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Short Communication

A Theoretical Study of Some Schiff Bases as 304 Stainless Steel Inhibitors in HCl Solution

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For four types of molecular Schiff inhibitors, the relationships between their corrosion inhibition efficiencies (IE) and some specific molecular property-related parameters, are investigated by using three different theoretical *ab initio* methods: Hartree-Fock (HF), Möller-Plesset perturbation theory on the 2nd order (MP2), and density functional theory (DFT). The parameters calculated include the energy of the highest occupied molecular orbital (E_{HOMO}) , the energy of the lowest unoccupied molecular orbital (E_{LUMO}), the energy difference between E_{HOMO} and E_{LUMO} (ΔE), the dipole moment (μ), the electronegativity value (x), the global hardness (η), the softness (σ), the fraction of transferred electrons between the molecular inhibitor and Fe (ΔN), and Mulliken atomic charges (Q). By using linear regression analysis, the relationships between *IE* and each of these parameters are carefully studied with the purpose to find the most effective parameters for the best inhibition efficiency. As a result, the comparison between the three different theoretical methods shows that the Hartree Fock (HF) method, with the 6-31++G(d, p) basis set, gives the most accurate results. In addition, the corrosion inhibition performances of all four molecular Schiff inhibitors show a linear relationship with the E_{HOMO} , E_{LUMO} , ΔE , μ , x, η , σ , and ΔN parameters. In conclusion, this work provides a theoretical method by which it is possible to predict the corrosion inhibition performance of molecules with geometrical structures like the Schiff inhibitors.

Keywords: modeling studies; corrosion inhibition; Schiff base

1. INTRODUCTION

A 304 stainless steel is one type of universal stainless steel. It is a common stainless-steel material with the characteristics of good processing performances and high toughness. It has, thus, been widely used in ship parts, for pipeline transportation, and for other industrial applications where it is important

to protect against corrosion. This type of stainless steel is, however, easily corroded in an acidic environment, especially in the presence of chloride ions. In fact, the corrosion rate even exceeds that of ordinary low carbon steel. To prevent the occurrence of corrosion, a certain amount of corrosion inhibitors is added to the solution [1-3]. Due to its high-qualitative performances, one type of widely used inhibitor is the molecular Schiff base corrosion inhibitor [4-5]. Behpour *et al.* [5] used electrochemical and weight loss methods in the search for a stainless-steel corrosion inhibitor with excellent performances. They found that the bis-N,S-bidentate Schiff base would meet the necessary demands.

Also, theoretical studies based on quantum chemistry calculations, have been used in the search for high-quality corrosion inhibitors [6-9]. The main goals of these studies were to deepen the understanding of the relationship between the structures and performances of corrosion inhibitors, and to gain knowledge about the corrosion inhibition mechanism at the micro level [10-13]. These types of knowledge are particularly useful for the development of improved corrosion inhibitors.

The purpose of the present study is to look for a correlation between the most relevant propertyrelated molecular parameters, and the experimental inhibition efficiency data, for some specific bis-N,Sbidentate Schiff bases [5]. With a deep knowledge about these relationships, it will be possible to understand the corrosion inhibition mechanism. In addition, this acquired knowledge will also lead to the development of similar inhibitors with even more pronounced corrosion inhibition performances [10, 14-15]. Some specific property-related parameters (from here on called the parameters) are calculated for the inhibitor molecules in the present study, including the highest occupied molecular orbital (E_{HOMO}), the energy of the lowest unoccupied molecular orbital (E_{LUMO}), the energy difference between E_{HOMO} and E_{LUMO} (ΔE), the dipole moment (μ), the electronegativity value (x), the global hardness (η), the softness (σ), the fraction of transferred electrons between the molecular inhibitor and Fe in a steel surface (ΔN), and Mulliken atomic charges (z). The results from these theoretical calculations were, thereafter, analyzed by using a linear regression method. The purpose of this analysis was to find those parameters that have a linear relationship with the inhibition efficiency. This type of direct correlations is, furthermore, especially important for future development and design of new inhibitors with improved corrosion efficiencies.



Table 1. Molecular structures and abbreviation[5]



2. THEORY AND COMPUTATIONAL DETAILS

Here, three different *ab initio* quantum chemistry methods are used in the optimization of the molecular structures, and in the calculations of the various parameters: Hartree Fock (HF), Möller-Plesset perturbation theory on the 2^{nd} order (MP2), and density functional theory (DFT). The structures of the inhibitor molecules were optimized by first using the semiempirical Parametric Method 3 (PM3) method. These optimized structures were then used as input structures for a continued optimization by using the following high-level methods: HF/6-31++G(d,p), MP2/3-21G*, and DFT/B3LYP/6-31++G(d,p) [16]. The molecular-specific parameters were calculated for the optimized molecular structures by using all four types of theoretical methods (PM3, HF, MP2, and DFT). In addition, the solvent effect was considered by using the Polarizable Continuum Model (PCM) [17] variant of the integral formula formalism (IEFPCM). The Gaussian09 software was used for all calculations in the present study [18].

3. RESULTS AND DISCUSSION



Figure 1. The molecular schematic of inhibitor

The geometrical structures, with the atomic (or group) numbering scheme, are presented in Fig. 1. Moreover, Table 2 presents the structural parameters of the molecular inhibitors, as obtained from calculations using different quantum chemistry methods. The HOMO, LUMO, and ΔE energies are also presented in Table 2.

Table 2. Quantum chemical parameters of the studied inhibitors with different calculated methods

Method	Molecule	E _{HOMO} ⁄ ev	E _{LUMO} ⁄ ev	ΔE/ev	µ(debye)	η/eV	x/ev	σ/ev^{-1}	ΔN	Q _{S1}	Q _{N1}	Q _{R1}	Q _{R2}	IE ^a
	M1	-5.822	-2.417	3.405	3.290	1.702	4.120	0.587	0.846	-0.109	-0.177	-0.631	0.102	96.4
DFT/B3LYP/	M2	-6.004	-2.196	3.808	3.818	1.904	4.100	0.525	0.762	-0.106	-0.176	-1.364	0.297	95.4
6-31++G(d,p)	M3	-5.809	-2.192	3.617	2.540	1.809	4.001	0.553	0.829	-0.110	-0.181	-0.463	0.457	92.9

	M4	-6.348	-2.506	3.842	9.748	1.921	4.427	0.521	0.670	-0.099	-0.144	-0.697	0.293	84.7
	M1	-7.935	1.145	9.080	2.730	4.540	3.395	0.220	0.397	-0.182	-0.176	-0.916	0.186	96.4
HF/6-	M2	-8.089	1.099	9.188	2.997	4.594	3.495	0.218	0.381	-0.176	-0.170	-1.050	0.171	95.4
31++G(d,p)	M3	-8.098	1.102	9.199	3.638	4.600	3.498	0.217	0.381	-0.200	-0.175	-0.761	0.435	92.9
	M4	-8.561	1.060	9.621	8.838	4.811	3.751	0.208	0.338	-0.194	-0.147	-0.925	0.509	84.7
MP2/3-21G*	M1	-7.829	1.274	9.102	3.046	4.551	3.278	0.220	0.409	0.461	-0.674	-0.581	-0.015	96.4
	M2	-7.961	1.531	9.492	3.135	4.746	3.215	0.211	0.399	0.459	-0.673	-0.814	-0.021	95.4
	M3	-7.968	1.529	9.497	2.688	4.749	3.220	0.211	0.398	0.461	-0.675	-0.499	-0.015	92.9
	M4	-8.264	0.891	9.155	9.712	4.578	3.686	0.218	0.362	0.473	-0.728	-1.132	0.009	84.7

a Experimental values from Ref.[5] the inhibition efficiency (*IE*) for the corrosion of *304 stainless steel* tested in 1M HCl solution with addition of 1mM of various Schiff base inhibitors at 25°C.

According to Koopman's theorem [19], the ionization potential (*I*) and the electron affinity (*A*) can be obtained from the HOMO and LUMO energies: $I = -E_{HOMO}$ and $A = -E_{LUMO}$. The concept of electronegativity values (χ) and global hardness (η) can also be related to *I* and *A*: $\chi = (I+A)/2$; $\eta = (I-A)/2$ (*I=A* (since these atoms are softer than the neutral metallic atoms) [20]. Also, the reverse of the global hardness is defined as softness: $\sigma = 1/\eta$. The electronegativity value (χ) and global hardness (η) are often used in calculating the fraction of electrons that are being transferred from the inhibitor molecule to the metallic atom (e.g., Fe): $\Delta N = (\chi_{Fe} - \chi_{inh})/2(\eta_{Fe} + \eta_{inh})$ ($\chi_{Fe} = 7.0$ eV/mol and $\eta_{Fe} = 0$ eV/mol, under the assumption of a bulk metal) [21-22]. Moreover, Q_{R1} refers to the net charge of each C atom in the benzene ring R1, Q_{R2} refers to the total charge of ring R2, and Q_{N1} and Q_{S1} refer to the net charges of N and S, respectively.

Table 3. The regression equations of corrosion inhibition efficiency and their quantum chemical parameters

	DFT			HF			MP2				
Variable	Equation		\mathbb{R}^2	Equation		\mathbb{R}^2	Equation		\mathbb{R}^2		
E _{HOMO}	<i>IE</i> =202.531+18.376* <i>E</i> _{НОМО}	(1)	0.756	<i>IE</i> =249.514+19.235* <i>E</i> _{НОМО}	(14)	0.962	<i>IE</i> =317.178+28.085* <i>E</i> _{HOMO}	(27)	0.947		
$E_{ m LUMO}$	IE=137.790+19.520*ELUMO	(2)	0.342	<i>IE</i> =-55.928+134.636* <i>E</i> _{LUMO}	(15)	0.770	IE=73.965+14.074*E _{LUMO}	(28)	0.641		
E _{HOMO} & E _{LUMO}	$IE=202.715+17.103*E_{HOMO}+3.$ $359*E_{LUMO}$	(3)	0.762	$IE=329.853+23.840*E_{HOMO}-38.777*E_{LUMO}$	(16)	0.971	$IE=277.524+23.733*E_{HOMO}+3.$ 686* E_{LUMO}	(29)	0.968		
ΔE	<i>IE</i> =152.506-16.400* <i>∆E</i>	(4)	0.387	<i>IE</i> =295.184-21.875*⊿E	(17)	0.969	<i>IE</i> =23.503+7.394* <i>∆E</i>	(30)	0.088		
μ	IE=99.470-1.468*µ	(5)	0.837	IE=99.470-1.468*µ	(18)	0.673	IE=99.238-1.483*µ	(31)	0.893		
η	<i>IE</i> =152.506-32.800*η	(6)	0.387	<i>IE</i> =295.184-43.751*η	(19)	0.969	<i>IE</i> =23.503+14.787*η	(32)	0.088		
x	IE=193.370-24.272*x	(7)	0.712	<i>IE</i> =213.194-34.187* <i>x</i>	(20)	0.953	<i>IE</i> =165.378-21.802* <i>x</i>	(33)	0.864		
σ	<i>IE</i> =34.150+106.493*σ	(8)	0.381	<i>IE</i> =-114.811+959.961*σ	(21)	0.969	<i>IE</i> =160.291-316.196*σ	(34)	0.085		
ΔN	<i>IE</i> =48.662+56.258*∆N	(9)	0.720	<i>IE</i> =15.932+204.214*∆N	(22)	0.959	<i>IE</i> =-6.912+253.261* <i>∆N</i>	(35)	0.967		
Q _{S1}	<i>IE</i> =-4.912-917.568*Q _{S1}	(10)	0.737	IE=144.677+278.333*Q _{S1}	(23)	0.330	<i>IE</i> =461.266-795.935*Q ₈₁	(36)	0.922		
Q_{N1}	<i>IE</i> =43.943-285.585*Q _{N1}	(11)	0.850	IE=31.157-366.426*Q _{N1}	(24)	0.880	IE=222.878+189.858*Q _{N1}	(37)	0.933		
Q_{R1}	<i>IE</i> =89.602-3.483*Q _{R1}	(12)	0.068	IE=86.819-6.058*Q _{R1}	(25)	0.018	IE=103.473+14.703*Q _{R1}	(38)	0.617		
Q _{R2}	<i>IE</i> =95.398-10.609*Q _{R2}	(13)	0.084	IE=101.047-26.741*Q _{R2}	(26)	0.753	IE=88.358-380.226*Q _{R2}	(39)	0.908		

By using linear regression analysis on the results obtained by the different calculations methods, the relationships between each of the molecular-specific parameters and the corrosion inhibitor efficiency (*IE*) are thoroughly analyzed with the purpose to find the most effective parameters for an improved inhibition efficiency. Regression equations (for the molecular structure-to-activity relationship) were, thereby, established, and the squares of the multiple correlation coefficients (R^2) were obtained (see Table 3).

3.1 Correlation between corrosion inhibition efficiency and frontier molecular orbital energies

By using a linear regression analysis method, the correlation between inhibition efficiency (*IE*) and the parameters E_{HOMO} , E_{LUMO} , and ΔE are investigated. As can be seen in Table 3, unary regression analysis showed that the correlations between *IE* and E_{HOMO} were good, but that the correlations between *IE* and the parameters E_{LUMO} and ΔE , were poor. By using binary regression analysis in studying the eventual correlation between *IE* and the energy parameters E_{HOMO} and E_{LUMO} , it was found that the corrosion inhibition efficiency experienced a good correlation with E_{HOMO} and E_{LUMO} . Hence, by tuning any of these frontier molecular orbital energy levels, it will be possible to directly affect the inhibition of corrosions. Moreover, the Eqs. (3) and (29) show that the coefficient of E_{HOMO} is about ten times and four times, respectively larger than that of E_{LUMO} . Also, the coefficient of E_{HOMO} in Eq. (16) is positive, while that of E_{LUMO} is negative. Hence, the effect of E_{HOMO} is found to be larger than that of E_{LUMO} , which is consistent with the regression results.

The molecular orbitals at the E_{HOMO} levels were found to be especially important for the chemical adsorption of the Schiff base molecules to the Fe atoms. These filled orbitals overlap with the empty Fe *3d* orbitals in the formation of coordination bonds (i.e., where the electrons have been provided by the Schiff base molecule). It should here be noted that a higher value of E_{HOMO} (for the Schiff base molecule) is strongly correlated with a higher ability to provide electrons. Hence, the ability to form coordination bonds will increase, and the inhibition rate of iron will be improved.





Figure 1. The frontier molecule orbital density distribution of four inhibitors after optimization using DFT B3LYP/6-31+G(d,p) method

According to the frontier orbital theory, the coupling between HOMO and LUMO orbitals of two molecules is solely responsible for their overall interactions with respect to each other [23-24]. To analyze the adsorption process of corrosion inhibitors onto the stainless-steel surface, one has therefore to consider the HOMO and LUMO levels of the inhibitor molecules and of a Fe atom (in the steel surface). [The steel surface Fe atoms will from here on be denoted as Fe atoms]. The distribution of HOMO and LUMO level orbitals for the four Schiff base molecules are shown in Fig. 2. The HOMO and LUMO distribution centers of the four molecules are similar, with mainly delocalized R1 and R2 rings. This facilitates easier adsorption of the molecules onto the Fe atoms. As can be seen in Fig. 2, the adsorption process involves successive adsorption of the R1 and R2 rings. The inhibitor molecules will overlap with their filled π orbitals with the empty 3d orbitals in the Fe atoms, thereby transferring a fraction of electrons from the molecule to the surface. There is also an overlap between the empty π orbitals in the inhibitor molecules with the filled 3d orbitals in the Fe atoms, which will lead to the transfer of a fraction of electrons from the steel surface to the inhibitor molecule. These coupled electron transfer processes are generally known as the bonding-back bonding process. The inhibitor molecules can thereby form very stable covalently bonded adsorbates on the Fe atoms. Furthermore, the lone-pair electrons on the N atom (between the R1 ring and the R2 ring), and the lone-pair electrons on the S atom (in the R2 ring), will increase the electron densities in the strong π bonds within the benzene rings (R1 and R2 rings). This increase in electron densities will further increase the total adsorption bond strength between the molecule and the Fe atom. Hence, the inhibitor molecules will most probably form a protective film on the metal surface, thereby playing an important role in the process of corrosion inhibition.

In summary, the inhibition efficiency is mainly determined by studying the ability of electron transfer between the inhibitor molecule and the stainless-steel surface [12, 25]. In the present study, the existence of lone pair electrons in the N and S atoms (in the Schiff base molecules) will increase the molecular E_{HOMO} level and, thereby, enhance the electron donating ability and the corrosion inhibition performances.

Some other parameters, such as the dipole moment (μ), the electronegativity value (χ), the global hardness (η), and the softness (σ), are also calculated in the present study (see Table 2). The relationships

between these parameters and the corrosion inhibition efficiency were obtained by using regression analysis functions, and these results can be seen in Table 3. It was found that the inhibition efficiency experiences strong correlations with the dipole moment (μ) (see Eq. (5)), the electronegativity value (χ) (see Eq. (21)), the global hardness (η) (see Eq. (22)), and the softness (σ) (see Eq. (23)). The square of the respective correlation coefficient was observed to reach a value of about 0.837~0.969. These parameters are, therefore, particularly useful in the modification of corrosion inhibitor performances.

3.2 Correlations between the corrosion inhibition efficiency and the Mulliken charges

The possibility for correlations between the experimental corrosion inhibition performance and the Mulliken charges of various atoms (Q_{N1} , Q_{S1} , QR_1 , and Q_{R2}) are also investigated in the present study. As can be seen in Table 3, the corrosion inhibition efficiency shows a noticeably clear correlation with the net charge of the N atom. When this net charge increased, the corrosion inhibition efficiency also increased. Moreover, this net charge corresponded to a specific electron density (on N) which interacted strongly with the 3d orbital of Fe, thereby forming a strong coordination bond. This new bond formation is strongly beneficial for the formation of a protective film on the steel surface, thereby playing an important role in the inhibition of corrosion inhibition (i.e., in enhancing the corrosion inhibition efficiency).

The ΔN parameter is another important factor that might affect the corrosion inhibition performances [26]. With an increased value of ΔN (i.e., a larger fraction of electrons has been transferred from the molecular inhibitor to the steel surface), the inhibition efficiency is expected to also increase. As can be seen in Table 2, the strongly bonded molecular inhibitors act as donators of electrons, while the iron atoms are the acceptors. The ΔN value of the M1 molecule was found to be the highest among the four studied inhibitor molecules, independent of the method used in calculations. This observation indicates that when these inhibitor molecules became adsorbed to the steel surface, it was the M1 molecule that transferred the largest portion of electrons to the surface. This result strongly supports the experimental observation, which shows that it is the M1 molecule that gives the best corrosion inhibition performance. This result is also consistent with the observation that the M1 molecule has the highest HOMO energy level among the four molecules studied in the present investigation. In fact, the highest ΔN value is generally associated with the best corrosion inhibitor performance [26]. The relationship between IE and ΔN showed that the corrosion inhibition efficiency experiences an exceptionally good correlation with ΔN . Consequently, as the electron density in steel increases, the corrosion resistance increases as well. This is due to fact that the inhibitor molecule, and then especially the N atom in this molecule, will provide a larger electron density to the metal atoms, thereby preventing the corrosion of the metal. As discussed in Section 3.1, we also found that if the HOMO energy of the inhibitor molecule is higher, these frontier orbital electrons will become more efficiently transferred to the LUMO orbital of the Fe atoms in the metal.

To also find out which parts of the inhibitor that play an important role in the efficiency of the surface adsorption process, the molecular electrostatic potential surface was calculated by using the DFT B3LYP/6-311+G(d,p) method [27]. As can be seen in Figure 3, the electronic charges in all four corrosion inhibitor molecules were mainly concentrated on the nitrogen atoms (N_1 and N_2). It was,

therefore, possible to draw the conclusion that when the molecules adsorb onto the metal surface, the lone pair electrons on the N atoms will play a major role in the adsorption process. In addition, the negative charge of the R1 ring will have a synergistic effect. This explains why the charge of N correlates that strongly with the inhibition efficiencies of the Schiff bases molecules (see Eqs. (11), (24), and (37)).

As shown in Table 2, the HF calculations resulted in 6 regression equations, whose R^2 values reached 0.9. When using the MP2 method, the corresponding calculations resulted in 5 equations, while the DFT method gave none. It can, therefore, be concluded that when studying the relationship between molecular structure and corrosion inhibitor performance, the calculations which are based on the HF/6-31++G(d,p) method will provide the best result (among the three methods that are used in the present study).



- **Figure 3.** The molecular electrostatic potential surface of four inhibitors (using DFT/B3LYP/6-31++G(d,p) method) with isopotential value of 1.50 a.u. Negative regions were shown in red, positive in blue
- 3.3 Prediction of corrosion inhibition efficiency for some similar molecular structures

Table 4. Structures of some similar molecules



In the present theoretical study, it was not only possible to establish a relationship between the

corrosion inhibitor efficiency (*IE*) and some molecular-specific parameters, and to learn more about the inhibitor adsorption process on the metal surface. It was also possible to predict the performance of some similar corrosion inhibitor molecules [28].

 Table 5. Some quantum chemical parameters and prediction of inhibition efficiency for similar molecules

molecular	E _{HOMO}	$E_{\rm HOMO}$ $E_{\rm LUMO}$ ΔE		µ(deby	/ 37		(** 1	437		Equation for Prediction of inhibition efficiency ^a							
	/eV	/eV	/eV	e)	η/ev	x/eV	σ/eV^{-1}	ΔN	(14)	(16)	(17)	(19)	(20)	(21)	(22)	IE%	
M5	-7.799	1.143	8.943	1.958	4.471	3.328	0.224	0.411	99.49	99.58	99.38	99.37	99.42	99.67	99.70	99.52	
M6	-8.029	1.144	9.173	2.236	4.587	3.443	0.218	0.388	95.07	94.07	94.33	94.33	95.50	94.29	95.04	94.66	
M7	-7.936	1.071	9.007	2.260	4.504	3.432	0.222	0.396	96.87	99.13	97.97	97.97	95.85	98.14	96.73	97.52	
M8	-8.131	1.110	9.241	5.069	4.621	3.511	0.216	0.378	93.11	92.97	92.85	92.85	93.17	92.75	92.96	92.95	

^{*a*} Equation (14), (16), (17), (19), (20), (21), (22) presented in Table 3.

For these predictions, four additional molecules (M5 - M8) were screened, and each of them had similar molecular structures as M1 – M4 (Table 4). The molecular parameters that were used for the M1 – M4 molecules, were also used in the calculations for these new compounds. The prediction of these new molecules' inhibition efficiencies were calculated using the HF/6-31++G(d, p) method and Eqs. (4), (16), (17), (19), (20), (21), and (22). These equations were chosen since they were found to be the best ones in the study of the M1 – M4 molecules.

As shown in Table 5, the molecules M5 and M7 show the best performances (with *IEs* close to 99%). These molecules have higher HOMO energies, and are, therefore, more likely to provide electrons to the metal surface. In addition, the optimized geometrical structure of M5 was flatter than for the other molecules, which made it easier to adsorb onto the metal surface (and, thereby, to achieve an improved corrosion inhibition effect). Moreover, the M7 molecule contained two NH₂ groups. Since an N atom usually provides one lone pair of electrons, the two N atoms in the M7 molecule, with their two lone pairs of electrons, enhances the possibilities for a very large corrosion inhibition effect when using the M7 molecule.

In the development of effective corrosion inhibitors, the traditional design of these types of molecules (with suitable evaluation methods) is generally based on speculation and many exploratory experiments (e.g., electrochemical experiments), which most often results in high costs, long cycles, and a lot of "blind" work. A screening procedure was, instead, used in the present study and four corrosion inhibitor molecules were selected. In the screening procedure, some specific molecular parameters were calculated, and compared, with their inherent corrosion inhibition performances. In the prediction of the best corrosion inhibitor molecule, structure-activity equations were used in searching for the best correlations between the molecular-specific parameters and the inhibitor efficiency. It was found that all four proposed molecular candidates (M5 – M8) have excellent corrosion inhibitor molecules with improved corrosion inhibition performances.

4. CONCLUSIONS

Three different *ab initio* quantum chemical methods (HF, MP2, DFT) were used in calculating the relationships between molecular-specific parameters and corrosion inhibition performances. The molecules that were used in these calculations were four types of Schiff inhibitor compounds, and their property-related parameters were investigated by using regression analysis (i.e., in establishing structureactivity equations). The property-related parameters, such as the level of the highest occupied molecular orbital HOMO), level of the lowest unoccupied molecular orbital (LUMO), energy gap (ΔE) between HOMO and LUMO, dipole moment (μ), electronegativity (x), global hardness (η), softness (σ), fraction of transferred electrons (ΔN), and Mulliken charges (Q), were thereby calculated. The structure-activity equations showed that the HF method, with the 6-31++G(d, p) basis set, most probably will provide the most accurate calculation results. Moreover, these equations showed that the corrosion inhibition efficiency experiences a strong correlation with most of the molecular property-related parameters (E_{HOMO} , E_{LUMO} , ΔE , μ , η , x, σ , and ΔN). The corrosion inhibition performances, of the investigated molecular inhibitors, were mainly determined by the electron donating capacities of the HOMO states in the molecules. The higher the HOMO energy, the stronger the electron donating capacity and the better the corrosion inhibition performance.

Based on similarities in molecular structures, four additional molecular inhibitors were chosen for the prediction of their most relevant structure-activity equations. By performing HF calculations, it was found that two of these molecules (M5 and M7) showed excellent corrosion inhibition performances, and that the predicted inhibition efficiency could reach 99% (M5). Thus, the present study provides theoretical guidance for discovering molecular corrosion inhibitors with improved corrosion inhibition effects.

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