ISSN 1392–1320 MATERIALS SCIENCE (MEDŽIAGOTYRA). Vol. 29, No. 4. 2023

The Quantum Chemical Investigation on the Structure-Activity Relationship of a Schiff Base Corrosion Inhibitor

Hong JU*, Di ZHU, Shufa LIU, Hanzhi LI

School of Materials Science and Engineering, China University of Petroleum (East China), Qingdao, China

http://doi.org/10.5755/j02.ms.33818

Received 18 May 2023; accepted 30 June 2023

This study investigated the relationship between the molecular structure and the corrosion inhibition efficiency of three corrosion inhibitors for steel in acidic media using the DFT method. First, the molecular conformations of the three compounds were optimized and the populations of charges and frontier orbitals were obtained at the B3LYP/6-311G level. Quantum chemical parameters were also obtained by calculations, including the highest occupied molecular orbital energy (E_{HOMO}), the energy gap (E_{LUMO}-E_{HOMO}), the total energy of the molecule, the dipole moment and the number of electrons transferred (ΔN). The results of the correlation between quantum chemical parameters and inhibition efficiencies demonstrated that the inhibition efficiency of the inhibitors increased with the decrease of E_{LUMO}-E_{HOMO} and the increase of ΔN. The regions with nitrogen and oxygen atoms are the sites most likely to bond with iron atoms by donating electrons.

Keywords: corrosion, inhibitor, quantum chemical, DFT method, molecular orbital.

1. INTRODUCTION

Corrosion inhibitors are affordable, efficient, and adaptable. They are extremely important in the petroleum, petrochemical, energy, transportation, electromechanical, and construction industries [1 – 5]. The current synthesis and screening of metal corrosion inhibitors use many experiments, but there are no examples of successful design or synthesis of corrosion inhibitors directly for specific corrosion-inhibition environments. The structure of organic-type corrosion inhibitors has a decisive role in their performance and is the precondition that determines the corrosion inhibition performance. Therefore, the establishment of qualitative and quantitative relationships between chemical structure and corrosion inhibition performance is of broad interest [6 – 11].

Quantum chemical calculation methods [12 – 15] can quickly and intuitively provide insight into molecular structure and can be used for rapid screening of corrosion inhibitors and inhibition mechanism studies. When organic corrosion inhibitors prevent corrosion on a metal surface, they often interact with metal atoms via their frontier orbitals [16, 17]. The ability of target organic corrosion inhibitors to interact with metal atoms can be determined rapidly and intuitively by calculating the charge density distribution, the frontier orbital distribution and energy, the dipole moment, the total molecular energy, and the number of electrons transferred [17, 18]. Thus, these quantum chemical parameters of inhibitors can be compared to other established inhibitors under the same conditions. The calculation of quantum chemical parameters for organic corrosion inhibitors can guide the rapid screening and evaluation of corrosion inhibitors and can direct more rational synthetic schemes. This saves time, money, and reagents. This relationship between corrosion inhibition and quantum chemistry can explain the inhibition mechanisms of organic compounds onto the electrode surfaces at the molecular level.

The quantitative structure-activity relationship of organic compounds allows researchers to purposely design and prepare new types of highly efficient corrosion inhibitors depending on adsorption, solubility, and chemical properties. This broadens the scope of corrosion inhibitor research. Applications of theoretical chemistry in corrosion inhibitor research can direct synthetic efforts and can create more effective chemical tools.

Previous studies on corrosion inhibitors have used ab initio or semi-empirical methods (such as complete neglect of differential overlap (CNDO), modified intermediate neglect of differential overlap (MNDO), parametric model number 3 (PM3) and Austin model 1 (AM1)) [19 – 21]. However, these methods lack sufficient accuracy and are unreliable. We used the relatively accurate density functional theory (DFT) [17, 22] to investigate the molecular structures of several compounds. DFT was suitable because of the electronic correlation. We also studied the active sites in the molecules and explored the possible mechanism underlying corrosion inhibition as a function of molecular characteristics.

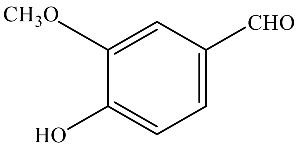
DFT is a mainstream quantum chemistry tool because electron correlation effects are considered, and its accuracy is usually better than Hartree-Fock methods (electron correlation is not considered). This work used Becke's three parameter hybrid method with the Lee, Yang, and Parr (LYP) correlation functional (B3LYP) [23]. This DFT method was adopted to perform a relatively high-level calculation on the molecules and optimize the molecular geometry and electronic structure. The LYP functional is a widely used gradient-corrected functional in DFT. Based on this, Becke added a three-parameter hybrid functional and combined it with the Lee-Yang-Parr for a non-local

---

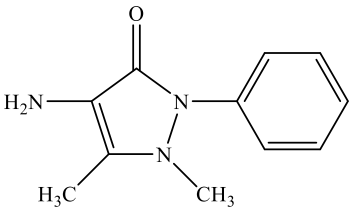
* Corresponding author. Tel.: +86-18724733900.
E-mail: *juhong@upc.edu.cn* (H. Ju)

correlation function to form B3LYP. The B3LYP functional fully considers the electron correlation, retains the advantages of the ab initio MO method, and saves a considerable amount of calculation time. The advantages of this functional are widely accepted and have been widely used for heterocyclic corrosion inhibitors [22, 24].

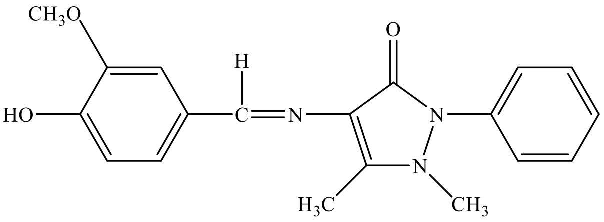
Three corrosion inhibitors used for steel in acidic media are shown in Fig. 1 [25]. 4-[(4-hydroxy-3-hydroxymethyl-benzylidene)-amino]-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (phv), as the Schiff base compound, was obtained by the synthesis of 4-hydroxy-3-methoxy-benzaldehyde (vn) and 4-amino-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (phz). At constant temperature and concentration, the order of corrosion inhibition efficiency was: phv > phz > vn. However, the corrosion inhibition mechanism was not explained or analyzed further. Therefore, we investigated the quantitative structure-activity relationships of these three compounds using quantum chemical calculations to explain their corrosion inhibition mechanisms.



4-hydroxy-3-methoxy-benzaldehyde (vn)



4-amino-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (phz)



4-[(4-hydroxy-3-hydroxymethyl-benzylidene)-amino]-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (phv)

Fig. 1. Molecular structures of the three compounds

2. CALCULATION MODEL AND METHOD

The molecular structures of the three compounds were constructed in GaussView 6.0; Gaussian09W was used as the quantum chemical calculation software, and all calculations were performed at the B3LYP/6-311G level to obtain the optimal spatial configuration and related quantum chemical parameters. The geometric configuration was optimized with the energy gradient method based on the Berny algorithm [26]. This is an optimal method to calculate the system with the lowest energy. The charges were analyzed using the Mulliken population analysis.

3. RESULTS AND DISCUSSION

3.1. Optimization of structures and the population distribution of charges

The electronic structure of a molecule can affect various properties of the molecule, including surface adsorption. Some studies [27 – 30] have shown that corrosion inhibitors undergo adsorption through the interaction of negatively charged atoms in the molecule with the positive charges on the metal surface. The calculations resulted in optimized structures and Mulliken charges populations for the three molecules (Fig. 2). In the Mulliken charge population analysis, the more negative charges on the atoms, the more favorable the adsorption of inhibitor molecules on the metal surface, and these negatively charged atoms are the adsorption centers of inhibitor molecules [28]. As can be seen in Fig. 2, the electronegativity of heteroatoms is higher compared to carbon and hydrogen atoms, therefore, these sites are the active adsorption sites for corrosion inhibitors.

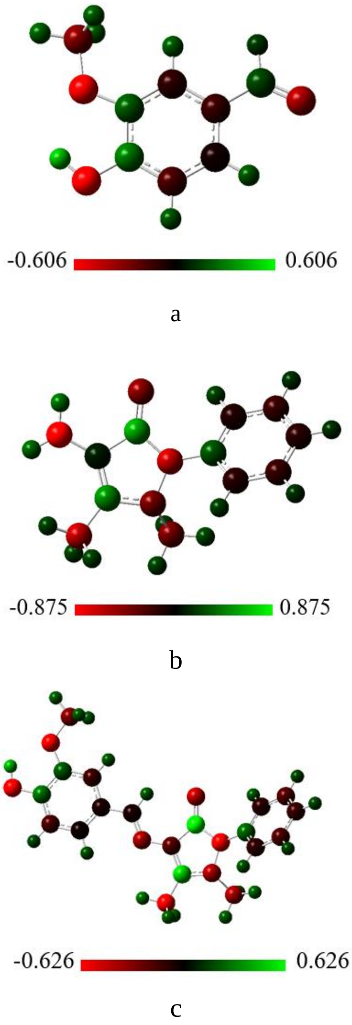


Fig. 2. Optimized structures and Mulliken charges of three molecules: a – vn; b – phz; c – phv

3.2. Frontier orbital distribution

In electrolyte solutions, organic molecules inhibit the corrosion of metals by adsorption. The adsorption mechanism is divided into physisorption and chemisorption.

In general, both physisorption and chemisorption should be considered. Physisorption requires mutual interaction between the corrosion inhibitor molecules and the charged metal through electrostatic attraction. Chemisorption requires electron transfer or charge sharing between the metal and corrosion inhibitor molecules, i.e., chemical bonding. The chloride ion in the hydrochloric acid solution has a certain degree of hydration – it can form ‘specific adsorption’ onto the metal surface that will allow the metal surface to have negative charges [29]. Protonated corrosion inhibitors interact with metals via their mutual attraction with the negatively charged chloride ions. Concurrently, the negatively charged active centers in the organic molecules can provide electrons to metal atoms, making the adsorption of corrosion inhibitors stronger [22, 30]. Therefore, there may be both physisorption and chemisorption during corrosion inhibition.

Frontier orbital theory plays an important role in predicting the interactions between metal atoms and adsorption centers of corrosion inhibitor molecules [30, 31]. Chemical bonding is generally believed to be the most effective overlap between the HOMO of one molecule and the LUMO of another molecule. Therefore, in this paper, the distributions of the HOMO and LUMO for the three compounds were calculated (Fig. 3). The HOMO orbital for vn was evenly distributed throughout the molecular structure, whereas the LUMO orbital was distributed at positions except for methoxy. Phz had the HOMO orbital distributed at sites except for the benzene ring, while the LUMO orbital was evenly distributed all over the molecule. For phv, the frontier orbitals were distributed at positions except for the benzene ring, such as heterocyclic ring, nitrogen atoms, oxygen atoms, and -C=N- bond. The three corrosion inhibitors adsorbed onto the steel surface by providing electrons to iron atoms to form coordination bonds through the HOMO distribution sites and accepting free electrons to form feedback bonds through the LUMO distribution sites, respectively. Both the Mulliken charges population and the frontier orbitals distribution show that all three compounds have multiple adsorption centers.

The orbitals of all atoms in the compound molecules were combined as the sum of the squares of the molecular orbital coefficients. After normalization, the contribution of each atom in the frontier molecular orbitals and nearby molecular orbitals was obtained (Table 1). There were large changes in energy based on the energies of HOMO−1, HOMO occupied orbitals, LUMO, and LUMO+1 unoccupied orbitals – these are the main orbitals involved in the reactions [32].

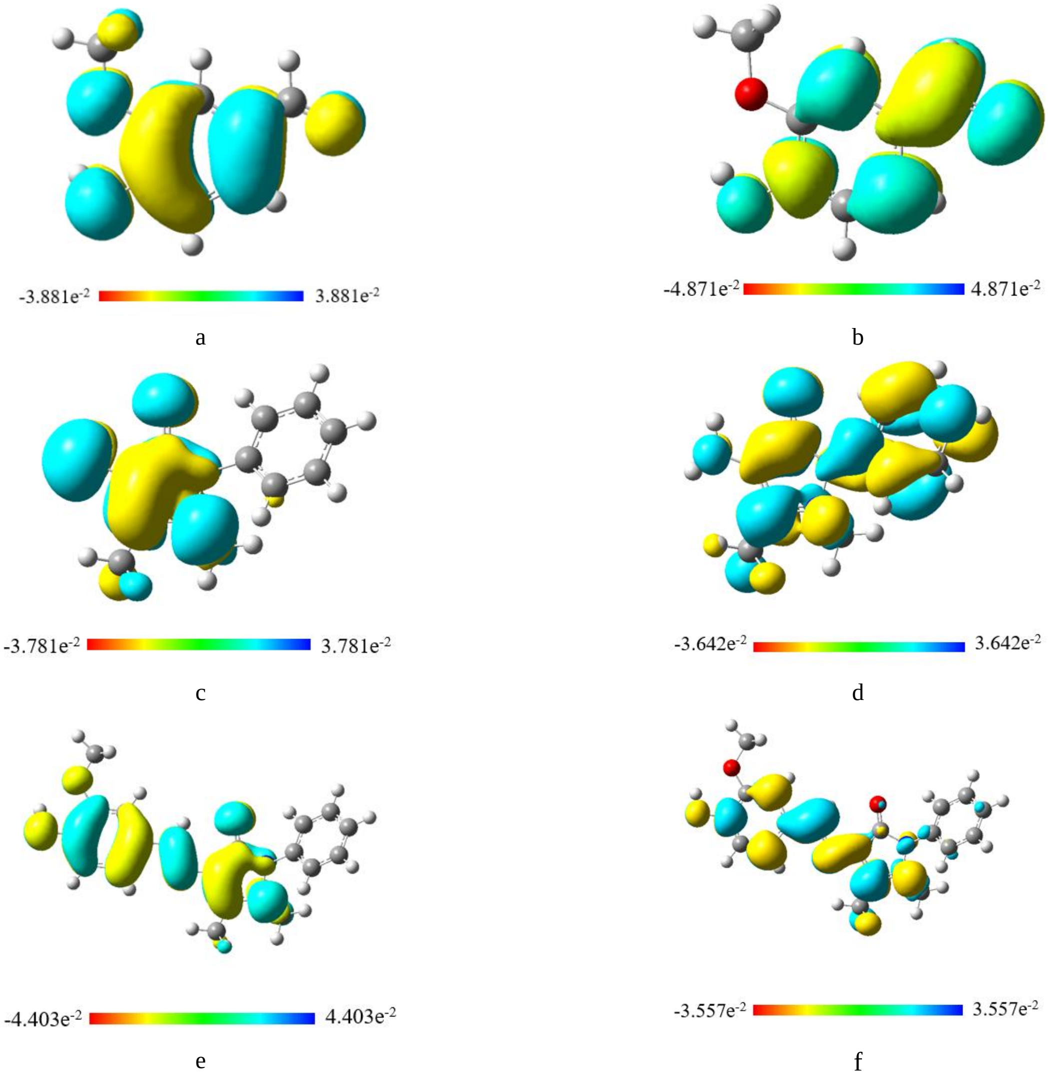


Fig. 3. The distributions of frontier orbitals for the three molecules (left: HOMO; right: LUMO): a, b – vn; c, d – phz; e, f – phv

Table 1. Energy of the molecular orbitals

	HOMO-2, a.u.	HOMO-1, a.u.	HOMO, a.u.	LUMO, a.u.	LUMO+1, a.u.	LUMO+2, a.u.
vn	-0.26883	-0.26000	-0.23639	-0.06979	-0.01908	0.02571
phz	-0.25177	-0.22065	-0.19151	-0.02871	-0.00704	0.00700
phv	-0.23166	-0.22467	-0.19714	-0.05383	-0.03059	-0.01448

Frontier orbital theory shows that the higher energy of the HOMO indicates a weaker attraction of the nucleus to the electrons. These electrons are more easily released; LUMOs with lower energy can more easily accept the external electrons. A smaller energy gap allows the molecules to form bonds more easily. Several previous studies [7 – 11] have shown that the corrosion inhibition efficiency increases with the increasing E_{HOMO} and the decreasing energy gap. Table 2 shows the quantum parameters obtained by Gaussion09W. Versus the quantum chemical parameters of high efficiency corrosion inhibitors in the literature [7 – 12], all three compounds shown here had relatively high HOMO orbital energies and small HOMO-LUMO energy gaps. This demonstrates that these three compounds can inhibit corrosion by forming bonds with the metals. Compared to vn and phz, phv had the smallest HOMO-LUMO energy gap and the lowest total energy value, indicating that it is most easily bound to metals. The resulting bond strength is the strongest, which means phv offers the best corrosion inhibition.

3.3. Discussion

3.3.1. Relationship between E_{HOMO} and inhibition efficiency

E_{HOMO} and inhibition efficiency of three corrosion inhibitors are correlated in Fig. 4. Although the fitted result showed a positive correlation, the inhibition efficiency did not strictly increase with increasing E_{HOMO} values, which suggested that the high inhibition efficiency of phv was not merely influenced by the electron giving ability.

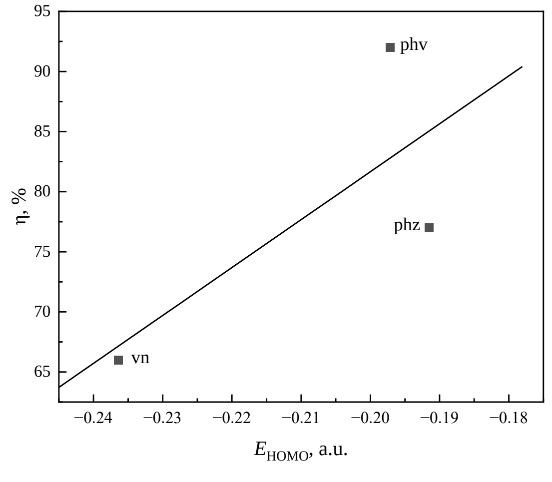


Fig. 4. Correlation between E_{HOMO} and inhibition efficiency of three inhibitors

3.3.2. Relationship between energy gap (E_{LUMO}-E_{HOMO}) and inhibition efficiency

In Fig. 5. The corrosion inhibition efficiency gradually reduced with increasing E_{LUMO}-E_{HOMO}. Phv had the smallest E_{LUMO}-E_{HOMO}, and the electrons in its frontier orbitals were the most likely to undergo transitions and interact with the metal atoms to protect the metal.

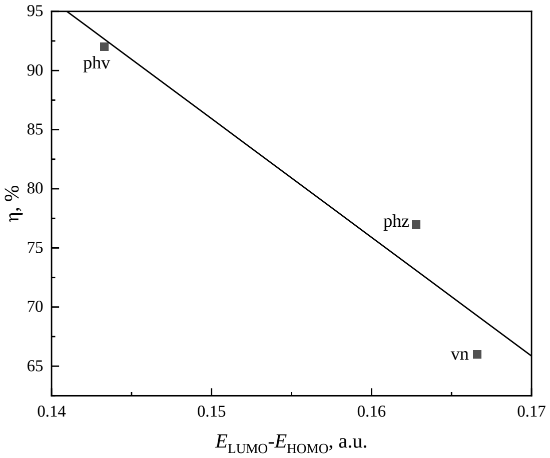


Fig. 5. Correlation between E_{LUMO}-E_{HOMO} and inhibition efficiency of three inhibitors

3.3.3. Relationship between total energy and inhibition efficiency

Fig. 6 shows the correlation between total energy and inhibition efficiency. As the total molecular energy increased, the corrosion inhibition efficiency gradually decreased. Phv had the lowest total energy value, which indicated that the phv molecule was the most active and more easily bonded to metals.

3.3.4. Relationship between dipole moment and inhibition efficiency

There are some controversies regarding the effect of dipole moment on the corrosion inhibition properties. Some scholars believe that low dipole moment values favor the compounds' accumulation on metal surfaces [33, 34], while others believe that high values imply strong corrosion inhibition properties [35, 36].

Table 2. Quantum parameters obtained by Gaussion09W

Compound	E_{HOMO}, a.u.	E_{LUMO}, a.u.	E_{LUMO}-E_{HOMO}, a.u.	Total energy, a.u.	Dipole moment, debye	Inhibition efficiency [22] η, %
vn	-0.23639	-0.06979	0.16660	-535.30	5.4325	66
phz	-0.19151	-0.02871	0.16280	-666.42	4.4580	77
phv	-0.19714	-0.05383	0.14331	-1125.30	3.9011	92

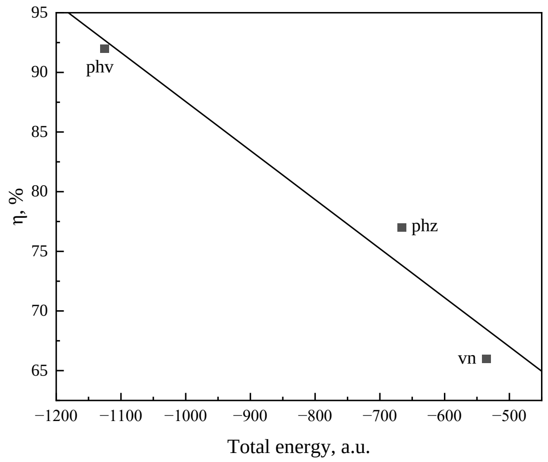


Fig. 6. Correlation between total energy and inhibition efficiency of three inhibitors

In Fig. 7, as the dipole moment values increased, the corrosion inhibition efficiency significantly decreased, this result is more in line with the former view that phv molecules are more likely to accumulate on the metal surface.

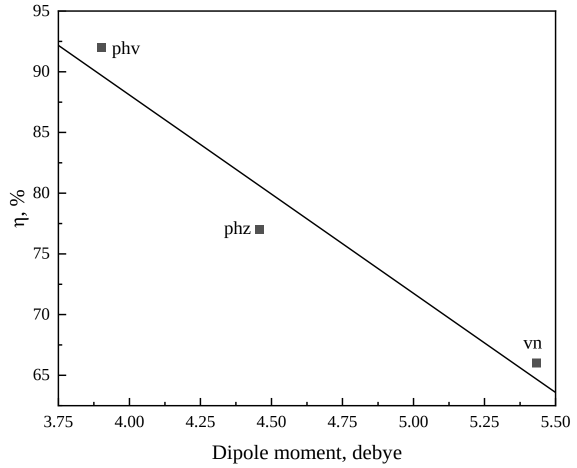


Fig. 7. Correlation between dipole moment and inhibition efficiency of three inhibitors

3.3.5. Relationship between ΔN and inhibition efficiency

ΔN is the number of transferred electrons between the corrosion inhibitor molecules and the metal atoms. When the corrosion inhibitor acts on the steel surface, the number of transferred electrons can be obtained from the formula as follows [12, 37]:

$$\Delta N = \frac{(\chi_{Fe} - \chi_{inh})}{[2(\eta_{Fe} + \eta_{inh})]}, \tag{1}$$

where χ_{Fe} and χ_{inh} represent the absolute electronegativity of the iron atom and corrosion inhibitor, respectively; η_{Fe} and η_{inh} denote the absolute hardness values of the iron atom and the corrosion inhibitor, respectively. The values of χ_{Fe} and η_{Fe} are 7 eV/mol and 0 eV/mol, respectively. The χ and η of the corrosion inhibitor can be obtained from the formulas as follows [22, 37]:

$$\chi = \frac{(I + A)}{2}; \tag{2}$$

$$\eta = \frac{(I - A)}{2}. \tag{3}$$

Meanwhile, I and A can be calculated from the values of E_{HOMO} and E_{LUMO} [22, 37]:

$$I = -E_{\mathrm{HOMO}}; \tag{4}$$

$$A = -E_{\mathrm{LUMO}}, \tag{5}$$

where η represents the absolute hardness, which is an important parameter for evaluating the stability of inhibitor molecules. It is widely accepted that compounds with low hardness are easier to bond with metals [37]. In Table 3, η followed the order of vn > phz > phv, indicating that phv had the highest reactivity and was more likely to bond with Fe atoms. Meanwhile, the higher number of electrons transferred means the stronger corrosion inhibition properties of the molecules. In Table 3, phv had the highest ΔN value, indicating that its corrosion inhibition property was stronger than that of vn and phz.

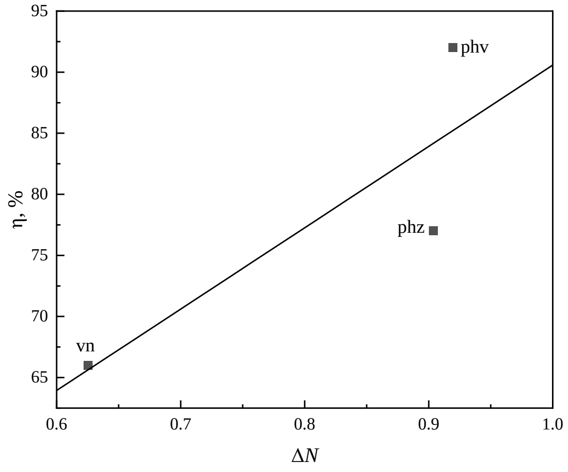


Fig. 8. Correlation between ΔN and inhibition efficiency of three inhibitors

The research result [12] indicated that when the value of ΔN is lower than 3.6, the corrosion inhibition efficiency increases as the electron transfer capability of corrosion inhibitors increases, which confirmed our conclusion. As seen in Fig. 8, the inhibition efficiency gradually increased with the value of ΔN increasing.

Table 3. Number of transferred electrons (ΔN) of three inhibitors.

Compound	I, eV/mol	A, eV/mol	χ, eV/mol	η, eV/mol	ΔN
vn	6.433	1.899	4.166	2.267	0.625
phz	5.211	0.781	2.996	2.215	0.904
phv	5.364	1.465	3.415	1.950	0.919

4. CONCLUSIONS

The calculated results show that 4-[(4-hydroxy-3-hydroxymethyl-benzylidene)-amino]-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (phv) chemisorbed better onto the steel surface. The corrosion inhibition efficiency increased with the decrease of the frontal orbital energy gap (E_{LUMO}-E_{HOMO}). Subsequent calculations of ΔN and its relationship with corrosion inhibition efficiency indicated that these three compounds formed bonds with iron atoms by transferring electrons, thus exerting corrosion inhibition. 4-[(4-hydroxy-3-hydroxymethyl-benzylidene)-amino]-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (phv) had the highest number of transferred electrons and therefore had the best inhibition performance, which was consistent with the tests.

The population distribution of the charges shows that the three compounds have numerous negatively charged active sites. In sites with nitrogen and oxygen atoms, electrons are most likely to be donated to metal atoms. 4-[(4-hydroxy-3-hydroxymethyl-benzylidene)-amino]-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (phv) has one more nitrogen-containing heterocyclic ring than 4-hydroxy-3-methoxy-benzaldehyde (vn) and one more -C=N- bond than 4-hydroxy-3-methoxy-benzaldehyde (vn) and 4-amino-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (phz). Thus, it is easier to form complexes with metal atoms by forming chemical bonds, which results in good adsorption.

Acknowledgments

This study was funded by the National Natural Science Foundation of China (NSFC, No. 52171092). We thank LetPub (www.letpub.com) for its linguistic assistance during the preparation of this manuscript.

REFERENCES

1. **Rodríguez-Valdez, L.M., Villamisar, W., Casales, M., González-Rodriguez, J.G., Martínez-Villafañe, A., Martinez, L., Glossman-Mitnik, D.** Computational Simulations of the Molecular Structure and Corrosion Properties of Amidoethyl, Aminoethyl and Hydroxyethyl Imidazolines Inhibitors *Corrosion Science* 48 (12) 2006: pp. 4053 – 4064. https://doi.org/10.1016/j.corsci.2006.05.036
2. **Issaadi, S., Douadi, T., Zouaoui, A., Chafaa, S., Khan, M.A., Bouet, G.** Novel Thiophene Symmetrical Schiff Base Compounds as Corrosion Inhibitor for Mild Steel in Acidic Media *Corrosion Science* 53 (4) 2011: pp. 1484 – 1488. https://doi.org/10.1016/j.corsci.2011.01.022
3. **Finšgar, M., Jackson, J.** Application of Corrosion Inhibitors for Steels in Acidic Media for the Oil and Gas Industry: A Review *Corrosion Science* 86 2014: pp. 17 – 41. https://doi.org/10.1016/j.corsci.2014.04.044
4. **El-Faham, A., Osman, S.M., Al-Lohedan, H.A., El-Mahdy, G.A.** Hydrazino-methoxy-1,3,5-triazine Derivatives' Excellent Corrosion Organic Inhibitors of Steel in Acidic Chloride Solution *Molecules* 21 (6) 2016: pp. 714. https://doi.org/10.3390/molecules21060714
5. **Obot, I.B., Onyeachu, I.B., Umoren, S.A.** Alternative Corrosion Inhibitor Formulation for Carbon Steel in CO_2-Saturated Brine Solution Under High Turbulent Flow Condition for Use in Oil and Gas Transportation Pipelines *Corrosion Science* 159 2019: pp. 108140. https://doi.org/10.1016/j.corsci.2019.108140
6. **Bentiss, F., Mernari, B., Traisnel, M., Vezin, H., Lagrenée, M.** On the Relationship between Corrosion Inhibiting Effect and Molecular Structure of 2,5-bis(n-pyridyl)-1,3,4-thiadiazole Derivatives in Acidic Media: Ac Impedance and DFT Studies *Corrosion Science* 53 (1) 2011: pp. 487 – 495. https://doi.org/10.1016/j.corsci.2010.09.063
7. **Ju, H., Li, Y.** Nicotinic Acid as a Nontoxic Corrosion Inhibitor for Hot Dipped Zn and Zn-Al Alloy Coatings on Steels in Diluted Hydrochloric Acid *Corrosion Science* 49 (11) 2007: pp. 4185 – 4201. https://doi.org/10.1016/j.corsci.2007.05.015
8. **Ju, H., Kai, Z.P., Li, Y.** Aminic Nitrogen-bearing Polydentate Schiff Base Compounds as Corrosion Inhibitors for Iron in Acidic Media: A Quantum Chemical Calculation *Corrosion Science* 50 (3) 2008: pp. 865 – 871. https://doi.org/10.1016/j.corsci.2007.10.009
9. **Obi-Egbedi, N.O., Obot, I.B.** Inhibitive Properties, Thermodynamic and Quantum Chemical Studies of Alloxazine on Mild Steel Corrosion in H_2SO_4 *Corrosion Science* 53 (1) 2011: pp. 263 – 275. https://doi.org/10.1016/j.corsci.2010.09.020
10. **El Ashry, E.S.H., Senior, S.A.** QSAR of Lauric Hydrazide and its Salts as Corrosion Inhibitors by using the Quantum Chemical and Topological Descriptors *Corrosion Science* 53 (3) 2011: pp. 1025 – 1034. https://doi.org/10.1016/j.corsci.2010.11.037
11. **Eddy, N.O.** Experimental and Theoretical Studies on some Smino Scids and their Potential Activity as Inhibitors for the Corrosion of Mild Steel, part 2 *Journal of Advanced Research* 2 (1) 2011: pp. 35 – 47. https://doi.org/10.1016/j.jare.2010.08.005
12. **Lukovits, I., Kálmán, E., Zucchi, F.** Corrosion Inhibitors – Correlation between Electronic Structure and Efficiency *Corrosion* 57 (1) 2001: pp. 3 – 8. https://doi.org/10.5006/1.3290328
13. **Qiang, Y., Zhang, S., Tan, B., Chen, S.** Evaluation of Ginkgo Leaf Extract as an Eco-friendly Corrosion Inhibitor of X70 Steel in HCl Solution *Corrosion Science* 133 2018: pp. 6 – 16. https://doi.org/10.1016/j.corsci.2018.01.008
14. **Fei, J., Mao, Q., Peng, L., Ye, T., Yang, Y., Luo, S.** The Internal Relation between Quantum Chemical Descriptors and Empirical Constants of Polychlorinated Compounds *Molecules* 23 (11) 2018: pp. 2935. https://doi.org/10.3390/molecules23112935
15. **Ebenso, E.E., Arslan, T., Kandemirlı, F., Love, I., Öğretır, C., Saracoğlu, M., Umoren, S.A.** Theoretical Studies of some Sulphonamides as Corrosion Inhibitors for Mild Steel in Acidic Medium *International Journal of Quantum Chemistry* 110 (14) 2010: pp. 2614 – 2636. https://doi.org/10.1002/qua.22430
16. **Verma, C., Obot, I.B., Bahadur, I., Sherif, E.M., Ebenso, E.E.** Choline Based Ionic Liquids as Sustainable Corrosion Inhibitors on Mild Steel Surface in Acidic Medium: Gravimetric, Electrochemical, Surface Morphology, DFT and Monte Carlo Simulation Studies *Applied Surface Science* 457 2018: pp. 134 – 149. https://doi.org/10.1016/j.apsusc.2018.06.035
17. **Murmu, M., Saha, S.K., Bhaumick, P., Murmu, N.C., Hirani, H., Banerjee, P.** Corrosion Inhibition Property of Azomethine Functionalized Triazole Derivatives in 1 mol L^{-1} HCl Medium for Mild Steel: Experimental and Theoretical Exploration *Journal of Molecular Liquids* 313 2020: pp. 113508. https://doi.org/10.1016/j.molliq.2020.113508

18. **Mamand, D.M., Anwer, T.M.K., Qadr, H.M.** Electronic Structure and Quantum Chemical Analysis of the Corrosion Inhibition Efficiency of Quinoxalines *Journal of the Indian Chemical Society* 100 (6) 2023: pp. 101018. https://doi.org/10.1016/j.jics.2023.101018
19. **Eddy, N.O., Momoh-Yahaya, H., Oguzie, E.E.** Theoretical and Experimental Studies on the Corrosion Inhibition Potentials of some Purines for Aluminum in 0.1M HCl *Journal of Advanced Research* 6 (2) 2015: pp. 203 – 217. https://doi.org/10.1016/j.jare.2014.01.004
20. **Kazansky, L.P.** DFT & PM3 Calculated Charges on Atoms in Heterocyclic Molecules and XPS *Corrosion Science* 112 2016: pp. 724 – 727. https://doi.org/10.1016/j.corsci.2016.09.003
21. **Quadri, T.W., Olasunkanmi, L.O., Fayemi, O.E., Akpan, E.D., Verma, C., Sherif, E.M., Khaled, K.F., Ebenso, E.E.** Quantitative Structure Activity Relationship and Artificial Neural Network as Vital Tools in Predicting Coordination Capabilities of Organic Compounds with Metal Surface: A Review *Coordination Chemistry Reviews* 446 2021: pp. 214101. https://doi.org/10.1016/j.ccr.2021.214101
22. **Aslam, R., Serdaroglu, G., Zehra, S., Kumar Verma, D., Aslam, J., Guo, L., Verma, C., Ebenso, E.E., Quraishi, M.A.** Corrosion Inhibition of Steel Using Different Families of Organic Compounds: Past and Present Progress *Journal of Molecular Liquids* 348 2022: pp. 118373. https://doi.org/10.1016/j.molliq.2021.118373
23. **Lee, C., Yang, W., Parr, R.G.** Development of the Colle-Salvetti Correlation-energy Formula into a Functional of the Electron Density *Physical Review B* 37 (2) 1988: pp. 785 – 789. https://doi.org/10.1103/physrevb.37.785
24. **Hou, B.S., Zhang, Q.H., Li, Y.Y., Zhu, G.Y., Lei, Y., Wang, X., Liu, H.F., Zhang, G.A.** In-depth Insight into the Inhibition Mechanism of Pyrimidine Derivatives on the Corrosion of Carbon Steel in CO_2-containing Environment Based on Experiments and Theoretical Calculations *Corrosion Science* 181 2021: pp. 109236. https://doi.org/10.1016/j.corsci.2021.109236
25. **Emregül, K.C., Hayvalí, M.** Studies on the Effect of a Newly Synthesized Schiff Base Compound from Phenazone and Vanillin on the Corrosion of Steel in 2M HCl *Corrosion Science* 48 (4) 2006: pp. 797 – 812. https://doi.org/10.1016/j.corsci.2005.03.001
26. **Schlegel, H.B.** A Comparison of Geometry Optimization with Internal, Cartesian, and Mixed Coordinates *International Journal of Quantum Chemistry* 44 (S26) 1992: pp. 243 – 252. https://doi.org/10.1002/qua.560440821
27. **Dibetsoe, M., Olasunkanmi, L.O., Fayemi, O.E., Yesudass, S., Ramaganthan, B., Bahadur, I., Adekunle, A.S., Kabanda, M.M., Ebenso, E.E.** Some Phthalocyanine and Naphthalocyanine Derivatives as Corrosion Inhibitors for Aluminium in Acidic Medium: Experimental, Quantum Chemical Calculations, QSAR Studies and Synergistic Effect of Iodide Ions *Molecules* 20 (9) 2015: pp. 15701 – 15734. https://doi.org/10.3390/molecules200915701
28. **Prakashaiah, B.G., Vinaya Kumara, D., Anup Pandith, A., Nityananda Shetty, A., Amitha Rani, B.E.** Corrosion Inhibition of 2024-T3 Aluminum Alloy in 3.5 % NaCl by Thiosemicarbazone Derivatives *Corrosion Science* 136 2018: pp. 326 – 338. https://doi.org/10.1016/j.corsci.2018.03.021
29. **El Azhar, M., Traisnel, M., Mernari, B., Gengembre, L., Bentiss, F., Lagrenée, M.** Electrochemical and XPS Studies of 2,5-bis(n-pyridyl)-1,3,4-thiadiazoles Adsorption on Mild Steel in Perchloric Acid Solution *Applied Surface Science* 185 (3) 2002: pp. 197 – 205. https://doi.org/10.1016/S0169-4332(01)00650-X
30. **Shahmoradi, A.R., Talebibahmanbigloo, N., Nickhil, C., Nisha, R., Javidparvar, A.A., Ghahremani, P., Bahlakeh, G., Ramezanzadeh, B.** Molecular-MD/atomic-DFT Theoretical and Experimental Studies on the Quince Seed Extract Corrosion Inhibition Performance on the Acidic-solution Attack of Mild-steel *Journal of Molecular Liquids* 346 2022: pp. 117921. https://doi.org/10.1016/j.molliq.2021.117921
31. **Haque, J., Srivastava, V., Quraishi, M.A., Singh Chauhan, D., Lgaz, H., Chung, I.M.** Polar Group Substituted Imidazolium Zwitterions as Eco-friendly Corrosion Inhibitors for Mild Steel in Acid Solution *Corrosion Science* 172 2020: pp. 108665. https://doi.org/10.1016/j.corsci.2020.108665
32. **Geng, S., Hu, J., Yu, J., Zhang, C., Wang, H., Zhang, X.** Rosin Imidazoline as an Eco-friendly Corrosion Inhibitor for the Carbon Steel in CO_2-containing Solution and its Synergistic Effect with Thiourea *Journal of Molecular Structure* 1250 2022: pp. 131778. https://doi.org/10.1016/j.molstruc.2021.131778
33. **Guo, G., Liang, C.** Electrochemical and DFT Studies of β-amino-alcohols as Corrosion Inhibitors for Brass *Electrochimica Acta* 52 (13) 2007: pp. 4554 – 4559. https://doi.org/10.1016/j.electacta.2006.12.058
34. **Al-Sabagh, A.M., Nasser, N.M., Farag, A.A., Migahed, M.A., Eissa, A.M.F., Mahmoud, T.** Structure Effect of some Amine Derivatives on Corrosion Inhibition Efficiency for Carbon Steel in Acidic Media using Electrochemical and Quantum Theory Methods *Egyptian Journal of Petroleum* 22 (1) 2013: pp. 101 – 116. https://doi.org/10.1016/j.ejpe.2012.09.004
35. **Rasheeda, K., Alamri, A.H., Krishnaprasad, P.A., Swathi, N.P., Alva, V.D.P., Aljohani, T.A.** Efficiency of a Pyrimidine Derivative for the Corrosion Inhibition of C1018 Carbon Steel in Aqueous Acidic Medium: Experimental and Theoretical Approach *Colloids and Surfaces A: Physicochemical and Engineering Aspects* 642 2022: pp. 128631. https://doi.org/10.1016/j.colsurfa.2022.128631
36. **Ferigita, K.S.M., Saracoglu, M., AlFalah, M.G.K., Yilmazer, M.I., Kokbudak, Z., Kaya, S., Kandemirli, F.** Corrosion Inhibition of Mild Steel in Acidic Media using New Oxo-pyrimidine Derivatives: Experimental and Theoretical Insights *Journal of Molecular Structure* 1284 2023: pp. 135361. https://doi.org/10.1016/j.molstruc.2023.135361
37. **Toghan, A., Khairy, M., Huang, M., Farag, A.A.** Electrochemical, Chemical and Theoretical Exploration of the Corrosion Inhibition of Carbon Steel with New Imidazole-Carboxamide Derivatives in An Acidic Environment *International Journal of Electrochemical Science* 18 (3) 2023: pp. 100072. https://doi.org/10.1016/j.ijoes.2023.10007