

# Case Study in a Conceptual DFT Investigation of New Corrosion Inhibitor

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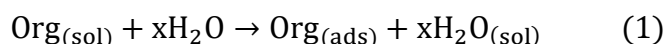
**Abstract:** Inhibition efficiency of thiosemicarbazide derivative, namely 4-ethyl-1-(4-oxo-4-phenylbutanoyl)thiosemicarbazide (EOPT) on corrosion of mild steel, was investigated utilizing the density functional theory (DFT) modeling techniques in the aqueous phase. Chemical parameters at the quantum level, such as energies of highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), dipole moment ( $\mu$ ), absolute electronegativity ( $\chi$ ), global hardness ( $\eta$ ), softness ( $\sigma$ ), and the fraction of electrons transferred ( $\Delta N$ ) have been determined at the B3LYP level of theory with 6-31G (d, p) basis set.

**Keywords:** corrosion inhibition; DFT; simulation; mild steel; thiosemicarbazide derivative.

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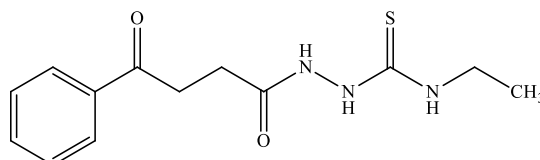
## 1. Introduction

Mild steel is a popular choice due to its inexpensive cost and ease of supply. Acids are used in various applications, including pickling, boiler cleaning, descaling, and oil well acidification. Corrosion inhibitors are commonly used to reduce the undesirable dissolution of base metals resulting from these processes [1-14]. The association between the structure of the inhibitor and its sorption properties has been the subject of studies on organic corrosion inhibitors. It has been discovered that the adsorption of inhibitor molecules is significantly influenced by physical and chemical features such as functional groups, esterifying agents, odors, the electron density in donor atoms, and the pi orbital nature of donor electrons [15-23]. It also depends on the electrical structure of the molecules. As a result, the efficiency of an organic compound is largely determined by its ability to adsorb on the metal surface [24-31]. Displacement of water molecules adsorbed by inhibitor species leads to selective adsorption of the inhibitor on the metal surface, which leads to corrosion inhibition (Equation 1).



Moreover, experimental procedures are expensive and time-consuming; as a result, the process of lighting wear usually suffers. Computer simulation has become a useful tool for investigating complex corrosion resistance systems due to advances in software and technology. The corrosion mechanism is now fully understood by examining the structure, electron distribution, and molecular adsorption on metal and oxide surfaces [32]. In 1971, Vosta and Eliasek [33-35] established the topic of quantum corrosion electrochemistry by introducing quantum chemical approaches to research corrosion blocking. Subsequently, the primary goal of quantitative chemical approaches was to identify and establish relationships

between molecular structure and activity, and many useful results have since been published. Quantitative chemical analysis has long been shown to be useful in determining the structure of molecules, interactions, and apparent electronic structures [36-38]. As a result, the computation of the chemical corrosion investigation to evaluate the efficiency of corrosion inhibitors with the help of mathematical modeling using chemical compounds to find compounds with preferred properties based on experience in mathematical quantum and the relationship between molecular structure once it is computed and worked. Found, any number of compounds became normal practice. Those not yet synthesized can be easily tested using a computational approach [39-48] and a set of mathematical equations that accurately display the chemical incident under investigation. The inhibitive characteristics of the 4-ethyl-1-(4-oxo-4-phenylbutanoyl)thiosemicarbazide (Figure 1) have been studied on the mild steel utilizing energies of highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), dipole moment ( $\mu$ ), absolute electronegativity ( $\chi$ ), global hardness ( $\eta$ ), softness ( $\sigma$ ), and the fraction of electrons transferred ( $\Delta N$ ) as quantum chemical parameters. The current investigation found that the DFT method can be efficiently utilized to screen organic corrosion inhibitor molecules preparatory to experimental analysis.



**Figure 1.** The chemical structure of the studied inhibitor.

## 2. Materials and Methods

### 2.1. Computational details.

The optimized molecular structure of PMO molecule was geometrically by DFT method with the 6-31G (d, p) basis set. Gaussian 09 software was used. The quantum electronic parameters of the most stable conformers were calculated of the DFT. HOMO, LUMO,  $\Delta E$ ,  $\eta$ ,  $\sigma$ ,  $\chi$ , and  $\Delta N$  were calculated using equations (2-6) [49, 50].

$$\Delta E = E_{\text{HOMO}} - E_{\text{LUMO}} \quad (2)$$

$$\eta = -\frac{E_{\text{HOMO}} - E_{\text{LUMO}}}{2} \quad (3)$$

$$\sigma = \frac{1}{\eta} \quad (4)$$

$$\chi = -\frac{E_{\text{HOMO}} + E_{\text{LUMO}}}{2} \quad (5)$$

$$\Delta N = \frac{\chi_{\text{Fe}} - \chi_{\text{inh}}}{2(\eta_{\text{Fe}} + \eta_{\text{inh}})} \quad (6)$$

where  $\chi_{\text{Fe}}$  and  $\eta_{\text{Fe}}$  were 7 eV/mol and 0 eV/mol, respectively.

## 3. Results and Discussion

### 3.1. Quantum chemical calculations.

The global molecular interaction was investigated using the study of frontier molecular orbitals (FMO) in terms of the interaction between the frontier orbitals, including HOMO and LUMO. The ability of a molecule to donate electrons is referred to as EHOMO. As a result,

large EHOMO values aid electron transport to an acceptor that has an empty orbital. LUMO energy, on the other hand, relates to a molecule's ability to receive electrons. The inhibitory efficacy improves when EHOMO values climb. High EHOMO values imply that a low-energy empty molecular orbital molecule tends to give electrons to the right acceptor molecules. Absolute stiffness is a key parameter in molecular interaction and stability research. The softest base inhibitors are the most effective in eroding the softest materials, according to published studies; according to Wu *et al.* [51], 's damper sections with higher smoothness and lower hardness are helpful. The tendency of an atom in a molecule to attract electrons is described by its electronegativity. As a result, electrons from a lower electronegative molecule will be partially transferred to a greater electronegative molecule (electrons flow from a high chemical potential to a lower chemical potential). Excellent inhibitors contribute electrons to the metal substrate, and thus the electronegativity values are expected to decrease as the inhibitory efficacy improves. In addition, Table 1 summarizes the  $\chi$  value of the current system. The trend in the  $\chi$  value of the respective inhibitor indicates that the tested inhibitor has a low electronegativity. Its adsorption on the surface of mild steel increases due to this process, and its anti-corrosion efficiency improves. Each species' quantity of electrons transported ( $\Delta N$ ) is likewise identified and reported in Table 1. Molecules that have a positive number of transferred electrons ( $\Delta N$ ) are electron donors, while those with a negative number of transferred electrons ( $\Delta N$ ) are electron acceptors [52]. As a result, in the current system, all species operate as electron donors. Corrosion inhibitors with a higher N content have a stronger desire to interact with the metal surface. The tested inhibitor has the highest  $\Delta N$  value according to the  $\Delta N$  value for species. As a result, the best inhibitor is closely associated with the biggest percent of electrons transferred, whereas the lowest fraction is linked to the inhibitor with the lowest inhibitory efficacy [53]. Density function theory (DFT) as a quantitative chemical calculation method can be used to investigate the adsorption capacity of EOPT composite on mild steel surfaces [54]. The adsorption of the investigated inhibitor may be demonstrated by the interactions between the donor and the acceptor (EOPT). On the surface of mild steel, electrons are moved from the highly electronegative centers of organic molecules (oxygen, sulfur, nitrogen, and pi-electrons) to the vacant 3d-orbital of iron atoms. The quantum chemical properties produced from the EOPT optimization molecular structure, as shown in Figure 2 and summarized in Table 1, will be discussed in more detail below. The highest occupied molecular orbital energy represents the investigated compound's electron donating activity (EHOMO).

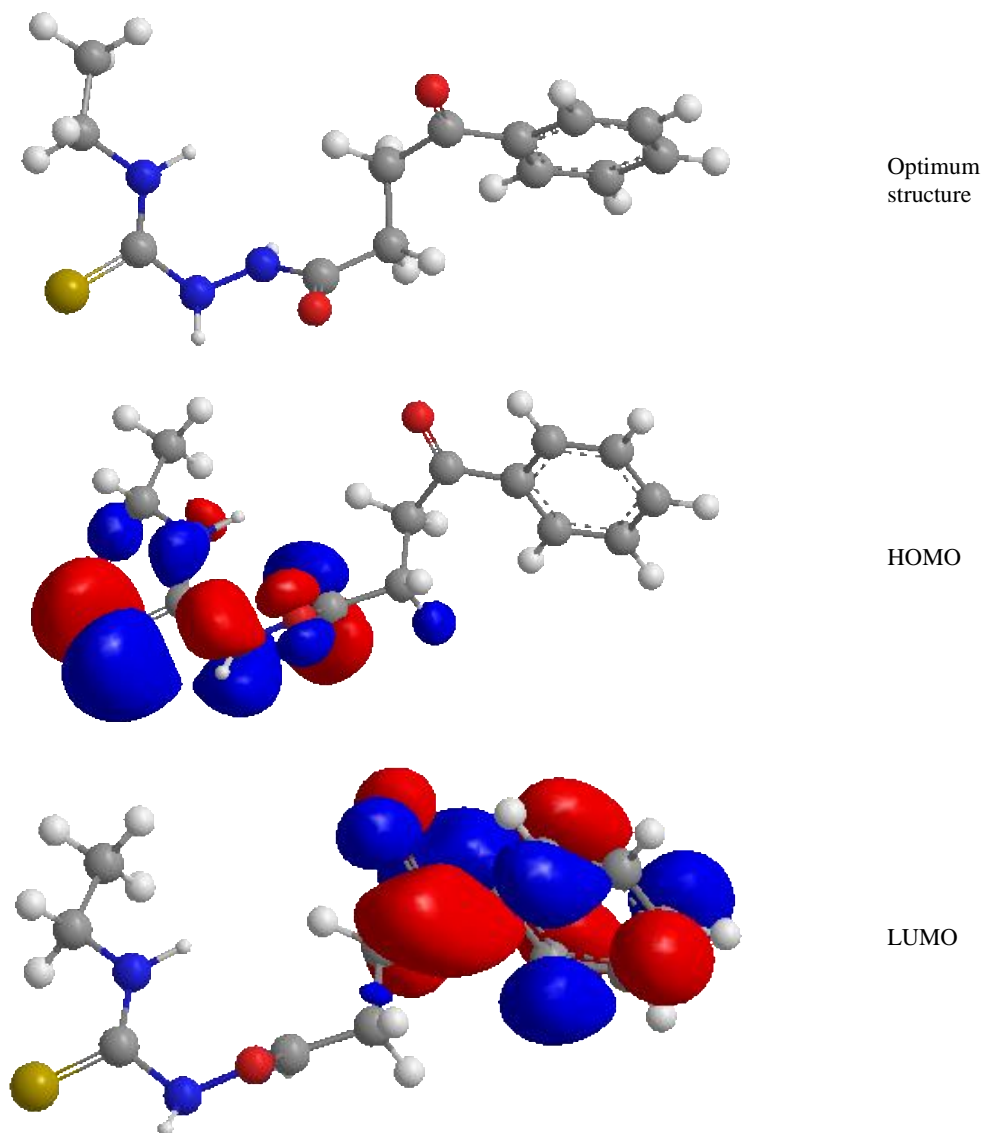
A lower ELUMO value indicates the inhibitor molecules' capacity to absorb electrons from donating the iron backing, hence enhancing the binding energy between the mild steel surface and the inhibitor molecules.

The more successful the adsorption/bonding of the investigated inhibitor with the metallic surface, the higher the HOMO energy value and the lower the LUMO energy value [55].

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The more successful the adsorption/bonding of the investigated inhibitor with the metallic surface, the higher the HOMO energy value and the lower the LUMO energy value [55]. The EOPT molecules aggregate on the mild steel surface when the dipole moment decreases, increasing the adsorption capacity of the EOPT molecules [57]. The global hardness

( $\eta$ ), softness ( $\sigma$ ), electronegativity ( $\chi$ ), and the fraction of electron transfer ( $\Delta N$ ) collectively describe the dynamic parameters that are calculated as presented in Table 1. The soft molecule has a smaller energy gap and higher basicity than the hard one, according to the hard-soft acid-base principle [58]. As a result of its easier electron transfer and better corrosion inhibitor than the hard molecule, the soft molecule possesses adsorption capability. According to Lukovit's research, the inhibitory effectiveness as a function of electron transfer improves when the number of electrons communicated ( $\Delta N$ ) is smaller than 3.6 [59]. The higher the electron transfer fraction ( $\Delta N$ ), the better the corrosion inhibitor. As indicated in Table 1,  $N$  increases as the number of inhibitor molecules increases, indicating that the electroadsorption efficiency is greater. Ionization energy [60] represents the chemical reaction of atoms and molecules.



**Figure 2.** Optimized structure, highest occupied molecular orbital (HOMO), and lowest unoccupied molecular orbital (LUMO).

**Table 1.** Chemical parameters of the studied Inhibitor.

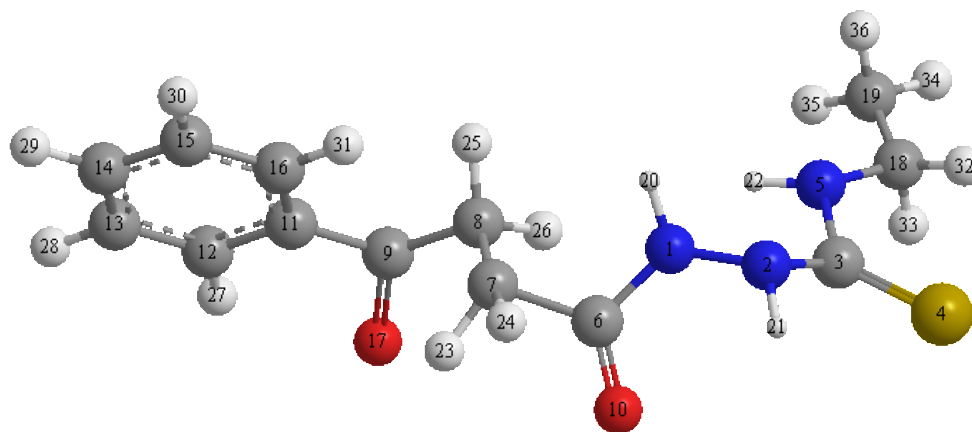
Inhibitor	$E_{HOMO}$	$E_{LUMO}$	$\Delta E$ (eV)	$A$	$I$	$\chi$ (eV)	$\eta$ (eV)	$\Delta N$ (eV)	$\mu$ (D)
EOPT	-8.785	-4.940	3.845	4.940	8.785	6.862	1.922	1.517	4.265

### 3.2. Mulliken charges.

When it comes to determining inhibitor adsorption sites, the Mulliken charge measurement is crucial. As the negatively charged heteroatom becomes increasingly negatively

charged, the ability to be adsorbed on the metallic surface rises. In EOPT, higher negative charges surround nitrogen, sulfur, oxygen, and some carbon atoms, indicating that these are the inhibitors' coordinating sites. The nitrogen connected as N-amide and N-thioamide, on the other hand, shows that the binding sites with higher negative Mulliken charges were chosen. Mulliken charges are summarised in Table 2.

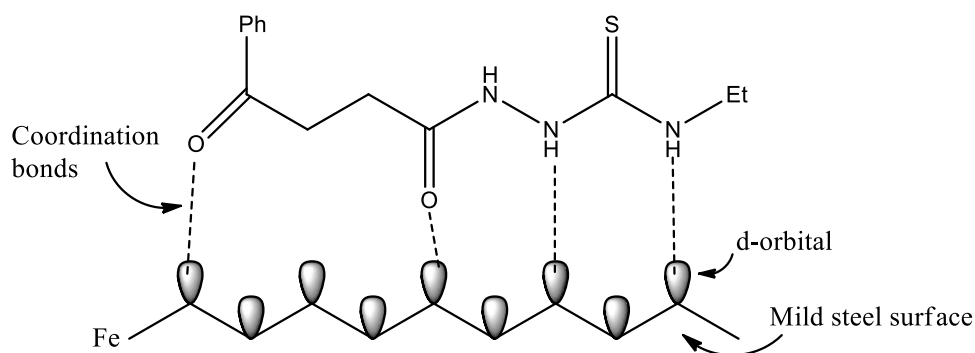
**Table 2.** The Mulliken charges of EOPT molecules.



No.	Atom	Atom type	Mulliken Charges
1	N(1)	N Amide	-0.3415
2	N(2)	N Thioamide	-0.1582
3	C(3)	C Thiocarbonyl	0.0873
4	S(4)	S Thiocarbonyl	-0.2471
5	N(5)	N Thioamide	-0.3011
6	C(6)	C Carbonyl	0.287
7	C(7)	C Alkane	-0.1721
8	C(8)	C Alkane	-0.2055
9	C(9)	C Carbonyl	0.2658
10	O(10)	O Carbonyl	-0.324
11	C(11)	C Alkene	-0.1579
12	C(12)	C Alkene	-0.0709
13	C(13)	C Alkene	-0.142
14	C(14)	C Alkene	-0.096
15	C(15)	C Alkene	-0.1444
16	C(16)	C Alkene	-0.0906
17	O(17)	O Carbonyl	-0.2815
18	C(18)	C Alkane	-0.0365
19	C(19)	C Alkane	-0.232

### 3.3. Suggested mechanism of inhibition.

The initial step in any corrosion inhibition is the adsorption of the inhibitor on the mild steel surface. According to theoretical findings, EOPT is adsorbed on a mild steel surface through a chemical reaction in which unpaired electrons (on the N, S, and O atoms) are transferred from inhibitor molecules (EOPT) to the vacant d-orbital of iron atoms at the mild steel surface, forming coordination bonds, and a very stable complex from inhibitor molecules covers the mild steel surface as a protected layer. The inhibitor is a charged molecule with a strong inductive and extremely strong resonance effect due to the position of the benzene ring and the functional groups thion, carbonyl, and amino. The aromatic ring, which contains thion and carbonyl groups, boosts electron delocalization, making it more reactive. Despite the fact that the carbonyl, thion, and amine (oxygen, sulfur, and nitrogen atoms) each have only one pair of electrons, the inhibitor is preferentially adsorbed onto the metal surface via these functional groups. Figure 3 depicts the proposed chemisorption-based inhibitory mechanism.



**Figure 3.** The suggested inhibition mechanism of EOPT molecules.

#### 4. Conclusions

The corrosion inhibitor 4-ethyl-1-(4-oxo-4-phenylbutanoyl)thiosemicarbazide (EOPT) was explored using DFT theoretical results. The results of the calculations show that the tested inhibitor is a promising and important corrosion inhibitor. At the B3LYP level of theory using the 6-31G (d, p) basis set, quantum chemical parameters such as frontier molecular orbitals (HOMO and LUMO), dipole moment, absolute electronegativity, global hardness, softness, and the proportion of electrons transported have been determined. The results back up the validity of the quantum chemical technique adopted in this research. The investigated inhibitor had the strongest tendency to adsorb strongly onto the metal surface, according to quantum chemical calculations..

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#### Conflicts of Interest

The authors declare no conflict of interest.

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