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Theoretical study of a new oxazolidine -5- one derivative as a corrosion inhibitor for carbon steel surface

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Abstract

A newly derivative of oxazolidin-5- one namely [2-(2-biphenyl-4-yl-imidazo [1,2-a] pyridine-3-yl)-3-(4-nitro-phenyl)-oxazolidin-5-one (BIPNO5)] was examined as an corrosion inhibitor for carbon steel surface. Quantum mechanical method of Density Functional Theory (DFT) with (B3LYP (6-311++G (2d, 2p)) level of theory was used to calculate the minimize structure, physical properties and inhibition chemical parameters, in vacuum and two solvents (DMSO and H_2O), all at equilibrium geometry. The results indicated that the new derivative could adsorb on the surface of carbon steel through the heteroatom, showing that the new inhibitor has good corrosion inhibition performance.

Keywords: DFT, Corrosion inhibitor, Quantum chemical calculations, Oxazolidin.

دراسة نظرية لمشتق جديد للأوكسازوليدين −5 أون كمثبط لتآكل سطح حديد الصلب الكربوني

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الخلاصة

تم إختبار مشتق جديد للأوكسازوليدين −5 أون وهو: [2−(2−biphenyl−4−yl−imidazo [1,2−a] pyridine−3−yl)−3−(4−nitro−phenyl)−oxazolidin−5−one (BIPNO5)] كمثبط لتآكل سطح حديد الصلب الكربوني. تم استخدام حسابات ميكانيك الكم لنظرية دوال الكثافة (DFT) عند مسوى الحساب [(B3LYP (6−311++G (2d, 2p)] للحصول على الشكل الفراغي والخواص الفيزيائية ومعلمات التثبيط الكيميائي، في الفراغ وفي المذيبين (DMSO وH_2O)، عند الشكل الهندسي التوازني. أشارت النتائج إلى أن المشتق الجديد يمكن أن يمتز على سطح الفولاذ الكربوني من خلال الكترونات الذرات الهجينة heteroatom والكترونات الحلقات العطرية ثنائية الفينيل. وقد تبين أن المثبط الجديد لديه أداء تثبيط تآكل جيد للغاية.

Introduction

Quantum chemistry as a device in the design and improvement of organic corrosion inhibitors has been extraordinarily upgraded by the evolution of the density functional theory (DFT). Quantum chemical methods are capable to accurately predict the inhibition characteristics of inhibitor molecules using molecular/ electronic properties and nucleophilic and/or eletrophilic active sites [1].

Recently (DFT) has been utilized to investigate the attributes of the (inhibitor/surface) and to characterize the nature of the inhibitor that adsorbed in the corrosion process [2]. On the other hand, (DFT) is viewed as a helpful technique to test the inhibitor/surface association as well as to

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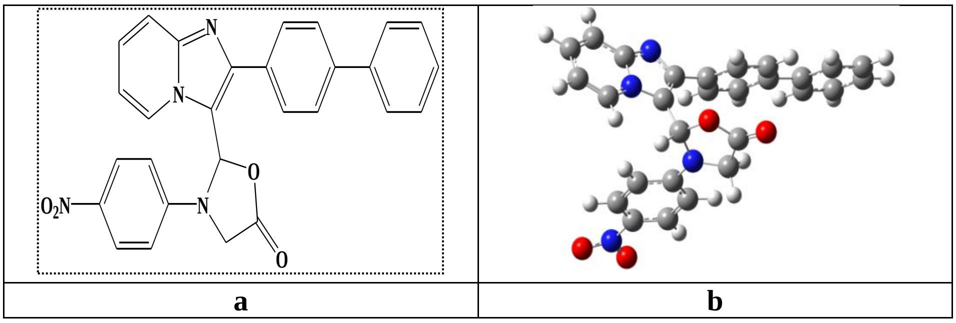
characterize the experimental data. Scientists have been identified a new corrosion inhibitors by examining hundreds of compounds in the lab., this exploratory are frequently pricey and tedious. Subsequently, continuous advances of the equipment and programming have opened the entryway for incredible utilization of theoretical chemistry in the researches of corrosion inhibition at a diminished expense and time [3]. The investigation of the corrosion processes and their inhibition by the organic inhibitors was a very significant field of the research. Numerous scientists report that the inhibition effect mainly relies upon some electronic and physicochemical properties of the inhibitor which relate to its planarity, functional groups, electronic density of donor atoms and orbital character of donating electrons. The mechanism of inhibiting is generally demonstrated by forming chemically [and/ or] physically film that adsorbed on the surface of metal. The compounds which act as the corrosion inhibitors are rich in the heteroatom, like, oxygen, nitrogen and sulfur. Organic inhibitors and their derivatives are premium corrosion inhibitors in the wide scope of media [4]. Oxazolidinones are five-member heterocyclic compounds that containing two hetero atoms oxygen and nitrogen, heterocyclic compounds with oxygen and nitrogen are important compounds in the medicinal chemistry, industry and biological materials, which help to understand life processes. Oxazolidinones has also biological efficacy; used for gram-positive infections and can be bacteriostatic or bactericidal depending on bacteria being treated. (BIPNO5) was a new synthesis derivative of oxazolidin-5-one prepared recently by Sallom, K.J [5]. The aim of this work is to study a newly derivative of oxazolidin-5- one (BIPNO5)] as a corrosion inhibitor depending on calculating and studying its quantum mechanical inhibition efficiency parameters computed using DFT methods with (6-311 basis set) and (B3LYP ++ G (2d, 2p) level of theory.

Results and Discussion:

Molecular geometry

The two dimension **s**tructure of the organic inhibitor was established by Chem. Draw Mopac program, see Figure-(1a). Gaussian 09 package [6] was utilized to calculate the fully optimize structure in vacuum, using quantum mechanical method of DFT (Density Functional Theory) with (6-311 basis set) and Becke's three-parameters of the [Lee, Yang and Parr (B3LYP ++ G (2d, 2p)) level of theory [7]. In addition to vacuum, the equilibrium geometry was calculated in two solvents (DMSO and H_2O).



a **b**

Figure 1- a; Two dimension **s**tructure of (BIPNO5), and, **b;** Three dimension optimize structure of (BIPNO5) inhibitor calculated by DFT method.

Table-1 displays the geometrical structure of compound (BIPNO5), such as (bond lengths, bond angels and dihedral angles), in vacuum, DMSO, and H_2O that studied by DFT method. The optimized geometrical structure observed to be the same in the three media (vacuum, DMSO, and H_2O). Figure (2) shows the numbering of atoms of compound (BIPNO5). From Table (1), C18-C19 (1.500Å) was the longest bond length and C1-H (1.080Å) was the shortest bond length that found in BIPNO5 compound. The bond angles calculated between (104.430 deg) for N18C19C20 and (132.553 deg) for C3N4C7. Values of dihedral angles (cis and trans) were showed that the compound was not planar with point group of C_1 [the cis dihedral angles are not 0.0 degree, and all trans dihedral angles are more or less than 180.0 degree].

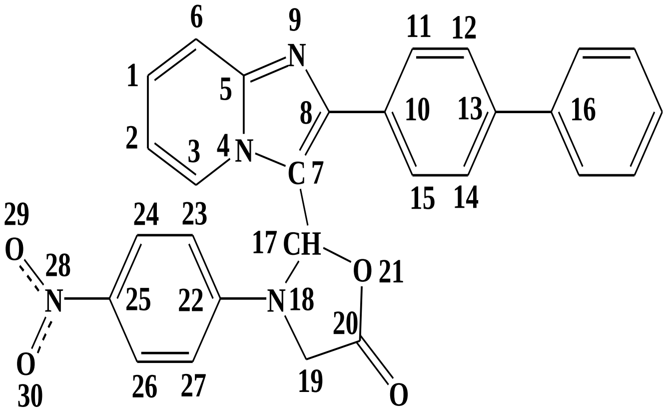
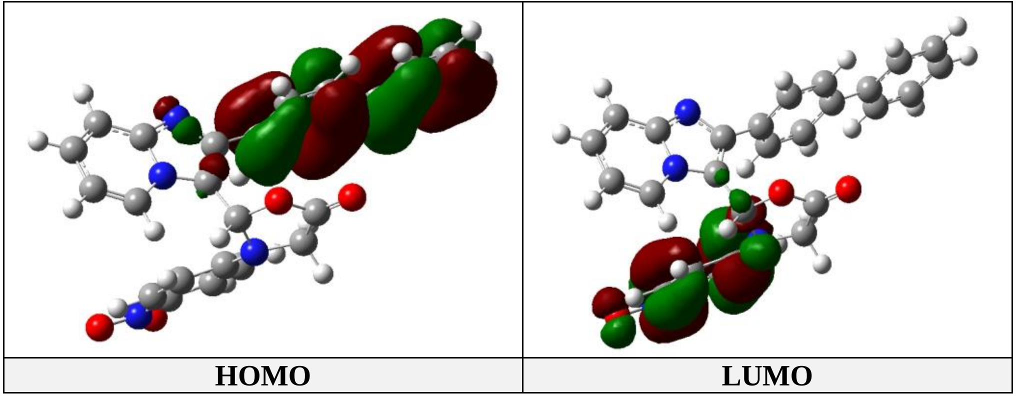


Figure 2- Label of atoms for (BIPNO5) compound.

Table 1- Calculated geometrical structure of (BIPNO5) compound by DFT in the three media (vacuum, DMSO, and H_2O).

Description bond	Bond length (Å)	Description angle	Bond angle (deg)	Description Dihedral angle	Dihedral angle (deg)
C1-C2	1.418	**C2C1C6**	120.043	**HC1C2H**	-0.474
C1-C6	1.368	**C2C1H**	119.576	**HC1C2C3**	179.996
C1-H	1.080	**C1C2C3**	120.589	**HC2C3H**	-0.873
C2-C3	1.361	**C2C3N4**	119.632	**HC2C3N4**	-179.966
C3-N4	1.372	**C3N4C7**	132.553	**HC3N4C7**	1.377
N4-C5	1.403	**C3N4C5**	121.242	**HC3N4C5**	-177.928
N4-C7	1.390	**N4C5C6**	118.878	**C7N4C5N9**	-0.739
C5-C6	1.408	**N4C5N9**	111.062	**C7N4C5C6**	179.318
C5-N9	1.328	**C5C6C1**	119.601	**N9C5C6H**	0.422
C7-C8	1.386	**N4C7C8**	105.277	**N9C5C6C1**	-179.502
C7-C16	1.491	**N4C7C17**	122.673	**N4C7C8N9**	-1.276
C8-N9	1.360	**C7C8N9**	111.446	**N4C7C8C10**	179.579
C8-C10	1.480	**C7C8C10**	128.125	**C7C8N9C5**	0.831
C10-C11	1.395	**C8N9C5**	105.996	**C8C10C11H**	-1.979
C12-C13	1.392	**C10C11H**	119.493	**HC12C13C14**	179.724
C13-C14	1.392	**C11C12C13**	119.818	**HC12C13C16**	-0.098
C17-N18	1.475	**C13C14C15**	119.781	**HC14C15H**	0.005
C17-H	1.091	**C7C17N18**	114.403	**HC14C15C10**	179.549
C17-O	1.447	**C7C17O21**	112.702	**O21C17N18C19**	-2.591
N18-C22	1.392	**C17N18C22**	123.714	**O21C17N18C22**	177.533
N18-C19	1.426	**C17N18C19**	111.801	**C17N18C19C20**	-0.366
C18-C19	1.500	**N18C19C20**	104.430	**N18C19C20O21**	3.352
C20-O	1.202	**C19C20O**	128.862	**N18C19C20O**	-176.169
C20-O21	1.401	**C19C20O21**	108.496	**C19C20O21C17**	-5.224
C22-C23	1.404	**C20O21C17**	111.098	**N18C22C23C24**	179.699
C23-C24	1.385	**N18C22C23**	121.094	**N18C22C23H**	-0.658
C24-C25	1.388	**C24C25N28**	119.375	**C22C23C24C25**	0.483
C25-C26	1.388	**C25C26C27**	119.899	**C23C24C25N28**	-179.629
N28-O29	1.235	**C25N28O29**	117.093	**N28C25C26C27**	179.354
N28-O30	1.236	**C25N28O30**	116.025	**C25C26C27C22**	0.056

Figure-3 shows geometrical optimization of the calculated inhibitor in vacuum included the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) density distributions. The HOMO is mainly located on the (2-(2-Biphenyl-4-yl-imidazo [1, 2-a] pyridine-3-yl)) moiety. This indicates that the preferred actives sites for an electrophilic attack are located within the region around the nitrogen atoms. Moreover, the electronic density of LUMO was distributed at the aromatic ring and around the ring of (4-nitro-phenyl) moiety (which is the most planar region in the compound).



HOMO **LUMO**

Figure 3-Frontier molecular orbital distributions of (BIPNO5) compound using DFT method. [Red color: negatively charged lobe; blue color: positive charge lobe].

Global molecular reactivity

To study the influence of the molecular structure on the efficiency and inhibition mechanism, several chemical quantum parameters were discussed.

The quantum parameters like; energy of the highest occupied molecular orbital (E_{HOMO}), the energy of lowest unoccupied molecular orbital (E_{LUMO}), HOMO-LUMO energy gap (ΔE_{gap}), dipole moment (μ) and other quantum chemical parameters, all are shown in Tables-(2a, 2b).

The Frontier Orbital Theory was used in portends the centers of adsorption of the inhibitor that responsible of the reaction metal surface and molecule [8].

According to this hypothesis, the transition state was formed due to the interaction between Frontier orbital's (HOMO and LUMO) of the reactants. The energy of HOMO (E_{HOMO}) is regularly connected with the electron giving capacity of the particle, so, the compounds that have high values of (E_{HOMO}) tend to give electrons to appropriate acceptor with low empty molecular orbital energy. Contrariwise, the energy of LUMO (E_{LUMO}) means the accepting capacity of an electron in the particle, lowest value indicate higher capability of accepting electrons. The energy gap between the Frontier orbital's [$\Delta E_{HOMO\text{-}LUMO}$] is another significant parameter in characterizing the molecular activity, thus, when this parameter decreased, the efficiency of an inhibitor increased [9]. The activation hardness was also characterized on the basis of the $\Delta E_{HOMO-LUMO}$ energy gap. The qualitative characterization of the hardness is widely related to the polarizability, so, any decrease in the energy gap prompts simpler polarization of the particle. The quantum chemical parameters expense attached to the efficiency of the inhibition of a molecule, like, values of HOMO and LUMO energy, Electronegativity (χ), Frontier Orbital Energy gap (ΔE_{gap}), Dipole Moment (μ), Softness (S), Global Hardness (η), The fraction of the electron transferred (ΔN) were studied by using density functional theory (DFT) and has been utilized to understood the activity and properties of the newly prepared organic compounds and to assist in the demonstration of the experimental data obtained for the process of corrosion. Due to Koopman's theorem [10], the ionization potential (IP) and electron affinity (EA) and of the inhibitors are studied by the Equations below [11]:

$$IP = -E_{HOMO} \qquad (1)$$

$$EA = -E_{LUMO} \qquad (2)$$

Chemical hardness (η) and electronegativity (χ) due to, operational, Pearson and approximate definitions can be calculated by the Equations below [11]:

$$\chi = (IP + EA)/2 \qquad (3)$$

$$\eta = (IP - EA)/2 \qquad (4)$$

Global chemical softness (S), which characterized the ability of an atom or group of atoms to accept electrons [6], was calculated by Equation 5:

$$S = 1/\eta \qquad (5)$$

The Global electrophilicity index (**ω**) which introduced by Parr [12], electronegativity and chemical hardness parameters are calculated by Equation 6:

$$(\boldsymbol{\omega}) = (-\chi)^2/2\eta = \mu^2/2\eta \qquad (6)$$

The fraction of the electrons transferred (ΔN) from the inhibitor particle to the surface of carbon steel was also estimated theoretically, by using (χ_{Fe}) and (η_{Fe}) values of carbon steel of (7.0 eV mol^{-1}) and (0.0 eV mol^{-1}), respectively. Number of the transferred electrons (ΔN) was also estimated [12] by using Equation (7):

$$\Delta N = (\chi_{Fe} - \chi_{inhib.})/[2(\eta_{Fe} + \eta_{inhib.})] \qquad (7)$$

Tables (2a, 2b) show that (BIPNO5) compound was a good inhibitor depending on the values of quantum chemical parameters in three media (vacuum, DMSO and H_2O). (E_{HOMO}) in vacuum was (-6.430eV), decreased in both DMSO and H_2O solvents, the (E_{LUMO}) in the vacuum (-2.834 eV), decreased in both DMSO and H_2O solvents and the value of ($\Delta E_{HOMO-LUMO}$) is (3.596 eV) in vacuum, be lower in DMSO and H_2O, indicating that the stability of the inhibitor in the solvents is lower than that in the vacuum.

The dipole moment (μ in Debye) is another significant electronic parameter that product from the non-uniform distribution of charges on the different atoms in the particle. High value of the dipole moment caused increase in the adsorption between the inhibitor molecule and the metal surface [13]. The dipole moment for (BIPNO5) inhibitor in vacuum is (3.797 Debye), increased in both DMSO and H_2O as a result of increasing polarity of the solvent.

The ionization potential (IP), was approximated as the negative value of the highest occupied molecular orbital energy (E_{HOMO}) [4]. Low values of (IP) increase the effectiveness of the inhibitor. The IP for (BIPNO5) inhibitor in the vacuum is (6.430 eV), decrease in the DMSO and H_2O solvents.

The electron affinity (EA) was the amount of energy freed when adding an electron to an atom or molecule [14]. A high value of (EA) indicates a less stable inhibitor (good corrosion inhibitor). The electron affinity of (BIPNO5) in the vacuum is (2.834 eV), be a higher on using DMSO and H_2O solvents.

Chemical Hardness (η) is a measure of the ability of atom or molecule to transfer the charge. Increasing (η) decreases the stability of molecule [13], so the inhibitor possessed a high value of (η) is considered to be a good inhibitor. (η) Value for (BIPNO5) in the vacuum is (1.798eV), be a lower in DMSO and H_2O solvents. The chemical Softness (S) is a measure of the flexibility of an atom to receive electrons (S), Molecules having a high value of (S) are considered to be a good inhibitor. The values of (S) in the vacuum is (0.556 eV), increase in both DMSO and H_2O [13].

The electronegativity (**χ**) is the ability of an atom or a group to pull electrons, High electronegativity indicates a good inhibitor. The calculated (**χ**) for (BIPNO5) in the vacuum was found to be (4.6320eV), decreased in both DMSO and H_2O solvents [15].

Global electrophilicity index (**ω**) is the measure of the stability of an atom after gaining an electron, Low value of (ω) meaning the molecule has a good inhibition. In the vacuum is (5.966 eV), increased in both DMSO and H_2O [16].

(ΔN); is the difference in number of electrons transferred. (BIPNO5) has (ΔN) value up to (0.658) in vacuum phase and this value increase in the solvents. This ability increases the inhibition efficiency, when two systems, Fe, and inhibitor, are brought together [4].

Table 2a- Some physical properties of (Oxazolidin-5-one derivative (BIPNO5)) calculated at equilibrium geometry, using DFT method.

Inhib. medium	P. G.	M. formula	E_{HOMO} (eV)	E_{LUMO} (eV)	$\Delta E_{HOMO-LUMO}$ (eV)	μ (Debye)	E_{total} (eV)
Vacuum	C_1	$C_{28}H_{22}N_4O_4$	-6.430	-2.834	3.596	3.797	-43519.293
DMSO	C_1		-6.302	-3.009	3.293	5.436	-43520.655
Water	C_1		-6.302	-3.011	3.291	5.466	-43520.641

Table 2b- Corrosion quantum chemical parameters for (Oxazolidin-5-one derivative (BIPNO5)) calculated at the equilibrium geometry utilizing by DFT.

Inhib. medium	IP (eV)	EA (eV)	□ (eV)	□ (eV)	S (eV)	ω (eV)	□□
Vacuum	6.430	2.834	1.798	4.6320	0.556	5.966	0.658
DMSO	6.302	3.009	1.646	4.655	0.607	6.582	0.712
Water	6.302	3.011	1.645	4.656	0.607	6.589	0.713

Mulliken charges of (BIPNO5) inhibitor

Mulliken charges distributions analysis, which gave a significance of the active centers of the particles (electrophilic and nucleophilic) centers. For that, the area that have large electronic charges are chemically softer than the area have small electronic charges. It can be readily noticed that oxygen, nitrogen and some carbon atoms have higher charge densities. The chemical adsorption interactions are either by orbital interactions or electrostatic. The sites of nucleophilic attack will be the position where the positive charge value is a maximum, thus only the charges on the oxygen (O), nitrogen (N), and some carbon atoms of biphenyl moiety are presented. In order, the position of the electrophilic attack was controlled by the negative charge value.

The nucleophilic and electrophilic electronic charge values of compounds are higher in the solvent (DMSO and H_2O) than in vacuum. Table-3 shows the Mulliken charges population (ecu) for the (BIPNO5) inhibitor in the three media (vacuum, DMSO, and H_2O). According to this table, the order of the nucleophihic reactive sites of (BIPNO5**)** inhibitor is:

C15> O21> C7> C24> N9> C1> C14> C12> C26> C11> C2, and the order of the electrophihic reactive sites order is: C16> C13> C5> C20> C22> C10.

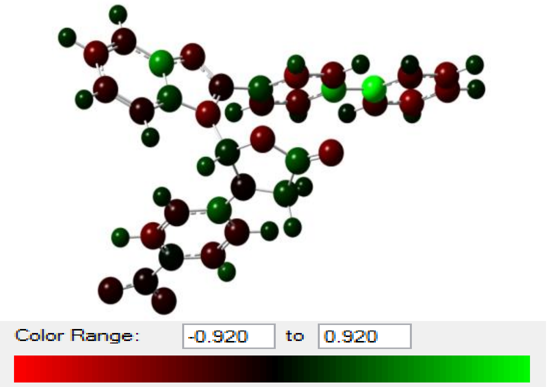


Figure 4: Charges distribution for atoms of (BIPNO5) inhibitor.

Table 3- Mulliken charges population **(ecu)** analysis for (BIPNO5) compound in three media (vacuum, DMSO, and H_2O).

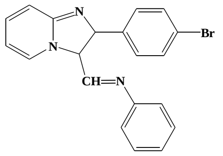
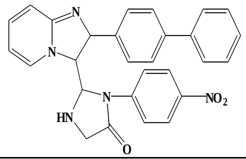
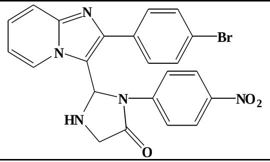
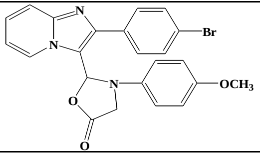
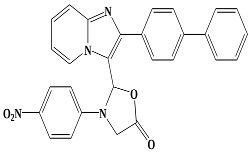
Atom no.	Electronic charge/ecu	Atom no.	Electronic charge/ ecu	Atom no.	Electronic charge/ ecu	Atom no.	Electronic charge/ecu
C1	-0.296V -0.329D -0.329W	C10	0.219V 0.225D 0.225W	C16	0.920V 0.852D 0.851W	C24	-0.311V -0.304D -0.304W
C2	-0.188V -0.227D -0.228W	C11	0.183V -0.229D -0.230W	N18	-0.047V -0.021D -0.020W	C26	-0.194V -0.235D -0.235W
N4	0.190V 0.190D 0.190W	C12	-0.254V -0.280D -0.280W	C19	0.168V 0.134D 0.134W	C27	-0.164V -0.139D -0.139W
C5	0.433V 0.452D 0.452W	C13	0.606V 0.586D 0.585W	C20	0.258V 0.334D 0.335W	N28	-0.052V 0.002D 0.003W

C7	-0.347V -0.319D -0.318W	C14	-0.288V -0.322D -0.323W	O21	-0.328V -0.360D -0.361W	O29	-0.128V -0.190D -0.186W
N9	-0.248V -0..375D -0.377W	C15	-0.394V -0.419D -0.419W	C22	0.263V 0.231D 0.230W	O30	-0.124V -0.185D -0.191W

V: vacuum phase, D: dimethyl sulfoxide (DMSO), W: water, ecu: electron controstatic unit.

Good relationships have been observed between the theoretical results of this research and the theoretical and experimental results of previous studies all of which are due to the new imidazo derivatives (1,2,a) that have been studied experimentally Table 4 (using potentiometric polarization measurements) in saline or acidic environments. From them it can be asserted that the derivative studied in this work, which is characterized by theoretical inhibition parameters is better than some of them, especially the dipole moment (in vacuum or solvents of DMSO and H_2O) of insufficiency which is one of the most important parameters to infer the efficiency of the inhibitor (the inhibition efficiency (IE%) of the inhibitor increases with increasing the dipole moment). It is noticeable that the dipole moments gradient corresponds with the sequence of the process of inhibition of the process in the following sequence as shown in Table 4, and in the following sequence:
3> 2> 4> 5 >1

Table 4- A comparison of the inhibition efficiency of new imidazo (1,2-a) pyridine derivatives,

Inhib. No.	Name	Structure	Exp. IE%	μ (Debye)
1	2-(4-Bromo-phenyl)-2,3-dihydro imidazo [1,2-a]pyridine-3-yl methylene]-phenyl-amine		77.39 in sea water	3.085V 4.023D 4.035W
2	2-(2-Biphenyl-4-yl-2,3-dihydro-imidazo [1,2-a]pyridine-3-yl)-3-(4-nitro-phenyl)-imidazolidin-4-one		89.093 in sea water	08.191V 11.363D 11.423W
3	2-[2-(4-Bromo-phenyl)-imidazo [1,2-a] pyridine-3-yl]-3-(4-nitro-phenyl)-imidazolidin-4-one		90.67 in sea water 83.52 in 0.5M HCl	08.831V 12.1458D 12.2054W
4	2-[2-(4-Bromo-phenyl)-imidazo [1,2-a] pyridine-3-yl]-3-(4-methoxy-phenyl)-oxazolidin-5-one		80.973 in sea water	6.2248V 8.4695D 8.5095W
5	2-(2-Biphenyl-4-yl-imidazo [1,2-a]pyridine-3-yl)-3-(4-nitro-phenyl)-oxazolidin-5-one		The studied derivative	3.797V 5.436D 5.466W

Conclusions

- The theoretical studies, using DFT method, were used to gain much information about the reactivity of (BIPNO5) as a corrosion inhibitor. The new synthesized (BIPNO5) derivative was theoretically established as a good organic inhibitor for carbon steel surface against corrosion. The locations containing (2-(2-Biphenyl-4-yl-)) moiety with atoms of O and N have a higher electron density. They are the most possible sites for the bonding the carbon steel surface by donating electron to the metal surface. The quantum chemical calculations have shown that the fraction from (4-nitro-phenyl) moiety adsorbing as cationic species on the carbon steel surface, the adsorption of the particle is taken place by O, N atoms and some carbon atoms. The high value of (E_{HOMO}) of the inhibitor molecule means the ability of the particle to offer electrons to the (d) orbital's of the metallic steel and a higher efficiency of inhibition of the inhibitor for carbon steel in the corrosive media. Negative coefficients of (E_{LUMO}) means that the (d) orbital's of the metal surface donate electrons to the (d) orbital of the Schiff bases leading to the presence of a feedback bond. The presence of feedback bonds promote the chemical adsorption of inhibitor molecule at the metal surface, so, increasing efficiency of inhibition of this compound.

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