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Research Article

Determination of electronic characteristics of tetrahydro pyrimidine derivatives and investigation of usability as anti-corrosion

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ABSTRACT

Corrosion of metallic structures is a serious problem in most industries worldwide. This problem can be controlled by the addition of chemicals capable of adsorption onto the metal surface. The metal can be isolated from the corrosive environment. These chemicals are often selected from groups containing free electron pairs and / or π electrons, which are rich in functional groups. In this study, electronic structures Highest Molecular Orbital (HOMO), Lowest Occupied Molecular Orbital (LUMO), MEP, energy gap (ΔE), ionization potential (I), electron affinity (A), chemical structure of pyrimidine derivative compounds containing unpaired electron pairs, π electrons, functional groups such as N, O and S hardness and softness (S), general electrophilic index (ω), transmitted electron fraction index (ΔN) and recovery (backEback-donation) properties of quantum chemical calculation methods to investigate the properties of the selected compounds in this direction and adsorbed to the surface with the quantum chemical calculation methods. The aim of this study is to determine the efficiency of synthesized compounds as anti-corrosion materials and to provide new gains to the industry in this sense.

Keywords: Pyrimidine, DFT, Corrosion, Quantum chemical studies.

Tetrahidro pirimidin türevlerinin elektronik özelliklerinin belirlenmesi ve korozyon önleyici olarak kullanılabilirliğinin araştırılması

ÖZ

Metalik yapıların korozyonu, dünya çapındaki endüstrilerin çoğunda ciddi bir problemdir. Bu problem, metal yüzey üzerine, adsorpsiyon kabiliyetine sahip kimyasalların ilavesiyle kontrol edilebilir. İlgili kimyasallar sayesinde metal, bulunduğu korozif ortamdan izole edilebilir. Bu kimyasallar çoğunlukla işlevsel grup açısından zengin, serbest elektron çiftleri ve/veya π elektronları içeren gruplardan seçilir. Bu çalışmada yapısında eşleşmemiş elektron çiftleri, π elektronları, N, O ve S gibi fonksiyonel gruplar bulunduran pirimidin türevi bileşiklerin elektronik yapıları en yüksek dolu molekül orbitali (HOMO), en düşük boş molekül orbitali (LUMO), MEP, enerji gap (ΔE), iyonizasyon potansiyeli (I), elektron afinitesi (A), kimyasal sertlik ve yumuşaklığı (S), genel elektrofilik indeksi (ω), iletilen elektron fraksiyonindeksi (ΔN) ve geri kazanım ($\Delta E_{back\text{-}donation}$) özelliklerinin kuantum kimyasal hesaplama yöntemleri ile incelenmesi amaçlanmış ve bu doğrultuda seçilen bileşiklerin kuantum kimyasal hesaplama yöntemleri ile demir yüzeyine adsorbe olma yetenekleri ve korozyon önleyici etkileri çalışılmıştır. Bu çalışma ile sentezlenmiş bileşiklerin anti-korozyon malzeme olarak kullanım verimliliği tespit edilerek bu anlamda endüstriye yeni kazanımlar sağlanması hedeflenmiştir.

Anahtar Kelimeler: DFT, Elektronik özellikler, Korozyon, Pirimidin.

1. INTRODUCTION

Corrosion is the deterioration of metal by reacting with chemicals or the environment. Corrosive solutions are used in many industrial applications. Acid solutions widely used in industry, especially in cleaning process causes significant mass loss on the surface.[1-3] There are very different techniques used to intercept corrosion. One

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of the techniques of preventing corrosion is to use protective materials. Organic compounds are also one of the important materials used as protective materials. The organic compounds show high inhibition property when containing aromatic rings, heteroatoms and π electrons.[4-8] Generally, inhibition between heteroatoms increases in the O <N <S sequence.[9,10] Heteroatoms and π-bonds are capable of forming coordinate covalent bond with metal surface and thus exhibit excellent inhibitory properties.[11]

It is preferred that the compounds used for corrosion inhibiting purpose are not harmful to nature. For this reason, pyrimidine derivatives have attracted great attention due to their less environmentally damaging properties.[12] Pyrimidine derivatives exhibit wide biochemical effects due to the activity of aromatic ring system, N atoms and π electrons.[13] Due to these properties, pyrimidine compounds are promising for corrosion inhibition.[14,15]

Many different methods are used in the development of corrosion inhibitors. Most of these methods are based on expensive experimental methods such as weight-loss, electrochemical impedance (*EI*), potentio dynamic polarization, etc.[16,17] Although experiments mostly are time-consuming, costly, and lacking in explaining the mechanism of inhibition of the corrosion.[18,19] Recently, it has been used frequently in computational methods as an alternative to expensive and time, consuming experimental methods. The quantum chemical calculation (QCC) method is one of these computational methods. This method was endorsed as a potent and easy tool to reduce the cost and time and can help in the interpretation of the experimental findings.[20,21]

Heakal et al.[22] used QCCs to determine the structural and electronic properties of imidazole-pyrimidine-based new ionic compounds. They compared the theoretical inhibition yields of the compounds prepared in this way. Molecules chosen as inhibitors must be capable of donating electrons to the empty *d*-orbital of the metal and also be suitable for forming anti-feedback bonds. Pyrimidine compounds have these properties. Therefore, these molecules are waited to be perfect corrosion inhibitors at industrial level.[23]

The inhibition effect of the molecule is mostly related to the electronic structure of the compounds. QCC is widely used to find the electronic properties of compounds. According to the frontier orbital theory, the reaction is due to an interaction between the Highest Molecular Orbital (HOMO) and Lowest Occupied Molecular Orbital (LUMO) boundary orbits of the compounds. Therefore, correct interpretation of these energy levels is important to understand the inhibition effect. To understand the mechanism, it must be calculated in the energy gap (ΔE). The energy gap equals the difference between E_{LUMO} and E_{HOMO} energies. Low values of ΔE will provide perfect inhibition effect.

In order to determine the ability of the molecule to prevent corrosion that may occur on the metal surface, the absolute I, A, S, ω, ΔN and $\Delta E_{back\text{-}donation}$ properties must be calculated. In this study, all these calculations were carried out according to Shojaie *et al.*[24] using Gaussian09.6 [25-29]

2. MATERIALS AND METHODS

In this study, Gaussian 09 package program was used. The Gaussian 09 program is a product of the Gauss series. Gauss is the most widely used program for theoretical and density functional calculations and can also perform semi-empirical calculations. The first version of Gauss appeared in 1970 and Gaussian 09 appeared in 2009. It was developed by Gauss, John Pople et al, and has had a significant impact on the increasing use of QCCs by chemists. It is an easy to use program that allows many calculations that can be done with almost any quantum-mechanical method available.

Based on the fundamental laws of quantum mechanics, Gaussian09 enables us to predict the molecular properties, molecular structures, vibrational frequencies of compounds and reactions in a wide variety of chemical environments.

To find the optimum geometry theoretically, the molecular wave function and electronic energy are calculated for many different configurations of nuclei by varying bond lengths, bond angles and dihedral angles to find the minimum energy sequence. The geometric optimization calculation continues until the magnitude of the gradient is close to zero, indicating the presence of an energy minimum. In the vibration frequency calculation, the program calculates the molecular vibration frequencies. The vibration frequency calculation should follow the geometry optimization. Because it is unnecessary to calculate vibration frequency for a geometry where energy is not at minimum.

As the geometric optimization calculations of large molecules are made with high level methods, they are very time consuming processes. Large molecules can have a large number of conformers whose global minimum and energies make it difficult to find local minimums as low as fairly large molecules can have. There are many special methods for conformational scanning whose aim is to find the low energy conformer. Due to the large number of conformers in question, energy calculations in conformational scanning with large molecules are usually made by molecular mechanics.

In this work, the potentials of pyrimidine derivatives as corrosion inhibitors were calculated by density functional

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theory (DFT) at the B3LYP / 6-31G (d, p) level using the Gaussian package program.

The aim of this study is to determine the efficiency of pyrimidine compounds as anti-corrosion materials and to provide new gains to the industry in this sense. For this purpose, the electronic structures; HOMO, LUMO, MEP, ΔE, I and A chemical structure of pyrimidine derivative compounds containing unpaired electron pairs, π electrons, functional groups such as N, O and S hardness and softness (S), general electrophilic index (ω), transmitted electron fraction index (ΔN) and recovery (backEback-donation) properties investigate the properties of the selected compounds in this direction and adsorbed to the surface with the quantum chemical calculation methods.

3. RESULTS AND DISCUSSION

In this work, geometric optimizations and quantum chemical parameters used to determine their corrosion inhibition potential of previously synthesized pyrimidine compounds[30] (Figure 1) has been studied by DFT calculations

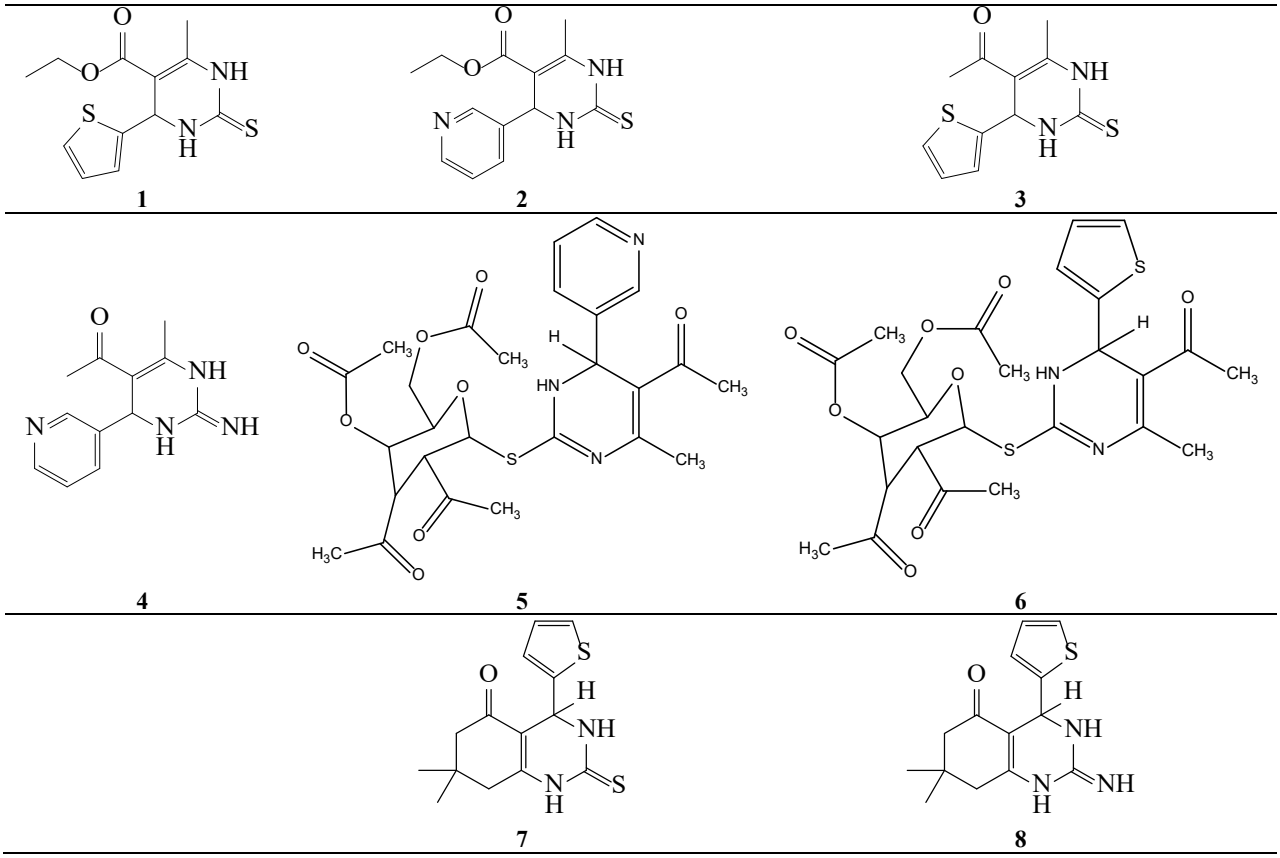

Figure 1. Molecular structures and schematic representation of pyrimidine derivatives

Theoretical calculations led to the development of experimental work. With theoretical calculations, corrosion activity parameters of the analyzed molecules against metal atoms can be calculated. Theoretical calculations have demonstrated that the molecule's filled highest energy orbital and empty lowest energy orbital values are the most important parameters in estimating the corrosion inhibition activity of the molecules against metal atoms. It can be found that molecules for which quantum chemical calculations are made are active molecules with parameters like E_{HOMO}, E_{LUMO}, ΔE, χ, μ, η, ω, σ. [31]

$$\mu = -\chi = \left(\frac{\partial E}{\partial N}\right)_{\vartheta(r)} \quad (1)$$

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{\vartheta(r)} = \frac{1}{2}\left(\frac{\partial \mu}{\partial N}\right) \quad (2)$$

The I, A, χ, σ, η values of the studied molecules are obtained by E_{HOMO} and E_{LUMO} with the following equations are obtained: [32]

$$\chi = -\mu = \left(\frac{-E_{HOMO}-E_{LUMO}}{2}\right) = \left(\frac{I+A}{2}\right) \quad (3)$$

$$\eta = \left(\frac{E_{LUMO}-E_{HOMO}}{2}\right) = \left(\frac{I-A}{2}\right) \quad (4)$$

σ is a chemical illustrator that surveys molecular stability and reactivity. σ is defined as the reverse of η. [33]

$$\sigma = \frac{1}{\eta} \quad (5)$$

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The ω is a survey of the energy drop because of the maximum electron run between donor and acceptor. It can be represented as a function of χ and η as shown in Eq. (6). [34]

$$\omega=\frac{\mu^2}{2\eta}=\frac{\chi 2}{2\eta} \quad (6)$$

The ω surveys the ability of molecules to receive electrons. As the ω value of a molecule increases, its electrophilic character increases, and as it decreases, its nucleophilic character increases.

The electronegativity value of molecules is a parameter that helps to compare the reactivity of molecules. The value of this parameter is given to estimate the electron transfer between metal and inhibitor. The molecule with a high electronegativity value hardly gives any valence electrons to this molecule. Because these electrons are attracted to the nucleus more than other molecules. According to Sanderson's electronegativity equation,[35,36] we calculate the value of the electrons transferred from the anti-corrosion molecule with the following equation.

$$\Delta N=\frac{\chi_M-\chi_{inh}}{2(\eta_M+\eta_{inh})} \quad (7)$$

Here χ_M and χ_{inh} are the electronegativity value of the metal and the inhibitor molecule, respectively. η_M and η_{inh} are the chemical hardness of the metal and the inhibitor molecule, respectively.

According to the simple charge transfer model, the electron donation and recovery process can be expressed as an electronic donation back process between the inhibitor molecule and the metal surface. [37]

$$\Delta E_{back\ donation}=-\frac{\eta}{4} \quad (8)$$

The $\Delta E_{back\ donation}$ implies that When $\eta > 0$ and $\Delta E_{back\ donation} < 0$ the charge transfer to a molecule, followed by a back donation from the molecule, is energetically favored.

Fully geometric optimizations of all molecules, HOMO-LUMO diagrams, molecular electrostatic potential maps (MEPs) and corrosion inhibition parameters were calculated with DFT and B3LYP (d, p) base set in Gaussian09 program (Figure 2 and Table 1).

It has been determined in some studies that this calculation method, which is carried out theoretically, is used to examine the relationship between corrosion inhibition efficiency and electronic properties of molecules.[38]

MEPs that provide information about the molecular distribution of electrons are represented by different colors. In Figure 1, the negative (red) areas of the MEPs are associated with electrophilic reactivity and positive (blue) areas with nucleophilic reactivity. Electrostatic potential increases during red> orange> yellow> green> blue. The highest potential is on oxygen atoms.[39]

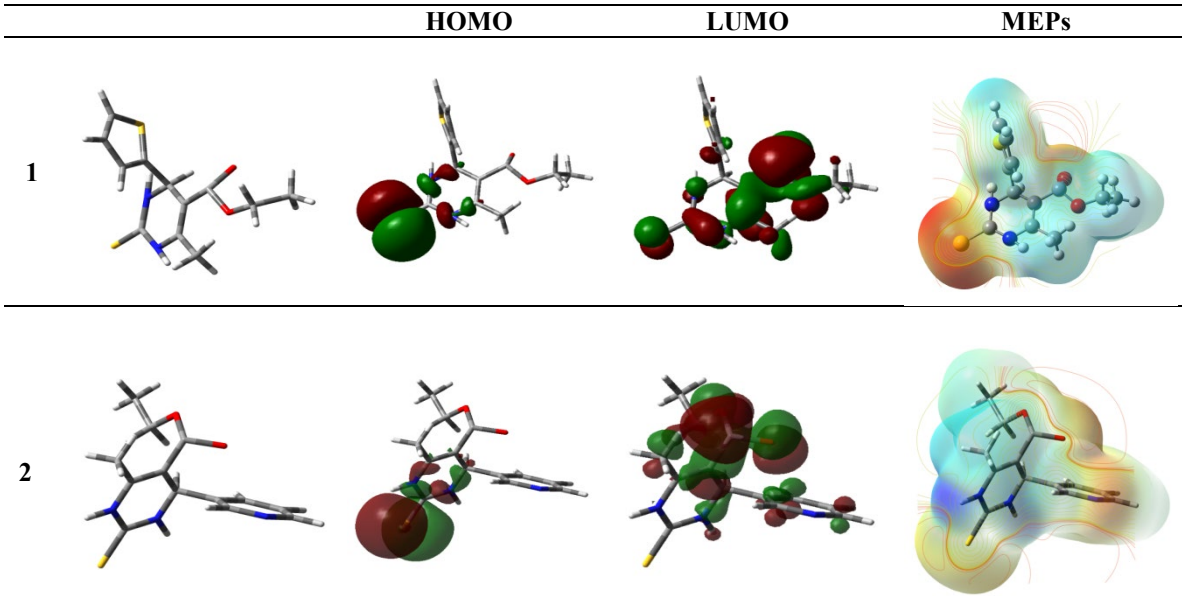

Figure 2. Structures, HOMO-LUMO diagrams and MEPs of optimized pyrimidine molecules

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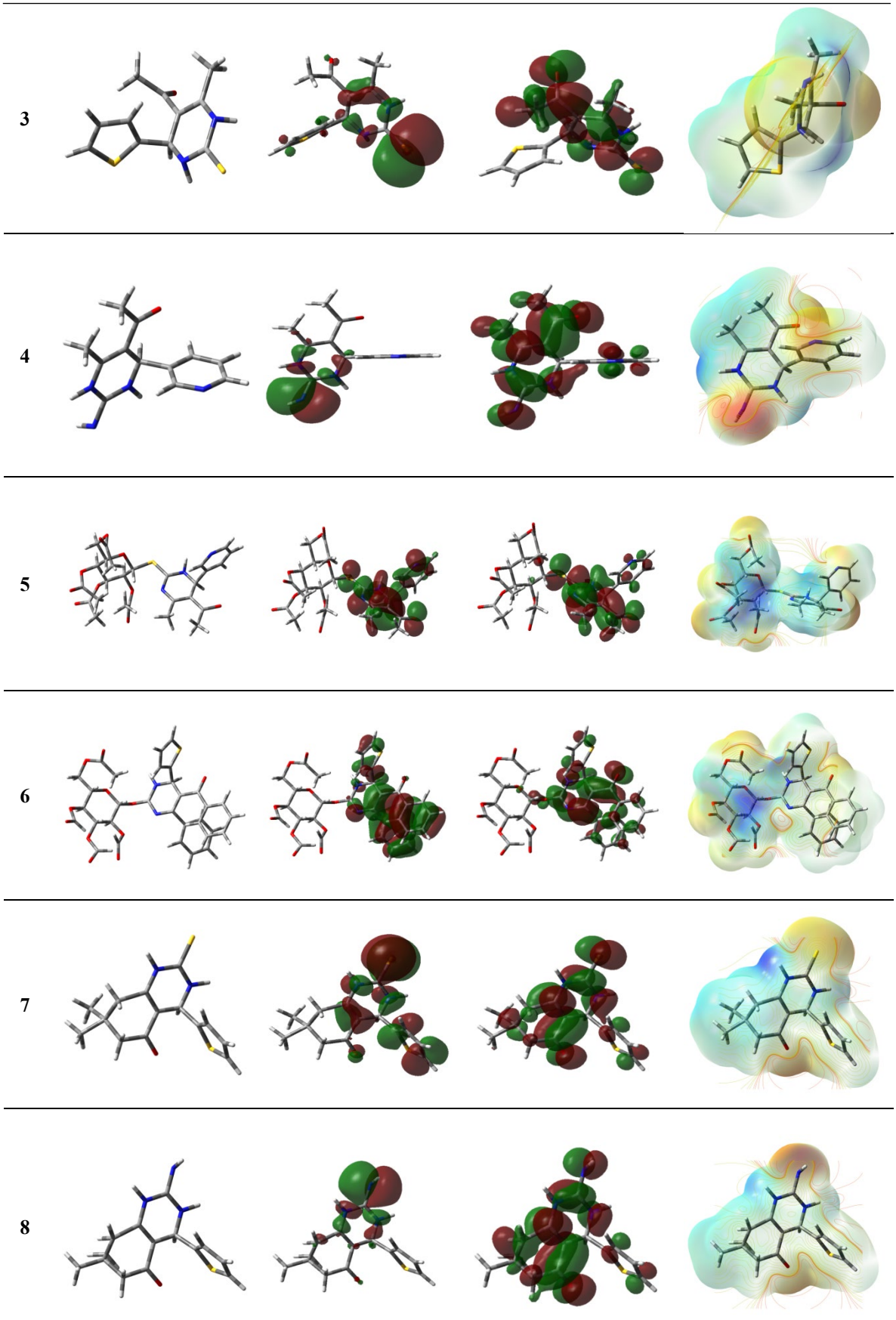

Figure 2. Continued

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Table 1. Calculated quantum chemical parameters of the studied molecules in gas phase (e*V*)

Compound	E_{HOMO}	E_{LUMO}	ΔE	I	A	η
1	-5.2995	-3.2518	2.0477	5.2995	3.2518	2.0477
2	-5.8046	-3.4603	2.3443	5.8046	3.4603	2.3443
3	-5.8174	-2.2074	3.6099	5.8174	2.2074	3.6100
4	-4.5629	-1.7851	2.7478	4.5629	1.7851	2.7778
5	-6.1366	-2.8254	3.3112	6.1366	2.8254	3.3112
6	-5.7711	-2.9677	2.8034	5.7711	2.9677	2.8034
7	-5.6549	-1.8795	3.7754	5.6549	1.8795	3.7754
8	-4.3874	-1.6131	2.7743	4.3874	1.6131	2.7743

Compound	S	χ	*μ*	ω	ΔN	$\Delta E_{back\text{-}donation}$
1	0.4884	6.9254	7.7544	14.6825	0.0182	-0.5119
2	0.4266	7.5347	4.4066	4.1416	-0.1140	-0.5860
3	0.2770	6.9211	3.6135	1.8085	0.0109	-0.9025
4	0.3599	6.4555	4.6522	3.8957	0.0980	-0.6944
5	0.3020	7.5493	3.1698	1.5172	-0.0829	-0.8278
6	0.3567	7.2549	4.9994	4.4578	-0.0454	-0.7008
7	0.2648	6.5946	5.3217	3.7506	0.0536	-0.94385
8	0.3605	5.1939	5.0076	4.5193	0.3255	-0.6935

The chemical reactivity properties of the inhibitor molecule depend on the interaction between HOMO and LUMO orbitals. The energy level of HOMO is defined as the skill of a molecule to donate electrons. Therefore, the molecule with a higher E_{HOMO} value shows a better tendency to electron donation and increases the adsorption on the metal. Therefore, it provides better inhibition efficiency. The LUMO energy level of molecules is the molecule's ability to accept electrons. When the LUMO energy level of the inhibitor molecule is lower, it is capable of accepting more electrons. The skill of the inhibitor to bind to the metal surface increases with increasing HOMO energy values and decreasing LUMO energy values.

The energy gap (ΔE_{gap}) between the E_{HOMO} and E_{LUMO} energy levels of molecules is one of the most important parameters used to determine the reactivity of the inhibitor molecule. The energy gap value (ΔE_{gap}) of the inhibitor molecule indicates its ability to bind to the metal surface. The term chemical hardness (η) is used against electron cloud polarization and chemical degradation. Chemical hardness (η) is an important parameter investigating the reactivity of molecules in experimental and theoretical chemistry. Global softness (σ), ΔE_{gap} and chemical hardness are interrelated. The chemical hardness, global softness values of the Koopman theory[40] replaced the HOMO and LUMO energy values. If hard molecules have a high ΔE_{gap} value, this molecule is not a good corrosion inhibitor. Therefore, this molecule cannot easily donate HOMO's electron to metal. The global electrophilic index (ω) surveys the ability of molecules to receive electrons. As the ω value of a molecule increases, its electrophilic character increases, and as it decreases, its nucleophilic character increases. If the transferred electron (ΔN) is < 3.6, it helps to increase the inhibitory efficiency by increasing the skill of these inhibitors to donate electrons to the metal surface. The highest electron fraction is connected with the best inhibitor. In the light of this information it can be said that the compounds **1** and **2** may have high inhibition potential.

CONCLUSIONS

In this study, quantum chemical calculations of previously synthesized pyrimidine compounds[30] were studied. The electronic properties of the molecules, corrosion prevention parameters and electrostatic potential maps (MEP) properties were theoretically calculated on the DFT-B3LYP / 6-31 G (d, p) base set. As a result, it was determined that compound **1,2** is theoretically the most active structure in terms of corrosion prevention potential.

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Conflict of interests

Authors declare that there is no a conflict of interest with any person, institute, company, etc.

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