Journal of Physical Chemistry and Functional Materials

Home Page of Journal: https://dergipark.org.tr/jphcfum

1H-Pyrrole, Furan, and Thiophene Molecule Corrosion Inhibitor Behaviors

[a]*Lana Ahmed**, [a]*Rebaz Omer*

[a] *Department of Physics, Faculty of Science, Firat University, 23169, Elazig, Turkey*
[b] *Department of Chemistry, Faculty of Science, Firat University, 23169, Elazig, Turkey*
** Corresponding author: Lana AHMED (E-mail: lana.omer@koyauniversity.org)*

ABSTRACT

The corrosion inhibitor behaviors of the molecules 1H-Pyrrole, Furan, and Thiophene were examined using the computational quantum method. The density functional theory (DFT) was applied to the 6-31G (d, p) basis set, parameters such as the energy of the highest occupied molecular orbital (E_{HOMO}), the energy of the lowest unoccupied molecular orbital (E_{LUMO}), the energy difference (ΔE) and the dipole moment (μ) were calculated. These parameters are correlated with the corrosion effects of organic compounds that are mainly investigated in molecular geometry and electronics. Besides, the chemical hardness (η), softness (σ), electronegativity (χ) has been determined. The transmitted electrons fraction (ΔN) has been determined between cupper surface and the 1H-Pyrrol, Furan and the Thiophene molecule. The parameters that have a direct relation with inhibition efficiency are described. The collected data indicate that 1H-Pyrrole inhibitor provides a good inhibition activity which can be used as a good anti-corrosion agent. There is an inverse relationship between the transmitted electrons fraction (ΔN) and electronegativity (χ) of inhibitor. The behavior of the corrosion inhibitor can therefore be predicted without an experimental analysis.

ARTICLE INFO

Keywords:
1H-Pyrrol
Furan
Thiophene
DFT
Corrosion

Received: 01-09-2021,
Accepted: 10-15-2021
ISSN: 2651-3080
DOI: 10.54565/jphcfum.989851

1. INTRODUCTION

Corrosion inhibitors prevent metals from the corrosion. Inhibitors are substances that are added to corrosive media to slow or stop metal corrosion [1-4]. Corrosion processes cause multiple casualties, mostly in the manufacturing sector. It is obvious that the only way to deal with it is to discourage it. Of the different strategies for avoiding or preventing the destruction or oxidation of metal surfaces, the corrosion inhibitors are one of the most well-known and effective in the industry [5-7].

Inhibitors have long been used in industry because of their excellent anti-corrosive properties. However, many occurred as a side effect, causing environmental damage. As a result, scientists started looking for environmentally friendly agents, such as organic inhibitors [8-15].

Experimentally and/or by theoretically using calculation chemistry, the efficiency of the inhibitor can be examined. Various methods are typically used to perform experimental measurements of corrosion inhibition efficiency and to monitor the inhibition mechanism such as weight loss, linear polarization, potentiodynamic polarization, electrochemical impedance spectroscopy (EIS), UV−visible spectroscopy, scanning electron microscope (SEM), X-ray spectroscopy (EDX) [16] and cyclic voltammetry [17]. Using just experimental procedures, on the other hand, is costly, time-consuming, and dangerous to the environment [18]. For this cause, many researchers have been involved in computational chemistry [19].

Structure properties of organic corrosion inhibitors, which are related to corrosion inhibition properties, are determined using quantum chemical calculations [19]. Density functional theory (DFT) is a quantum chemical method that is used to measure a molecule's electronic parameters and analyze inhibitor/surface relationships in corrosion inhibition studies. For theoretical studies of corrosion inhibition properties and to help experimental measurements, different electronic parameters obtained by quantum chemistry methodologies are used [20-28].

In this research, the computational quantum method was used to investigate the corrosion inhibitor characteristics of the molecules 1H-pyrrole, Furan, and Thiophene using the density functional theory (DFT) at 6-31G (d, p) basis set. The parameters that are directly related to inhibition efficiency are defined.

2. METHODOLOGY

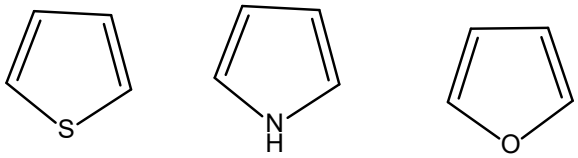
Multiple calculations can be done with the Gaussian 09 software [23-28]. The energy of the maximum occupied molecular orbital (E_{HOMO}), the energy of the lowest unoccupied molecular orbital (E_{LUMO}) [29-31], the energy difference (E),

and the dipole moment (μ) were all determined using density functional theory (DFT) at the 6-31G (d, p) basis set. Chemical hardness (η), softness (σ), and electronegativity (χ) have also been determined. The transmitted electron fraction (ΔN) between the copper surface and the 1H-pyrrol, Furan, and Thiophene molecules has been calculated.

3. Results

The structure of 1H-pyrrol, Furan, and Thiophene molecules were drawn by Chem. Bio Ultra Draw 14.0 (Fig. 1). The first step of the computational research is to find the optimized molecular structure. The quantum chemical parameters of the molecules such as the energies of highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbital (E_{LUMO}), the energy gap (ΔE), dipole moment (μ), absolute electronegativity (χ), chemical hardness (η), global electrophilicity index (ω), chemical softness (S) and fraction of electrons transferred (ΔN) were calculated (Table 1)

The relation between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) determines chemical reactivity, according to the frontier molecular orbital theory. Figure 2 displays the frontier molecular orbital diagrams of molecule 1, 2, and 3. The order of E_{HOMO} for the three compounds is 1> 2 > 3, meaning that 1 has the most electrons transferred (ΔN). The better inhibitor is correlated with the largest fraction of electrons transferred.



thiophene 1*H*-pyrrole furan

Figure 1: The chemical structure of the molecules

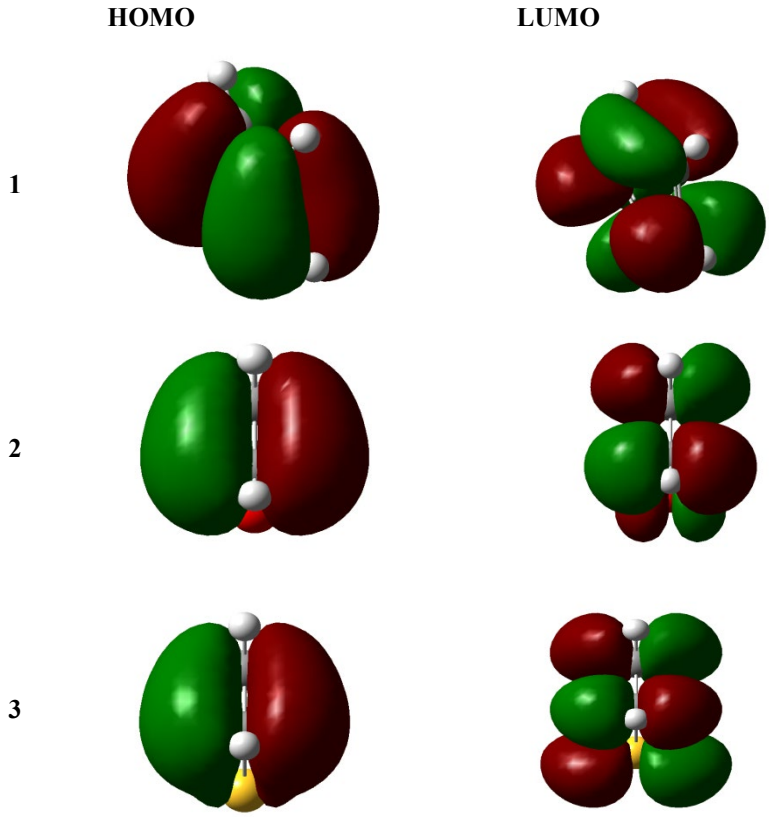


Figure 2: Frontier molecular orbital diagrams of 1, 2 and 3

Table 1: Quantum chemical parameters of the molecules using B3YLP/ 6-31G (d, p) basis set

Molecule Name	1H-Pyrrole (1)	Furan (2)	Thiophene (3)
Total Energy (a.u)	-210.176	-230.027	-553.009
μ (D)	1.902	0.63	0.623
E_{HOMO} (eV)	-5.503	-6.122	-6.35
E_{LUMO} (eV)	1.346	0.505	-0.229
ΔE (eV)	6.849	6.627	6.121
χ (eV)	2.079	2.809	3.29
η (eV)	3.424	3.314	3.06
σ (eV)	0.292	0.302	0.327
Pi (eV)	-2.079	-2.809	-3.29
ω (eV)	0.631	1.19	1.768
ε (eV)	-7.118	-9.306	-10.068

ΔN	0.825	0.742	0.725

4. . Conclusion

As per the data obtained, it is reported that the inhibitor of Molecule 1 (1H-Pyrrole) has good inhibition activity that can be used as a good anti-corrosion agent, using density functional theory (DFT) at B3LYP/6-31G(d,p) level.

Acknowledgements

First, we would like to thank Firat University, Physics Department. And secondly, we would also like to thank Prof. Dr. Niyazi Bulut for his excellent guidance and support

References

1. M. Hegazy, et al., Synthesis, surface properties and inhibition behavior of novel cationic gemini surfactant for corrosion of carbon steel tubes in acidic solution. Journal of Molecular Liquids, 2015. 211: p. 126-134.
2. S. Deng and X. Li, Inhibition by Ginkgo leaves extract of the corrosion of steel in HCl and H2SO4 solutions. Corrosion Science, 2012. 55: p. 407-415.
3. N. Muthukumar, et al., 1-Aminoanthraquinone derivatives as a novel corrosion inhibitor for carbon steel API 5L-X60 in white petrol–water mixtures. Materials chemistry and physics, 2009. 115(1): p. 444-452.
4. R. Saratha and V. Vasudha, Inhibition of mild steel corrosion in 1N H2SO4 medium by acid extract of Nyctanthes arbortristis leaves. E-journal of Chemistry, 2009. 6(4): p. 1003-1008.
5. M. Al-Otaibi, et al., Corrosion inhibitory action of some plant extracts on the corrosion of mild steel in acidic media. Arabian Journal of Chemistry, 2014. 7(3): p. 340-346.
6. I. Obot, N. Obi-Egbedi, and S. Umoren, Antifungal drugs as corrosion inhibitors for aluminium in 0.1 M HCl. Corrosion Science, 2009. 51(8): p. 1868-1875.
7. A. Yıldırım and M. Cetin, Synthesis and evaluation of new long alkyl side chain acetamide, isoxazolidine and isoxazoline derivatives as corrosion inhibitors. Corrosion Science, 2008. 50(1): p. 155-165.
8. C. Hansson, L. Mammoliti, and B. Hope, Corrosion inhibitors in concrete—part I: the principles. Cement and concrete research, 1998. 28(12): p. 1775-1781.
9. A. Abdel-Gaber, et al., A natural extract as scale and corrosion inhibitor for steel surface in brine solution. Desalination, 2011. 278(1-3): p. 337-342.
10. M. Salasi, et al., The electrochemical behaviour of environment-friendly inhibitors of silicate and phosphonate in corrosion control of carbon steel in soft water media. Materials Chemistry and physics, 2007. 104(1): p. 183-190.
11. G. Blustein, et al., Zinc basic benzoate as eco-friendly steel corrosion inhibitor pigment for anticorrosive epoxy-coatings. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2006. 290(1-3): p. 7-18.
12. P. Bommersbach, et al., Formation and behaviour study of an environment-friendly corrosion inhibitor by electrochemical methods. Electrochimica Acta, 2005. 51(6): p. 1076-1084.
13. A. Lecante, et al., Anti-corrosive properties of S. tinctoria and G. ouregou alkaloid extracts on low carbon steel. Current Applied Physics, 2011. 11(3): p. 714-724.
14. I. Radojčić, et al., Natural honey and black radish juice as tin corrosion inhibitors. Corrosion Science, 2008. 50(5): p. 1498-1504.
15. R. Omar, P. Koparir, and M. Koparir, Synthesis Of 1, 3-Thiazole Derivatives. 2021.
16. D.K. Yadav and M.A. Quraishi, Application of some condensed uracils as corrosion inhibitors for mild steel: gravimetric, electrochemical, surface morphological, UV–visible, and theoretical investigations. Industrial & engineering chemistry research, 2012. 51(46): p. 14966-14979.
17. M. Bobina, et al., Corrosion resistance of carbon steel in weak acid solutions in the presence of l-histidine as corrosion inhibitor. Corrosion Science, 2013. 69: p. 389-395.
18. H. El Sayed and S.A. Senior, QSAR of lauric hydrazide and its salts as corrosion inhibitors by using the quantum chemical and topological descriptors. Corrosion Science, 2011. 53(3): p. 1025-1034.
19. H. Zhao, et al., Quantitative structure–activity relationship model for amino acids as corrosion inhibitors based on the support vector machine and molecular design. Corrosion Science, 2014. 83: p. 261-271.
20. F. Bentiss, et al., On the relationship between corrosion inhibiting effect and molecular structure of 2, 5-bis (n-pyridyl)-1, 3, 4-thiadiazole derivatives in acidic media: Ac impedance and DFT studies. Corrosion Science, 2011. 53(1): p. 487-495.
21. I. Ahamad, R. Prasad, and M. Quraishi, Adsorption and inhibitive properties of some new Mannich bases of Isatin derivatives on corrosion of mild steel in acidic media. Corrosion Science, 2010. 52(4): p. 1472-1481.
22. I. Obot and Z. Gasem, Theoretical evaluation of corrosion inhibition performance of some pyrazine derivatives. Corrosion Science, 2014. 83: p. 359-366.
23. L. Ahmed and O. Rebaz, Spectroscopic properties of Vitamin C: A theoretical work. Cumhuriyet Science Journal, 2020. 41(4): p. 916-928.
24. L.A. Omer and R.O. Anwer, Population Analysis and UV-Vis spectra of Dopamine Molecule Using Gaussian 09. Journal of Physical Chemistry and Functional Materials, 2020. 3(2): p. 48-58.
25. R.A. Omer, et al., Theoretical analysis of the reactivity of chloroquine and hydroxychloroquine. Indian Journal of Chemistry-Section A (IJCA), 2020. 59(12): p. 1828-1834.
26. O. Rebaz, et al., Computational determination the reactivity of salbutamol and propranolol drugs. Turkish Computational and Theoretical Chemistry, 2020. 4(2): p. 67-75.
27. L.A. Omer and O. Rebaz, Computational Study on Paracetamol Drug. Journal of Physical Chemistry and Functional Materials, 2020. 3(1): p. 9-13.
28. L. Ahmed and O. Rebaz, A theoretical study on Dopamine molecule. Journal of Physical Chemistry and Functional Materials, 2019. 2(2): p. 66-72.
29. P. Koparir, et al., Synthesis, Characterization, and theoretical inhibitor study for (1E, 1'E)-2, 2'-thiobis (1-(3-mesityl-3-methylcyclobutyl) ethan-1-one) dioxime. El-Cezeri. 8(3): p. 1495-1510.
30. R.A. Omer, et al., Computational and spectroscopy study of melatonin. Indian Journal of Chemistry-Section B (IJC-B), 2021. 60(5): p. 732-741.

31. O. Rebaz, et al., Structure reactivity analysis for Phenylalanine and Tyrosine. Cumhuriyet Science Journal. 42(3): p. 576-585