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RESEARCH ARTICLE

INHIBITION OF ALUMINUM CORROSION IN HYDROCHLORICACID BY 2-(1H-BENZO(D)IMIDAZOL-2-YL)-3-PHENYLACRYLONITRILE: AN EXPERIMENTAL AND THEORETICAL APPROACH.

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ABSTRACT

The molecule 2-(1H-benzo(d)imidazol-2-yl)-3-phenylacrylonitrile) or BIPHA-4-H was investigated as an inhibitor of aluminum corrosion in a 1 M hydrochloric acid solution using the mass loss technique and quantum chemical studies based on density functional theory (DFT) at the B3LYP level with the B3LYP/6-31G(d) basis set. The results obtained show that the inhibitory efficiency increases with the concentration of the inhibitor, while it decreases as the temperature of the corrosive medium rises. DFT at the 6-31G(d,p) level allowed for the analysis of global parameters and local reactivity, which revealed the sites of electrophilic and nucleophilic attack.

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INTRODUCTION

Aluminum corrosion in acidic environments remains a major concern in many industrial sectors, even though this metal naturally possesses a protective passive layer on its surface (1). To limit this degradation, organic inhibitors, particularly benzimidazole derivatives, are of great interest due to their high adsorption capacity on metal surfaces, attributed to the presence of heteroatoms and π-conjugated systems (2-4). In this context, the molecule 2-(1H-benzo(d)imidazol-2-yl)-3-phenylacrylonitrile (BIPHA-4-H) has emerged as a potential corrosion inhibitor. The combination of the benzimidazole ring with the acrylonitrile group promotes interactions with the aluminum surface, thereby enhancing its anticorrosive properties.

MATERIALS AND METHODS

Aluminum Specimens : The material used in these tests consists of a 99.6 % pure aluminum rod with a density of 2.7g/cm^3 (0.1325 ± 0.0001), having a cylindrical shape with a height of 1 cm and a diameter of 0.25 cm. The molecule under study, 2-(1H-benzo(d)imidazol-2-yl)-3-phenylacrylonitrile (BIPHA-4-H), is a synthesized organic molecule with the molecular formula $C_{16}H_{11}N_3$ and a molecular weight of 245.10 g/mol. Its percentage composition is as follows: C: 78.35 %, H: 4.52 %, N: 17.13 %. Its structure is shown in Figure 1.

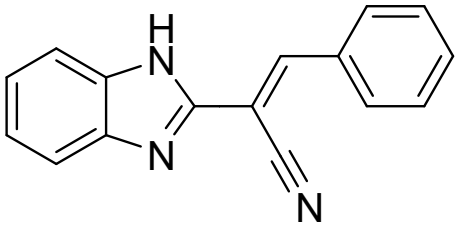

Figure 1 : Structure of 2-(1H-benzo(d)imidazol-2-yl)-3-phénylacrylonitrile)

g·mol⁻¹, was used to prepare the corrosive solution. From this stock solution, a 1 M HCl solution was prepared. In addition, various BIPHA-4-H solutions were prepared at the following concentrations: 0.005 mM; 0.01 mM; 0.05 mM; 0.1 mM; and 0.5 mM.

Mass Loss Method : The gravimetric method (5–7) is a simple and reliable technique commonly used to evaluate corrosion inhibition. It involves immersing a pre-weighed metal sample in a test solution at temperatures ranging from 298 K to 338 K. After immersion, the sample is rinsed, dried, and then reweighed to determine the mass loss. The values obtained are then used to calculate the corrosion rate, the inhibition efficiency, and the coverage rate using the appropriate equations.

$$W = \frac{\Delta m}{St} \quad (1)$$

$$EI(\%) = \frac{W_0 - W}{W_0} \times 100 \quad (2)$$

$$\theta = \frac{W_0 - W}{W_0} \quad (3)$$

where W_0 and W are the corrosion rates in the absence and presence of the inhibitor, respectively
Δm is the mass loss, S is the total surface area of the copper sample, and t is the immersion time.

Quantum calculation method

Electronic parameters : Gravimetry evaluates the effectiveness of corrosion inhibitors but does not explain the molecular mechanisms. To this end, quantum chemistry calculations based on DFT (Gaussian 09W, B3LYP/6-31G) were used to study the reactivity and inhibitor/surface interaction (8). This approach, combining modeling (GaussView) and DFT calculations, provides electronic descriptors (EHOMO, ELUMO, ΔE, I, A, χ, η, S, μ, ω) as well as local parameters (Fukui functions, local softness), to better understand the electronic structure and the mechanism of corrosion inhibition (9).

$$I = -E_{HOMO} \quad (4)$$

$$A = -E_{LUMO} \quad (5)$$

$$\chi = \frac{I+A}{2} = -\frac{E_{LUMO}+E_{HOMO}}{2} \quad (6)$$

$$\eta = \frac{I-A}{2} = \frac{E_{LUMO}-E_{HOMO}}{2} \quad (7)$$

$$\Delta E = I - A = E_{LUMO} - E_{HOMO} \quad (8)$$

$$\sigma = \frac{1}{\eta} = \frac{2}{I-A} \quad (9)$$

$$\omega^+ = \frac{(I+3A)^2}{16(I-A)} \quad (11)$$

$$\omega^- = \frac{(3I+A)^2}{16(I-A)} \quad (12)$$

Based on these values, the fraction of transferred electrons (ΔN) was calculated using the equation**:**

$$\Delta N = \frac{\chi_{Al} - \chi_{inh}}{2(\eta_{Al} + \eta_{inh})} \quad (13)$$

The calculations were performed using the following theoretical values: $\chi_{Al} = 4.28\ eV$; $\eta_{Al} = 0$ [8].

This quantity allows us to consider the following cases

- If $\Delta N < 0$, this means that electrons are transferred from the metal to the inhibitor.
- If $\Delta N > 0$, then electron transfer occurs from the inhibitor to the metal.
- If $\Delta N = 0$, there is no possibility of electron transfer between the metal and the inhibitor molecule.

Techniques for Calculating Local Reactivity Descriptors : Fukui functions are used to identify the reactive sites of a molecule with respect to nucleophilic and electrophilic attacks. They are defined by changes in electron density upon the addition or removal of an electron, and are then localized to specific atoms to analyze local reactivity. The site with the highest Fukui function value is generally the most reactive. However, these descriptors have limitations in clearly distinguishing certain sites. To address this, improved indices such as local softness and, most notably, the dual reactivity descriptor have been introduced. The latter, based on the difference between the nucleophilic and electrophilic Fukui functions ($\Delta f_k = f_k^+ - f_k^-$), allows for a more reliable identification of reactive sites: $\Delta f_k > 0$ indicates a nucleophilic attack (electrophilic site), while $\Delta f_k < 0$ corresponds to an electrophilic attack (nucleophilic site) (9). This descriptor thus offers a clearer and physically consistent interpretation of molecular reactivity.

RESULTS AND DISCUSSION

Corrosion Rate and Inhibitory Efficiency of BIPHA-4-H in HCl: Figures 2, 3, and 4 show, respectively, the evolution of the corrosion inhibition rate as a function of concentration and temperature, the influence of inhibitory efficiency on concentration and temperature, and the evolution of inhibitory efficiency as a function of immersion time for BIPHA-4-H.

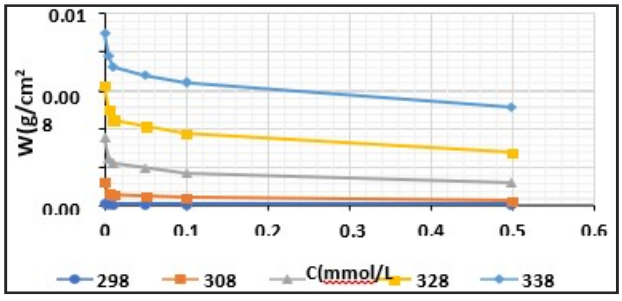

Figure 2. Corrosion rate as a function of BIPHA-4-H concentration at different temperatures

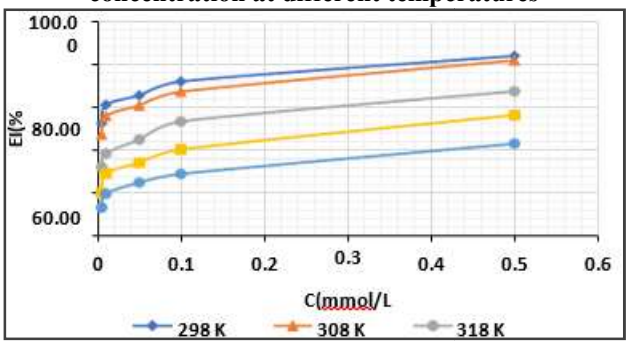

Figure 3. Changes in inhibitory activity as a function of BIPHA-4-H concentration at different temperatures

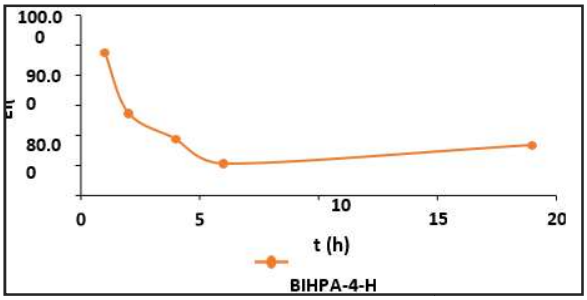

Figure 4. Changes in the inhibitory efficacy of BIPHA-4-H as a function of immersion time.

The BIPHA-4-H molecule exhibits strong inhibitory efficacy against aluminum corrosion in 1 M HCl solution; this efficacy increases with concentration due to its adsorption onto the metal surface and the formation of a protective film (10,13). However, an increase in temperature leads to a decrease in this protection due to the destabilization of the adsorbed layer (11), a result similar to that reported by Yeo et al. (12). This inhibitory performance is primarily linked to the presence of nitrogen atoms, which promote interaction with the aluminum surface. Furthermore, El-Awady's model shows excellent correlation ($R^2 \approx 1$), confirming the effective adsorption of BIPHA-4-H, while the value of $1/y > 1$ indicates the occupation of multiple active sites by a single molecule (14). Finally, the slight decrease in effectiveness between 1 h and 6 h of immersion, followed by stabilization up to 19 h, reflects rapid initial adsorption followed by an adsorption–desorption equilibrium of the protective film, consistent with the observations of Yeo et al. (12).

Theoretical Study : To study the reactivity of the BIPHA-4-H molecule and its ability to act as effective corrosion inhibitors, quantum chemistry calculations were performed using the Gaussian 09 software with the B3LYP hybrid functional and the 6-31G(d,p) basis set. This functional was chosen because it provides accurate electronic properties and geometries for many organic molecules (15).

Optimized structures of the BIPHA-4-H molecule

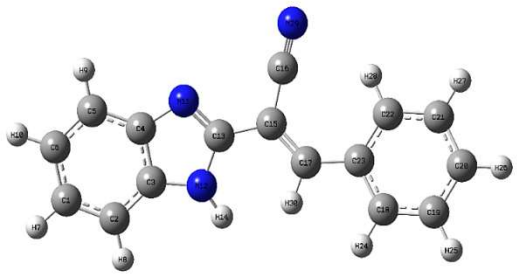

Figure 5 : Optimized structure of the 2-(1H-benzo[d]imidazol-2-yl) -3-phénylacrylonitrile

Descriptor Parameters: Molecular reactivity descriptors for the molecule under study were calculated to explain the experimental values obtained. Table 1 presents the various quantum parameters examined using the B3LYP/6-31G(d,p) method.

Table 1. Descriptor parameters of the molecule obtained from B3LYP/6-31G (d,p)Table 1:

Descripteurs			BIPHA-4-H
E_{HOMO} (eV)			-5.929
E_{LUMO} (eV)			-2.384
Energy gap (ΔE) (eV)			3.545
Dipole moment μ (D)			6.5540063
Ionization energy I (eV)			5.929
Electron affinity A (eV)			2.384
Electronegativity χ (eV)			4.157
Overall hardness η (eV)			1.773
Overall softness σ (eV^{-1})			0.564
Electron transfer fraction ΔN			0.0347
Electrophilicity index ω (eV)			4.873
Total energy ET (eV)			- 780.588

The energy of the highest occupied molecular orbital (HOMO) is a measure of a molecule's tendency to donate its HOMO electrons to the appropriate vacant orbital of an electron acceptor during donor-acceptor interactions; the higher the HOMO value, the greater the probability that the donor molecule will donate electrons (16). The results in Table 1 show that the HOMO tendency for the molecule in the database is high. The BIPHA-4-OH molecule is therefore favorable for donating its electrons to our aluminum metal (17). These theoretical data correspond to the trend in inhibition efficiency observed experimentally. On the other hand, the energy of the lowest unoccupied molecular orbital (ELUMO) is a measure of a molecule's tendency to accept electrons from the occupied orbital of an electron donor (16). In other words, the lower the ELUMO value, the greater the probability that the acceptor molecule will accept electrons. The ELUMO values obtained for the compound under study do not correlate with the observed inhibition efficiency (EI (%)). The opposite trends in the ELUMO and (EI (%)) values suggest that the inhibitory potentials of the studied BIPHA-4-H are not determined by their ability to accept electrons from the occupied orbitals of aluminum (17). Similarly, the values of the energy gap (ΔE) and overall hardness (η), often used as indicators of a molecule's reactivity or relative stability, do not correlate with the observed inhibition efficiency (EI (%)). Similar results were observed by (17). However, the values of overall electronegativity (χ) compared to that of aluminum ($\chi Al = 4.28$ eV) show that BIPHA-4-H ($\chi = 4.157$ eV in the 6-31G (d, p) database) has a tendency to retain its electrons or a greater propensity to release its electrons in a favorable donor-acceptor mechanism. The trend in the total electronegativity (χ) results is in perfect agreement with the observed inhibition efficiency (IE (%)). The positive value of the transferred electron fraction ($\Delta N > 0$) for the BIPHA-4-H molecule in the 6-31G (d, p) basis set highlights a strong donor-acceptor interaction between these molecules and the aluminum surface (16). This strong attraction possessed by aluminum will contribute to the replacement of its electrons lost during oxidation in the 1M HCl corrosive medium; this electron sharing between the BIPHA-4-H molecule and the metal surface would justify the establishment of chemical adsorption (chemisorption) (18). The trend in the results for the transferred electron fraction (ΔN) shows a strong correlation

molecule observed experimentally (19). of Applied Organometallic Chemistry, 4(2), 100–118

Table 2: Parameters describing the overall reactivity of the various molecule

Molecule	AtomN	q_k(N-1)	q_k(N)	q_k(N+1)	f_k^+	f_k^-	Δf_k
BIPHA-4-H	**C (4)**	0.251538	0.220346	0.233665	0.031192	-0.013319	0.044511
	H (7)	0.154699	0.087349	0.038538	0.067350	0.048811	0.018539
	C (16)	0.308115	0.297045	0.241986	0.011070	0.055059	-0.043989
	N (29)	-0.456897	-0.504221	-0.583445	0.047324	0.079224	-0.031900

Local Reactivity Parameters: To identify the local reactivity sites of the molecule (BIPHA-4-H), we have chosen to use the dual descriptor (Δf_k) and the Fukui functions Fukui (f_k^+, f_k^-). Fukui functions are the appropriate method for studying the local nucleophilic and electrophilic reactive sites responsible for the behavior of an inhibitor (20). As for the dual descriptor, it clearly facilitates the comparison of the relative attractiveness of sites for nucleophilic and electrophilic attacks on a given k atom. The most likely site for nucleophilic attacks is determined by the atom with the highest values of f_k^+ and Δfk,, while the atom with the highest value of $f_k^-$and the lowest value of Δfk, determines the most likely site for electrophilic attacks (20). Examination of Table 2 reveals that the atoms in BIPHA-4-H with the maximum values of f_k^+ et f_k^- are H(7) and N(29), respectively. According to the dual descriptor, carbon atoms C(4) and C(16) have the highest and lowest values of Δfk, respectively. Consequently, C(4) constitutes the nucleophilic attack center and C(16) the electrophilic attack center in the BIPHA-4-H molecule. Indeed, the C(4) carbon atom of BIPHA-4-H has a virtually non-existent electron cloud (LUMO) and can accept electrons from aluminum. This is why it is the likely site for nucleophilic attacks (Figure 6).

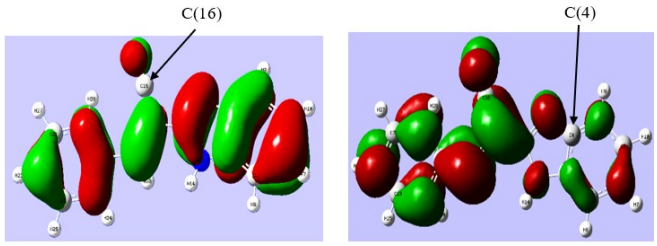

Figure 6. HOMO and LUMO Orbital to BIPHA-4-H at the level of B3LYP/6-31G (d, p).

CONCLUSION

We can conclude that, for our molecule, corrosion inhibition efficiency increases with rising concentration but decreases as the temperature of the corrosive medium rises. BIPHA-4-H acts as an effective inhibitor of aluminum corrosion in 1 M HCl, and its inhibition efficiency increases with both concentration and temperature. The adsorption process is dominated by chemisorption. Based on the overall parameters, we also note that the molecule possesses excellent corrosion inhibition capacity and acts predominantly as an electron donor to the metal.

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