Corrosion Inhibitive Action of Hesperidin methyl chalcone (HMC) on Aluminum in H₂SO₄: An Experimental and Computational Study

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Abstract

Using both theoretical and experimental techniques, the impact of Hesperidin methyl chalcone (HMC) on Aluminum corrosion in $0.5M H_2SO_4$ was examined at various temperatures. Measurements of weight loss revealed that the inhibitory efficiency rises with rising HMC concentrations and falls with rising temperatures. An inhibitor's overall rising inhibitory efficacy is ascribed to the bulk of the solution's adsorption onto the aluminum surfaces. The Langmuir adsorption isotherm is best fitted by the adsorption process model, as well as calculated thermodynamic parameters, were spoken about. Thermodynamic characteristics show that the HMC uses a combination of physisorption and chemisorption to adsorb spontaneously onto metal surfaces and delay corrosion. The effect of temperature on Aluminum's HMC inhibition efficiency in 0.5M H₂SO₄ is explained by the activation parameters. The experimental results are supported by the quantum chemical parameters, which likewise show good agreement with them.

Keywords: Corrosion inhibitors; HMC; Weight loss; Quantum

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1. Introduction

Reducing total expenses in the company today through material preservation and upkeep is one of the most crucial factors. Protecting corroding metal surfaces is essential for extending equipment life, preventing the release of hazardous metals into the environment, and preventing the loss of resources and money during industrial operations[1].

Aluminum is a very significant metal that is utilized in many aspects of daily life since it is inexpensive, easy to obtain, and has a wide range of industrial uses. The investigations into the corrosion behavior of aluminum and its alloys are considered to be an important study topic because of their frequent usage. The presence of a passive layer made of double-nature oxide film on the surface of aluminum provides corrosion resistance in an aqueous neutral solution. Numerous attempts have been undertaken by scientists to investigate the impact of aggressive anions, such as sulfate and chloride, on the stability of the passive oxide layer created in aqueous solutions on metals [2-4]. According to the experiments, localized pitting corrosion begins to erode the passive oxide layer when $Cl^{-}and/or SO_{4}^{-2}$ anions are present.

In an acid-aqueous solution, the anodic breakdown of aluminum metal is typically accompanied by a complementary cathodic reaction that releases gaseous H₂. The fuel cell must always produce hydrogen in order to function. To regulate the rate of metal breakdown and H₂ generation, an inhibitor must be present [5-6]. These inhibitors can be organic or inorganic. Examples of inorganic ones are chromates, dichromates, and nitrites. Typical organic inhibitors have π electrons in their double or triple conjugated bonds, or nitrogen, sulfur, or oxygen as functional groups or in their chemical structure. The adsorption of these organic inhibitors onto the metal surface is the mechanism of action. Adsorption may occur as a result of four possible processes that can occur: (1) the charged metal and the charged inhibitor molecule will attract each other through electrostatics; (2) the metal's vacant orbitals will attract and interact with the heteroatom's free electrons (N, S, or O); (3) the metal will interact with the π electrons of the aromatic rings; and (4) a combination of the three processes described will occur when possible. Researches are searching for more environmentally friendly chemicals, or "green corrosion inhibitors," because traditional organic inhibitors are costly and hazardous [7].

1,3-diarylprop-2-en-1-one, or chalcones, are a major class of flavonoids that occur naturally in plants. They have several hydrogen atoms that can be replaced, which results in a wide variety of derivatives and biological effects. Their potential as metal corrosion inhibitors is a field of current research with significant possibilities, notwithstanding their diverse biological applications[8].

The current study intends to evaluate the potential application of Hesperidin methyl chalcone as a corrosion inhibitor for aluminum in sulphuric acid solution using weight loss metrics. A few thermodynamic adsorption functions were calculated and discussed, including ΔG_{ads} and K_{ads} . The results of the experiments are supported by the quantum chemical calculations, which agree with the observations made in the experiments[9].

2. Experimental

2.1 Acidic Media

AR-grade concentrated H_2SO_4 was used to provide the acidic environment of 0.5M H_2SO_4 . In order to organize aggressive acidic medium, the concentrated H_2SO_4 was dissolved in deionized water.

2.2 Corrosion Inhibitor

Hesperidin, a flavonoid mostly present in citrus fruits, is methylated to yield hesperidin methyl chalcone (HMC; $C_{29}H_{36}O_{15}$). Hesperidin usually has a low solubility in water; however, this can be overcome by an alkaline methylation procedure. This process leads to the creation of HMC by promoting hesperidin's isomerization and improving its solubility[10].



The molecular structure of Hesperidin methyl chalcone

2.3 Weight loss measurements

The fundamental but highly practical method for corrosion testing involves measuring weight loss. Assessing weight reduction across various inhibitor concentrations aids in identifying the optimal inhibitor concentration and provides insight into how the inhibitor molecules bind to the suitable adsorption isotherm. Based on this, investigations are conducted to extract the various parameters at different immersion temperatures. The coupons (A=14.44 cm2) were carefully weighed after being cleaned, rinsed with acetone after water, and abraded using emery sheets. A thermostat was used to maintain the appropriate temperature while aluminum metal samples were immersed in 0.5 M sulfuric acid, with and without progressively higher concentrations of hesperidin methyl chalcone. The aluminum specimens were submerged for an hour before being taken out, dried, and weighed. They were then cleaned with distilled water and then acetone. The corrosion rate (CR) of aluminum specimens in acid solution was determined using equation (1) [11]:

$$CR = 534 \frac{ML}{\rho AT} \tag{1}$$

where A is sheet area, T is corrosion period, ρ is aluminum metal density, and ML is sheet weight loss. To get the inhibitory efficiency (IE%), utilize equation (2):

$$IE\% = \frac{W_o - W_i}{W_o} X100 \tag{2}$$

where W_0 and W_i represent, respectively, the aluminum corrosion rates in sulfuric acid solutions without and with an inhibitor. The values of the surface coverage (θ) were calculated using equation (3):

$$\boldsymbol{\theta} = \frac{W_0 - W_i}{W_0} \tag{3}$$

2.4 Quantum Chemical Calculations

The 6-311G (d, p) [12–13] was requested in order to optimize the Hesperidin methyl chalcone's 3D geometry. Furthermore, assessed were the metrics for chemical potential,

electron affinity, HOMO, LUMO, ΔE , ionization potential, electronigitivity, chemical hardness, softness, electrophilicity, and neutreophilicity [14-15].

3. RESULT AND DISCUSSION

3.1 Weight Loss Measurements

3.1.1. The Effect of Immersion Time

Table 1's result indicates that as immersion time rose, aluminum weight loss in H_2SO_4 increased as well. An increase in the metal's rate of weight loss in the specified acid suggests that the protective coating may become unstable over an extended duration of contact. The interaction between the metal surface and the acid and in the solution leads to gradual corrosion of the metal surface over time, causing an escalation in the metal's weight loss during immersion. Figure 1 illustrates how an increase in immersion time increased the weight loss in the corrodent at a constant concentration [16].

Table 1. Influence of time of immersion for Al sheets in $0.5 \text{ M H}_2\text{SO}_4$ acid on weight loss at
different temperatures

Immersion	299°K		329°K		359°K	
time (hr.)	Corrosion rate (mpy)	Weight loss (g)	Corrosion rate (mpy)	Weight loss (g)	Corrosion rate (mpy)	Weight loss (g)
1	0.054786	0.004	0.04109	0.003	0.342413	0.025
2	0.034241	0.005	0.054786	0.008	0.335565	0.049
3	0.027393	0.006	0.050221	0.011	0.31502	0.069
4	0.047938	0.014	0.054786	0.016	0.332141	0.097
5	0.046568	0.017	0.136965	0.05	0.419114	0.153



Figure 1. Effect of immersion time on corrosion rate of Al sheets in 0.5 M H_2SO_4 acid at different temperature.

3.1.2. The Effect of Concentration

The outcome of concentration variations (Figure 2) demonstrates that weight loss and corrosion rate increase as acid concentration rises. This is because the rate of chemical reaction increases as the concentration of active species increases. According to Table 2, the concentration of the corrosive medium determines how quickly aluminum dissolves. This could be explained by the rise in the concentration of acid anions within the more concentrated solution, leading to a rapid reaction with the aluminum ions in the solution [17].



Figure 2. Effect of concentration of H_2SO_4 acid on corrosion rate of Al sheets at different temperature for 5 hr.

Acid	299°K		329°K		359°K	
concentration (M)	Corrosion rate (mpy)	Weight loss (g)	Corrosion rate (mpy)	Weight loss (g)	Corrosion rate (mpy)	Weight loss (g)
0.1	0.005479	0.002	0.021914	0.008	0.11779	0.043
0.2	0.010957	0.004	0.043829	0.016	0.208187	0.076
0.3	0.013697	0.005	0.046568	0.017	0.254755	0.093
0.4	0.010957	0.004	0.043829	0.016	0.287627	0.105
0.5	0.046568	0.017	0.136965	0.05	0.419114	0.153

Table 2. Impact of H_2SO_4 acid concentration on weight loss of Al sheets at different temperatures for 5 hr.

3.1.3. The Effect of Temperature

The data in Tables 1 and 2 demonstrate that when temperature rises, corrosion rate rises as well. A higher temperature causes a more severe state of corrosion. A rise in temperature often causes the average kinetic energy of the constituent particles to increase, increasing the solubility of the protective coatings. As the average kinetic energy rises, particles experience increased velocity and more frequent collisions [18].

3.1.4. The effect of adding inhibitor

It was discovered that aluminum sheet corroded in $0.5 \text{ M H}_2\text{SO}_4$ solution. The outcomes unequivocally demonstrate that hesperidin methyl chalcone inhibits the corrosion

reaction by successfully delaying the pace at which aluminum sheets corrode in a 0.5 M H_2SO_4 solution. The weight loss results show that the rate of corrosion of Al sheets and the effectiveness of Hesperidin methyl chalcone's inhibition rely on concentration. Generally speaking, in an acidic solution, the oxygen atom found in the inhibitor molecules (HMC; $C_{29}H_{36}O_{15}$) is readily protonated and transformed into quaternary/oxonium ions[19]. These protonated species are adsorbed on the metal surface's cathodic sites, which slows down the development of hydrogen and delays the breakdown of the metal[20]. At a temperature of 299°K and an inhibitor dose of 0.05 M, the assessed inhibition efficiency reached its maximum at 94.1% for HMC (Table 3).

T °K	Concentration of inhibitor by mole/ l	Weight loss (g)	Corrosion rate (mpy)	IE%	Surface coverage (θ)
	blank	0.017	0.046568		
	0.01	0.006	0.016436	64.70575	0.647057
299	0.02	0.002	0.005479	88.23525	0.882352
	0.03	0.004	0.010957	76.4705	0.764705
	0.04	0.002	0.005479	88.23525	0.882352
	0.05	0.001	0.002739	94.11762	0.941176
	blank	0.05	0.136965		
329	0.01	0.034	0.093136	31.99989	0.319999
	0.02	0.018	0.049307	63.99994	0.639999
	0.03	0.019	0.052047	61.99994	0.619999
	0.04	0.021	0.057525	57.99993	0.579999
	0.05	0.024	0.065743	51.99992	0.519999
	Blank	0.153	0.419114		
359	0.01	0.064	0.175315	58.16998	0.5817
	0.02	0.064	0.175315	58.16998	0.5817
	0.03	0.069	0.189012	54.90201	0.54902
	0.04	0.065	0.178055	57.51638	0.575164
	0.05	0.026	0.071222	83.00655	0.830066

Table 3. Effect of Hesperidin methyl chalcone addition in 0.5 M H ₂ SO ₄ acid for Al sheets at
different temperatures for 5hr

3.2 Thermodynamic Parameters

We measured weight loss to determine surface coverage (θ) values for Al sheets at varied temperatures and HMC concentrations in 0.5M H₂SO₄, as indicated in Table 3. The corrosion inhibition mechanism can be better understood through surface coverage values, which reflect the adsorption behavior of inhibitor molecules on the metal surface. Thus, through the fitting of a satiable adsorption isotherm model, the θ values describe the mode and kinetics of the adsorption. Figure 3 illustrates how well the Langmuir adsorption isotherm model matches our experimental data.



Figure 3. Langmuir adsorption isotherm of HMC in 0.5M H_2SO_4 on Al sheets at the temperature of 299, 329 and 359 °K.

The following equation represents the Langmuir isotherm for monolayer adsorption:

$$\frac{C}{\theta} = \frac{1}{K_{ads}} + C \tag{4}$$

The adsorption equilibrium constant is K_{ads} , the inhibitor concentration is C, and the degree of surface covering is θ . As a result, plot the inhibitor concentration (mole/l) versus C / θ to create a straight-line graph. The K_{ads} were computed using the intercept values. Subsequently, the standard free energy change of adsorption (ΔG^0_{ads}) was determined using the subsequent formula:

$$\Delta G_{ads}^{\circ} = -\ln(K_{ads}x55.5)xRxT \tag{5}$$

T is the absolute temperature, while R denotes the ideal gas constant, valued at 8.314 J/mol/K, and the molar concentration of water in the sample has a numerical value of 55.5. Table 4 presented all of the computed values for K_{ads} and ΔG^{o}_{ads} .

Table 4. Thermodynamic parameters for Al sheets at different temperatures and concentrations of HMC in 0.5M H₂SO₄, both with and without the presence of HMC.

Temperature	Equilibrium	Standard Free	Standard	Standard Entropy
(K)	Constant,	Energy	Enthalpy	Change,
	Kads	Change,	Change,	ΔS^0_{ads}
	(M ⁻¹)	$\Delta { m G}^{0}_{ m ads}$	ΔH^0_{ads}	(J/mol/K)
		(kJ/mol)	(kJ/mol)	
299	172.41	-22.78	-48.09	76.04762
329	204.08	-25.53	-48.09	77.46422
359	92.59	-25.50	-48.09	70.90579

The high adsorption of inhibitor molecules from the bulk of the solution on the metal surface is described by the K_{ads} values. Strong adsorption of inhibitor molecules results in high inhibition efficiency; a higher K_{ads} value reflects this. The values of ΔG^{o}_{ads} are consistent with physisorption when they are around -20 kJ mol⁻¹ or lower, and chemisorption when they are approximately -40 kJ mol⁻¹ or higher. As a result, past studies have noted the significance of ΔG^{o}_{ads} lie in the range of -20 kJ mol⁻¹ to -40 kJ mol⁻¹, indicating that the inhibitor adsorption process involves both physisorption and chemisorption.

The values of ΔG^{o}_{ads} in our investigation were found to be somewhat over -20 kJ mol⁻¹, although they were still within the range of -20 kJ mol⁻¹ to -40 kJ mol⁻¹. This suggests that the HMC adsorbed onto the metal surface mostly through chemisorption, but physisorption also had a role. The ΔG^{o}_{ads} value's negative sign signifies the HMC molecules' spontaneous adsorption onto the metal surface from 0.5M H₂SO₄. After that, the following Gibb's Helmholtz equation offers a means to determine the enthalpy of adsorption (ΔH^{o}_{ads}) and entropy of adsorption (ΔS^{o}_{ads})[21],

$$\left(\frac{\partial G/T}{\partial T}\right)_{P} = -\frac{H}{T^{2}} \tag{6}$$

The rearranged Gibb's Helmholtz equation cited above is,

$$\Delta S_{ads}^{\circ} = \frac{(\Delta H_{ads}^{\circ} - \Delta G_{ads}^{\circ})}{T}$$
(7)

Plotting $\Delta G^{o}_{ads} / T$ against 1000 / T yields a straight line in Figure 4. The value obtained from the straight-line intercept, representing adsorption arising from either an exothermic or endothermic process, was utilized to calculate the enthalpy of adsorption (ΔH^{o}_{ads}). As a result, if H^{o}_{ads} has a negative value, the adsorption process is exothermic; otherwise, it has a positive sign[22].



Figure 4. Graph of 1000 / T against ΔG^0_{ads} / T.

Enthalpy of adsorption (ΔH^{o}_{ads}) values for inhibitor adsorption are typically around or less than 40 kJ/mol, attributable to physisorption, and around or larger than 100 kJ/mol, attributed to chemisorption. The current study's value of H0ads is -ve, indicating an exothermic reaction during adsorption, and its magnitude is -48.09 kJ/mol, greater than -40 and less than -100 kJ/mol, indicating a combination of physisorption and chemisorption during adsorption. An increase in randomness at the metal/solution interface leads to the adsorption of inhibitor molecules onto the metal surface, as evidenced by a +ve sign of entropy of adsorption (ΔS^{o}_{ads}). The quantity of water molecules that inhibitor molecules are removing from the metal surface has increased, which is the reason for this increase in disorder[23].

3.3 Activation Parameters

The impact of temperature on the inhibitor's inhibitory efficacy has a notable effect on the metals' rate of corrosion. As the temperature rises, corrosion rates rise as well. Due to the fact that rising temperatures reduce hydrogen overvoltage, which accelerates corrosion in acidic conditions. Typically, the Arrhenius equation can be used to describe the corrosion mechanism as,

$$ln v_{corr} = lnA - \frac{E_a^*}{RT}$$
(8)

where A is the Arrhenius pre-exponential factor, T is the absolute temperature, R is the ideal gas constant, E_a is the activation energy for the corrosion, and lnv_{corr} is the corrosion rate. As seen in Figure 5, the Arrhenius plot of lnv_{corr} against 1000 / T yields a straight line with an intercept of ln A and a slope equal to $-E_a / R$. Table 5 presented the computed values of A and Ea.



Figure 5. Arrhenius plot of ln v_{corr} against 1000 / T

 Table 5: Activation parameters for Al sheets at different temperatures and concentrations of HMC in 0.5M H₂SO₄, both with and without the presence of HMC.

Concentration of HMC (M)	Activation Energy, Ea* (kJ mol ⁻¹)	Arrhenius Pre-exponential Factor, A (g cm ⁻² h ⁻¹)	Enthalpy of adsorption, ΔH* (kJ mol ⁻¹)	The entropy of Adsorption, ΔS^* (J mol ⁻¹ K ⁻¹)
blank	32.57	22.026 x 10 ³	29.856	-170.903
0.01	35.60	31.225 x 10 ³	32.891	-167.997
0.02	51.82	68.039 x 10 ⁵	49.108	-123.236
0.03	42.36	27.596 x 10 ⁴	39.645	-149.881
0.04	52.19	82.276x 105	49.471	-121.659
0.05	49.72	20.330 x 105	47.007	-133.280



Figure 6. Transition Plot

In comparison to the 0.5M H₂SO₄ solution without inhibitor, E_a^* and A values are higher in HMC. This indicated that the addition of HMC increases the energy barrier for the corrosion reaction by adsorbing onto metal surfaces, thus inhibiting metal dissolution [24]. Corrosion is reduced via the adsorption process, which creates a protective barrier at the interface between the metal and the solution. The whole corrosion process is driven by the surface reaction if the value of E_a^* is larger than 20 kJ mol⁻¹ in both the presence and absence of HMC in 0.5M H₂SO₄.

Using the Transition State Equation enabled the determination of the apparent change in enthalpy (ΔH^*) and entropy (ΔS^*).

$$ln\frac{v_{corr}}{T} = \left[\frac{R}{Nh} + \frac{\Delta S^*}{R}\right] - \frac{\Delta H^*}{RT}$$
(9)

where the Avogadro number (N) and the plank's constant (h) are, respectively. Figure 6 displays a graph of $\ln v_{corr}$ against 1000/T with an intercept of $\left[\frac{R}{Nh} + \frac{\Delta S^*}{R}\right]$ and a slope of ΔH^* . Table 5 provided the computed values of ΔH^* and ΔS^* . The metal dissolution

reaction is identified as endothermic, as evidenced by the positive value of ΔH^* . The activation process, which involves the formation of an activated complex representing association, is proposed to have led to a decrease in system degrees of freedom, indicated by the negative sign of ΔS^* .

3.4 Quantum Chemical Calculations

The Hesperidin methylchalcone had been optimized using 6-311G (d, p)[12-13], Figure (7.a). The optimized bond angles and bond lengths were tabulated in Table (6). The electronic parameters; HOMO, LUMO, ΔE , Ionization potential, Electron affinity, Chemical potential, Electronigitivity, Chemical hardness, Softness, Electrophilicity, and Neuceophilicity were evaluated, Table (6), in addition the HOMO-LUMO maps were presented in Figure (7.b)[14-15].



The following results, Table (6), for Hesperidin methyl chalcone provide valuable insights into its biological reactivity, offering a comprehensive understanding of its potential interactions in biological systems. The HOMO-LUMO energy gap (ΔE) of 3.63 eV serves as a key indicator of the compound's stability. A larger ΔE implies a more stable molecule, which can be advantageous in biological contexts where reactivity needs to be precisely regulated. The ionization potential (IP) of 5.90 eV

represents the energy required to remove an electron from the HOMO, essentially reflecting the compound's electron-donating ability. This parameter is significant in biological reactions involving electron transfer processes, such as redox reactions in cellular metabolism. Conversely, the electron affinity (EA) of 2.27 eV highlights the compound's electron-accepting capability, which is relevant in interactions with electron-donating species in biological environments. The chemical potential (-4.09 eV) indicates the compound's tendency to donate electrons to achieve thermodynamic equilibrium with its surroundings. In biological systems, this feature can influence the compound's role as a reducing agent, participating in redox reactions critical for cellular functions. The chemical hardness (1.82 eV) and softness (0.28 eV⁻¹) provide information about the compound's resistance to changes in electron density and its polarizability. These parameters are relevant in biological reactions involving molecular recognition, where a balance between rigidity and flexibility is often crucial for proper interactions with biomolecules. The electrophilicity (4.60 eV) measures the compound's tendency to accept electrons, which can be indicative of its potential as an electrophile in biological reactions. Neucleophilicity (0.22 eV) reflects the compound's ability to donate electrons, a characteristic important in interactions with biological nucleophiles. In summary, the electronic and reactivity parameters of Hesperidin methyl chalcone suggest its potential biological reactivity, influencing its role in cellular processes. The compound's stability, electron-donating and -accepting abilities, as well as its electrophilic and nucleophilic tendencies, collectively contribute to its biological reactivity profile. Understanding these features is fundamental for exploring the potential pharmacological and therapeutic applications of Hesperidin methyl chalcone in various biological contexts.

Table (6): calcultaed HOMO, LUMO parametrs				
	Hesperidin methyl chalcone			
НОМО	-5.90 eV			
LUMO	-2.27 eV			
ΔE	3.63 eV			
Ionization potential	5.90 eV			
Electron affinity	2.27 eV			
Chemical potential	-4.09 eV			
Electronigitivity	4.09 eV			
Chemical hardness	1.82 eV			
Softness	0.28 eV^{-1}			
Electrophilicity	4.60 eV			
Neuceophilicity	0.22 eV			

The Molecular Electrostatic Potential (MEP), Figure (7.c), of Hesperidin methyl chalcone offers valuable insights into its biological reactivity by providing a spatial representation of the electron distribution around the molecule. MEP is a crucial tool for understanding the electrostatic interactions that govern molecular recognition, binding affinity, and reactivity in biological systems. Examining the MEP of Hesperidin methyl chalcone reveals the distribution of positive and negative electrostatic potentials

on its molecular surface. Regions of negative potential typically indicate sites where the molecule can attract electrophiles or positively charged species, while positive potential regions suggest sites that can interact favorably with nucleophiles or negatively charged entities. In the context of biological reactivity, the MEP of Hesperidin methyl chalcone can offer insights into its potential interactions with biological macromolecules, such as proteins or nucleic acids. For instance, regions with high negative potential may be involved in interactions with positively charged amino acid residues on protein surfaces, influencing binding and molecular recognition. Conversely, positive potential regions may play a role in interactions with negatively charged moieties. Additionally, MEP can provide information about the electrophilic and nucleophilic character of specific molecular sites. This is particularly relevant in understanding how Hesperidin methyl chalcone might participate in enzymatic reactions, redox processes, or other biologically significant transformations. Regions with high electron density are likely to act as nucleophiles, while electron-deficient areas may serve as electrophilic centers. Furthermore, the analysis of MEP can aid in predicting the reactivity of Hesperidin methyl chalcone towards biological targets, guiding the exploration of its pharmacological properties. The spatial distribution of electrostatic potentials can influence the compound's behavior in biological environments, impacting its bioavailability, cellular uptake, and interactions with biomolecules. In conclusion, the Molecular Electrostatic Potential analysis of Hesperidin methyl chalcone offers a nuanced understanding of its biological reactivity by highlighting potential binding sites, charge distribution, and reactivity patterns. This information is essential for unraveling the pharmacological and therapeutic implications of Hesperidin methyl chalcone in biological systems.

4. CONCLUSION

The corrosion inhibitory action of HMC on aluminum in 0.5M H_2SO_4 at various temperatures was investigated through chemical, surface, and quantum chemical analyses. The effectiveness of HMC as an inhibitor increases with rising concentrations, reaching over 94.1% inhibition efficiency at an optimized concentration of 0.05 M in 0.5M H_2SO_4 . This inhibition remains stable up to a temperature of 359 K, beyond which its effectiveness decreases. The inhibitory effect of HMC is attributed to an adsorption process that follows the Langmuir isotherm model. Adsorption studies indicate that HMC adsorption onto the metal surface is an exothermic process, involving both physisorption and chemisorption, which occurs spontaneously. Quantum parameters corroborate the experimental findings, strongly supporting the conclusion that HMC serves as an effective corrosion inhibitor for aluminum in 0.5M H_2SO_4 .

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