies. The inhibition efficiency of TMCATP obtained at the optimum inhibitor concentration (1.0 mM) from polarization measurement was 97.0%. The value of inhibition efficiency obtained *via* the electrochemical analyses for the inhibitor was comparable. The data from polarization measurement implies the TMCATP operated as a mixed-type inhibitor in the

tested media but mostly minimized the cathodic reaction. The data obtained experimentally fitted well into Langmuir adsorption isotherm with R^2 values and slopes close to unity. The results of DFT calculations showed that the molecules had high tendency to interact with the steel surface. The value of energy gap (eV) obtained was 3.58 while the estimated adsorption energy obtained from molecular dynamic simulation studies was $-951.9 \text{ kJ}\cdot\text{mol}^{-1}$ for TMCATP [55].

3. DFT

Quantum chemical methods have already proven to be very helpful in evaluating the molecular structure as well as in elucidating the electronic structure and reactivity that could be realistic in the quantitative structure-activity relationship (QSAR) approach for the design of novel high-efficiency inhibitors [56–59]. These quantum-chemical computational simulations based on DFT of acceptable models have increasingly made this prevailing method available to corrosion scientists for theoretical corrosion inhibition mechanism investigation. Using a variety of quantum chemical descriptors, such computations have been commonly used to examine the molecular electronic structures of a wide range of adsorption-type inhibitors, which have provided valuable physical insights into corrosion inhibition mechanisms [60]. The efficiency of inhibition is therefore associated with the molecular and structural parameters that can be accomplished through theoretical calculations such as chemical selectivity, reactivity, and distribution of charges. The frontier molecular orbital, HOMO (higher occupied molecular orbital) energy, LUMO (lower unoccupied molecular orbital) energy, chemical potential and hardness, electronegativity, and a number of electron transfers are other quantum chemical effects, among others. The main objective of computational corrosion inhibitor research is to gain insight into the mechanisms by which the metal-corrodent interaction is retarded by inhibitors applied to a fluid aggressive environment. Indeed, the efficacy of the overall process depends on the surface of the metal, the corrosive media, the molecular and electronic structure, and the inhibitor concentration, as well as the temperature. and other environmental considerations [61]. The frontier molecular orbital of some corrosion inhibitors namely DMPO, and azelaic acid dihydrazide were postulated in Figure 11.

A molecule's ability to donate electrons to the free d orbital of metal is correlated with the energy of the highest occupied molecular orbital (HOMO). Compounds are more capable of donating electrons with higher EHOMO. The energy of the lowest unoccupied molecular orbital (LUMO) is linked to the ability of the metal to receive electrons. Lower values show a greater propensity to accept electrons. Furthermore, positive values are associated with chemisorption, whereas negative physisorption values are associated with chemisorption [62]. The energy gap is another important parameter:

$$\Delta E = E_{\text{HOMO}} - E_{\text{LUMO}}$$

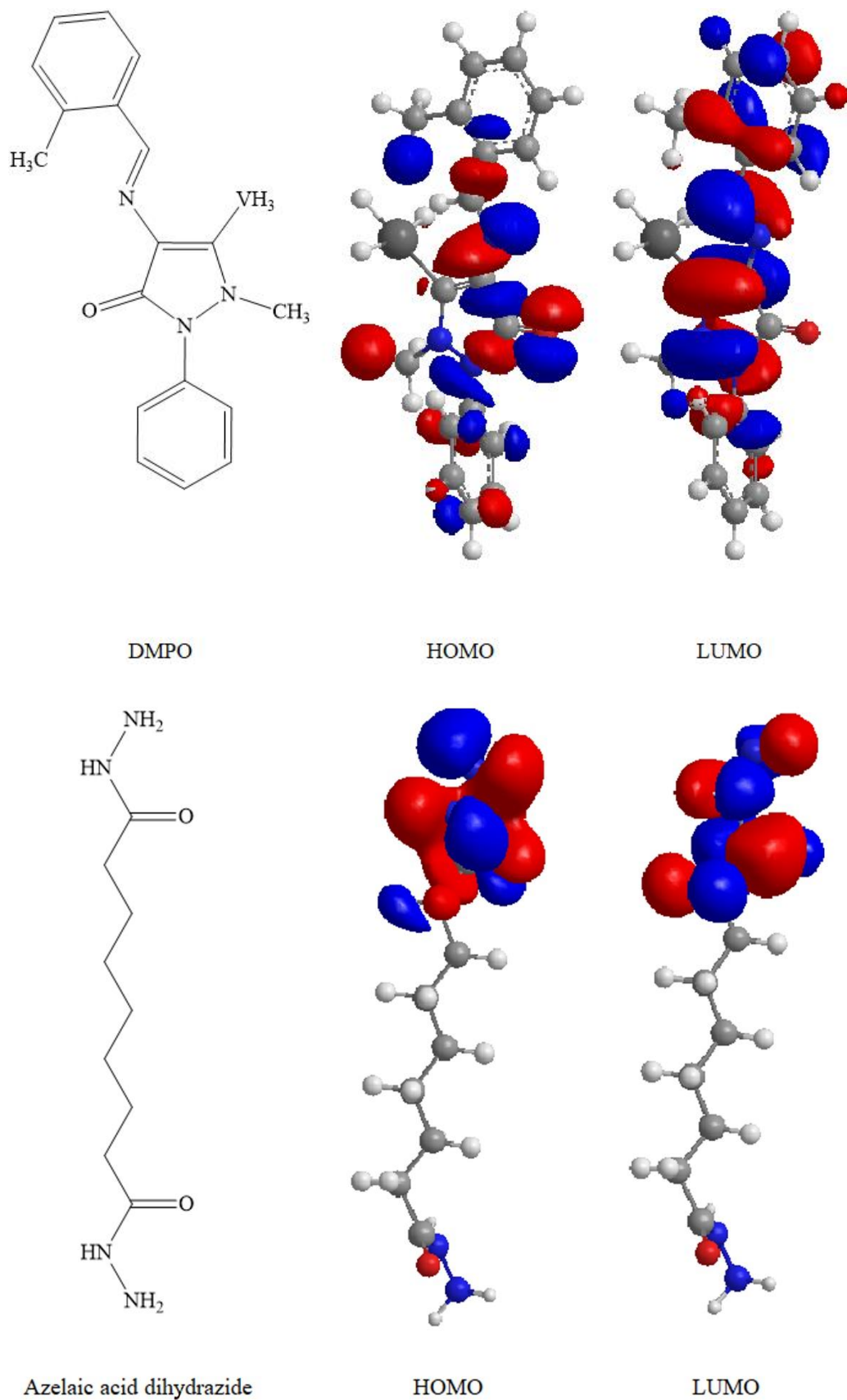


Figure 11. The HOMO and LUMO MOs for DMPO and azelaic acid dihydrazide.

The lower E , the more reactive molecule, is associated with increased adsorption of inhibitor molecules to the surface of the metal [63]. A significant parameter which gives information about polarity in a bond is also the dipole moment (μ). As the value of μ increases, corrosion inhibition performance increases due to stronger dipole–dipole interactions with the metal surface, resulting in stronger adsorption and effective inhibition of corrosion [64]. Information on the resistance of a molecule to charge transfer and on the capacity of a molecule to receive electrons is given by chemical hardness (η) and softness (σ). They are evaluated based on these equations:

$$\eta = -\frac{E_{\text{HOMO}} - E_{\text{LUMO}}}{2}$$

$$\sigma = \frac{1}{\eta}$$

The higher σ value means that the molecule is weaker and has a greater propensity to donate electrons to the metal [65]. For the measurement of ionization potential (I_P) and electron affinity (E_A), the energy of HOMO and LUMO orbitals can be used using the following equations:

$$I_P = -E_{\text{HOMO}}$$

$$E_A = -E_{\text{LUMO}}$$

The determined values are utilized for calculating the electronegativity (χ) [65]:

$$\chi = -\frac{E_{\text{HOMO}} + E_{\text{LUMO}}}{2}$$

The high χ value implies a good ability to draw electrons from the metal, leading to higher interactions and greater protection from corrosion. The last measured parameter is the electron fraction transferred (ΔN):

$$\Delta N = \frac{\chi_{\text{Fe}} - \chi_{\text{in}}}{2(\eta_{\text{Fe}} + \eta_{\text{in}})}$$

where χ_{Fe} equals 7 eV and $\eta_{\text{Fe}} = 0$.

If $\Delta N > 0$, the electrons are passed to the metal from the molecule and if $\Delta N < 0$, to the molecule from the metal. For the compounds tested, the electron fraction values were transferred if the transmission from the metal to the molecules was negative [66–71].

As an example (Figure 12) for theoretical studies herein theoretical calculations with all parameters for 4-benzyl-1-(4-oxo-4-phenylbutanoyl)thiosemicarbazide (BOT) have been postulated. To calculate the ground-state geometries, Gaussian 03, Revision C.01 was optimized to a local minimum without symmetry restrictions using the valence and polarization basis set (6-31G++(d,p)). A combination of the Becke three-parameter hybrid (B3) exchange functional and the Lee–Yang–Parr (LYP) correlation functional (B3LYP), a

version of the (DFT) method was used in gas phase to determine all optimized geometries, HOMO energies (E_{HOMO}), LUMO energies (E_{LUMO}) and physical properties [72].

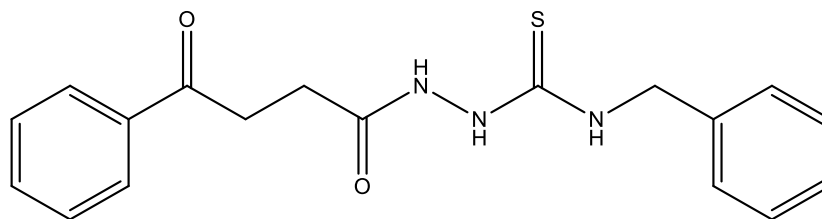


Figure 12. The structure of BOT.

The results demonstrate that BOT low ΔE value (2.608 eV) and is thus the most reactive molecule [73]. The polarity is determined by the dipole moment. The polarity of a molecule is proportional to its dipole moment [74]. The orbital electron energies were spread uniformly across the molecules, according to the BOT's HOMO and LUMO diagrams (Figure 13).

The global hardness (η), softness (σ), electronegativity (χ), and the fraction of electron transfer (ΔN) collectively describe the dynamic parameters that are calculated as presented in Table 1. In the estimation of the specified chemical parameters, Koopmans Theorem [75] presents excellent abilities to theoretical and computational researchers. Based on this theory, the values of electron affinity and ionization energy of chemical species are connected with values of E_{HOMO} and E_{LUMO} .

The principle of hard-soft acid and base (HSAB) [76, 77] presented by Pearson declares that “hard acids prefer to coordinate to hard bases and soft acids prefer to coordinate to soft bases.” As can be understood from Pearson classification, nitrogen-containing structure contributes its electrons readily to d-orbital of iron atoms on the surface of mild steel [78]. As a result, the soft molecule has adsorption capability owing to its easier electron transfer and excellent corrosion inhibitor than the hard one. As per Lukovit's research, when the number of electrons transmitted (ΔN) is less than 3.6, the inhibitory effectiveness as a function of electron transfer improves [79]. The better the corrosion inhibitor, the higher the electron transfer fraction (ΔN).

Table 1. Quantum chemical parameters of BTO.

E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE ($E_{\text{HOMO}} - E_{\text{LUMO}}$)	η	σ	χ	ΔN	μ (D)	$IE\%$
-7.284	-4.676	-2.608	1.304	0.7668	5.98	0.3911	7.0311	96.2

* $IE(\%)$ value was calculated from weight loss measurement.

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