DFT analysis of salicylideneaniline derivatives as corrosion inhibitors for mild steel

Yumuşak çelik için korozyon inhibitörleri olarak salisilidenanilin türevlerinin DFT analizi

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Abstract

Schiff bases are important in corrosion inhibition due to their ability to form stable complexes with metal ions and create protective layers on metal surfaces, thereby extending the lifespan of structural materials in various industrial applications. In this study the Salicylideneaniline and its derivatives were analyzed as corrosion inhibitor versus mild steel corrosion via DFT analysis. The eight molecules were chosen; salicylideneaniline, 2-(benzylideneamino)phenol, 4-(benzylideneamino)phenol, 2-phenyldiazenylphenol, 2-Phenylazo-4-methylphenol, 3-methyl-2-phenyldiazenyl phenol, 2-[(2-methylphenyl)diazenyl]phenol, 4-phenyldiazenylbenzene-1,3-diol), for this purpose. The Gaussian 03 program and the 6-311++G (d, p) basis set was used. Electronic properties such as the energy of the highest occupied molecular orbital (E_{HOMO}), energy of the lowest unoccupied molecular orbital (E_{LUMO}), energy gap (ΔE) between LUMO and HOMO, dipole moment, and charges on the backbone atoms, ESP were determined.

Keywords: Corrosion, Green inhibitör, DFT, ESP

Öz

Schiff bazları, metal iyonları ile stabil kompleksler oluşturma yetenekleri ve metal yüzeylerinde koruyucu tabakalar oluşturma kapasiteleri sayesinde, çeşitli endüstriyel uygulamalarda yapısal malzemelerin ömrünü uzatmada korozyon inhibisyonunda önemlidirler. Bu çalışmada, Salisilidenanilin ve türevleri, DFT analizi yoluyla yumuşak çelik korozyon inhibitörü olarak incelendi. Bu amaçla salisilidenanilin, (2-(benzilidenamino)fenol, 4-(benzilidenamino)fenol, 2-fenildiazanilfenol, 2-fenilazo-4-metilfenol, 3-metil-2-fenildiazanilfenol, 2-[(2-metilfenil)diazenil]fenol, 4-fenildiazanilbenzen-1,3-diol) sekiz molekül seçildi. Gaussian 03 programı ve 6-311++G(d,p) temel seti kullanıldı. En yüksek dolu moleküler orbital enerjisi (E_{HOMO}), en düşük dolu olmayan moleküler orbital enerjisi (E_{LUMO}), LUMO ve HOMO arasındaki enerji farkı (ΔE), dipol momenti ve atomları üzerindeki yükler gibi elektronik özellikler ve ESP belirlendi.

Anahtar kelimeler: Korozyon, Yeşil inhibitör, DFT, ESP

1 Introduction

Salicylideneaniline is an important Schiff base widely utilized in numerous scientific and industrial applications due to its chemical properties [1, 2]. It is prominently utilized in the development of liquid crystal materials, which are essential in modern display technologies, including televisions, computer monitors, and smartphones [3-5]. Additionally, salicylideneaniline serves as a key component in the synthesis of coordination compounds, where it acts as a bidentate ligand, forming stable complexes with various metal ions [6-8] . These complexes are studied for their potential catalytic, magnetic, and luminescent properties, which play an important role in advancing catalysis, materials science, and sensor technology. Furthermore, the study of salicylideneaniline derivatives aids in understanding the structure-property relationships in Schiff bases, providing insights that are valuable in the design of new functional materials [9-12]. Salicylideneaniline and its derivatives have garnered significant attention in academic research as corrosion inhibitors for metals, particularly in

acidic environments [13, 14]. These compounds possess a structurally advantageous configuration that facilitates strong adsorption onto metal surfaces, crucial for forming protective layers against corrosion. The imine group in salicylideneaniline plays an important role in its effectiveness as a corrosion inhibitor, primarily due to its polarity and coordination capabilities. This functional group, characterized by a carbon-nitrogen double bond, imparts a polar nature to the molecule, enabling it to interact strongly with metal surfaces and metal ions in solution. The nitrogen atom in the imine group possesses a lone pair of electrons that can coordinate with metal ions, facilitating the formation of coordinate bonds. This interaction enhances the adsorption of salicylideneaniline onto metal surfaces, where it forms a stable protective layer. By covering active sites on the metal, this layer impedes corrosive agents from reaching and deteriorating the metal surface. Furthermore, the adsorption of salicylideneaniline alters the electrochemical properties of the metal surface, contributing to a reduction in the overall corrosion rate. This mechanism underscores the

compound's ability to effectively mitigate corrosion through both physical and chemical interactions, making it a valuable agent in various industrial applications where metal protection is important [1, 15]. Additionally, the presence of phenolic hydroxyl groups enables hydrogen bonding interactions with metal atoms, further stabilizing the protective film [16-20]. The aromatic rings in the molecular structure contribute π-electron interactions, enhancing the inhibitor's ability to adhere to the metal surface effectively [6, 21-24]. Ongoing research into salicylideneaniline derivatives focuses on exploring various chemical modifications and their effects on corrosion inhibition efficiency, with the goal of enhancing their performance in industrial applications like metal coatings and corrosion-resistant materials [13, 14, 24]. Thus, salicylideneaniline represents a importanat class of compounds in the ongoing quest for effective and environmentally friendly corrosion control strategies.

Investigating the corrosion inhibition potential of compounds such as Salicylideneaniline and its derivatives (2-(benzylideneamino)phenol, 4-(benzylideneamino) phenol, 2-phenyldiazenylphenol, 2-Phenylazo-4-methylphenol, 3-methyl-2-phenyldiazenylphenol, 2-[(2-methylphenyl)diazenyl]phenol, 4-phenyldiazenylbenzene-1,3-diol) using Density Functional Theory (DFT) analysis holds significant academic importance. These compounds, known as Schiff bases, vary structurally and are recognized for their ability to form protective layers on metal surfaces, thereby mitigating corrosion processes, particularly in acidic environments where metal degradation is prevalent. The diversity in their structural configurations influences their adsorption behavior on metal surfaces, a critical aspect elucidated by DFT analysis. This theoretical approach provides detailed insights into molecular interactions at the atomic level, predicting adsorption energies, charge transfer phenomena, and electronic properties relevant to corrosion inhibition mechanisms. Through theoretical calculations, researchers can determine the most efficient Schiff bases, which in turn can direct the synthesis and development of corrosion inhibitors customized for certain industrial uses. Industries reliant on mild steel infrastructure benefit from prolonged asset lifespan, reduced maintenance costs, and minimized environmental impact associated with corrosion-related failures. Enhancing corrosion inhibition chemistry also helps with sustainability initiatives by encouraging resource efficiency and minimizing material waste. This scholarly endeavor not only broadens the theoretical framework in surface chemistry and materials science, but it also encourages creativity in the creation of new inhibitors that function better and are more environmentally friendly.

2 Materials and methods

The calculations of the molecules were achieved with the Gaussian 03W. We operated the program for Salicylideneaniline and its some derivatives (2-(benzylideneamino)phenol, 4-(benzylideneamino)phenol, 2-phenyldiazenylphenol, 2-Phenylazo-4-methylphenol, 3-methyl-2-phenyldiazenylphenol, 2-[(2-methylphenyl)diazenyl]phenol, 4-phenyldiazenylbenzene-1,3-diol). For

the optimized molecules the energy calculations were carried out at 6-311++G (d, p) basis set. The energy of highest occupied molecular orbital (E_{HOMO}), energy of the lowest unoccupied molecular orbital (E_{LUMO}), energy gap (ΔE) between LUMO and HOMO and Mulliken charges on the backbone atoms for molecules were determined. The obtained energy gap values were compared with the literature data. The optimized molecular structures and HOMO, LUMO surfaces were visualized using Gauss View.

3 Results and discussion

Density Functional Theory (DFT) with the B3LYP functional and 6-311++G(d,p) basis set is important for accurately predicting how Schiff bases like salicylideneaniline and its derivatives inhibit corrosion. This method balances computational efficiency with precision, providing insights into electronic structures and interactions at metal surfaces [25-28]. DFT provides guidance in the design of efficient corrosion inhibitors for industrial applications by simulating adsorption energies and charge transfers [29-32]. The obtained results (Mulliken charges of atoms in au unit; electrostatic potential_ESP, HOMO and LUMO surfaces) were presented in Figures 1-8.
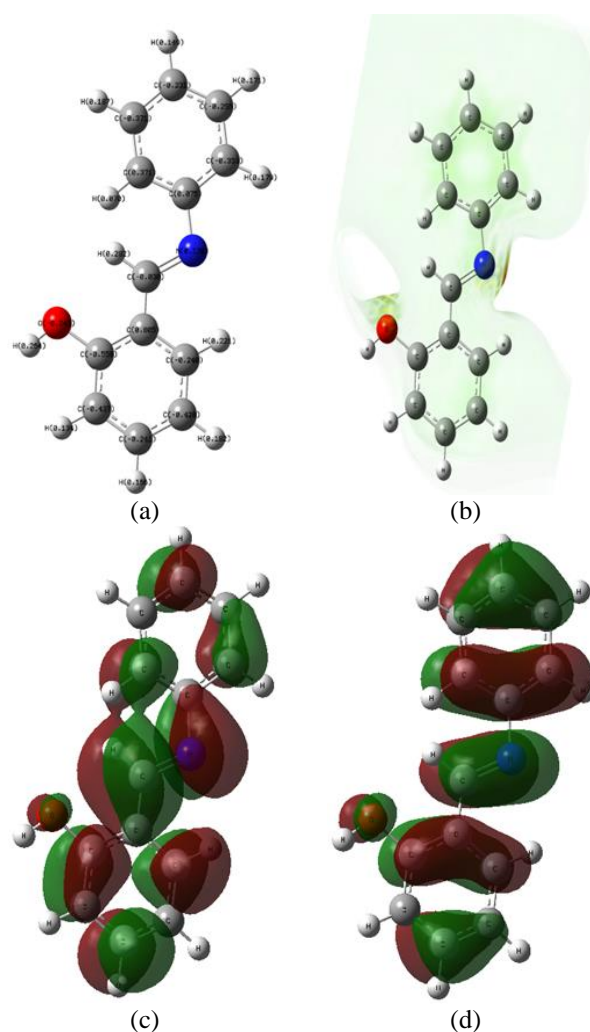

Figure 1. The Mulliken charges (a), ESP (b), LUMO (c) and HOMO (d) of salicylideneaniline

In Figure 1, Salicylideneaniline exhibits a varied distribution of Mulliken charges across its molecular structure, which influences its potential as a corrosion inhibitor. The C atoms range from slightly negative to positive charges (-0.371 to 0.805), indicating different degrees of electron density and potential interactions with metal surfaces. This diversity suggests that salicylideneaniline may form complex coordination bonds or adsorption layers on metal surfaces, depending on the specific carbon atom involved. The N atom shows a small positive charge (0.120), suggesting a region capable of accepting electrons, potentially contributing to stabilizing metal ions on the surface. Meanwhile, oxygen (O) exhibits a negative charge (-0.241), enhancing its ability to interact with metal cations or form hydrogen bonds with the surrounding environment, aiding in corrosion inhibition. The H atoms generally display positive charges, indicating their role in stabilizing the molecule through intramolecular interactions or participating in hydrogen bonding with water molecules or acidic species in the corrosion environment. The distribution of Mulliken charges and ESP in salicylideneaniline underscores its potential as a corrosion inhibitor, highlighting its complex molecular interactions that contribute to protective mechanisms against metal degradation in corrosive environments. In Figure 1, the widespread distribution of the HOMO and LUMO across the entire structure of salicylideneaniline is significant in the context of its potential as a corrosion inhibitor. This extensive distribution suggests that salicylideneaniline can effectively donate and accept electrons from metal surfaces, facilitating strong adsorption and the formation of stable protective layers. This wide-ranging contact capability improves the molecule's ability to connect with metal ions, stable metal surfaces, and effectively prevent corrosive processes in a variety of environmental circumstances by covering the full molecule [33-38].

In Figure 2, the Mulliken charges for 2-(benzylamino)phenol reveal a distribution of electron density across its molecular structure, which is important for understanding its potential as a corrosion inhibitor. The C atoms exhibit a range of charges from positive to negative values, indicating different degrees of electron donation and acceptance capabilities throughout the molecule. This variability suggests diverse interactions with metal surfaces, where certain carbon atoms may facilitate strong coordination or adsorption processes, contributing to corrosion inhibition mechanisms. The N atom shows a positive charge (0.187841), suggesting it can donate electrons to stabilize metal ions or participate in hydrogen bonding interactions, potentially enhancing the molecule's effectiveness in corrosive environments. The O atom exhibits a negative charge (-0.250701), which could facilitate interactions with metal cations or water molecules, further contributing to corrosion inhibition. The H atoms generally display positive charges, indicating their role in stabilizing the molecule's structure through intramolecular interactions or forming hydrogen bonds with the surrounding environment [39-41].

The similarity in the shape of the HOMO and LUMO between 2-(benzylamino)phenol and salicylideneaniline,

despite their differing values, indicates comparable electronic structure characteristics relevant to their corrosion inhibition potential. Both molecules likely exhibit HOMO and LUMO distributions that are delocalized over their aromatic ring systems and functional groups. This extensive distribution suggests that both can effectively interact with metal surfaces through electron donation and acceptance, crucial for forming stable adsorption layers and inhibiting corrosion processes. The specific differences in HOMO and LUMO energies and their distribution may influence their exact mechanism of interaction with metal ions and the surrounding environment in corrosion inhibition [42, 43].
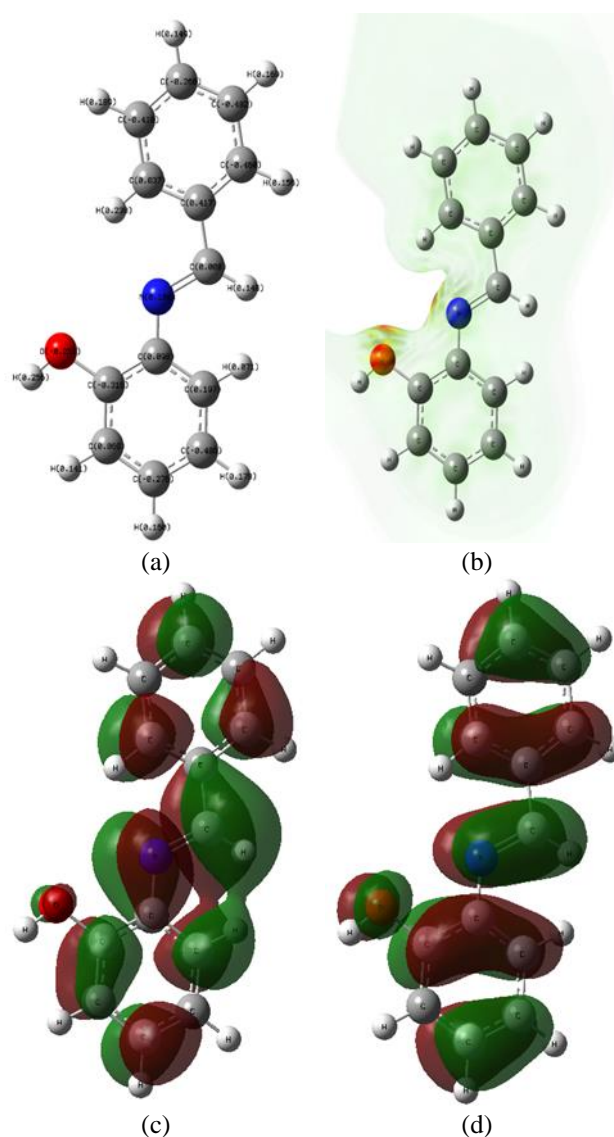

(a)　　　　　(b)

(c)　　　　　(d)

Figure 2. The Mulliken charges (a), ESP (b), LUMO (c) and HOMO (d) of 2-(benzylideneamino)phenol

In Figure 3, the Mulliken charges for 4-benzylideneaminophenol illustrate a distribution of electron density across its molecular structure, which is critical for understanding its potential as a corrosion inhibitor. The C atoms exhibit varying charges from positive to negative values, indicating different degrees of electron donation and

acceptance capabilities throughout the molecule. This variability suggests diverse interactions with metal surfaces, where certain carbon atoms may facilitate strong coordination or adsorption processes, contributing to corrosion inhibition mechanisms. The N atom has positive charge (0.172624), suggesting it can donate electrons to stabilize metal ions or participate in hydrogen bonding interactions, potentially enhancing the molecule's effectiveness in corrosive environments. The O atom exhibits a negative charge (-0.321571), which could facilitate interactions with metal cations or water molecules, further contributing to corrosion inhibition. The ESP and frontier orbitals shapes correlate this claim.
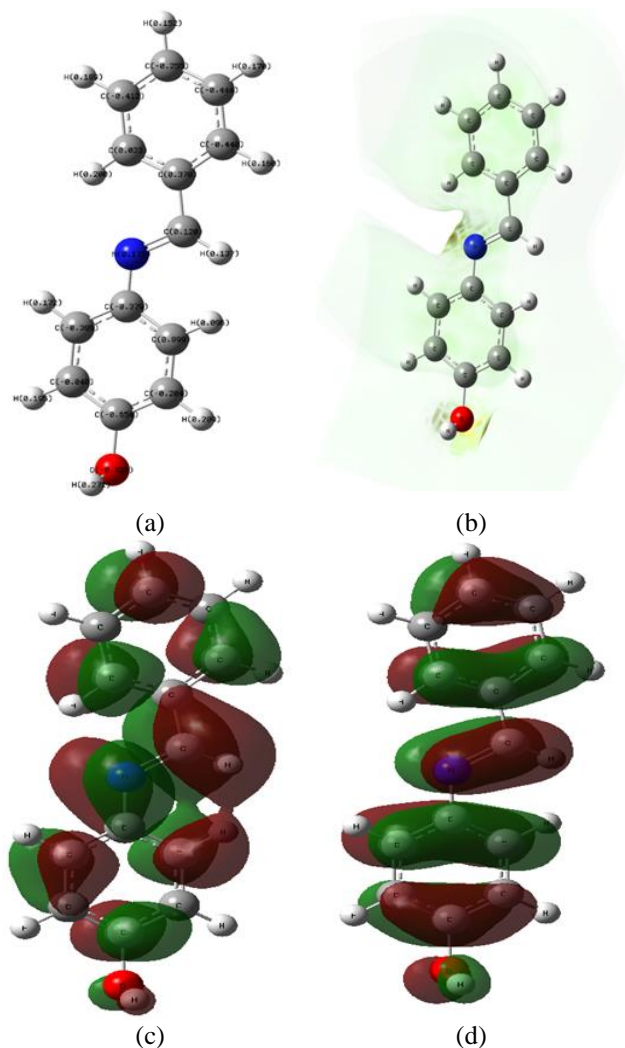
metal surfaces, where specific carbon atoms may facilitate robust coordination or adsorption processes, thereby contributing significantly to corrosion inhibition mechanisms. The N atoms display mixed charges: one nitrogen atom showing a slight negative charge (-0.021678) and the other exhibiting a positive charge (0.116187). These contrasting charges suggest potential sites for electron donation and participation in hydrogen bonding interactions, crucial for stabilizing metal ions on the surface and enhancing corrosion inhibition effectiveness [44-46].

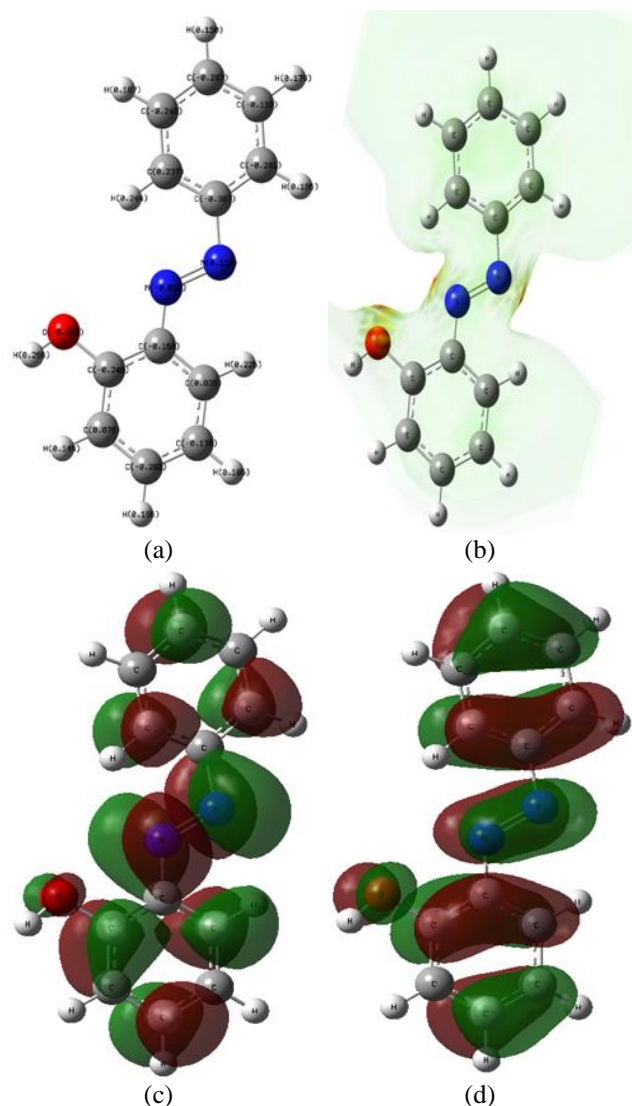(a)   (b)

(c)   (d)

Figure 3. The Mulliken charges (a), ESP (b), LUMO (c) and HOMO (d) of 4-(benzylideneamino)phenol

(a)   (b)

(c)   (d)

Figure 4. The Mulliken charges (a), ESP (b), LUMO (c) and HOMO (d) of 2-phenyldiazenylphenol

In Figure 4, the Mulliken charges for 2-phenyldiazenylphenol reveal a nuanced distribution of electron density across its molecular structure, which is important for assessing its potential as a corrosion inhibitor. The C atoms exhibit a range of charges, spanning from negative to positive values, indicating varying degrees of electron donation and acceptance capabilities throughout the molecule. This variability suggests diverse interactions with

Additionally, in Figure 4, the O atom has negative charge (-0.235083), likely promoting interactions with metal cations or water molecules, further bolstering the molecule's corrosion inhibition properties. The H atoms generally present positive charges, indicative of their role in stabilizing the molecule through intra-molecular interactions or forming hydrogen bonds with the surrounding environment [47, 48].

In Figure 5, the Mulliken charges for 2-Phenylazo-4-methylphenol exhibit a varied distribution of electron density

across its molecular structure, which is critical for evaluating its effectiveness as a corrosion inhibitor. The C atoms display a range of charges from negative to positive, indicating differing electron donation and acceptance capabilities. This variation suggests diverse interactions with metal surfaces, with specific carbon atoms potentially facilitating strong coordination or adsorption processes that contribute to the corrosion inhibition mechanism. The N atoms have different charges, with one nitrogen atom slightly negative (-0.015939) and the other slightly positive (0.126024). These charges indicate potential sites for electron donation and acceptance, important for forming stable bonds with metal surfaces and participating in hydrogen bonding interactions that enhance the molecule's inhibition effectiveness. The O atom carries a negative charge (-0.238246), suggesting a high potential for interactions with metal cations or water molecules, which is essential for the corrosion inhibition process.
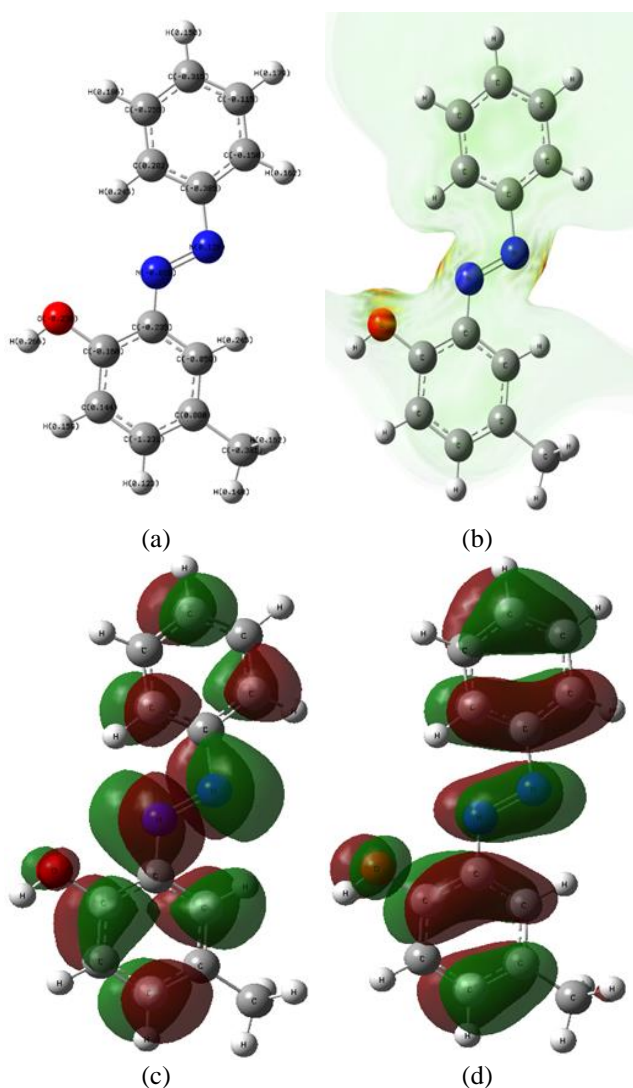
interactions and forming hydrogen bonds with the surrounding environment. The effect of charge distribution was correlated in ESP. The localized LUMO and HOMO proved the high potential inhibitor behavior [46, 49, 50].

In Figure 6, the Mulliken charges for 3-methyl-2-phenyldiazenylphenol reveal a complex distribution of electron density across its molecular structure, which is essential for understanding its potential as a corrosion inhibitor. The C atoms exhibit a wide range of charges from highly negative (-0.516012) to slightly positive (0.278585), indicating various degrees of electron donation and acceptance throughout the molecule. This variability suggests that different carbon atoms may engage in diverse interactions with metal surfaces, enhancing the molecule's ability to inhibit corrosion through adsorption and coordination processes.

Figure 5. The Mulliken charges (a), ESP (b), LUMO (c) and HOMO (d) of 2-Phenylazo-4-methylphenol

H atoms generally display positive charges, indicating their role in stabilizing the molecule through intramolecular
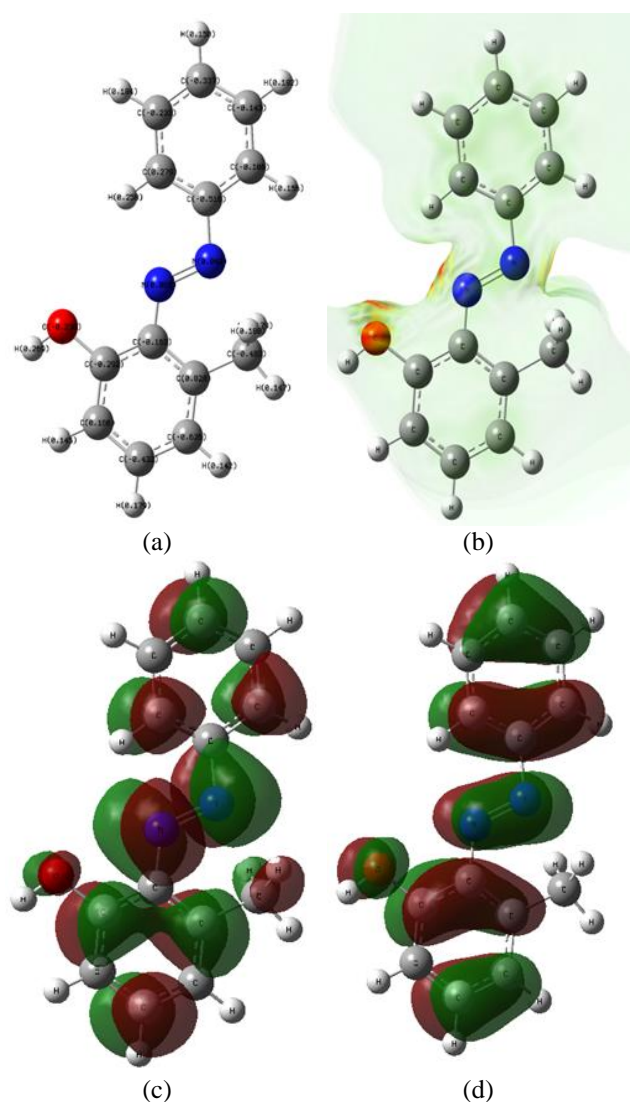

Figure 6. The Mulliken charges (a), ESP (b), LUMO (c) and HOMO (d) of 3-methyl-2-phenyldiazenylphenol

The N atoms display slightly positive charges (0.065483 and 0.049167), suggesting potential sites for electron donation and hydrogen bonding interactions. These

interactions are important for stabilizing metal ions on the surface and improving the overall effectiveness of the corrosion inhibition. The O atom has a negative charge (-0.229808), indicating a strong potential for interactions with metal cations or water molecules, which plays a significant role in the corrosion inhibition process. In ESP, the distribution of charges had a correlating effect. Localized LUMO and HOMO demonstrate the behavior of a strong potential inhibitor [51]. In 3-methyl-2-phenyldiazenylphenol, the localization of the LUMO is notable not only across the entire molecule but also particularly on the methyl group. This distribution is slightly different from other molecules where the LUMO is more uniformly spread across the molecule. The presence of the LUMO on the methyl group suggests that this group could play a significant role in the molecule's electronic interactions with metal surfaces. From a corrosion inhibition perspective, the LUMO distribution enhances the molecule's ability to accept electrons from the metal surface, thus contributing to the adsorption process.
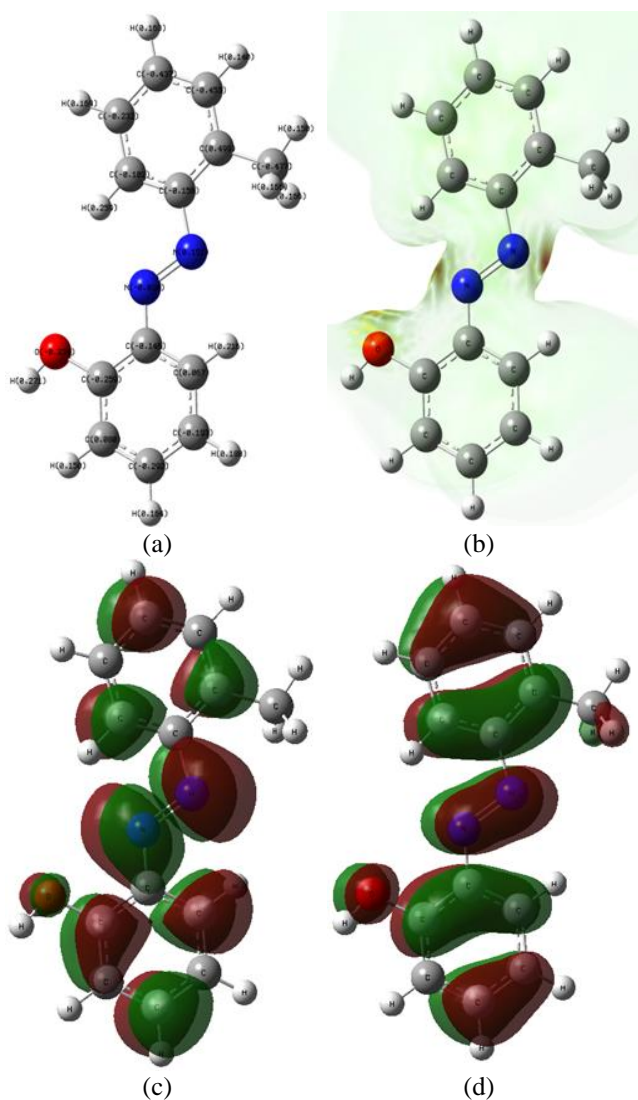

(a) (b)

(c) (d)

Figure 7. The Mulliken charges (a), ESP (b), LUMO (c) and HOMO (d) of 2-[(2-methylphenyl)diazenyl]phenol

The methyl group, typically considered inert in many chemical reactions, becomes an active site due to this LUMO localization, potentially increasing the overall efficiency of the molecule as a corrosion inhibitor. The electronic interactions facilitated by the LUMO on the methyl group may lead to a more stable and protective layer formation on the metal surface, thereby improving the inhibition performance against corrosive agents [52].

In Figure 7, for 2-[(2-methylphenyl)diazenyl]phenol, the Mulliken charges show a complex distribution of electron density, which is need for understanding its effectiveness as a corrosion inhibitor. The C atoms exhibit a range of charges from highly negative (-0.477234) to positive (0.499092), indicating various electron-donating and electron-accepting capabilities. This distribution suggests potential diverse interactions with metal surfaces, enhancing the adsorption and coordination processes that are vital for corrosion inhibition. The N atoms have charges of -0.018258 and 0.151003, indicating potential sites for electron donation and acceptance, which are essential for forming stable bonds with metal surfaces and participating in hydrogen bonding interactions that improve corrosion inhibition. The oxygen atom (O) has a negative charge (-0.234416), highlighting its role in interacting with metal cations or water molecules, which is a critical aspect of the inhibition process. In Figure 7, the HOMO is localized on the methyl group, which is unusual as methyl groups are typically considered less reactive in many chemical contexts. The methyl group may actively contribute to electron donation to the metal surface, increasing the molecule's adsorption efficiency, according to the existence of the HOMO on this group. Stronger interactions with the metal surface resulting from this localization may make it easier for a stable protective layer to form, hence reducing corrosion [53].

In Figure 8, for 4-phenyldiazenylbenzene-1,3-diol, the Mulliken charge distribution shows the C atoms exhibit a range of charges, with some being significantly negative (e.g., -0.583712) and others positive (e.g., 0.379117). This variation in charge indicates diverse electron-donating and electron-accepting abilities, which are essential for strong adsorption to metal surfaces and effective corrosion inhibition. The N atoms have relatively small charges (-0.013791 and 0.109692), suggesting their roles as minor sites for electron donation and acceptance. The O atoms, with charges of -0.233462 and -0.316361, are likely involved in hydrogen bonding and interactions with metal cations, which are critical for forming a protective barrier against corrosion [52, 54].

Furthermore, the absolute electronegativity (χ), absolute hardness (η) and softness ($\vartheta=1/\eta$) values were calculated [55-58];

$$A = -E_{LUMO} \quad (1)$$

$$I = -E_{HOMO} \quad (2)$$

$$\chi = \frac{I + A}{2} \quad (3)$$
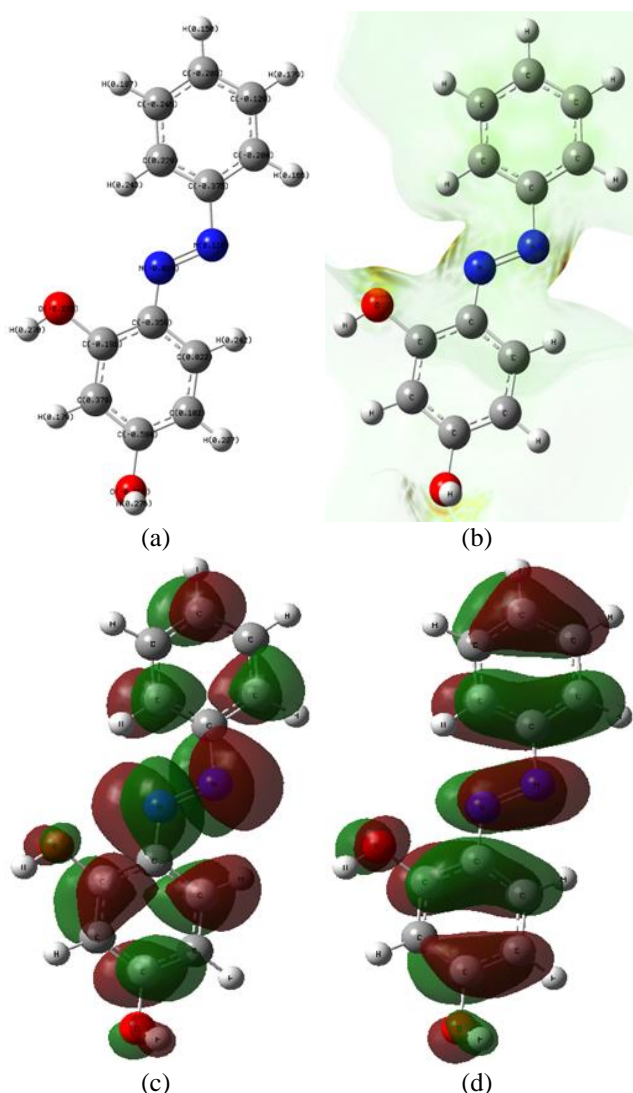
$$\eta = \frac{I - A}{2} \qquad (4)$$

(a)   (b)

(c)   (d)

Figure 8. The Mulliken charges (a), ESP (b), LUMO (c) and HOMO (d) of 4-phenyldiazenylbenzene-1,3-diol

Salicylideneaniline and its derivatives—2-(benzylideneamino)phenol, 4-(benzylideneamino)phenol, 2-phenyldiazenylphenol, 2-phenylazo-4-methylphenol, 3-methyl-2-phenyldiazenylphenol, 2-[(2-methylphenyl) diazenyl]phenol, and 4-phenyldiazenylbenzene-1,3-diol demonstrate varied electronic properties that are significant for their application as corrosion inhibitors. The Mulliken charge analysis indicates substantial differences in electron distribution, which directly influences their interaction with metal surfaces. For instance, salicylideneaniline demonstrates a diverse range of charges, with some carbon atoms being positively charged and others negatively charged, suggesting its potential for both electron donation and acceptance. Conversely, derivatives such as 2-phenyldiazenylphenol show more pronounced negative charges on certain carbons, enhancing their electron-accepting capabilities. As seen from Table 1, quantum chemical parameters, including electronegativity (χ),

absolute hardness (η), softness (ϑ), and dipole moment (μ), provide further insights into the reactivity and interaction potential of these molecules. Salicylideneaniline has an electronegativity of 3.160 eV and an absolute hardness of 1.580 eV, indicative of its balanced electron affinity and resistance to deformation. In contrast, 2-phenyldiazenylphenol has a higher electronegativity (4.644 eV) and lower absolute hardness (1.455 eV), reflecting its stronger tendency to attract electrons and greater flexibility in electronic configuration. The softness values (ϑ) suggest that these molecules possess the adaptability required for effective metal surface interaction, with 2-[(2-methylphenyl)diazenyl]phenol having the highest softness (0.702 eV^{-1}), indicating its superior capability to distribute electron density upon interaction. Additionally, the dipole moments (μ) ranging from 1.5768 D to 3.5540 D across these molecules denote their varying degrees of polarity, which affects their solubility and adsorption behavior on metal surfaces. Salicylideneaniline, with a dipole moment of 3.5540 D, demonstrates the highest polarity, potentially enhancing its surface interaction and inhibitory effectiveness. To calculate the number of electrons transferred (ΔN) from the inhibitor molecules to iron (Fe), the equation considers the absolute electronegativity (χ) and absolute hardness (η) of both iron and the inhibitor. Iron's absolute electronegativity (χFe) is 7.87 eV, with an absolute hardness (ηFe) of 0, reflecting its relatively inert nature [56]. Inhibitor molecules such as salicylideneaniline derivatives exhibit varying electronegativities and hardness values, influencing their electron-donating or accepting capacities when interacting with iron surfaces. For Salicylideneaniline, χ and η were determined as 4.187 eV and 1.580 eV, so the $\Delta N \approx 4.29$, indicating a moderate electron transfer capability from Salicylideneaniline to iron. For 2-(benzylideneamino)phenol $\Delta N \approx 4.68$; for 4-(benzylideneamino)phenol $\Delta N \approx 4.39$; for 2-phenyldiazenylphenol $\Delta N \approx 3.57$; for 2-phenylazo-4-methylphenol $\Delta N \approx 3.71$; for 3-methyl-2-phenyldiazenylphenol $\Delta N \approx 5.61$; for 2-[(2-methylphenyl)diazenyl]phenol $\Delta N \approx 5.08$ and for 4-phenyldiazenylbenzene-1,3-diol $\Delta N \approx 3.39$. As the structural complexity and substituent groups vary among the molecules analyzed, the ΔN values show distinct trends. For instance, molecules like 3-methyl-2-phenyldiazenylphenol and 2-[(2-methylphenyl)diazenyl]phenol exhibit higher ΔN values of approximately 5.61 and 5.08, respectively, suggesting a stronger electron transfer capability to iron due to the presence of methyl groups. Conversely, molecules with fewer or no methyl groups, such as 2-phenyldiazenylphenol with $\Delta N \approx 3.57$, demonstrate comparatively lower electron donation potential. The comparison of salicylideneaniline and derivatives versus literature is seen in Table 2 [59-63].

The comparison of the energy gap (ΔE) values among various inhibitors provides insight into their reactivity and effectiveness as corrosion inhibitors. In this study, several salicylideneaniline derivatives exhibited relatively low ΔE values, ranging from 2.850 eV for 2-[(2-methylphenyl)diazenyl]phenol to 3.160 eV for salicylideneaniline itself, indicating moderate reactivity.

These values are generally lower than those reported by Abdelsalam et al. [59], such as N-(furan-2-ylmethylene)-1H-1,2,4-triazol-3-amine (4.249 eV) and N-(thiophen-2-ylmethylene)-1H-1,2,4-triazol-3-amine (4.151 eV), suggesting that the these compounds might exhibit lower reactivity as corrosion inhibitors. The compound 2-pyrrolidin-1-yl-1,3-thiazole-5-carboxylic acid, studied by Karazehir et al. [61], has a high ΔE value of 6.416 eV, indicating significantly lower reactivity and suggesting less effective corrosion inhibition. Similarly, Hamood et al. [60] reports an even higher ΔE for 7-mercapto-4-methylcoumarin at 6.637 eV, reinforcing its characterization as a less reactive molecule. Conversely, compounds studied by Golafshani et al. [62], such as 3-O-caffeoylquinic acid (2.590 eV) and 4-O-caffeoylquinic acid (2.440 eV), display the lowest ΔE values, indicating higher reactivity and potential effectiveness as corrosion inhibitors. The ΔE values suggest a range of reactivity among these compounds, which may inform their suitability and efficiency as corrosion inhibitors under specific conditions [63]. The lower ΔE values typically correlate with better performance in inhibiting corrosion due to increased electronic interactions with metal surfaces.

Table 1. The quantum chemical parameters (electronegativity (χ), absolute hardness (η), softness (ϑ) and dipole moment=μ) of molecules

Molecule	E_{LUMO}/ eV	E_{HOMO}/ eV	ΔE/ eV	χ/ eV	η/ eV	ϑ/ eV^{-1}	μ/ D
Salicylideneaniline	-5.767	-2.607	3.160	4.187	1.580	0.633	3.5540
2-(benzylideneamino)phenol	-5.695	-2.595	3.101	4.145	1.550	0.645	1.5768
4-(benzylideneamino)phenol	-5.810	-2.680	3.130	4.245	1.565	0.639	2.0577
2-phenyldiazenylphenol	-6.099	-3.189	2.909	4.644	1.455	0.687	2.4971
2-Phenylazo-4-methylphenol	-6.028	-3.144	2.884	4.586	1.442	0.693	2.6696
3-methyl-2-phenyldiazenylphenol	-6.089	-3.020	3.068	4.555	1.534	0.652	2.2138
2-[(2-methylphenyl)diazenyl]phenol	-6.020	-3.170	2.850	4.595	1.425	0.702	2.4406
4-phenyldiazenylbenzene-1,3-diol)	-6.096	-3.200	2.896	4.648	1.448	0.691	2.3149

Table 2. The comparison of ΔE for several corrosion inhibitors

Molecule	ΔE/ eV	References
1-((1H-1,2,4-triazol-3-ylimino)methyl)naphthalen-2-ol	3.673	
N-(furan-2-ylmethylene)-1H-1,2,4-triazol-3-amine	4.249	[59]
N-(thiophen-2-ylmethylene)-1H-1,2,4-triazol-3-amine	4.151	
7-mercapto-4-methylcoumarin	6.637	[60]
2-pyrrolidin-1-yl-1,3-thiazole-5-carboxylic acid	6.416	[61]
3-O-Caffeoylquinic acid	2.590	
4-O-Caffeoylquinic acid	2.440	[62]
5-O-Caffeoylquinic acid	2.610	
(E)-4-(((4-propylphenyl) imino)methyl)phenol	4.141	[63]
(E)-4-((o-tolylimino)methyl)phenol	4.194	
Salicylideneaniline	3.160	In this study
2-(benzylideneamino)phenol	3.101	In this study
4-(benzylideneamino)phenol	3.130	In this study
2-phenyldiazenylphenol	2.909	In this study
2-Phenylazo-4-methylphenol	2.884	In this study
3-methyl-2-phenyldiazenylphenol	3.068	In this study
2-[(2-methylphenyl)diazenyl]phenol	2.850	In this study
4-phenyldiazenylbenzene-1,3-diol)	2.896	In this study

4 Conclusion

This study focuses on salicylideneaniline and its derivatives as potential corrosion inhibitor candidates. The Mulliken charge analysis revealed significant variations in electron distribution across the molecules, which influence their ability to donate or accept electrons when interacting with metal surfaces. Quantum chemical parameters such as electronegativity, absolute hardness, softness, and dipole moment provided further insights into the reactivity, adaptability, and interaction potential of these inhibitors. Salicylideneaniline exhibited a balanced electron affinity and notable polarity, while derivatives like 2-phenyldiazenylphenol demonstrated stronger electron-attracting capabilities and greater electronic flexibility. These findings emphasize the importance of tailoring molecular properties to enhance corrosion inhibition performance, suggesting that the strategic modification of electronic characteristics can lead to the development of more effective and targeted corrosion inhibitors.

Conflict of interest

The authors declare that there is no conflict of interest.

Similarity rate (iThenticate): 14%

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