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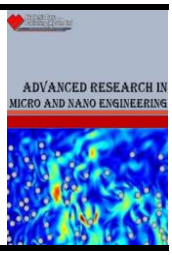

Theoretical Investigation of New Possible Fatty Hydrazides Corrosion Inhibitors Via Density Functional Theory

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ABSTRACT

In this study, two new possible corrosion inhibitors derived from fatty hydrazides were investigated via the density functional theory (DFT) to measure the quantum chemical calculation of these new molecules and analyse their corrosion inhibition ability. The quantum calculation parameters included the calculation for the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) and the energy gap (ΔE_{gap}) between HOMO and LUMO. Other chemical descriptors were also measured, including the global hardness (η), electronegativity (χ), and the fraction of transferred electrons (ΔN). The results revealed that both new possible corrosion inhibitors, TADHS11 and TADHS12, showed excellent chemical reactivity and inhibition efficiency based on the calculation of electronic properties, with band gap energy of 4.35 eV for TADHS10 and 4.18 eV for TADHS11. The other chemical descriptor also revealed similar observations, which agree that these two compounds exhibit excellent corrosion inhibitor properties. Overall, all data were consistent with previously reported findings, proving the ability of these new possible fatty hydrazide derivatives as effective corrosion inhibitors.

1. Introduction

Over the decades, corrosion in pipelines has always been a challenge in many industries. Pipelines are the central circulatory system in all production and processing operations in the oil and gas industry. Oil, produce water and gas are generated from the wells and flow to central points through pipelines and transfer to processing, separation, and refineries facilities [1]. These produced oil, water and gas are always accompanied by various high impurities products such as carbon dioxide, hydrogen sulfide and other corrosive materials that affect the integrity of the pipelines and promote internal corrosion [2].

The use of corrosion inhibitors has been proven in many studies as an effective method of mitigating corrosion. Among many others, organic corrosion inhibitors are the most extensively employed in the chemical, petrochemical, and oil exploration industries [3]. This is because organic compound inhibitors can exhibit their inhibition performance by physically (physisorption) or

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chemically (chemisorption) adsorbed on the metal surface. Therefore, preventing the anodic or cathodic reaction or combination of the two-act as mixed-type inhibitors in corrosive media [4]. Most importantly, they are known to be more environmentally friendly and non-toxic compared to inorganic compounds [5,6]. Hydrazide derivatives are found to be the potential acid corrosion inhibitors of mild steel. Many researchers have studied various hydrazide derivatives and proved their effectiveness in mitigating corrosion [7,8]. Moreover, fatty hydrazides are produced using green technology from a renewable source [9].

In recent years, many studies have focused on using computational studies to develop new corrosion inhibitor molecules to mitigate corrosion with higher inhibition efficiency by modifying the chemical structure, which is highly related to the chemical adsorption ability and the inhibition efficiency. The use of computational simulation, such as density functional theory, DFT, has enabled accurate prediction of stability, chemical reactivity, and inhibition efficiency without using expensive chemicals and time-consuming laboratory testing [10,11]. The ability of corrosion inhibitors typically depends on the electron-donating tendency of the compounds as well as the nature of its interaction with the surface of the metal. These effects can be seen and validated via the quantum chemical calculation of the DFT method. The DFT method will be used to calculate the electronic properties of the inhibitors and establish the relationship between inhibitive effect and molecular structure and predict the most efficient inhibitors. These electronic properties include the energies of the highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbital (E_{LUMO}), the energy gap (ΔE) difference between E_{HOMO} and E_{LUMO}, ionization potential (I), electron affinity (A), global hardness (η), electronegativity (χ) and the number of electrons transferred (ΔN).

The E_{HOMO} and E_{LUMO} are the main values obtained used to calculate all the other parameters and determine the properties related to the reactivity and selectivity of the inhibitors. This is because the interaction between inhibitor and metal is through the donation of the electron from inhibitor occupied orbital (refers to the E_{HOMO}) to the d-orbital of the metal [12,13] and the acceptance of the electrons from the d-orbital of the metal to the unoccupied orbitals (refers to the E_{LUMO}) of the inhibitor. Therefore, the interaction and adsorption of the inhibitors on the surface of the metal will increase with the tendency to donate electrons but vice versa with the ability of the molecule to accept electrons. Meanwhile, the ΔE act as a significant parameter to predict the reactivity of the compounds and the efficiency of the inhibitors [14]. The smaller value of the ΔE indicated small values of energy required to remove an electron from the HOMO of the electron-donating species to the LUMO of the electron-acceptor and make the adsorption of these molecules easier [15].

However, the reactivity of the inhibitors can also be predicted using other parameters. Ionization energy is typically used to describe the chemical reactivity of atoms and molecules. Higher ionization energy represents greater stability and chemical inertness. Meanwhile, global hardness measures molecular stability and reactivity. The smaller the global hardness, the greater the inhibition performance and the polarization rate of the molecules. Electronegativity (χ) calculate the tendency of the molecule to attract electrons. A lower electronegativity value indicates greater electron transfer between the metal and the inhibitor molecules, thus leading to higher reactivity. Finally, ΔN represents the probability of electron transfer from the inhibitors to the metal surface. If the ΔN showed a positive value, meaning that the electron transfer takes place from the inhibitor molecule to the metal surface and vice-versa if the value shows a negative value. When $\Delta N = 3.6$, the inhibitor transfers electrons to the metal surface by forming coordination bonds, but when $\Delta N < 3.6$, the inhibition efficiency increases with increasing ΔN. Therefore, the ΔN values are strongly correlated to the inhibition efficiency as the highest ΔN is associated with the best inhibition efficiency [12,16,17].

It is apparent that the inhibition efficiency of corrosion inhibitors largely depends on the nature of the medium, the metal surface state, and the structure of the inhibitors [18]. Some factors

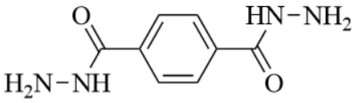
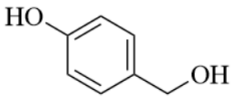
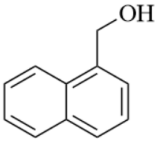
contribute to the action of organic inhibitors, including the chain length, size of the molecule, bonding, aromatic/conjugate, strength of bonding to the substrate, cross-linking ability, and solubility in the environment [19]. These effects can be analyzed using DFT methods. Therefore, two new possible corrosion inhibitors derived from fatty hydrazide compounds were examined to investigate the electronic properties of these two new potential corrosion inhibitors and establish the relationship between inhibitive effect and molecular structure and predict the most efficient inhibitors.

2. Methodology

2.1 Development of New Possible Corrosion Inhibitors from fatty Hydrazide Derivatives

Terephthalic acid dihydrazide was selected as the parent structure for this study due to its chemical composition containing an aromatic ring in the middle of its Gemini structure. These terephthalic dihydrazide will then be modified by adding new functional groups in their terminal chains to further increase their ability to inhibit corrosion. The combination of the selected spacer with two new functional groups will be computationally simulated to study their corrosion inhibition activities and their chemical reactivity. Table 1 listed the selected parent spacer, Terephthalic dihydrazide and two functional groups for the new combinations.

Table 1
New candidates' spacer and substituents for new possible corrosion inhibitors

Chemicals	Structure	Function
Terephthalic dihydrazide (TADH)		Spacer
4-hydroxybenzyl alcohol (S10)		Substituent terminal chain
1-naphthalenemethanol (S11)		Substituent terminal chain

2.2 Density Functional Theory (DFT) Calculation Methods

The density functional theory calculation method has followed the method used previously in a similar study by Mazlan *et al.,* [20]. The TmoleX program was used to conduct the geometry optimization and the subsequent electronic structure calculation of the newly designed combination in the non-aqueous environment using the def-SV(P).h basis set [21,22]. The function of B3LYP and ground state calculation was selected in order to generate the input file under the DFT setting [23, 24], and the program visualized and performed calculations on the molecular electronic structure. The value obtained on the highest occupied molecular orbital energy (HOMO) and the lowest unoccupied molecular orbital energy (LUMO), as well as the energy gap (ΔE), were then used to

calculate the global reactivity parameters such as electron affinity (A), ionization potential (I), electronegativity (χ), global hardness (η) and the fraction of electrons transferred (ΔN).

The calculation for each global reactivity is as stated below. Ionization energy is commonly associated with the HOMO, while electron affinity is related to the LUMO value.

$$I = -E_{HOMO}$$

$$A = -E_{LUMO}$$

To obtain the energy difference between the HOMO and LUMO, the calculation is expressed as below

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

The other parameters, such as global hardness (η), electronegativity (χ), and the fraction of transferred electrons (ΔN), can be calculated as follows

$$\eta = \frac{(I - A)}{2}$$

$$\chi = \frac{(I + A)}{2}$$

$$\Delta N = \frac{[\chi_{Fe} - \chi_{Inh}]}{2[\eta_{Fe} - \eta_{Inh}]}$$

where the electronegativity of metal, $\chi_{Fe} = 7$, and the global hardness of the metal, $\eta_{Fe} = 0$ [25-27].

3. Results and Discussions

3.1 Quantum Chemical Calculation of New Possible Corrosion Inhibitors from Fatty Hydrazides Derivatives

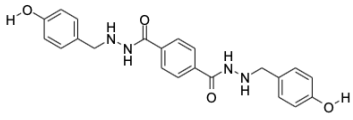
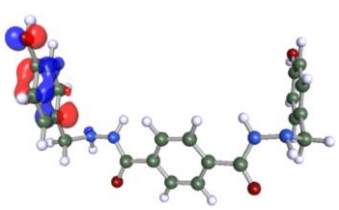
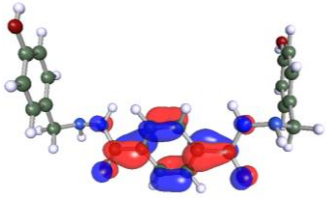
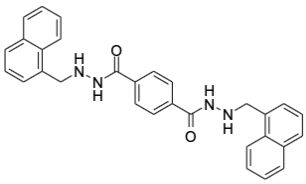
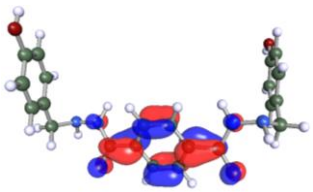
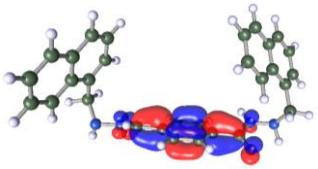
Table 2 reveals the DFT calculations of the new combination between terephthalic dihydrazide with 4-hydroxylbenzyl alcohol (TADHS10) and 1-napthalenemethanol (TADHS11) as substituents. The data indicate that the new combination of fatty hydrazide derivatives with functional groups containing active aromatic groups has further effect in increasing the ability of the molecules to inhibit corrosion. These can be reflected based on the E_{HOMO} and E_{LUMO} calculations obtained for both combinations. For TADHS10, the E_{HOMO} value obtained is -6.05 eV, while the E_{HOMO} value for TADHS11 is -5.94 eV. Both are higher in value, thus associated with a higher ability to donate electrons. On the other hand, the lowest E_{LUMO} values for both combinations, TADHS10 (-1.70 eV) and TADHS11 (-1.75 eV), are related to the highest tendency of both compounds to accept an electron. The lower the E_{LUMO} values, the higher the ability of the compound to adsorb on the metal surface, increasing its ability to inhibit corrosion. Both combinations also have lower energy differences (ΔE), reflecting higher chemical reactivity and binding ability of both compounds towards the metal surface. The lesser amount of energy difference implies greater inhibition efficiency, which means that TADHS11 (4.18 eV) has higher inhibition activities than TADHS10 (4.35 eV).

TADHS11 also shows lower ionization energy (TADHS10: 6.05, TADHS11: 5.94) and global hardness (TADHS10: 2.17, TADHS11: 2.09), implying that TADHS11 has superior reactivity than TADHS10. Besides, TADHS11 also has higher values for electron affinity (TADHS10: 1.70, TADHS11: 1.75), electronegativity (TADHS10: 3.88, TADHS11: 3.84) and the fraction of transferred electrons (TADHS10: -0.71, TADHS11: -0.75) due to the presence of an extra aromatic ring in its structure, allowing more specific binding and stronger interaction between the delocalized electron on the aromatic rings and the metal surface. Therefore, providing extra protection to the metal surface. These effects can also be seen clearly in Table 3, in which the configuration distribution of TADHS11 for both HOMO and LUMO is mainly focused on the aromatic ring structure, thus proving the ability of TADHS11 molecules to donate and accept electrons more efficiently. The stronger donor-acceptor interaction in TADHS11 indicated the excellent adsorption ability of TADHS11 on the metal surface and its inhibition efficiency. For TADHS10 molecules, the presence of electron-donating substituents like the hydroxy group has favoured the HOMO distribution to occur around the electron-donating group instead of the aromatic compound.

Table 2
Quantum chemical calculation of the new combination derived from fatty hydrazide derivatives

Compounds	E_{HOMO}, eV	E_{LUMO}, eV	ΔE, eV	I	A	η	χ	ΔN
TADHS10	-6.05716	-1.70340	4.35376	6.05716	1.70340	2.17688	3.88028	-0.71655
TADHS11	-5.94016	-1.75510	4.18505	5.94016	1.75510	2.09252	3.84763	-0.75324

Table 3
Optimized structure of the new combination derived from fatty hydrazide derivatives

Compounds	Chemical structures	E_{HOMO} configuration	E_{LUMO} configuration
TADHS10			
TADHS11			

3.2 The Effects of Aromatic Rings and Functional Groups

In this study, the effect of aromatic rings is highlighted in both the selected spacer and substituent groups, as it has contributed highly to increasing inhibition efficiency. Many studies have revealed that the presence of aromatic rings in inhibitor compounds can lead to the formation of protective layers on the metal surface due to the strong π-electron and the unoccupied d-orbital interaction on the metal surface (Reference). The contribution of aromatic rings is demonstrated in the combinations of spacers with substituents S11 (naphthalene group), in which the inhibition efficiency increased with the increasing number of rings. The same trend was also observed in the spacers-substituents combination having the ring structure and specific functional groups (TADHS10). Combining aromatic rings with a specific functional group elevated the inhibitive performance over

the combination containing just the specific functional group. The additional functional group presence in TADHS10 also contributed to increasing its chemical reactivity due to the ability of the hydroxy compound to form chelating complexes with metal ions and behave as strong corrosion inhibitors compared to their non-substituent analogues. Alamry *et al.,* [28] also noted the same outcome when studying novel benzenesulfonamide-based benzoxazine compounds (BSB) for X60 carbon steel corrosion in an acidizing environment. The BSB turned out to be an excellent inhibitor (90% efficiency), attributed to the ring structure of BSB, which formed a protective film over the substrates and blocked corrosive species from reaching the surface steel.

4. Conclusions

In conclusion, the inhibition ability of the new possible bio-based corrosion inhibitors derived from fatty hydrazides derivatives was successfully investigated. Based on the results obtained, it was revealed that both studied fatty hydrazides, TADHS10 and TADHS11, exhibit higher inhibition efficiency, with TADHS11 predicted as the most effective corrosion inhibitor. These are attributed to the presence of high number of aromatic rings in TADH11, which helped enhance the inhibitive performance of TADHS11 due to the presence of π-electron clouds in the rings, which form coordinate bonds with the metal steel. On the other hand, TADHS10 also exhibits promising results as a corrosion inhibitor due to its composition combined with a specific functional group such as hydroxy groups. Moreover, the presence of oxygen and nitrogen groups in the hydrazides further enhanced the ability of the molecules to bind with the metal surface since oxygen and nitrogen has proven to be the preferable active site of bindings. Finally, the study concluded that TADHS11, which consists of terephthalic dihydrazide as the spacer with 1-napthalenemethanol (TADHS11) as substituents, was predicted to be the most effective corrosion inhibitor, with the lowest energy gap of 4.18 eV, among the studied fatty hydrazide combinations with 4-hydroxylbenzyl alcohol (TADHS10).

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