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Quantum Chemical Calculations on Corrosion Inhibition Efficacy of Benzodiazepines on Mild Steel in Acid Medium

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RESEARCH ARTICLE

Quantum Chemical Calculations on Corrosion Inhibition Efficacy of Benzodiazepines on Mild Steel in Acid Medium

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ABSTRACT

One of the most important factors in preventing mild steel from deteriorating in acidic conditions is corrosion inhibition. This study examined the anti-corrosion properties of two benzodiazepine compounds, namely Dimethyl-[4-(4-phenyl-2,3-dihydro-1H-benzo[b][1,4] diazepin-2-yl] L-[4-(4-methyl-2,3-dihydro-1H-benzo[b][1,4]diazepin-2-yl)-phenyl] and dimethy-amine (DPBD) and toluene (DMBD), employing density functional theory (DFT)-based quantum chemical computations. Determining the corrosion inhibitors' active locations and contrasting their efficacy were the goals. The probable active sites of DPBD and DMBD as corrosion inhibitors were identified by the DFT calculations. The total corrosion inhibition performance of these two compounds did not significantly differ, according to the data. However, a slightly better performance was observed for DPBD compared to DMBD. These findings contribute to the understanding of the molecular-level interactions between benzodiazepine corrosion inhibitors and mild steel surfaces. The insights obtained from this study can aid in the design and development of more effective corrosion inhibitors for practical applications in the field of materials protection.

Keywords: Acid medium, Benzodiazepines, Corrosion inhibition, Density functional theory, Mild steel

Introduction

Due to the extensive usage of mild steel metals in most industrial processes, prophylaxis against metal corrosion is essential for environmental safety.[1,2] Effective corrosion control becomes a crucial undertaking because it can partially offset the enormous financial losses and industrial structural problems that are corrosion's obvious side effects.[1,3,4] Corrosion inhibitors are one method used to reduce the rate of corrosion from metallic surfaces, in addition to cathodic protection and the application of protective coatings.[5–8] It becomes necessary to look for and use new, efficient corrosion inhibitors as a result. Selecting effective inhibitors is influenced by their structure and potential applications in various situations.[5,8,9]

Due to its low cost, unique physical and mechanical characteristics, and wide range of applications, mild steel is frequently employed as a basic building material in a variety of sectors.[10–13] Despite their widespread use, mild steels are quite prone to corrosion, especially in acidic environments. As a result of mild steel's poor corrosion resistance, special corrosion protection methods must be developed. The most efficient chemicals for preventing corrosion are organic molecules. Because they have heteroatoms like O, N, and S and have numerous linkages, they can bind to the surface of metals.[1,3,5]

In this study, two benzodiazepines compounds as a corrosion inhibition are used. "The quantum calculations compounds based on density functional theory (DFT) is used to optimize the molecular structures of these benzodiazepines inhibitors. The atomic charge inherent in matter, the highest occupied molecular orbital (HOMO), and the lowest unoccupied molecular orbital (LUMO) are also tweaked in order to evaluate

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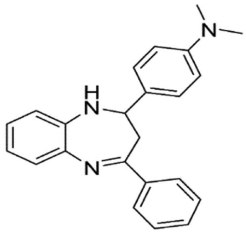
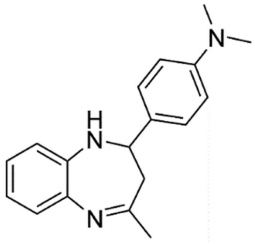
Table 1. The two benzodiazepines compounds description.

No.	Structure	IUPAC Name
1		Dimethyl-[4-(4- phenyl-2,3-dihydro- 1H-benzo[b] [1,4]diazepin-2-yl)- phenyl]-amine (DPBD)
2		Dimethyl-[4-(4- methyl-2,3-dihydro- 1H- benzo[b] [1,4]diazepin-2-yl)- phenyl]-amine (DMBD)

the electronic interaction between the mild steel surface and the inhibitors under research (MSS)".

Materials and methods

Quantum chemical calculations

Two benzodiazepines compounds, "Dimethyl-[4-(4-phenyl-2,3-dihydro-1H-benzo[b][1,4]diazepin-2-yl)-phenyl]-amine (DPBD) and Dimethyl-[4-(4-methyl-2,3-dihydro-1H- benzo[b][1,4]diazepin-2-yl)-phenyl]-amine (DMBD)", as a corrosion inhibition were taken from.[14] The names, molecular structure, and abbreviations are given in Table 1. The experimental measurements were conducted by.[14] Based on the potentiodynamic polarization measurements the measured corrosion inhibition efficiencies (IE%) were 67.77% and 64.26% for DPBD and DMBD, respectively at a concentration of 100 ppm of these inhibitors in 1 M H2SO4. These inhibitors were chosen for further investigations using quantum chemical calculations.

Using the Chem3D program, the molecular structures of DPBD and DMBD were developed. The software Gaussian09[15] was employed to calculate the quantum chemical parameters and optimize the geometry of the investigated inhibitors at the B3LYP level of the DFT theory using the 6-311 + + G(d,p) basis set. The EHOMO, ELUMO, ΔE, ionization potential (I), electronegativity (χ), electron affinity (A), softness (S), hardness (η), and the natural atomic charge were calculated. The gas phase was used for the quantum chemical calculations. The following formulae were used to calculate the values of the quantum chemical parameters Eqs Eqs. (1) to (6)".

$$\Delta E = E_{LUMO} - E_{HOMO} \tag{1}$$

$$I = -E_{HOMO} \tag{2}$$

$$A = -E_{LUMO} \tag{3}$$

$$\chi = -\frac{1}{2}\left(E_{HOMO} + E_{LUMO}\right) \tag{4}$$

$$\eta = -\frac{1}{2}\left(E_{HOMO} - E_{LUMO}\right) \tag{5}$$

$$S = \frac{1}{\eta} \tag{6}$$

Results and discussion

To identify the molecules of DPBD and DMBD's active locations, DFT calculations were performed. The atoms that serve as electrophilic or nucleophilic sites in the inhibitor compounds under investigation were allocated based on their inherent atomic charge. Organic inhibitors' lone pairs of electrons and the d-orbital of the Fe atom can interact to create coordination bonds. The behavior of an atom as a donor atom is improved by increasing its negative charge.[16] Fig. 1 depicts the DFT-optimized molecular structures for DPBD and DMBD molecules, while Table 2 lists the inherent atomic charges.

The inhibitor molecules contain a number of atoms with negative charges, as indicated in Table 2. However, for DPBD, the atoms with the largest

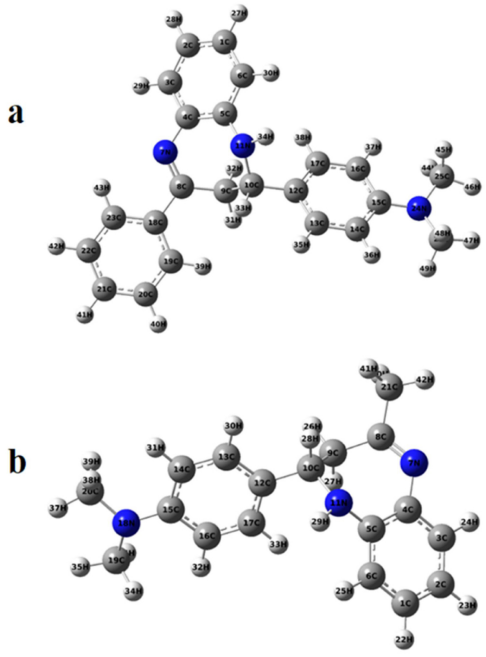


Fig. 1. The a) DPBD and b) DMBD optimized molecular structures.

negative charges are organized as follows: N(11), N(24), C(9), N(7), C(25), and C(26) in that order. Similar to DMBD, N(11), C(21), N(18), N(7), C(9), C(19), and C(20) have the most negative charges. The Fe atom's d-orbital on the surface of mild steel frequently receives electron donations from these atoms with higher negative charges. This indicates that multiple active sites, such as nitrogen, multiple methyl group carbon atoms, and the phenyl group on the Dimethyl-[4-(4-(4-(4-phenyl-2,3-dihydro- 1H-benzo[b] [1,4]diazepin-2-yl)-phenyl] compound, are used by DPBD and DMBD inhibitors to provide electrons to the Fe-amine's d-orbital, additionally active spots having propensity to donate electrons include the nitrogen and numerous carbon atoms of the methyl group on the DPBD and the carbon atoms on the phenyl group on the DPBD.

The electrons that Fe atoms on the mild steel surface may contribute may find better acceptor sites among the more positively charged atoms.[17] The atoms on the DPBD and DMBD molecules with the largest positive charges are C(8), C(15), C(10), and C(4), respectively, as in Table 2. These are all carbon atoms that are close to the nitrogen atoms of the investigated inhibitors. Nitrogen atom is more electronegative than the carbon atom next to it because two lone pairs of electrons are present. The neighboring carbon atom is then partially positive (electrophilic) and the nitrogen atom is partially negative (nucleophilic). These carbon atoms on the inhibitor molecules have stronger positive charges

Table 2. DPBD and DMBD atomic charge.

DPBD		DMBD	
Atom	Charge	Atom	Charge
“C (1)	–0.17931	C (1)	–0.19704
C (2)	–0.24179	C (2)	–0.23268
C (3)	–0.17608	C (3)	–0.1789
C (4)	0.09171	C (4)	0.09044
C (5)	0.14866	C (5)	0.14748
C (6)	–0.25091	C (6)	–0.24206
N (7)	–0.46038	N (7)	–0.47105
C (8)	0.28792	C (8)	0.31521
C (9)	–0.47283	C (9)	–0.45258
C (10)	0.1171	C (10)	0.0018
N (11)	–0.65462	N (11)	–0.63454
C (12)	–0.13603	C (12)	–0.09928
C (13)	–0.18367	C (13)	–0.17587
C (14)	–0.24703	C (14)	–0.25738
C (15)	0.18821	C (15)	0.19321
C (16)	–0.25412	C (16)	–0.25138
C (17)	–0.18113	C (17)	–0.18023
C (18)	–0.07892	N (18)	–0.49224
C (19)	–0.1927	C (19)	–0.3506
C (20)	–0.20339	C (20)	–0.35051
C (21)	–0.19349	C (21)	–0.6100”
C (22)	–0.20009	–	–
C (23)	–0.16877	–	–
N (24)	–0.49284	–	–
C (25)	–0.35075	–	–
C (26)	–0.35075	–	–

than the other atoms, as indicated in Table 2. As a result, these carbon atoms are better able to take electrons that Fe atoms on the MSS donate in order to establish a back-donating link.

Due to the presence of the -NCH3 group, both inhibitors operate as corrosion inhibitors. This nitrogen and the carbon atoms next to it function as electron donors and acceptors, respectively, to create donating and backdonation bonds. Additionally, aromatic rings' double bond electrons enhance the ability of corrosion inhibitors to stop corrosion. In contrast to DPBD, the DMBD inhibitor has a lower level of inhibitory performance. This is explained by the variations in their molecular structures. The fact that DPBD possesses a phenyl group instead of DMBD's methyl group can be credited with its superior experimental performance as a corrosion inhibitor. The addition of the phenyl group raises the number of electrons, which improved the effectiveness of inhibition of DPBD compared to DMBD.

Fig. 2 displays the HOMO and LUMO of the DPBD and DMBD molecules. As its seen in Fig. 2, the -Ph-N(CH3)2 group is where the density of HOMO electrons for the DPBD and DMBD molecules localizes, which includes the phenyl group, nitrogen atom, methyl groups, and π electrons of the double bond. This indicates that the characteristic of the nitrogen atom, phenyl and methyl groups on the DPBD and

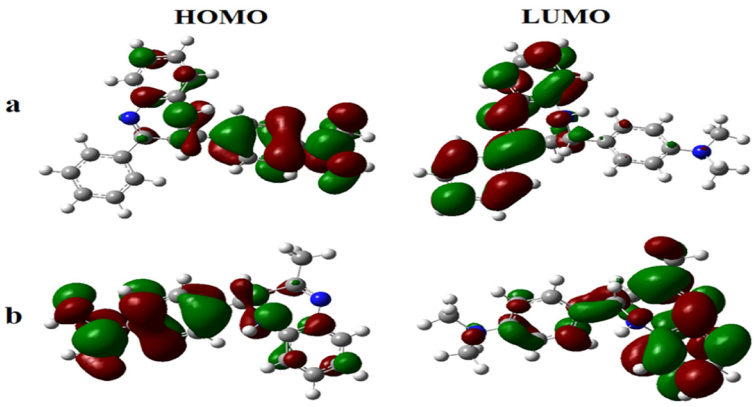


Fig. 2. HOMO and LUMO Localization on a) DPBD and b) DMBD molecules.

Table 3. Characteristics of DPBD and DMBD inhibitors' quantum chemistry.

Quantum parameter	DPBD	DMBD
E_{HOMO}	–5.3299	–5.3280
E_{LUMO}	–1.6370	–0.8892
ΔE	3.6929	4.4388
I	5.3299	5.3280
A	1.6370	0.8892
x	3.4834	3.1086
η	1.8464	2.2194
S	0.5416	0.4505
IE (%)	67.77%	64.26%

DMBD molecules behave as electron donors. These are the best active places for Fe atoms to donate electrons to vacant orbitals. These results indicate that nitrogen atom, phenyl and methyl groups are the most favorable sites for the effective adsorption of DPBD and DMBD molecules on the surface of Fe substrate. The LUMO electron density for the DPBD and DMBD molecules localizes on the dihydrobenzodiazepinyl group. This indicates that the atoms of this group on the DPBD and DMBD molecules behave as electron acceptors sites of the electrons from the metal surface that were contributed. These sites are the most favorable sites that accept electrons from Fe atoms on the MSS.

Table 3 is a list of the quantum chemical parameter values. "The EHOMO is connected to the molecule's capacity to transfer electrons. High EHOMO value inhibitors have a propensity to transfer electrons to vacant orbitals that have a lower energy than an appropriate recipient. The ELUMO demonstrates the molecule's ability to take electrons. A stronger ability of an inhibitor to accept electrons from the metal surface is indicated by a lower ELUMO.

ΔE = ELUMO - EHOMO gives the energy difference (ΔE) between HOMO and LUMO molecular orbitals. The inhibitor's IE is enhanced by a reduction in the ΔE.[18–20] The EHOMO values which are displayed in Table 3 of DPBD and DMBD are −5.3299, and −5.3280 eV. There is no significant difference between these two values. This indicates that almost same ability of DPBD and DMBD to contribute electrons to the acceptors' empty orbitals. These EHOMO values reflect very close experimental inhibition efficiencies (IE%) for DPBD and DMBD of 67.77% and 64.26%, respectively".

DPBD and DMBD have ELUMO values of 1.6370 and 0.8892 eV, respectively. The ELUMO value of the DPBD inhibitor is lower. This finding shows that DPBD has a greater ability to receive electrons from the MSS, followed by DMBD. Compared to the DMBD, the DPBD has a lower ΔE of 2.1810 eV. The lower values of ELUMO and ΔE found for DPBD indicate that it has a higher IE than DMBD. This outcome is consistent with the experimental IE of the inhibitors under investigation. The following formulas are used to determine an inhibitor's hardness (η) and electronegativity ((χ)) values[19,21,22]: $\eta = (I - A)/2$ and $\chi = (I + A)/2$, respectively, where A is the electron affinity and I is the ionization potential. The inverse of hardness is called softness (S): $S=1/\eta$. Previous research suggests that adsorption takes place at the location of the molecule where S is highest to promote the transfer of the electrons.[18,23,24] The DPBD has higher S value of 0.5416 as compared with DMBD of 0.4505. According to this finding, DPBD is a more effective inhibitor than DMBD, which is in line with the findings of the experiment. The results of the quantum analysis point to DPBD as the top corrosion inhibitor based on the explanation above. The experimental results are in agreement with the quantum calculation results.

Conclusion

The current work used DFT to examine the effectiveness of two benzodiazepine compounds, DPBD

and DMBD, in inhibiting corrosion on mild steel in an acidic environment. Finding these corrosion inhibitors' active locations and contrasting how well they worked were the goals. We were able to identify the probable active sites of DPBD and DMBD as corrosion inhibitors on mild steel surfaces in acidic environments by using the DFT calculations. The findings showed that the effectiveness of DPBD and DMBD in inhibiting corrosion was similar, with DPBD showing a minor advantage. The results imply that the benzodiazepine compounds' molecular makeup and characteristics are important factors in determining how well they inhibit corrosion. Comparable corrosion inhibition efficacy between DPBD and DMBD suggests that the mechanisms by which these compounds obstruct corrosion on mild steel surfaces are similar. Even though DPBD and DMBD show promise in inhibiting corrosion, more experimental research is necessary to confirm these computational findings and evaluate the inhibitors' effectiveness in practical settings. To sum up, the amalgamation of quantum chemical computations and empirical studies exhibits potential for propelling the field of corrosion inhibition studies forward and aiding in the creation of efficacious inhibitors that counteract the degradation of mild steel in acidic environments.

Acknowledgment

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Authors' declaration

- Conflicts of Interest: None.
- I hereby confirm that all the figures and tables in the manuscript are mine. Furthermore, any figures and images, that are not mine, have been included with the necessary permission for re-publication, which is attached to the manuscript.
- No animal studies are present in the manuscript.
- No human studies are present in the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at University of Mosul.

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الحسابات الكيميائية الكمية على فعالية تثبيط التآكل للبنزوديازيبينات على الفولاذ الطري في الوسط الحامضي

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المستخلص

يعد منع التآكل جانبًا مهمًا في حماية الفولاذ الطري من التدهور في البيئات الحامضية. في هذا البحث، تم دراسة فعالية مركبين من مركبات البنزوديازيبين في تثبيط التآكل، وتحديداً ثنائي ميثيل- [4- (4-فينيل -2، 3-ثنائي هيدرو-H1-بنزو [ب] [1،4] ديازيبين-2- يل] ديميثي و 2-(4-methyl) -4- [1،l] [b] 3-dihydro-1H-benzo، DPBD) -amine [phenyl- (2-yl-diazepin [4]) والتولوين (DMBD)، اذ تم فحصها باستخدام الحسابات الكيميائية الكمية لتحديد المواقع النشطة لمثبطات التآكل ومقارنة أدائها، وكشفت حسابات DFT عن المواقع النشطة المحتملة لـ DPBD و DMBD كمثبطات تآكل، ولم تظهر النتائج معنوية الاختلافات في فعالية تثبيط التآكل الإجمالي بين هذين المركبين. ومع ذلك، لوحظ أداء أفضل قليلاً بالنسبة لـ DPBD مقارنة بـ DMBD. تساهم هذه النتائج في فهم تفاعلات المستوى الجزيئي بين مثبطات التآكل البنزوديازيبين والأسطح الفولاذية الطرية. ان هذه الدراسة يمكن أن تساعد في تصميم وتطوير مثبطات تآكل أكثر فعالية للتطبيقات العملية في مجال حماية المواد.

الكلمات المفتاحية: وسط حامضي، البنزوديازيبين، تثبيط التآكل، نظرية الكثافة الوظيفية، الفولاذ الطري.