

Article

Furanyl Hydrazone Schiff Base as a Corrosion Inhibitor for Carbon Steel in HCl: Experimental and Theoretical Study

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Abstract

This study aims to investigate the performance and mechanism of N'-[(E)-phenylmethylidene]furan-2-carbohydrazide (FNH), a hydrazone Schiff base, as a corrosion inhibitor for carbon steel in 1.0 M HCl. The research was conducted by coupling electrochemical testing (Tafel analysis and Impedance spectroscopy) with surface characterization (SEM and AFM) and advanced computational tools, including quantum-chemical modeling and classical molecular dynamics (MD) simulations. Tafel analysis revealed that FNH acts as a mixed-type inhibitor, concurrently slowing iron oxidation and hydrogen reduction. Impedance data showed that the Faradaic resistance grew monotonically with FNH dosage, reaching 95% protection at 1×10^{-4} M. Fitting the results to the Langmuir model indicated a joint physical–chemical anchoring pathway, further confirmed by SEM/AFM inspection which disclosed a uniform organic deposit. Quantum-chemical modeling revealed that protonated species broaden the molecule's capacity for bidirectional electron exchange, while MD simulations on the Fe (110) slab confirmed a flat-lying geometry that maximizes heteroatom–metal contact. The consistency between laboratory observables and atomic-scale predictions provides a detailed, mechanism-oriented picture of how this organic protective layer curtails acid corrosion.

Keywords: electronic structure; hydrazone; corrosion inhibitor; density functional theory; molecular dynamics



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1. Introduction

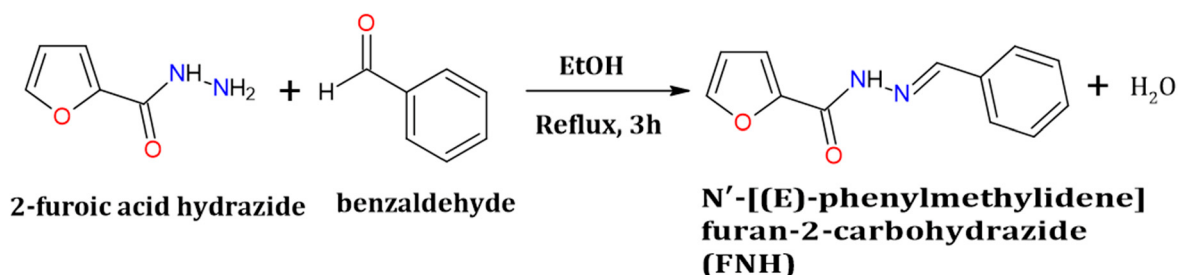
Metallic materials and their alloys underpin virtually every sector of modern infrastructure and manufacturing [1–3]. Despite their widespread utility, these materials are inherently susceptible to electrochemical degradation when exposed to media rich in aggressive species such as chloride and sulfate ions [4,5]. The economic and structural toll of such degradation, ranging from equipment failure to unplanned shutdowns, has spurred sustained efforts to develop protective strategies, among which the addition of organic inhibitors to the corrosive medium stands out for its simplicity, affordability, and demonstrated effectiveness [6–8]. The protective action of organic inhibitors stems from their ability to anchor onto metallic substrates and form a molecular barrier between the metal and its environment [9–11]. Efficient anchoring typically requires a conjugated backbone capable of π electron overlap with surface orbitals, together with heteroatoms (N, O, S) whose lone-pair electrons can coordinate directly with the partially vacant d-band of the metal [12–14]. Within this broad family, nitrogen-bearing heterocycles and their derivatives, including azines, amino acids, imines, Schiff bases, and hydrazides, have attracted particular attention over the past decade [15–17]. Recent literature has showcased the versatility of these compounds; for instance, Naveenkumar et al. (2026) [18] demonstrated that Schiff bases can achieve high inhibition efficiency using potentiodynamic polarization and EIS. Similarly, the work of Ahmed et al. (2026) [19] and El Hamri et al. (2026) [20] emphasized the role of functionalized nitrogen-bearing groups in enhancing the adsorption stability on carbon steel surfaces in 1 M HCl. Furthermore, Elaraby et al. (2025) [21] highlighted the importance of multi-scale quantum insights to validate these protective effects, while Al-Amiery et al. (2024) [22] underscored the shift toward more sustainable, environmentally responsible corrosion control strategies. However, many of these studies still rely predominantly on static quantum-chemical calculations, often overlooking the complex dynamic behavior of the inhibitor–metal interface under real service conditions. Hydrazones, defined by the characteristic C=N–N linkage, occupy a noteworthy position in this landscape [23]. The –NH–N=CH– fragment imparts an unusual dual character: the carbon center is simultaneously electrophilic and nucleophilic, while both nitrogen atoms function as nucleophilic donors. This combination confers mixed hard–soft Lewis base behavior that favors strong, multisite coordination with iron and steel surfaces [24–26]. Despite these promising features, a significant research gap remains: the precise electronic influence of the furanyl moiety when coupled with a hydrazone bridge, particularly the impact of protonation in highly acidic (1.0 M HCl) environments, is not yet fully understood. Most existing computational models fail to account for how the transition from neutral to cationic forms, which is typical during industrial acid pickling and cleaning processes, alters the binding geometry and orbital interactions at the corroding interface. While gravimetric and electrochemical measurements remain indispensable for quantifying protection levels, they offer limited visibility into the atomic-scale events that dictate how an organic molecule settles onto and interacts with a corroding interface. Computational chemistry has filled this gap. In particular, quantum-mechanical modeling at the DFT level can map the electronic landscape of an inhibitor, frontier orbitals, charge distribution, and local reactivity, while MD simulations capture the time-dependent behavior of the adsorbed layer under conditions that approximate the real service environment. Against this backdrop, the present study introduces the synthesis and multiscale evaluation of a new furanyl hydrazone derivative, FNH, as a high-performance inhibitor for XC70 carbon steel. The novelty of this work lies in its integrated approach; we bridge the gap between macroscopic electrochemical observables (Tafel and EIS) and microscopic insights (DFT and MD) to elucidate the bidirectional electron exchange mechanism. By focusing on both neutral and protonated states, this research provides a mechanistic blueprint that explains

how FNH achieves exceptional inhibition efficiency, offering a strategic framework for the future design of heteroatom-rich inhibitors in aggressive acidic media.

2. Methods and Materials

2.1. *N'*-[(*E*)-Phenylmethylidene] Furan-2-Carbohydrazide (FNH)

All chemicals used for the synthesis of FNH were of analytical grade, purchased from Sigma-Aldrich (St. Louis, MO, USA) and used without further purification. 2-furoic acid hydrazide (0.01 mol) was dissolved in 15 mL of heated ethanol. Benzaldehyde (0.01 mol) was then added, and the resulting mixture was refluxed for three hours. Thin layer chromatography with a CH₂Cl₂: MeOH (5:1) eluent system was used to track the progress of the reaction. After cooling, the precipitate was filtered out, cleaned with cold ethanol and purified by recrystallisation from a mixture of ethanol and water (Scheme 1).



Scheme 1. General procedure of the synthesis of *N'*-[(*E*)-phenylmethylidene]furan-2-carbohydrazide.

Analytical and spectroscopic data for the synthesized compound are presented below: Yield: 1.85 g (86.3%); m.p: 226.8 °C. Anal. Calcd. for C₁₂H₁₀N₂O₂ (%): C, 67.28; H, 4.71; N, 13.08. Found (%): C, 67.12; H, 4.65; N, 13.19. UV-Vis (EtOH) λ_{max} (nm): 219, 302. FT-IR (KBr, cm⁻¹): ν_{N-H} (hydrazine: CO-NH-N=) 3175, ν_{C-H} (arom) 3103, ν_{C=O} (CO-NH-) 1630, ν_{C=N} (-NH-N=CH-) 1584, ν_{C-N} (CO-N-H) 1282, δ_{C-H} (arom. mono-substituted) 756 and 691. ¹H NMR (DMSO-d₆, δppm): 11.92 (s, 1H, NH), 8.50 (s, 1H, CH=N), 7.98–7.95 (m, 2H, Ar-H), 7.74–7.70 (m, 2H, Ar-H), 7.47–7.43 (m, 3H, Ar-H), 6.73 (dd, *J* = 3.5, 1.8 Hz, 1H, furyl-H); ¹³C NMR decoupled (DMSO-d₆, δ(ppm): 148.3 (CH=N), 146.3 (CH-furyl), 130.6, 129.3, 127.5 (CH-phenyl), 115.4, 112.6 (CH-furyl). The SMILES code is O=C(N/N=C/c1ccccc1)c2ccco2.

2.2. Steel Coupons and Solutions

XC70 carbon steel, supplied by the mold-making unit of Setif, Algeria, was selected as the metallic substrate for all corrosion experiments. Its nominal composition, determined by optical emission spectrometry and expressed in weight percent, is: C 0.065, Si 0.245, Mn 1.685, Cr 0.042, Al 0.042, Ni 0.026, V 0.014, Cu 0.010, Mo 0.005, P 0.002, and S 0.001, with iron accounting for the remainder. The aggressive electrolyte consisted of 1 M hydrochloric acid, prepared by volumetric dilution of a 37% HCl stock solution (Sigma-Aldrich, St. Louis, MO, USA) with double-distilled water; the exact molarity was checked by acid–base titration before each experimental campaign. Inhibitor-containing media were prepared by dissolving weighed amounts of the synthesized FNH hydrazone directly in the 1 M HCl to yield a concentration series spanning four orders of magnitude, from 1 × 10⁻⁶ to 1 × 10⁻⁴ M.

2.3. Weight Loss Experiment

The effect of inhibitor concentration on corrosion protection performance was assessed through gravimetric measurements. XC70 carbon steel coupons of cylindrical geometry, presenting a total exposed area of 4 cm², were abraded using successive grades of emery

paper and subsequently degreased with acetone. Each coupon was then suspended in 50 mL of 1 M HCl maintained at ambient temperature for an exposure duration of 24 h, in the absence and presence of FNH at different concentrations. The mass of each coupon was determined before and after immersion on an analytical balance with a readability of 0.001 g. All trials were performed in triplicate, and the averaged values are reported.

2.4. Electrochemical Measurements

Electrochemical characterization was performed with a Bio-Logic SP-150 potentiostat/galvanostat controlled by EC-Lab software (version V11.42; Bio-Logic Science Instruments, Seyssinet-Pariset, France). The cell—a 100 mL double-walled Pyrex vessel connected to a thermostatic bath—housed three electrodes: a 2 cm² platinum plate serving as the auxiliary electrode, a saturated Ag/AgCl half-cell as the reference, and the XC70 carbon steel specimen (exposed area 0.2 cm²) as the working electrode. Prior to data acquisition, the steel electrode was held in the test solution for 60 min until the open-circuit potential (E_{OCP}) reached a stable value. EIS measurements followed: a 10 mV peak-to-peak sinusoidal signal was applied around E_{OCP} while the excitation frequency was logarithmically swept from 100 kHz to 10 mHz. Once the impedance acquisition was complete, the electrode potential was ramped linearly at 1 mV s^{−1} across a ±250 mV interval centered on E_{OCP} to record the potentiodynamic polarization response. Every measurement sequence was carried out three times on freshly prepared electrodes; the curves shown are representative of the triplicate set.

2.5. Surface Analysis Using AFM and SEM

To assess surface topography changes, AFM is frequently utilized alongside SEM. These techniques provide critical insights into the roughness of metal samples following immersion in corrosive electrolytes, both with and without the addition of inhibitors [27–29]. Carbon steel samples were immersed in 1 M HCl for 24 h at ambient temperature, both without inhibitor and with 1×10^{-4} mol L^{−1} FNH, which was identified from weight loss and electrochemical measurements as the concentration delivering the highest inhibition efficiencies. This optimal concentration was therefore selected for the surface roughness analysis in order to visualize the morphology of the steel under conditions where the protective film is most effective. Three-dimensional topographical images were captured using an Oxford Instruments AFM (Oxford Instruments plc, Oxford, UK), providing nanometric resolution. Additionally, SEM micrographs were obtained with a JOEL-JSM-7001F system (JEOL Ltd., Tokyo, Japan) to observe the adsorption of the hydrazone compound on the surface. The preparation and exposure conditions for the SEM samples were consistent with those applied for the AFM measurements.

2.6. DFT and MD Computations

The microspecies distribution of FNH as a function of pH was calculated using the MarvinSketch software package (ChemAxon, Budapest, Hungary, version 25.3.5), which predicts protonation equilibria based on calculated pK_a values and the Henderson–Hasselbalch equilibrium formalism. The software determines the relative abundance of each protonation state through thermodynamic acid–base equilibria according to

$$PH = PK_a + \log \frac{\text{conjugate base}}{\text{weak acid}} \quad (1)$$

Quantum-chemical modeling of FNH was conducted within the DFT framework as implemented in Materials Studio. Geometry optimizations and single-point property evaluations employed the B3LYP functional with the DNP...basis set and the COSMO implicit solvation model [30–32]. Once a stationary point on the potential energy surface

was confirmed, a suite of global descriptors was derived, specifically, the energies of the highest occupied and lowest unoccupied molecular orbitals, the gap separating them, Mulliken electronegativity, absolute hardness, and the fraction of transferred electrons ΔN and the back-donation energy, together with condensed Fukui indices derived from Hirshfeld charges [33,34].

The interfacial behavior of FNH on Fe (110) was examined using an MD simulation performed with the Forcite module. The simulation was carried out in a simulation box ($24.82 \times 24.82 \times 44.20 \text{ \AA}^3$) with periodic boundary conditions, and the COMPASSIII force field (Condensed Phase Optimized Molecular Potentials for Atomistic Simulation Studies) was used to optimize the structures of all components of the system [35]. The Fe (110) surface was selected to simulate the adsorption process, since it is the most stable low-Miller-index iron surface and therefore the most abundant. First, the Fe crystal was imported and cleaved along the (110) plane, and a $9.93 \text{ \AA}$ slab thickness was employed. The Fe (110) surface was relaxed by minimizing its energy using the smart minimizer method, and then enlarged to a (10×10) supercell to provide a large surface area for inhibitor interactions. A vacuum slab with zero thickness was built. Two independent cells were built in this way—one with neutral FNH and one with the protonated FNH-H^+ cation—to compare their adsorption. Each cell includes water (490 molecules), H_3O^+ (5 molecules), and Cl^- (5 molecules) for a more reliable system, and placed above the iron surface layer. All atoms in the Fe (110) surface were kept frozen during the simulation process; only the FNH and water molecules were allowed to contact the iron surface freely. Nonbonding, van der Waals, and electrostatic interactions were set as atom-based summations using the Ewald summation method, with a cutoff radius, spline width, and buffer width set to $15.5 \text{ \AA}$, $1 \text{ \AA}$, and $0.5 \text{ \AA}$, respectively. The Andersen algorithm was employed to control the simulation temperature at different levels. The simulation was performed at 298 K in the NVT ensemble, with a time step of 1 fs and a simulation time of 100 ps. The dynamics were run until the entire system reached equilibrium, at which point both the temperature and the energy of the system were balanced. The strength of the inhibitor–surface association was quantified through the interaction energy and the corresponding binding energy, calculated according to Equations (2) and (3) [36]:

$$E_{\text{interaction}} = E_{\text{total}} - (E_{\text{surface+solution}} + E_{\text{inhibitor}}) \quad (2)$$

$$E_{\text{binding}} = -E_{\text{interaction}} \quad (3)$$

In these expressions, E_{total} denotes the energy of the complete system, $E_{\text{surface+solution}}$ represents the combined energy of the Fe slab and the water phase, and $E_{\text{inhibitor}}$ is the energy of the free inhibitor molecule.

3. Results and Discussion

3.1. Gravimetric Measurements

Gravimetric data recorded after 24 h of immersion were used to quantify the protective action of FNH toward mild steel in 1 M HCl at ambient temperature. The corrosion rate, W ($\text{g cm}^{-2} \text{ h}^{-1}$), and the corresponding inhibition efficiency, IE_W (%), were derived from Equations (4) and (5), respectively:

$$W = \frac{m_1 - m_2}{S \cdot t} \quad (4)$$

$$IE_W = \left(\frac{W_0 - W}{W_0} \right) \times 100 \quad (5)$$

Here, m_1 and m_2 (g) are the masses of the steel coupon before and after exposure, S (cm^2) is the area in contact with the solution, and t (h) is the total immersion period. W_0 and W denote the corrosion rates obtained in the uninhibited and inhibited media, respectively.

The resulting corrosion parameters are compiled in Table 1. A clear concentration-dependent trend is observed: IE_W rises steadily with FNH concentration and attains 94.94 ± 1.2 at $1 \times 10^{-4} \text{ mol L}^{-1}$. Such pronounced protection originates from the adsorption of FNH molecules onto the steel substrate, where the nitrogen and oxygen heteroatoms supply lone-pair electrons to the partially filled d-orbitals of surface iron atoms. This electron donation facilitates the formation of a dense, adherent barrier film that effectively suppresses the corrosion process [37,38].

Table 1. Corrosion parameters obtained from weight loss measurements for XC70 steel in 1 M HCl after 24 h at room temperature, in the absence and presence of various concentrations of FNH.

C (M)	Δm (g)	W_{corr} ($\text{g cm}^{-2} \text{ h}^{-1}$)	θ	IE (%)
1×10^{-6}	0.0030 ± 0.0001	0.0146 ± 0.0005	0.697 ± 0.02	69.70 ± 2.1
1×10^{-5}	0.0014 ± 0.0001	0.0068 ± 0.0003	0.858 ± 0.01	85.86 ± 1.5
5×10^{-5}	0.0009 ± 0.0001	0.0044 ± 0.0002	0.909 ± 0.01	90.91 ± 1.5
1×10^{-4}	0.0005 ± 0.00005	0.0024 ± 0.0002	0.949 ± 0.01	94.94 ± 1.2

3.2. Potentiodynamic Polarization Curves

The influence of FNH on the anodic and cathodic half-reactions occurring at the steel surface was examined by potentiodynamic polarization. Prior to each scan, the carbon steel electrode was allowed to stabilize for 60 min in 1 M HCl containing FNH at concentrations between 1×10^{-6} and 1×10^{-4} M; a blank experiment without inhibitor was run under identical conditions. The recorded polarization curves are displayed in Figure 1.

Inspection of the curves shows that the addition of FNH over the entire concentration range produces a pronounced suppression of the corrosion current density relative to the uninhibited acid. Both the anodic and cathodic branches shift toward lower current values, whereas the corrosion potential undergoes only a modest displacement with respect to the blank. This dual retardation of metal dissolution and hydrogen evolution is characteristic of a mixed-type inhibitor. The gradual decline in current density at higher FNH concentrations reflects a progressive buildup of adsorbed molecules on the electrode surface, generating a protective film that restricts the access of chloride ions and protons to the underlying metal and, consequently, diminishes the overall dissolution rate [39].

The related electrochemical parameters, such as corrosion potential E_{corr} , corrosion current density i_{corr} , and Tafel slopes β_a , β_c , determined by extrapolation of the Tafel regions, surface coverage (θ) and the inhibitory effectiveness (IE_p (%)) are listed in Table 2.

Table 2. Electrochemical parameters obtained from Tafel plots at 293 K in 1 M HCl, in the absence and presence of various concentrations of FNH.

C (M)	$-E_{corr}$ (mV/Ag/AgCl)	i_{corr} (mA/cm ²)	β_a (mV/dec)	$-\beta_c$ (mV/dec)	R_p	θ	IE_p (%)
Blank	426.1 ± 0.8	2.64 ± 0.05	153.3	101.1	10.24	/	/
1×10^{-6}	436.54 ± 0.4	0.75 ± 0.008	143.7	48.58	21.00	0.7127	71.27 ± 0.85
1×10^{-5}	440.99 ± 0.12	0.27 ± 0.004	91.90	131.6	86.92	0.8976	89.76 ± 0.52
5×10^{-5}	402.64 ± 0.45	0.12 ± 0.005	40.40	83.60	100.16	0.9529	95.29 ± 0.35
1×10^{-4}	444.24 ± 0.15	0.06 ± 0.0071	48.60	55.20	187.03	0.9759	97.59 ± 0.22

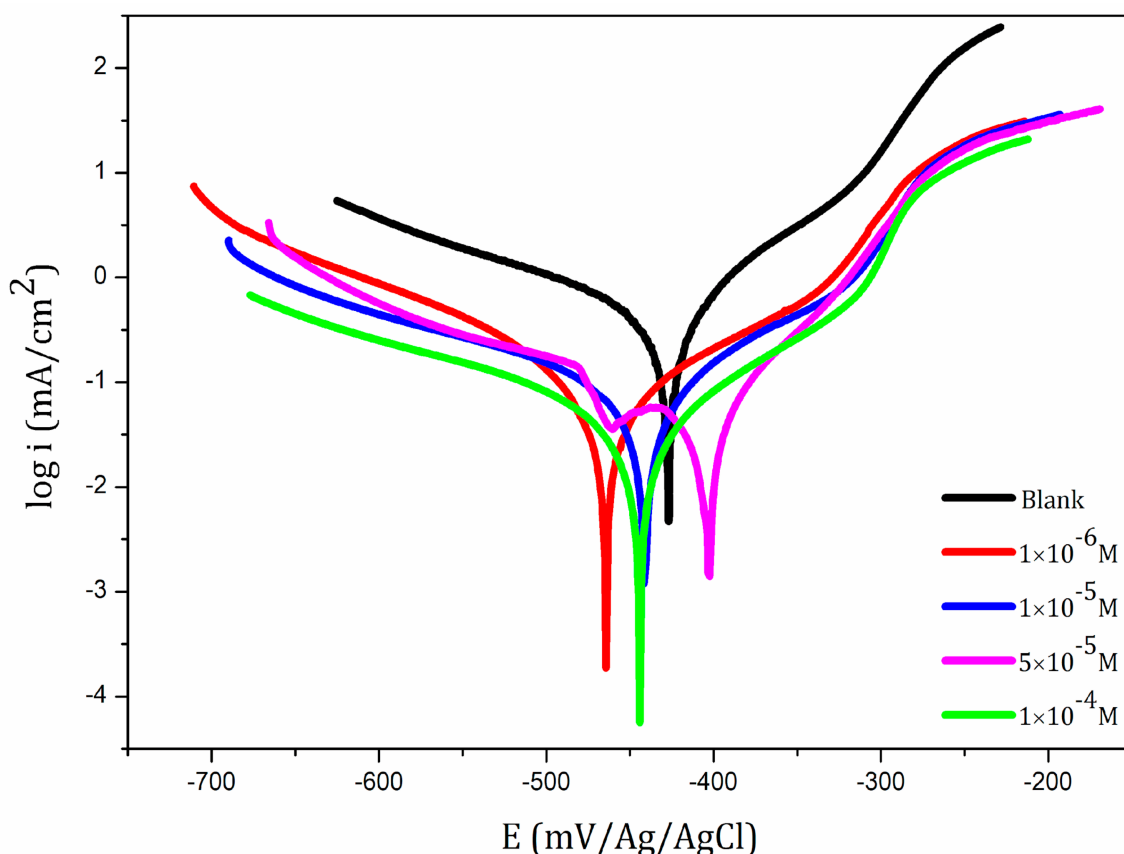


Figure 1. Polarization curves of XC70 carbon steel in 1 M HCl in the absence and presence of various concentrations of FNH inhibitor at 293 K.

The inhibitory effectiveness was calculated using the following equation:

$$IE_p = \frac{i_{corr}^{\circ} - i_{corr}^{inh}}{i_{corr}^{\circ}} \quad (6)$$

where i_{corr}° and i_{corr}^{inh} are the corrosion current density without and with inhibitor, respectively.

Quantitatively, i_{corr} falls from $2.64 \pm 0.05 \text{ mA cm}^{-2}$ in the blank solution to $0.06 \pm 0.0071 \text{ mA cm}^{-2}$ at $1 \times 10^{-4} \text{ M}$, confirming the strong corrosion-mitigating capacity of FNH in 1 M HCl. In parallel, IE_p (%) (%) and the fractional surface coverage θ increase with concentration, reaching $97.59 \pm 0.22\%$ and 0.9759 at the highest dosage examined, which points to the establishment of a dense and well-organized adsorbed layer over the steel surface. The net shift in E_{corr} does not exceed 85 mV (ranging from -403 to -444 mV), further corroborating the mixed inhibition character of FNH, with concurrent action on both the anodic and cathodic partial reactions [40]. The changes recorded in the anodic (β_a) and cathodic (β_c) Tafel slopes warrant a more detailed mechanistic interpretation. Two conceptually distinct inhibition mechanisms can be identified from the behavior of the Tafel slopes: (i) geometric site-blocking, in which the inhibitor physically occupies active surface sites without altering the intrinsic electrochemical reaction pathway, in this case, β_a and β_c remain essentially invariant with inhibitor concentration, and the suppression of i_{corr} solely reflects a reduction in the effective electroactive area ($\theta \rightarrow 1$); and (ii) modification of the charge-transfer mechanism, in which the adsorbed inhibitor participates in the electrode reaction by modifying the intermediate steps of the iron dissolution sequence ($\text{Fe} \rightarrow \text{Fe}^* \rightarrow \text{Fe}^{2+} + 2e^-$) or the hydrogen evolution mechanism ($\text{H}_3\text{O}^+ + e^- \rightarrow \text{Hads} \rightarrow \text{H}_2$), resulting in a systematic variation in the Tafel slopes with inhibitor concentration [41].

Applying this framework to the FNH data in Table 2, the values of β_a vary from 153.3 mV dec^{−1} (blank) to 40.4–91.9 mV dec^{−1} (inhibited), and β_c varies from 101.1 mV dec^{−1} to 48.6–131.6 mV dec^{−1}. The non-systematic variation in both Tafel slopes across the concentration series—rather than a clean invariance or a monotonic trend—indicates a mixed situation: FNH simultaneously reduces the accessible electroactive area (dominant effect, responsible for the large i_{corr} suppression) and exerts a moderate reorganizing influence on the charge-transfer kinetics at the Fe/solution interface. The occasional increase in β_c above the blank value is attributed to the partial blocking of cathodic hydrogen evolution sites by adsorbed FNH molecules, which modifies local proton availability and alters the apparent cathodic transfer coefficient. This behavior is consistent with the strong chemisorptive interaction of FNH with surface Fe atoms via its N and O donor centers. Consequently, FNH inhibits corrosion via a combination of geometric blocking of active sites and partial modification of the charge-transfer kinetics, with the former being the dominant mechanism [42].

The inhibition efficiency of FNH ($\text{IE}_p = 97.59\%$ at 1×10^{-4} M) represents a significant advancement relative to contemporary benchmarks. Recent studies by Danyaro et al. [43] on benzoic acid-based Schiff bases reported an efficiency of 89.9%, while Satarkar and Dubey [44] achieved 91.2% with 5-aryl-furan derivatives. The comprehensive review by Koushik et al. [45] highlights that many green inhibitors plateau around 85%–88% in aggressive acidic media. Even compared with the eco-friendly systems reported by Chaouiki et al. [46], which reached 93%, and the furfural-derived Schiff bases studied by Ginting et al. [47] (78.6%), FNH provides a more robust protective layer. This superior performance underscores the critical role of the electronic synergy between the furanyl moiety and the hydrazone bridge, which ensures stable interfacial anchoring and superior surface coverage relative to these recently reported scaffolds.

3.3. Electrochemical Impedance Spectroscopy (EIS)

EIS was employed to probe the interfacial processes governing the corrosion of the steel electrode in 1 M HCl, both in the uninhibited acid and in the presence of FNH at concentrations spanning 1×10^{-6} to 1×10^{-4} M. The resulting Nyquist and Bode representations are collected in Figure 2.

The Nyquist diagrams (Figure 2a) consist of a single, depressed capacitive arc for every solution examined, pointing to a corrosion process governed predominantly by charge-transfer kinetics [48]. In the inhibitor-free acid, the arc diameter is comparatively small, consistent with a low charge-transfer resistance (R_{ct}) and rapid metal dissolution. Upon successive introduction of FNH, the semicircle diameter expands considerably, with the enlargement becoming increasingly pronounced at higher concentrations [49]. This progressive growth in R_{ct} provides direct evidence for the effective protective action of the compound under study. The departure of the experimental arcs from perfect semicircular geometry is a well-known consequence of frequency dispersion originating from surface roughness, microscopic heterogeneities, grain boundaries, dislocations, and the fractal character of real electrode surfaces [50].

The Bode modulus representation (Figure 2b) offers complementary insight: the low-frequency impedance modulus $|Z|$ increases systematically with rising FNH concentration, corroborating the progressive buildup of an insulating adsorbed layer on the steel substrate [51]. In the corresponding phase-angle plots (Figure 2c), a single broad maximum is resolved for all systems, signifying a single relaxation time constant—fully consistent with the single capacitive loop in the Nyquist plane. The broadening and upward shift in the phase angle upon inhibitor addition reflect the displacement of water molecules from the metal–solution interface by adsorbed FNH species [52].

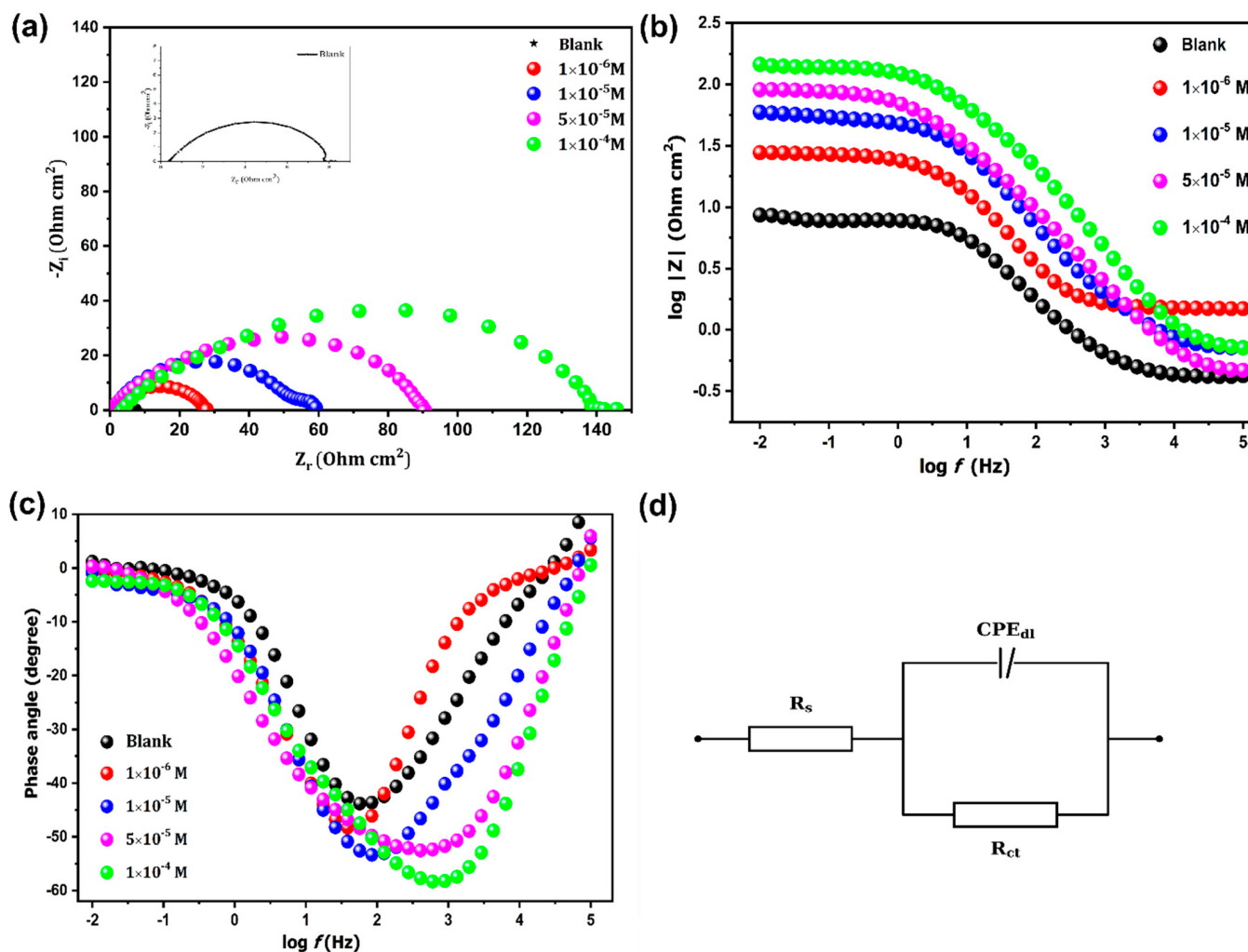


Figure 2. EIS diagrams for XC70 carbon steel in 1 M HCl solution containing different concentrations of FNH: (a) Nyquist plots, (b) Bode modulus plots, (c) Bode phase angle plots, and (d) the equivalent electrical circuit (EEC) used to fit the impedance data.

The collective impedance evidence leaves little doubt that FNH adsorption onto the steel substrate is the origin of the observed corrosion suppression. By occupying electrochemically active sites, the organic film raises the energetic cost of the interfacial charge-transfer step, which manifests experimentally as growing R_{ct} and rising low-frequency $|Z|$ values across the entire concentration series. Quantitative extraction of the kinetic parameters required fitting the measured Nyquist responses to an appropriate electrical analog. The equivalent circuit retained for this purpose (Figure 2d) couples R_s —representing the ohmic drop through the bulk electrolyte—in series with a parallel R_{ct} /CPE element that captures the faradaic and capacitive contributions of the corroding interface. A constant phase element was chosen over an ideal capacitor because real electrode surfaces, with their inherent roughness, grain-boundary network, and compositional gradients, invariably produce a frequency-dependent capacitive response that a single C_{dl} value cannot reproduce. The CPE impedance takes the form:

$$Z_{CPE} = \frac{1}{Q(j\omega)^n} \quad (7)$$

Here Q carries units of $\text{s}^n \Omega^{-1} \text{cm}^{-2}$ and sets the magnitude of the pseudo-capacitive response, $j = \sqrt{-1}$, ω is the angular frequency, and the exponent n —bounded between

0 and 1—serves as a diagnostic of surface ideality. When n approaches unity the element collapses to a classical parallel-plate capacitor; progressive departure toward lower n values signals increasing dispersion of relaxation times, a fingerprint of microscopic heterogeneity across the electrode area.

The parameters extracted from the EIS fitting are listed in Table 3. The effective double-layer capacitance was evaluated from the CPE parameters using [53]:

$$C_{dl} = \left(Q R_{ct}^{1-n} \right)^{\frac{1}{n}} \quad (8)$$

Table 3. EIS fitting parameters and corresponding inhibition efficiencies for XC70 steel in acidic medium at 293 K.

C (M)	R_s ($\Omega \cdot \text{cm}^2$)	R_{ct} ($\Omega \cdot \text{cm}^2$)	Q ($\mu\text{F} \cdot \text{s}^{(n-1)}$)	n	C_{dl} ($\mu\text{F} \cdot \text{cm}^{-2}$)	$\chi^2/ Z $	IE _{EIS} (%)
Blank	0.4140 ± 0.005	7.740 ± 0.08	1040 ± 15	0.7339 ± 1.05	205 ± 04	0.17	/
1×10^{-6}	1.4124 ± 0.015	26.26 ± 0.25	540 ± 10	0.7464 ± 1.10	83.5 ± 02	0.004497	70.52 ± 0.95
1×10^{-5}	0.5224 ± 0.008	57.32 ± 0.45	345 ± 08	0.6645 ± 0.95	8.96 ± 0.15	0.07282	86.49 ± 0.72
5×10^{-5}	0.6820 ± 0.010	91.26 ± 0.62	326 ± 07	0.6506 ± 0.90	4.80 ± 0.09	0.1105	91.51 ± 0.55
1×10^{-4}	0.5668 ± 0.009	143.66 ± 0.95	124 ± 05	0.6740 ± 0.92	1.89 ± 0.05	0.05304	94.61 ± 0.38

The inhibition efficiency was then determined according to [54]:

$$IE_{EIS}\% = \frac{R_{ct}^{inh} - R_{tc}^{\circ}}{R_{ct}^{inh}} \times 100 \quad (9)$$

where R_{ct}° and R_{ct}^{inh} are the charge-transfer resistances recorded in the absence and in the presence of FNH, respectively.

The quality of the equivalent circuit fitting was assessed through the normalized chi-squared values ($\chi^2/|Z|$) reported in Table 3. For all inhibited solutions, $\chi^2/|Z|$ values are satisfactorily low, ranging from 4.50×10^{-3} to 1.11×10^{-1} , confirming the excellent agreement between the experimental EIS spectra and the proposed $R_s(R_{ct}/CPE)$ equivalent circuit model and validating the reliability of the extracted impedance parameters. The slightly elevated $\chi^2/|Z|$ value observed for the blank solution (0.17) is attributed to the intrinsic complexity of the bare steel/HCl interface in the absence of an organic inhibitor film, where additional interfacial processes—including active pit initiation and oxide layer dissolution—contribute to deviations from the ideal circuit response. This behavior is well documented for bare carbon steel in aggressive acidic media [55] and does not affect the validity of the inhibited system analyses.

As seen in Table 3, R_{ct} undergoes a substantial increase upon inhibitor addition, rising nearly 19-fold from the blank solution to $1 \times 1 \times 10^{-4}$ M FNH. This trend signals the gradual development of a surface film that increasingly impedes the interfacial charge-transfer step.

In parallel, C_{dl} drops markedly from 205 ± 04 to $1.89 \pm 0.05 \mu\text{F cm}^{-2}$, a decrease that can be rationalized within the Helmholtz model (Equation (10)) by the substitution of adsorbed water—possessing a high dielectric constant—by organic inhibitor molecules of lower permittivity, and/or by an increase in the effective thickness of the electrical double layer [56].

$$C_{dl} = \frac{\epsilon_0 \epsilon S}{d} \quad (10)$$

In this expression, d represents the film thickness, S the electrode area, ϵ_0 the vacuum permittivity, and ϵ the local dielectric constant of the adsorbed layer.

The CPE exponent n provides additional insight into surface heterogeneity. When $n = 1$, the interface behaves as a perfect capacitor on a flat, homogeneous surface; values of $n < 1$ reflect frequency dispersion arising from microscopic roughness, chemical non-uniformity, grain-boundary effects, and variations in local adsorption density—all characteristic features of polycrystalline carbon steel [57]. In the uninhibited acid, $n = 0.734$, consistent with the known heterogeneous microstructure of XC70 steel. Upon successive addition of FNH, n decreases slightly to values in the range 0.651–0.674. This modest decrease is attributed to the preferential adsorption of FNH molecules onto the most energetically active surface sites (grain boundaries, dislocations), which creates lateral heterogeneity at the interface arising from the coexistence of FNH-covered and bare domains with distinct local dielectric properties. This broadening of the relaxation-time distribution is reflected in the slight reduction in n . Importantly, this trend does not contradict the strong protective performance of FNH: the n parameter quantifies the geometric uniformity of the interface, not its corrosion-suppression capacity. The absolute values of n remaining below 0.75 throughout confirm that XC70 steel retains intrinsic heterogeneity inherent to its polycrystalline microstructure—a well-documented behavior for technical-grade carbon steels in acidic media—irrespective of inhibitor coverage [58].

3.4. Temperature Effect

Temperature governs both the kinetics of electrochemical reactions and the stability of adsorbed inhibitor films, making it a key variable in evaluating corrosion inhibitor performance. To assess this influence, polarization and EIS measurements were carried out on XC70 steel in 1 M HCl containing the optimal FNH concentration (1×10^{-4} M) over the range 293–333 K; parallel experiments in the uninhibited acid served as reference (Figures 3 and 4). With rising temperature, the polarization curves show a progressive increase in i_{corr} accompanied by accelerated anodic and cathodic kinetics, while the Nyquist semicircle diameter contracts, indicating a decline in R_{ct} .

The quantitative electrochemical parameters extracted from polarization and impedance measurements at temperatures between 293 and 333 K are compiled in Tables 4 and 5, respectively, for the uninhibited acid and the solution containing the optimal FNH dosage.

Table 4. Tafel polarization–derived electrochemical parameters and corresponding inhibition efficiencies (IE%) for XC70 carbon steel in 1 M HCl at different temperatures, evaluated at the optimal FNH concentration (1×10^{-4} M).

	T (K)	$-E_{\text{corr}}$ (mV)	i_{corr} (mA/cm ²)	β_a (mV/dec)	$-\beta_c$ (mV/dec)	IE _p (%)
HCl 1 M	293	426.1 ± 0.8	2.64 ± 0.05	153.3	101.1	/
	303	419.1 ± 1.2	6.41 ± 0.11	142.9	165.8	/
	313	412.3 ± 1.4	22.50 ± 0.38	105.1	115.1	/
	323	393.2 ± 1.8	39.78 ± 0.62	101.9	129.7	/
	333	388.6 ± 2.1	62.91 ± 0.95	107.2	118.9	/
HCl 1 M + FNH 10^{-4} M	293	444.24 ± 0.15	0.060 ± 0.007	48.6	55.2	97.59 ± 0.22
	303	496.31 ± 0.12	0.110 ± 0.002	65.3	72.1	98.22 ± 0.25
	313	480.92 ± 0.25	0.180 ± 0.004	56.7	52.4	99.16 ± 0.18
	323	529.94 ± 0.18	0.470 ± 0.011	92.2	73.8	98.80 ± 0.28
	333	509.06 ± 0.31	0.560 ± 0.013	85.1	64.8	99.09 ± 0.24

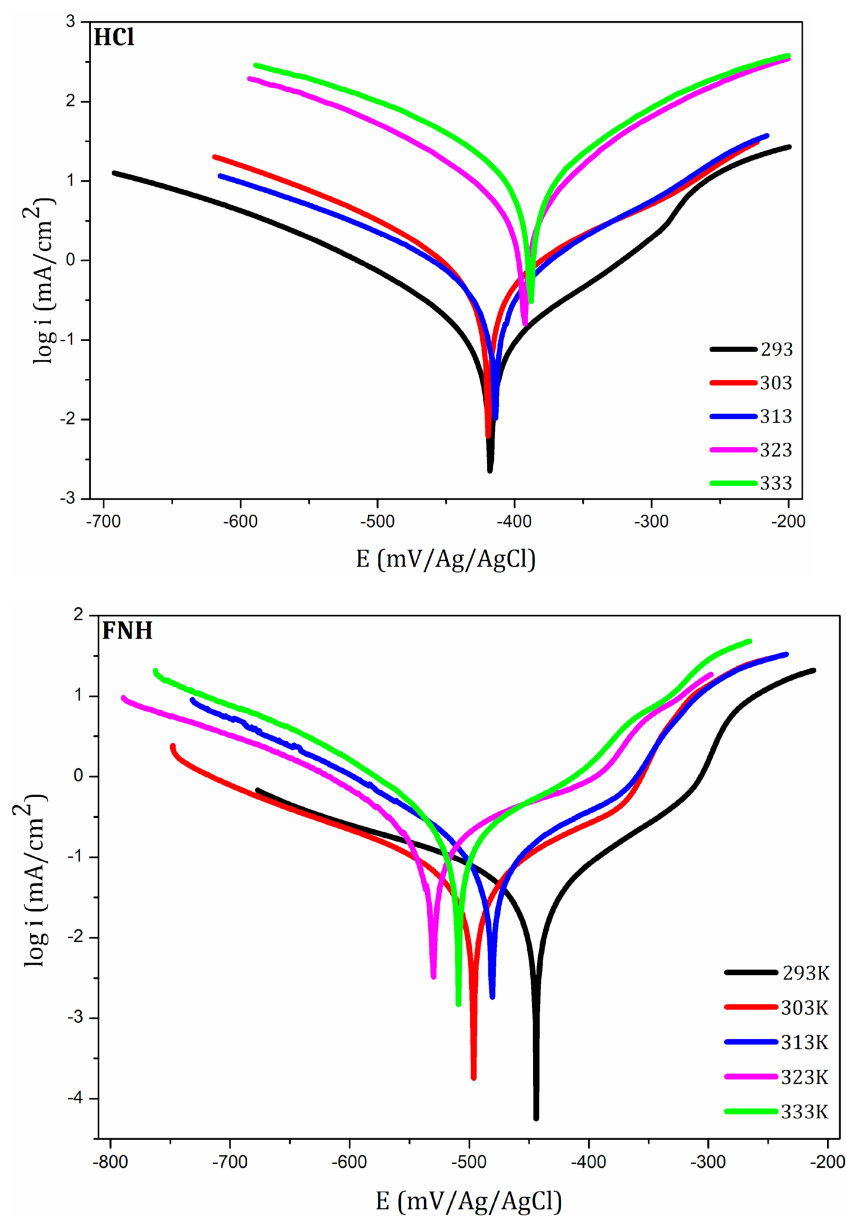


Figure 3. Temperature-dependent potentiodynamic polarization (PDP) profiles for XC70 carbon steel in 1 M HCl: (HCl) uninhibited solution and (FNH) solution containing 1×10^{-4} M FNH.

Table 5. EIS-derived parameters and corresponding inhibition efficiencies (IE%) for XC70 carbon steel in 1 M HCl, with and without 1×10^{-4} M FNH, evaluated across various temperatures.

	T (K)	R_s ($\Omega \cdot \text{cm}^2$)	R_c ($\Omega \cdot \text{cm}^2$)	Q ($\mu\text{F} \cdot \text{s}^{(n-1)}$)	n	C_{dl} ($\mu\text{F} \cdot \text{cm}^{-2}$)	IE (%)
Blank	293 K	0.414 ± 0.02	7.74 ± 0.21	1004	0.7339	114.5	/
	303 K	1.078 ± 0.05	2.168 ± 0.15	491	0.7810	148.4	/
	313 K	0.672 ± 0.03	1.320 ± 0.11	466	0.7353	74.6	/
	323 K	0.366 ± 0.02	0.672 ± 0.08	343	0.7325	59.8	/
	333 K	0.182 ± 0.01	0.274 ± 0.05	301	0.7235	60.2	/
FNH 10^{-4} M	293 K	0.566 ± 0.03	143.66 ± 0.52	124 ± 8	0.6740 ± 0.45	0.331 ± 0.02	94.61 ± 0.38
	303 K	0.453 ± 0.02	74.28 ± 0.42	88.1 ± 5	0.7892 ± 0.62	7.49 ± 0.25	97.08 ± 0.31
	313 K	0.571 ± 0.03	42.54 ± 0.38	603 ± 35	0.6284 ± 0.58	1.58 ± 0.12	96.86 ± 0.35
	323 K	0.393 ± 0.02	30.84 ± 0.25	351 ± 19	0.6713 ± 0.72	3.03 ± 0.18	97.82 ± 0.28
	333 K	0.309 ± 0.02	23.10 ± 0.19	570 ± 24	0.7003 ± 0.65	15.3 ± 0.31	98.81 ± 0.22

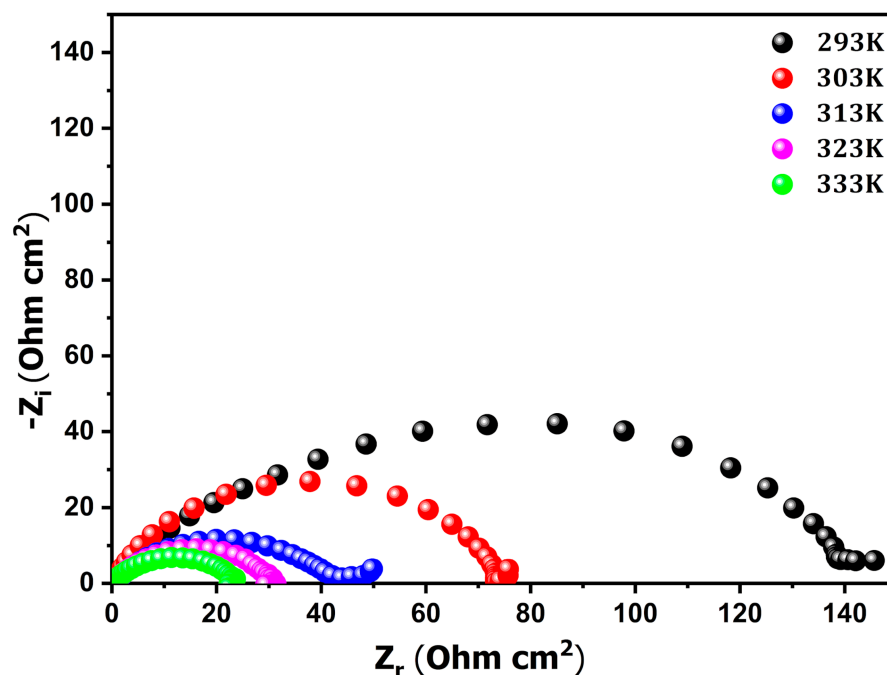


Figure 4. Nyquist plots for XC70 mild steel in 1 M HCl solution in the absence (HCl) and presence of FNH inhibitor at different temperatures.

A common feature across both media is the acceleration of corrosion kinetics at elevated temperatures, i_{corr} rises and R_{ct} contracts as the thermal energy input grows. However, the magnitude of these changes differs sharply between the two cases. In the plain acid, both trends are steep, i_{corr} climbs rapidly while R_{ct} undergoes a pronounced collapse, reflecting the increasingly aggressive dissolution of bare steel as the thermal barrier to charge transfer is progressively lowered. When FNH is present, the same trends persist but are substantially attenuated: i_{corr} increases at a much slower pace, and R_{ct} retains considerably higher values than those recorded in the blank at every temperature examined.

A noteworthy observation concerns E_{corr} , which shifts to more negative potentials with heating in the inhibited solution relative to the blank, suggesting that the thermal activation preferentially enhances the cathodic-site blocking ability of the adsorbed FNH layer and thus reinforces its influence on the anodic partial reaction. More importantly, the calculated inhibition efficiency does not decline with temperature but instead rises steadily, culminating at 99% at 333 K, a trend confirmed independently by both PDP and EIS datasets. Such behavior departs from the pattern typically observed for physically adsorbed inhibitors, where thermal desorption erodes protection at higher temperatures. The positive temperature dependence recorded here points instead to specific, chemically driven interactions between the FNH molecule and the iron substrate that are strengthened as more thermal energy becomes available [59–61]. The capacity of FNH to maintain, and indeed improve, its protective action even at elevated temperatures, and at relatively low dosage, underscores both the robustness of the adsorbed film and the practical viability of this compound under thermally demanding service conditions.

A complete kinetic and thermodynamic analysis was performed to provide quantitative evidence for the adsorption mechanism. The Arrhenius activation energy ($E_a = 47.23 \text{ kJ mol}^{-1}$ in the presence of FNH vs. $66.60 \text{ kJ mol}^{-1}$ for the blank), the transition-state parameters ($\Delta H_a = +44.64 \text{ kJ mol}^{-1}$, $\Delta S_a = -81.93 \text{ J mol}^{-1} \text{ K}^{-1}$ for the inhibited system), and the standard Gibbs free energy of adsorption ($\Delta G^\circ_{\text{ads}} = -43.39 \text{ kJ mol}^{-1}$) collectively confirm the chemisorptive nature of FNH adsorption on XC70 steel. It is noteworthy that the apparent activation energy E_a decreases from $66.60 \text{ kJ mol}^{-1}$ in the

uninhibited solution to $47.23 \text{ kJ mol}^{-1}$ in the presence of $1 \times 10^{-4} \text{ mol L}^{-1}$ FNH. Similar behavior has been reported for strongly chemisorbing organic inhibitors and is commonly attributed to the formation of a stable adsorbed film that alters the rate-determining step and the effective reaction pathway, rather than to a simple uniform increase in the intrinsic rate of metal dissolution. In our case, despite the lower E_a , the corrosion current density and charge-transfer rate decrease markedly over the entire temperature range (Tables 4 and 5), and the inhibition efficiency increases up to $\sim 99\%$, indicating that the overall corrosion process is strongly retarded and that the inhibitory action cannot be assessed on the basis of E_a alone. The negative $\Delta G^\circ_{\text{ads}}$ value ($|\Delta G^\circ_{\text{ads}}| > 40 \text{ kJ mol}^{-1}$) is consistent with spontaneous chemisorption involving charge transfer between FNH and surface Fe atoms. Full details, equations, and graphical representations (Arrhenius and Eyring plots, Langmuir isotherm) are provided in the Supplementary Materials (Table S1, Figures S1–S3).

3.5. Surface Characterization

3.5.1. Atomic Force Microscopy

AFM was used to probe how FNH modifies the nanoscale landscape of the steel surface. XC70 coupons were retrieved after 24 h of contact with 1 M HCl at room temperature—one set from the plain acid, the other from a solution containing $1 \times 10^{-4} \text{ M}$ FNH—and scanned alongside a freshly polished reference specimen. The three-dimensional height maps are collected in Figure 5a–c; Table 6 lists the corresponding mean roughness data.

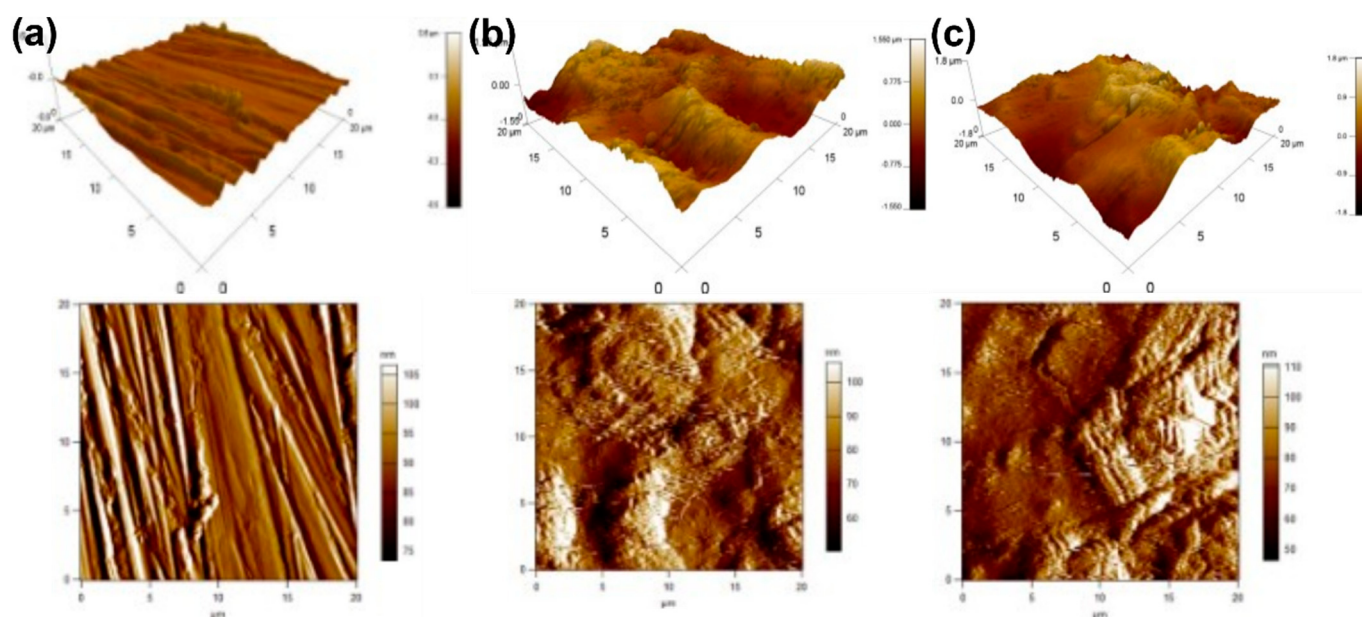


Figure 5. Three-dimensional AFM topographies of XC70 carbon steel: (a) as-polished reference surface, (b) after 24 h immersion in 1 M HCl, and (c) after 24 h immersion in 1 M HCl with $1 \times 10^{-4} \text{ M}$ FNH inhibitor.

Table 6. Average surface roughness of XC70 steel measured in 1 M HCl, reported for conditions with and without the addition of $1 \times 10^{-4} \text{ M}$ FNH inhibitor.

	Polished XC70	Uninhibited XC70	Inhibited XC70/FNH
RMS (nm)	39.192	419.981	356.186

The coupon withdrawn from the inhibitor-free acid (Figure 5b) exhibits a cratered terrain densely populated with pits of irregular shape and depth, a morphology that

reflects the sustained corrosive action of the HCl medium on the bare metal. A strikingly different picture emerges when FNH is present (Figure 5c): the topography is considerably flattened and the pit population is largely suppressed, pointing to effective mitigation of iron dissolution [62,63]. This leveling effect is consistent with the self-assembly of an organic barrier derived from adsorbed FNH molecules that shields the underlying substrate from direct acid contact. On a quantitative basis, the mean roughness drops from 419.981 nm for the unprotected surface to 356.186 nm under FNH coverage, numerically corroborating the visual evidence of surface preservation.

The interpretation of the residual roughness of 356 nm should be considered carefully. This value must be compared in relative, not absolute, terms: the uninhibited surface undergoes approximately a 10.7-fold increase in roughness relative to the polished reference (39.19 nm), while the inhibited surface shows only a 9.1-fold increase. Moreover, a 97.59% reduction in corrosion rate still permits 2.41% of the original dissolution rate to continue over 24 h in a highly aggressive 1 M HCl medium, which is sufficient to generate measurable surface damage. Additionally, AFM topography detects all surface features, including the texture of the deposited organic film itself, which contributes to the measured RMS value and is not a manifestation of corrosion damage.

3.5.2. Scanning Electron Microscopy

SEM micrographs of XC70 carbon steel after 24 h of exposure at ambient temperature to 1 M HCl, without and with 1×10^{-4} M FNH, are shown in Figure 6a–c. The coupon retrieved from the blank acid (Figure 6b) presents a heavily corroded surface characterized by deep attack features resulting from severe dissolution. In contrast, the specimen exposed to the inhibited solution (Figure 6c) is covered by a relatively continuous deposit exhibiting a platelet-like morphology, which is attributed to the chemisorption of hydrazone FNH molecules onto the active metallic sites. The resulting compact and adherent organic film restricts the transport of aggressive Cl^- and H^+ ions toward the underlying steel, thereby suppressing both anodic dissolution and cathodic hydrogen evolution and confirming the protective action of FNH [27].

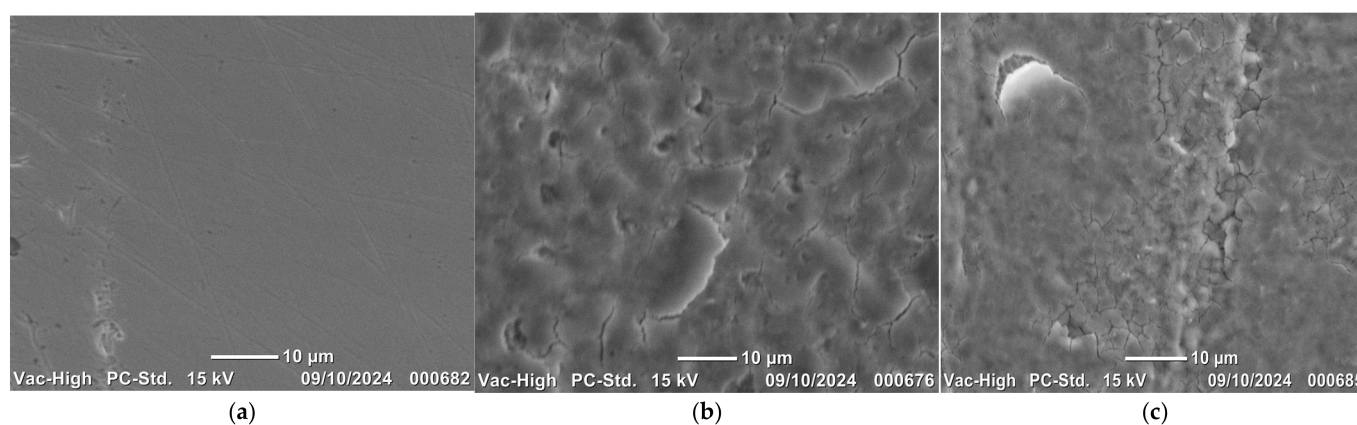


Figure 6. SEM micrographs of XC70 carbon steel surfaces: (a) polished condition, (b) after 24 h exposure to 1 M HCl, and (c) after 24 h exposure to 1 M HCl in the presence of 1×10^{-4} M FNH.

3.6. Computational Investigation

3.6.1. Prediction of the Major Micro Species in an Acidic Medium

The chemical behavior of a molecule in solution is fundamentally determined by the species it produces under aqueous conditions; therefore, a protonation study was carried out for FNH to clarify which microstates are relevant under the experimental conditions. This analysis, performed over a pH range of 0.0–14.0, allows identification of the major

and minor microspecies of the inhibitor in aqueous medium. The speciation calculations were conducted with the Protonation module of the MarvinSketch package (ChemAxon, version 25.3.5) using the standard aqueous pKa prediction protocol, in which intrinsic pKa values are first estimated for each ionizable center and the corresponding microstate populations are then obtained by solving the set of acid–base equilibria together with the mass-balance and electroneutrality conditions as a function of pH. Within this framework, the four species labeled Forms 1–4 in Figures 7 and 8 correspond to distinct protonation states of FNH (neutral and protonated forms) that share the same carbon skeleton but differ in the number and location of bound protons and in their total charge. Because the corrosive medium in this work is 1 M HCl ($\text{pH} \approx 0.0$), the equilibrium distribution was evaluated by fixing $\text{pH} = 0.0$ in the Marvin “distribution of species” routine; under these conditions, Form 3, which is generated by protonation at the azomethine nitrogen ($\text{C}=\text{N}$), is overwhelmingly dominant and accounts for 95.98% of the total species population. This protonated form is expected to alter the electronic structure and enhance electrostatic attraction toward the negatively charged chloride-rich interface [64], and it was therefore selected as the representative microspecies for the subsequent DFT and MD calculations.

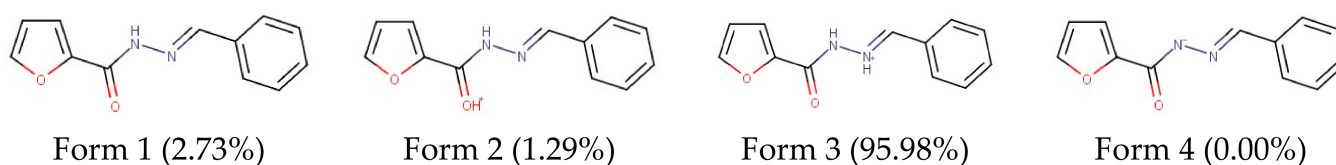


Figure 7. The percentage of microspecies of the investigated inhibitor at $\text{pH} = 0$ in acidic solution.

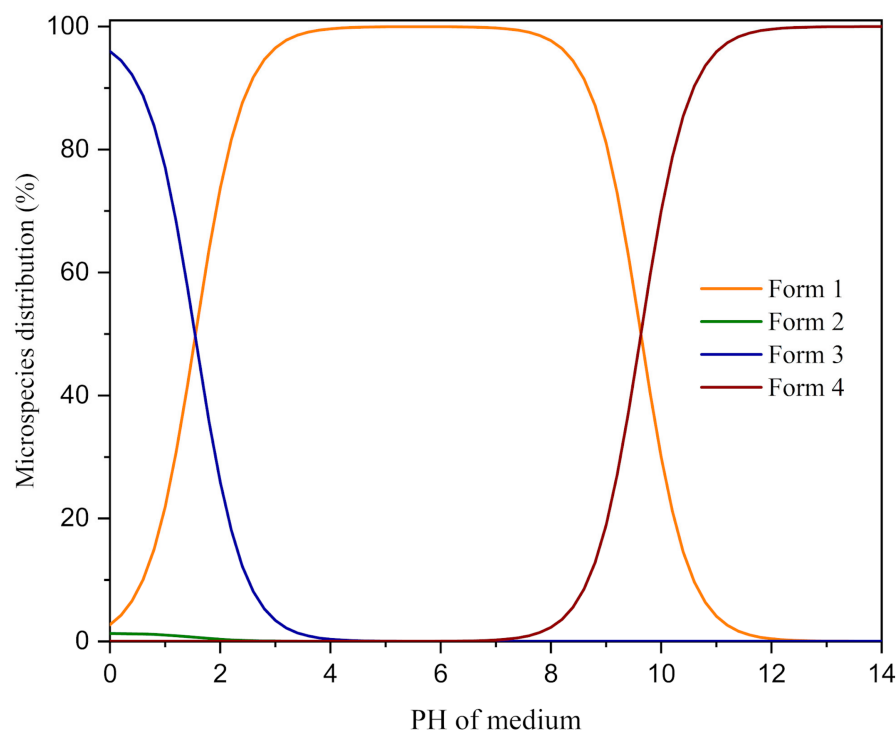


Figure 8. Identified microspecies of FNH in the 0–14 pH range.

3.6.2. DFT Descriptors and Frontier Molecular Orbitals

DFT calculations were performed on both the neutral (FNH) and protonated (FNH-H^+) forms to relate molecular electronic structure to inhibition performance [65]. The optimized geometries and corresponding HOMO/LUMO isosurfaces are depicted in Figure 9, and the derived quantum-chemical descriptors are listed in Table 7.

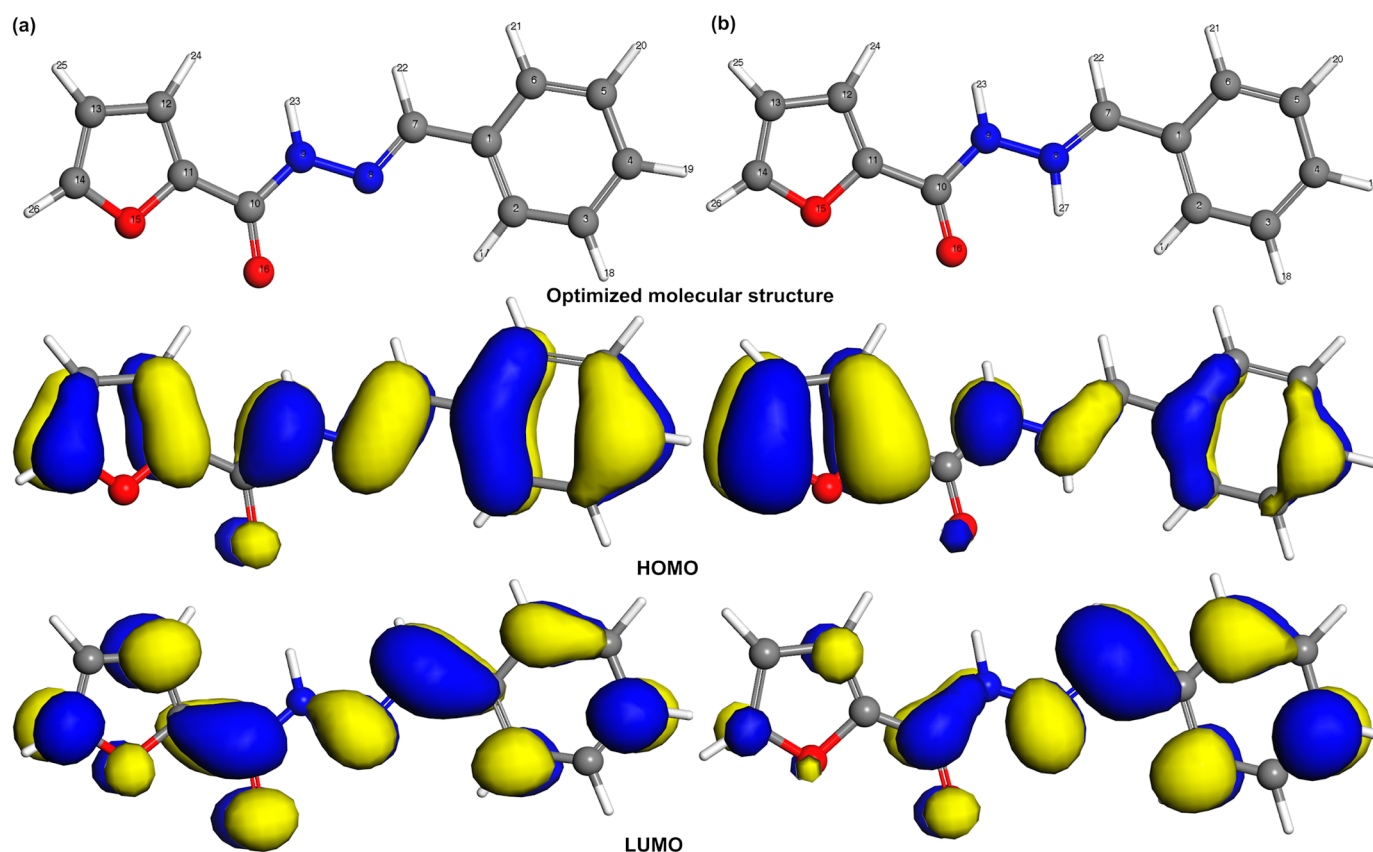


Figure 9. Optimized structure, HOMO-LUMO distributions in (a) neutral and (b) protonated forms of FNH (isovalue = 0.03 a.u.).

Table 7. Global quantum-chemical reactivity descriptors for the neutral and protonated inhibitor (B3LYP/DMol3). Δ denotes the change on protonation (protonated – neutral).

Parameter	Formula	Neutral	Protonated	Δ
E_{HOMO} (eV)	—	−6.274	−7.020	−0.746
E_{LUMO} (eV)	—	−1.981	−3.165	−1.184
Energy gap, ΔE (eV)	$\Delta E_{\text{GAP}} = E_{\text{LUMO}} - E_{\text{HOMO}}$	4.293	3.855	−0.438
Ionization potential, IP (eV)	$I_P = -E_{\text{HOMO}}$	6.274	7.020	+0.746
Electron affinity, EA (eV)	$E_A = -E_{\text{LUMO}}$	1.981	3.165	+1.184
Electronegativity, χ (eV)	$\chi = \frac{(I_P + E_A)}{2}$	4.128	5.093	+0.965
Chemical potential, μ (eV)	$-\chi$	−4.128	−5.093	−0.965
Global hardness, η (eV)	$\eta = \frac{(I_P - E_A)}{2}$	2.147	1.928	−0.219
Global softness, σ (eV ^{−1})	$\sigma = \frac{1}{\eta}$	0.466	0.519	+0.053
Electrophilicity, ω (eV)	$\omega = \frac{\mu^2}{2\eta}$	3.968	6.728	+2.760
Back-donation, $\Delta E_{\text{b-d}}$ (eV)	$\Delta E_{\text{b-d}} = -\frac{\eta}{4}$	−0.537	−0.482	+0.055
Fraction transferred, ΔN	$\Delta N = \frac{\chi_{\text{Fe}} - \chi_{\text{inh}}}{2(\eta_{\text{Fe}} + \eta_{\text{inh}})}$	0.669	0.495	−0.174
Initial Fe–inhibitor, $\Delta\Psi$ (eV)	$\Delta\Psi = \frac{(\chi_{\text{Fe}} - \chi_{\text{inh}})^2}{4(\eta_{\text{Fe}} + \eta_{\text{inh}})}$	0.960	0.472	−0.488

In both forms the HOMO is delocalized over the conjugated backbone with appreciable amplitude on the furan ring, the carbonyl group and the hydrazone bridge, identifying these electron-rich regions as the primary donor sites for coordination with vacant Fe d-orbitals [66]. The LUMO topology, by contrast, differs between the two species: in neutral FNH it is broadly delocalized across the carbonyl, hydrazone and aromatic fragments, whereas in FNH-H⁺ it contracts onto the azomethine bridge (C7=N8) and the adjacent

phenyl ring. These differences in acceptor topology are expected to affect how each form interacts with the metal surface.

Protonation produces a moderate narrowing of the HOMO–LUMO gap (from 4.293 eV in FNH to 3.855 eV in FNH-H⁺) which, together with a pronounced rise in electrophilicity, signals heightened electron-accepting reactivity and, by extension, stronger adsorption affinity for the protonated species. Both forms exhibit relatively low global hardness ($\eta = 2.147$ and 1.928 eV) and comparatively high softness, consistent with facile charge redistribution and favorable inhibitor–metal interaction [67]. The electrophilicity index follows the order $\omega(\text{FNH-H}^+) > \omega(\text{FNH})$ (6.728 vs. 3.968 eV), confirming the superior electron-accepting character of the protonated form [68]. Positive ΔN values for both species (0.669 and 0.495) indicate a net electron-donation capability toward the Fe surface, while the negative back-donation energy ($\Delta E_{\text{b-d}}$) shows that synergistic charge transfer from the metal to the inhibitor is thermodynamically favorable, reinforcing the stability of the adsorbed complex.

3.6.3. Fukui Function Analysis

Condensed Fukui indices were computed for both FNH and FNH-H⁺ to pinpoint the atomic centers most actively involved in inhibitor–metal electron exchange. The local indices were evaluated within the finite-difference approximation as:

$$f_k^+ = q_k(N + 1) - q_k(N) \quad (11)$$

$$f_k^- = q_k(N) - q_k(N - 1) \quad (12)$$

where $q_k(N + 1)$, $q_k(N)$, and $q_k(N - 1)$ are the atomic charges of the anionic, neutral, and cationic species, respectively. The charge analysis was carried out using the Hirshfeld scheme.

Local reactivity was resolved through the condensed Fukui functions. The electrophilic Fukui index (f_k^-), which maps the electron-donating propensity of individual atoms, attains its largest values at the hydrazone nitrogens N8 and N9 together with the aromatic carbon C4 in neutral FNH, identifying this set as the dominant donor centers responsible for coordination with vacant Fe d-orbitals during surface attachment [69]. Protonation reshapes this landscape: while f_k^- at the nitrogens drops sharply, the furan-ring carbons—C11, C13 and C14 in particular—gain appreciable donor character, reflecting a migration of the reactive electron density onto the heterocyclic ring. The net effect is a relocation of the molecular donor footprint available for metal binding, which is expected to sustain the anchoring of the adsorbed layer.

A complementary picture emerges from the nucleophilic Fukui index (f_k^+), which gauges the capacity of each atom to accommodate incoming electrons. In the neutral molecule the highest f_k^+ values reside on the azomethine carbon C7 and the carbonyl group (C10, O16), confirming their role as acceptor sites through which metal-to-ligand back-donation can occur. After protonation, the azomethine carbon C7 becomes by far the strongest acceptor, while the protonated nitrogen N8 and the phenyl-ring carbons (C2, C4, C6) acquire substantially elevated f_k^+ magnitudes relative to the neutral molecule, signaling a markedly enhanced electron-accepting ability redistributed toward the imine bridge and the aromatic framework.

Overall, the Fukui analysis shows that FNH already possesses multiple donor and acceptor centers suited to cooperative interaction with the steel surface, but protonation spatially reorganizes local reactivity—shifting electron-donating density toward the furan ring while concentrating electron-accepting density on the azomethine bridge and phenyl ring. This donor–acceptor partitioning within a single molecule is fully coherent with the

frontier-orbital results discussed above, and rationalizes the superior adsorption strength and inhibition efficiency observed experimentally for the protonated form under acidic conditions (Figure 10).



Figure 10. Condensed Fukui indices (f^+ and f^-) illustrating the (a) neutral and (b) protonated states of FNH.

3.6.4. MD Simulation

MD simulations were carried out to examine the adsorption of FNH and its protonated form FNH-H⁺ on the Fe(110) surface within a simulated corrosive aqueous environment at 298 K. Each inhibitor was initially positioned above the metal slab immersed in a solution box containing water molecules and chloride ions, and the system was allowed to evolve until the lowest-energy adsorption configuration was located. Equilibration was monitored through the temporal evolution of the total energy and temperature.

As shown in Figure 11, both the neutral and protonated forms adopt an almost flat, parallel orientation relative to the Fe(110) plane. This near-coplanar arrangement maximizes the contact area between the conjugated backbone—the furan ring, carbonyl, hydrazone bridge and phenyl ring—and the surface iron atoms, allowing the heteroatom lone pairs and the π -system to interact simultaneously with vacant Fe d-orbitals. Such a flat-lying geometry is characteristic of strong adsorption, since it enables a single molecule to shield the largest possible number of surface active sites from the aggressive electrolyte [36].

Small but discernible geometric differences distinguish the two species. In the protonated form the molecule lies slightly closer and flatter against the surface, with the protonated hydrazone segment tilting toward the metal, whereas the neutral form retains a marginally greater stand-off distance. These subtle reorientations illustrate how protonation modifies the local charge distribution and, in turn, the molecule–surface registry, without disrupting the favorable parallel adsorption mode.

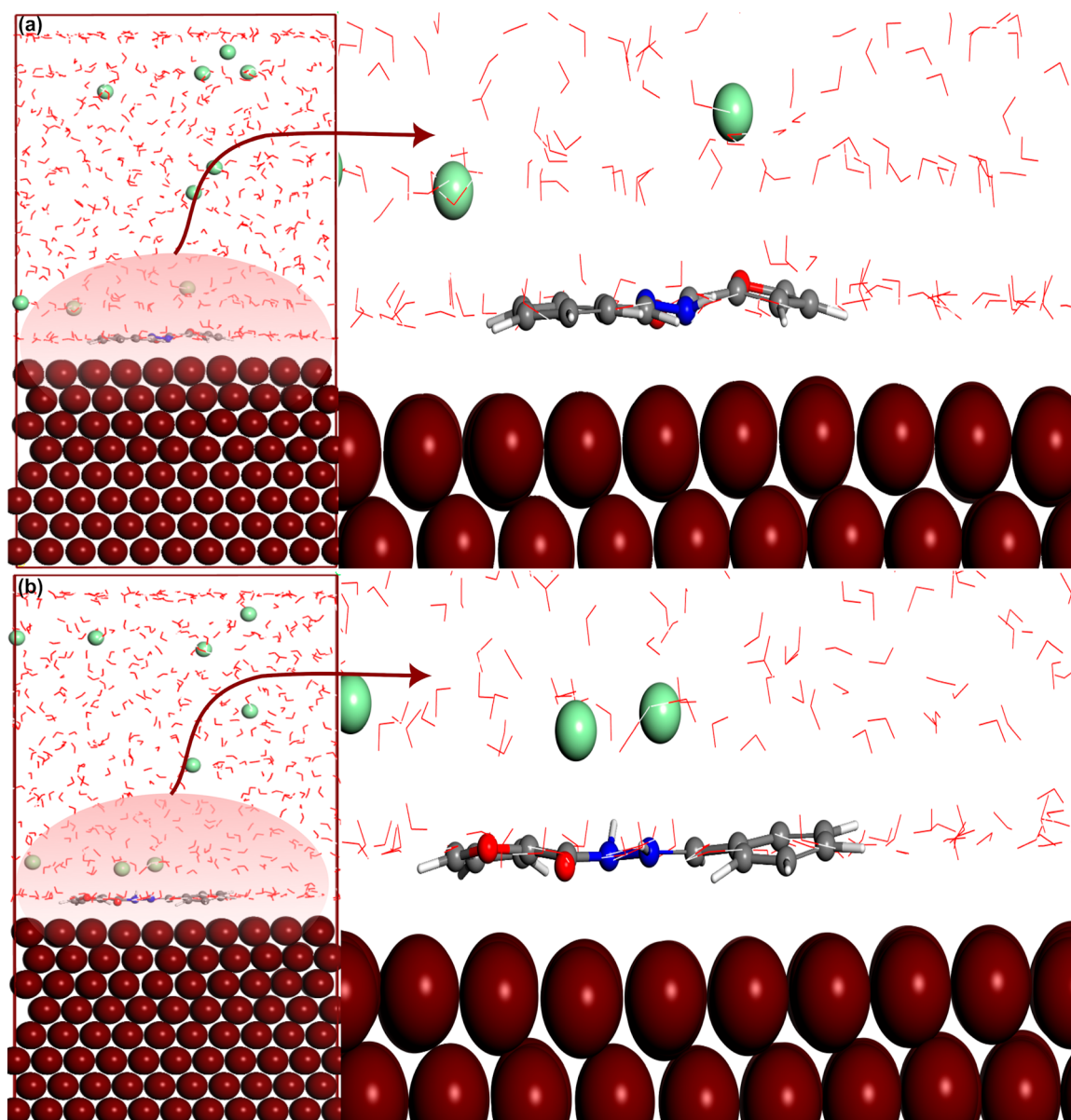


Figure 11. MD-Equilibrium adsorption configurations of the studied inhibitor (a) FNH and (b) FNH-H⁺ on Fe (110) surface.

The corresponding energetics reinforce the geometric picture. Both forms display large negative interaction energies (Table 8), confirming spontaneous and strong adsorption on Fe(110). The protonated species exhibits the more exothermic interaction energy and, equivalently, the larger binding energy, indicating a firmer attachment to the metal in the acidic medium. The magnitude of these energies is consistent with combined electrostatic and coordinative (donor–acceptor) bonding rather than weak physisorption alone, and supports the conclusion that the almost parallel adsorption of both molecules is energetically preferred and able to occupy a maximal fraction of surface sites [36].

Table 8. Interaction and binding energies for the adsorption of the neutral (FNH) and protonated (FNH-H⁺) inhibitor on the Fe(110) surface in the aqueous corrosive environment. Binding energy is defined as the negative of the interaction energy.

System	$E_{\text{interaction}}$ (kcal mol ^{−1})	E_{binding} (kcal mol ^{−1})
FNH (neutral)/Fe(110)	−518	518
FNH-H ⁺ (protonated)/Fe(110)	−612	612

4. Conclusions

This study establishes FNH as a highly effective and structurally robust inhibitor, bridging the gap between molecular design and industrial applicability for carbon steel protection in aggressive HCl environments. This work examined the anticorrosive properties of FNH, a hydrazone Schiff base whose structural integrity and chemical purity were verified to ensure the reliability of the subsequent multi-scale analysis. Beyond quantifying its high efficiency, the major contribution of this work lies in the synergistic integration of experimental and computational scales, providing a definitive blueprint for the adsorption mechanism. Electrochemical testing and impedance measurements revealed a superior protective capacity that remains resilient across the thermal range explored, reflecting an increasingly effective barrier at the metal–electrolyte boundary. A fundamental insight gained from this research is the critical role of the protonated species in acidic media. Contrary to traditional views, our theoretical analysis demonstrates that acid-induced protonation actually enhances the molecule’s electronic communication with the iron surface through a bidirectional electron exchange. This, combined with a confirmed ‘flat-lying’ geometry, ensures maximum surface coverage and explains the exceptional stability of the organic deposit observed by surface imaging. Ultimately, FNH represents more than just a potent inhibitor; it serves as a mechanistic model for the development of future eco-friendly, heteroatom-rich inhibitors. This study provides a strategic framework for designing sustainable corrosion mitigation solutions for infrastructure and manufacturing exposed to aggressive conditions. We note, however, that SEM/AFM offer only morphological insight into the protective film, and that the MD simulations employ an ideal Fe(110) slab with single-molecule adsorption, so the mechanistic picture should be regarded as a well-supported but still simplified representation of the real, heterogeneous steel–acid interface.

Supplementary Materials: The following supporting information can be downloaded at <https://www.mdpi.com/article/10.3390/coatings16060678/s1>, Figure S1: Arrhenius plots of the corrosion current density for X70 carbon steel in 1 M HCl solution in the absence and presence of FNH at different temperatures; Figure S2: Plot of $\ln(i_{\text{corr}}/T)$ versus the reciprocal of temperature ($1/T$) for X70 carbon steel in the absence and presence of 10^{-4} M FNH; Figure S3: Adsorption isotherm plots of (a) Temkin, (b) Frumkin, and (c) Langmuir models for XC70 carbon steel in 1 M HCl in the presence of the FNH inhibitor, obtained using the three methods at 293 °C; Table S1: Activation parameters of the corrosion process for carbon steel in 1 M HCl solution in the absence and presence of the inhibitor FNH at its optimal concentration (1×10^{-4} M). References [70–79] are cited in the Supplementary Materials.

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