

# A Simple and Fast Method for Comparison of Corrosion Inhibition Powers Between Pairs of Pyridine Derivative Molecules

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## ABSTRACT

*Ab initio quantum chemical calculations at the density functional theory (DFT) level were performed on eight pyridine derivative molecules as corrosion inhibitors for iron in an acidic solution. In this regard, the geometry of the molecules were optimized using the B3LYP/6-31G\*\* method first, and then interactions of these optimized structures with the iron atom were explored using the B3LYP/LANL1MB method. Two modes of adsorption were considered, i.e., planar adsorption (P) via the pyridine ring and vertical adsorption (V) through a nitrogen atom. The interaction energy was minimized through the variation of the inhibitor molecule-iron atom distance. These minimum energy values, along with the values of induced charge on the iron atom, were used to compare the inhibition power of various pairs of pyridine derivatives under consideration. Compared with the experimental data, the P orientation seems to be more satisfactory, if the minimum energy values are considered alone. However, the V orientation is in accordance with the experiment, if the induced charge on iron is considered. This is attributed to the effect of the induced charge on reducing the original surface charge of iron. It may be concluded that the P orientation is more favorable at low coverage and the V orientation at high coverage because of the excessive diminishing of the charge on the iron surface and area releasing through the P → V reorientation.*

**KEY WORDS:** adsorption modes, density functional theory calculations, iron, LANL1MB, pyridine corrosion inhibitors

## INTRODUCTION

It is well known that iron corrodes in acid solutions, and corrosion can be reduced through the addition of some compounds known as inhibitors. Pyridine and its derivatives are among the compounds that have been studied as corrosion inhibitors for iron-acid systems. These studies have been carried out experimentally and theoretically.<sup>1-4</sup> Most of these theoretical studies, which are based on semi-empirical quantum chemical calculations, the so-called "isolated inhibitor model," ignore the effect of the metallic surface.<sup>1-2</sup> The molecular parameters resulting from these calculations are then correlated to the inhibition efficiency. This isolated inhibitor model is deficient in the following areas:

- In inhibition evaluation, the effect of surface has not been accounted for.
- For prediction of the inhibition power of a certain molecule, a knowledge of inhibition efficiencies of a set of similar molecules is required.

Recently there have been a few papers published dealing with semi-empirical calculations of the inhibition properties of organic molecules in which the surface effect has been included.<sup>4-8</sup> However, as a result of the nature of the method used, not only the application is restricted to certain parameterized atoms but also an inherent error is associated with the approximations involved with them.<sup>9</sup>

Ab initio studies of the interacting surface-molecule have been applied by some investigators in the field of heterogeneous catalysis. In these studies, two

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powerful models have been innovated and developed. These are simple cluster and embedded cluster models.<sup>10-13</sup> Although the embedded cluster model is more reliable than the former, it is very complicated and time consuming. Thus, it is mostly used for small molecules.

In the present work, the authors have attempted to apply ab initio calculations along with the simple cluster model to investigate the inhibition properties of eight substituted pyridine molecules in an Fe-acid system. The minimum energy values obtained were used to compare the inhibition powers of various pairs of pyridine derivatives under consideration. Just as in the simple cluster model, the model applied here accounts for surface-inhibitor interaction, and ab initio calculations use the correct Hamiltonian but do not use experimental data other than the values of the fundamental physical constants. Furthermore, the calculations involved here can be carried out on a common personal computer. In these calculations, two extreme orientations were applied, namely, adsorption through the delocalized  $\pi$ -electrons of the ring and through the lone pair electrons of the nitrogen atom. These orientations were first considered by Ayers and Hackerman,<sup>3</sup> and then observed experimentally by others.<sup>14-17</sup>

The extension of this work for larger molecules (with multi-center adsorption sites) is currently under consideration in this laboratory, and some interesting results have been obtained, which will be reported in the near future.

## METHOD

The method used in this work involved the simplest possible form of a cluster model (iron atom-inhibitor molecule). As mentioned before, for the molecules under consideration here, two extreme adsorption modes were postulated. These are the planar (P) and vertical (V) adsorptions. Ab initio quantum chemical calculations at a modified density functional theory (DFT) level were performed via the B3LYP method.<sup>18-19</sup> This modification is a Hartree-Fock (HF)/DFT hybrid method, which used a Becke's 3-parameter functional (B3) and includes a mixture of HF with DFT exchange terms associated with the gradient corrected correlation functional of Lee, Yang, and Parr (LYP).<sup>20</sup> Although the three semi-empirical parameters in B3LYP fitted to produce thermo-chemistry of a set of small organic molecules, it has been shown to perform exceptionally well on transition metal systems and has much less convergence problems than those commonly found for pure DFT methods.<sup>21-22</sup> Transition metals systems are electron-rich; thus, their calculations are very time consuming and huge. Also, for a proper description of them, the relativistic effect must be considered. Therefore, for a reduction of computational efforts and consideration of relativistic

effects, a pseudo-potential method was used. So, for iron atoms, 18 inner shell electrons ( $1s^2$ ,  $2s^2$ ,  $2p^6$ ,  $3s^2$ ,  $3p^6$  core electrons) were substituted by an effective core potential (ECP) of Hay and Wadt.<sup>23-25</sup> The ECP used in this paper was LANL1, which includes the scalar, mass-velocity, and Darwin relativistic effects.<sup>24</sup> The eight remaining electrons of iron at the valance layer ( $3d^6$ ,  $4s^2$  shell electrons) are described with a single-exponent minimal basis (MB) set. Other atoms in iron-inhibitor systems were treated by the STO-3G basis set.<sup>26-27</sup> Alternatively, the above basis sets can be replaced by LANL1MB. Also, for geometry optimization of the inhibitor molecule, the standard 6-31G\*\*<sup>28</sup> basis set was used. Calculations were initiated using geometry optimization of the inhibitor molecules through symmetry constrictions, i.e., planar holding of pyridine ring and  $C_{3v}$  symmetry of methyl groups. Thus, optimization was performed only on the bond lengths and angles. Then, interaction of these optimized inhibitors with an iron atom was explored as a function of the distance of the inhibitor molecule from the iron atom. At the equilibrium distance, the energy of the systems was determined. All calculations were performed using the Gaussian98 computer code,<sup>28</sup> working with an 1,800-MHz processor.

## RESULTS AND DISCUSSION

The eight inhibitor molecules for which ab initio quantum chemical calculations were performed are given in Table 1. The experimental relative efficiency<sup>3</sup> are also included in this table. Table 2 contains quantum chemical results, which consist of the following:

- The minimum energy of the isolated inhibitor molecule,  $E_{iso}$ .
- The inhibitor molecule-iron atom distance at minimized energy,  $r_{min}$ , for both modes.
- The minimum energy of inhibitor molecule-iron atom system,  $E_{in-Fe}$ , calculated for the two modes of V and P.
- Interaction energies,  $E_{int} = E_{in-Fe} - (E_{iso} + E_{Fe})$ . In this relation,  $E_{Fe}$  is the total electronic energy of an iron atom and is equal to  $-22.31455$  hartree.
- Induced charge on an iron atom by the adsorbed inhibitor molecule at  $r_{min}$ ,  $N_{Fe}$ , calculated from the B3LYP/LANL1MB method for both modes.

All of the energies listed above, namely  $E_{in-Fe}$ ,  $E_{iso}$ , and  $E_{Fe}$ , were calculated using the B3LYP/LANL1MB method.

It can be easily shown that from the eight molecules given in Table 1, 24 pairs can be selected that differ in inhibition efficiency.<sup>29</sup> These pairs are listed in Table 3. In this table, m and n refer to the inhibitor's number given in Table 1. The interaction energy difference,  $\Delta E$ , for each pair are also tabulated. These values are calculated for both modes, V and P. The negative values of  $\Delta E$  indicate that Inhibitor m is ad-

**TABLE 1**  
*Experimental Data<sup>3</sup> for Relative Inhibition Efficiencies  
of Methyl-Substituted Pyridines (0.15 M) for Iron in Acidic Media<sup>(A)</sup>*

(1) 36	(2) 44	(3) 40	(4) 44
(5) 46	(6) 48	(7) 44	(8) 46

<sup>(A)</sup> Labels given to inhibitors are in parentheses.

**TABLE 2**  
*Quantum Chemical Results for Interaction Evaluation of Inhibitor Molecules with Iron Atom<sup>(A)</sup>*

No.	$E_{\text{iso}}^{(B)}$	$r_{\text{min}}^{(C)}$		$E_{\text{in-Fe}}^{(D)}$		$E_{\text{int}}^{(E)}$		$N_{\text{Fe}}^{(F)}$	
		V	P	V	P	V	P	V	P
1	-245.17900	1.9	2.6	-267.58505	-267.51619	-0.09150	-0.02264	-0.310736	-0.203872
2	-284.03279	1.9	2.6	-306.43891	-306.37112	-0.09157	-0.02378	-0.316749	-0.210781
3	-284.03188	1.9	2.6	-306.43929	-306.36920	-0.09286	-0.02277	-0.317782	-0.206248
4	-284.03222	1.9	2.6	-306.43968	-306.37032	-0.09291	-0.02355	-0.317998	-0.208881
5	-322.88633	2.0	2.6	-345.29263	-345.22560	-0.09175	-0.02472	-0.318818	-0.216928
6	-361.73926	2.0	2.6	-384.14462	-384.07903	-0.09081	-0.02522	-0.324978	-0.216439
7	-322.88463	1.9	2.6	-345.29341	-345.22161	-0.09423	-0.02243	-0.324591	-0.186490
8	-322.88591	1.9	2.6	-345.29332	-345.22476	-0.09286	-0.02430	-0.323614	-0.210135

<sup>(A)</sup> All data are given in atomic units, except distance which is given in Å.

<sup>(B)</sup>  $E(\text{RB+HF-LYP})$  energy of geometry optimized inhibitor molecules calculated via B3LYP/LANL1MB method.

<sup>(C)</sup> Distance of inhibitor to iron at equilibria.

<sup>(D)</sup>  $E(\text{RB+HF-LYP})$  energy of inhibitor-iron system at  $r_{\text{min}}$ .

<sup>(E)</sup> Interaction energy of inhibitor and iron;  $E_{\text{Fe}} = -22.31455$  hartree.

<sup>(F)</sup> Charge induced to iron atom.

sorbed on the iron surface more strongly than n (i.e., m is a better inhibitor than n). From the data given in Table 3 we can see that:

—For the planar orientation, we have 22 correct predictions out of 24 cases (91.7%), while the corresponding statistical probability is 0.016%.<sup>30</sup>

—For the perpendicular mode, the relative agreement is 10 out of 24 or 41.7%, compared with 11.7% for complete randomness.

The above observations indicate that, for the adsorption models considered here, the P mode is closer to reality. This is in accord with some experimental results, which indicate that parallel orientation is more probable for low coverage.<sup>14-17</sup> Considering the vertical orientation by itself, although the relative agreement seems to be low, it cannot be entirely ruled out when it is compared with the values obtained

from complete randomness (41.7% vs. 11.7%). The experimental studies show that the vertically adsorbed pyridine-substituted molecules are predominant at high coverage.<sup>14-17</sup> Moreover, this mode seems to be more suitable for real cases when adsorption and accumulation of inhibitor molecules at a metal/solution interface are considered. Thus, it may be concluded that, experimentally and theoretically, the initial adsorption prefers the parallel mode, but as this process continues a reorientation from P to V (P→V) will take place. This is due to the area releasing and the decrease in the ensemble adsorption energy caused by this reorientation.

In a real metal-adsorbate system, where the accumulation of inhibitor molecules at the interface is appreciable, besides the interaction energy given in Table 2, two other factors must also be considered. These are the lateral interaction between adsorbed

TABLE 3

Inhibition Efficiency Prediction on the Basis of Interaction Energies for Pairs of Inhibitors  $m$  and  $n$ ,  
Defined as  $\Delta E = E_{int}(m) - E_{int}(n)$  for Both Vertical (V) and Planer (P) Orientations

Pair (m, n)		$\Delta E$ (atomic units)		Prediction		Agreement with Experiment	
		V	P	V	P	V	P
2	1	-0.00007	-0.00114	2 > 1	2 > 1	Yes	Yes
3	1	-0.00136	-0.00013	3 > 1	3 > 1	Yes	Yes
3	2	-0.00129	0.00101	3 > 2	2 > 3	No	Yes
4	1	-0.00144	-0.00091	4 > 1	4 > 1	Yes	Yes
4	3	-0.00005	-0.00078	4 > 3	4 > 3	Yes	Yes
5	1	-0.00025	-0.00208	5 > 1	5 > 1	Yes	Yes
5	2	-0.00018	-0.00094	5 > 2	5 > 2	Yes	Yes
5	3	0.00111	-0.00195	3 > 5	5 > 3	No	Yes
5	4	0.00116	-0.00117	4 > 5	5 > 4	No	Yes
6	1	0.00069	-0.00258	1 > 6	6 > 1	No	Yes
6	2	0.00076	-0.00144	2 > 6	6 > 2	No	Yes
6	3	0.00205	-0.00245	3 > 6	6 > 3	No	Yes
6	4	0.00210	-0.00167	4 > 6	6 > 4	No	Yes
6	5	0.00094	-0.00050	5 > 6	6 > 5	No	Yes
7	1	-0.00273	0.00021	7 > 1	1 > 7	Yes	No
7	3	-0.00137	0.00034	7 > 3	3 > 7	Yes	No
7	5	-0.00248	0.00229	7 > 5	5 > 7	No	Yes
7	6	-0.00342	0.00279	7 > 6	6 > 7	No	Yes
8	1	-0.00136	-0.00166	8 > 1	8 > 1	Yes	Yes
8	2	-0.00129	-0.00052	8 > 2	8 > 2	Yes	Yes
8	3	0.00000	-0.00153	—	8 > 3	—	Yes
8	4	0.00005	-0.00075	4 > 8	8 > 4	No	Yes
8	6	-0.00205	0.00092	8 > 6	6 > 8	No	Yes
8	7	0.00137	-0.00187	7 > 8	8 > 7	No	Yes

molecules and the effect of the charge induced by the inhibitor molecule upon the surface charge of the metal,  $q_M$ . As the model applied here is a limiting case of low coverage, the first factor seems to be insignificant. However, since the maximum adsorption of organic molecules occurs at near  $q_M = 0$ ,<sup>31</sup> the second factor must not be ignored. It is well known that in acid environments,  $q_M$  for iron is positive.<sup>32</sup> Thus, induced charge by pyridine derivative molecules (Table 2) will diminish  $q_M$  and, hence, will facilitate further adsorption of inhibitor molecules. This phenomenon may be considered as a synergistic effect.<sup>33</sup> Following this argument, the induced charge values of Table 2 have been used to compare the inhibitor efficiencies of the compounds in Table 1. The results are presented in Table 4. This table shows that there are 23 true predictions out of 24 (96% compared to approximately zero statistical probability<sup>30</sup>) for the vertical mode and 20 out of 24 (83% compared to 0.06%) for the parallel mode. In summary, inhibition efficiency is related to both adsorption strength and the amount of inhibitors on the metal surface. In other words, the inhibition efficiency is decided by both the interaction energy,  $E_{int}$ , and the number of inhibitor molecules already present on the surface, which, in turn, is a function of the inhibitor concentration in the media. This point has been observed experimentally for a number of corrosion inhibitors in acidic media.<sup>33</sup>

As shown in Table 2, the calculated mean value of distance between substituted pyridine molecules

and the iron atom ( $r_{min}$ ) is about 1.95 Å. This is comparable with the experimental value of 1.97 Å reported previously.<sup>34</sup> This relatively constant value of  $r_{min}$  for different molecules under consideration here indicates that no definite hindrance effect because of the presence of the methyl group is observable. This fact can be attributed to the relatively long distance of the methyl group in the ortho position from the iron atom (around 3 Å). This can be observed in Figure 1, which is a optimized three-dimensional representative of 2-methyl pyridine, one of four ortho-substituted molecules of Table 1. For comparison, the calculated distances between the other atoms in the molecule are also given in this figure.

Finally, a multiple regression analysis for the eight methyl-substituted pyridine studied (Table 1) has been carried out and the results are represented by Equations (1) and (2):

$$\varepsilon = -2283.93E_{int,V} - 4402.57E_{int,P} - 271.568$$

Regression coefficient = 0.941 (1)  
Standard error = 1.526

$$\varepsilon = -680.874N_{Fe,V} - 178.02N_{Fe,P} - 210.911$$

Regression coefficient = 0.931 (2)  
Standard error = 1.646

where  $\varepsilon$  represents inhibitor efficiency, and other parameters have been defined previously.

TABLE 4

Inhibition Efficiency Comparison on the Basis of Induced Charge on Iron Atom for Both Vertical (V) and Planer (P) Adsorptions

Pair (m, n)		Prediction		Agreement with Experiment	
		V	P	V	P
2	1	2 > 1	2 > 1	Yes	Yes
3	1	3 > 1	3 > 1	Yes	Yes
3	2	3 > 2	3 < 2	No	Yes
4	1	4 > 1	4 > 1	Yes	Yes
4	3	4 > 3	4 > 3	Yes	Yes
5	1	5 > 1	5 > 1	Yes	Yes
5	2	5 > 2	5 > 2	Yes	Yes
5	3	5 > 3	5 > 3	Yes	Yes
5	4	5 > 4	5 > 4	Yes	Yes
6	1	6 > 1	6 > 1	Yes	Yes
6	2	6 > 2	6 > 2	Yes	Yes
6	3	6 > 3	6 > 3	Yes	Yes
6	4	6 > 4	6 > 4	Yes	Yes
6	5	6 > 5	6 < 5	Yes	No
7	1	7 > 1	7 < 1	Yes	No
7	3	7 > 3	7 < 3	Yes	No
7	5	7 > 5	7 < 5	Yes	Yes
7	6	7 < 6	7 < 6	Yes	Yes
8	1	8 > 1	8 > 1	Yes	Yes
8	2	8 > 2	8 < 2	Yes	No
8	3	8 > 3	8 > 3	Yes	Yes
8	4	8 > 4	8 > 4	Yes	Yes
8	6	8 < 6	8 < 6	Yes	Yes
8	7	8 > 7	8 > 7	Yes	Yes

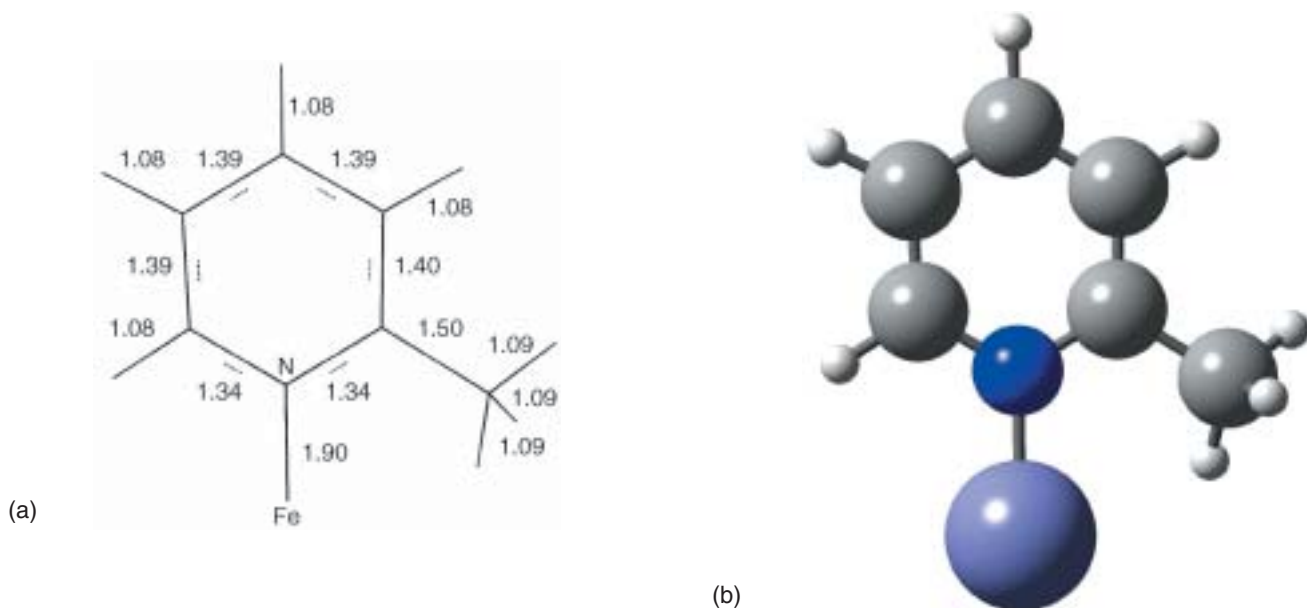


FIGURE 1. Optimized three-dimensional structure of *o*-methyl pyridine, which vertically adsorbed on the iron atom at a minimized iron-molecule distance: (a) wire frame with bond length and (b) ball and tube model with 75% scaled van der Waals' radii.

## CONCLUSIONS

❖ The theoretical calculation seems to be in line with the experimental observation that at a low coverage of the inhibitor, the planar orientation is preferred, and at a high coverage, the orientation of the inhibitor molecule will convert to a vertical form.

❖ Inhibition efficiencies of the pyridine derivative molecules are not only affected by the molecule-metal atom interaction energy, but the induced charge on the metal atom by the inhibitor molecule must also be considered. The second factor affects the original charge on the metal surface. This may be considered as a kind of synergistic effect.



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