Synthesis, Spectroscopic Characterization, Electrochemical Corrosion Inhibition, and DFT Analysis of a 1,2,4-Triazole-Derived Schiff Base

Ali Faris Al-Ghezi

Dhi Qar Directorate of Education, 64001 Nasiriyah, Dhi Qar, Iraq.

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ABSTRACT

A nitrogen-rich Schiff base, 1-(4-isopropylphenyl)-N-(4H-1,2,4-triazol-4-yl)methanimine (L), was prepared by condensation of 4-amino-1,2,4-triazole with 4-isopropylbenzaldehyde in ethanol. The source record reports orange crystalline material isolated in approximately 90% yield and a melting range of 185–188 °C. Its proposed molecular formula is C12H14N4 (molar mass approximately 214.27 g mol−1). The reported FTIR spectrum includes a band at 1590 cm−1 assigned to an imine-associated vibration; however, complete structure confirmation requires reconciliation of the mass-spectral assignments and verification of the experimental 1H NMR dataset. The source study also reports potentiodynamic polarization measurements on carbon steel in 0.1 M HCl. Using the tabulated corrosion-current densities, the calculated inhibition efficiencies are 80.64% at 298 K and 87.33% at 323 K for the entries labeled inhibitor 1. A reported B3LYP/6-31G calculation gives EHOMO = −6.511 eV and ELUMO = −2.180 eV, corresponding to a positive orbital energy gap of 4.331 eV. These preliminary findings suggest that the compound merits further investigation as an adsorption-based corrosion inhibitor, while incomplete experimental metadata and discrepancies in the original tables currently limit mechanistic conclusions.

Keywords: 1,2,4-triazole; Schiff base; carbon steel; corrosion inhibition; potentiodynamic polarization; density functional theory.

INTRODUCTION

Carbon steel is extensively used in chemical processing, structural systems and industrial infrastructure because of its availability and favorable mechanical properties. Its susceptibility to corrosion remains a major limitation, particularly during acid cleaning, descaling and related operations in which exposed steel comes into contact with chloride-containing solutions. Acidic attack can accelerate iron dissolution and the accompanying cathodic reactions, making effective interfacial protection essential for service reliability [1–3]. Organic corrosion inhibitors are attractive because comparatively small quantities of adsorbing molecules can modify the steel–electrolyte interface and suppress electrochemical reaction rates [2,3]. The protective performance of organic inhibitors depends on the nature and distribution of adsorption sites, electronic structure, molecular geometry, concentration and solution conditions. Heteroatoms with available electron density, aromatic π systems and polar substituents can facilitate interaction with iron-containing surfaces, although such structural features alone do not guarantee strong inhibition. Adsorption can involve electrostatic and donor–acceptor contributions, while the experimentally observed response may reflect simultaneous effects on anodic dissolution and cathodic hydrogen evolution [3,8,14–16]. Consequently, electrochemical data should be considered together with chemical characterization and appropriately qualified molecular modeling. Schiff bases contain an azomethine (C=N) functionality typically obtained through condensation of a primary amine with an aldehyde or ketone. Their readily varied aromatic substituents and nitrogen-donor environments have stimulated interest in synthesis, coordination chemistry and corrosion protection [4–9]. Among these structures, 1,2,4-triazole-based systems are particularly relevant because the nitrogen-rich five-membered ring offers several potential sites for interaction with metal surfaces. Prior studies of triazole-derived Schiff bases

under acidic conditions demonstrate that electrochemical response can vary substantially with substitution, the medium and the testing temperature [10–12]. Studies combining electrochemical measurements with quantum chemical analysis have attempted to explain inhibitor behavior through the energies and spatial distributions of frontier molecular orbitals and related electronic descriptors [11,14–16]. Such analyses are useful for formulating adsorption hypotheses but do not independently establish an adsorption mechanism or a quantitative structure–efficiency relationship. In addition, cross-study comparisons require caution: reported efficiencies are strongly dependent on steel composition, acid concentration, immersion time and inhibitor dosage [8,9,17–20]. In this context, the present study examines a Schiff base incorporating a 4-isopropylphenyl fragment and a 1,2,4-triazole ring. The work aims to (i) describe its condensation synthesis, (ii) evaluate the available spectroscopic and physical evidence for the proposed structure, (iii) assess the supplied polarization results for carbon steel in hydrochloric acid, and (iv) place the reported DFT descriptors in an appropriate chemical framework. Particular attention is paid to internal consistency of the experimental record, because reliable molecular identification and transparently reported electrochemical conditions are prerequisites for a defensible corrosion-inhibition claim.

EXPERIMENTAL

Materials and Synthesis

According to the original laboratory description, 4-amino-1,2,4-triazole (4.0 g, 0.0476 mol) and 4-isopropylbenzaldehyde (7.0 g, approximately 0.0472 mol) were mixed in absolute ethanol (100 mL). The mixture was heated for approximately 6 h, with reaction progress followed by thin-layer chromatography. The solution was concentrated to approximately half its initial volume and cooled. The resulting orange crystalline solid was collected by filtration, washed and recrystallized from absolute ethanol. The isolated mass was reported as 9 g (approximately 89%, reasonably rounded to 90% based on the stated reagent amounts). The source contains no TLC solvent system, Rf values, detailed heating setup or drying conditions; these must be supplied for a fully reproducible procedure. The anticipated condensation is: 4-isopropylbenzaldehyde + 4-amino-1,2,4-triazole → L + H2O. This describes a mono-imine product, not a bis-imine. The correctly balanced proposed product formula is C12H14N4 (molar mass ≈ 214.27 g mol^{-1}).

Instrumentation

The original manuscript reports melting-point measurement using an SMP31 instrument; FTIR measurement as a KBr disk over 250–4000 cm−1; and 1H NMR acquisition on a 500 MHz instrument described as “Bruker DXR AL500”. Exact models, NMR solvent, acquisition parameters and mass-spectrometric ionization mode require verification against the instrument outputs. An image labeled “ChemNMR 1H Estimation” is a prediction and must not be presented as experimentally acquired evidence.

Electrochemical and Computational Protocols

The supplied tables refer to potentiodynamic polarization of carbon steel in 0.1 M HCl at 298 and 323 K, with comparison of uninhibited and inhibited conditions. However, the composition and exposed area of the steel, inhibitor concentration units, reference/counter electrodes, equilibration period, scan rate, replicate count and uncertainty are not consistently stated. These missing parameters must be restored from the laboratory record before the results can be treated as reproducible. The original calculations are described as B3LYP/6-31G. The software, molecular charge and protonation state, optimization/convergence criteria, solvent treatment and frequency checks were not provided. Accordingly, computed values are reported descriptively rather than as validated predictors of inhibition.

RESULTS AND DISCUSSION

Physical and Spectroscopic Characterization

The obtained solid was described as orange crystals with a reported melting interval of 185–188 °C, compared with 86–88 °C for the starting amine. The different melting intervals are consistent with obtaining a material

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distinct from the precursor, but do not by themselves prove chemical identity or purity. The proposed empirical formula, expected formula mass and selected FTIR bands are summarized in Table 1.

Property	Reported value	Interpretive note
Formula / molar mass	C12H14N4 / 214.27 g mol−1	Consistent with mono-condensation product
Isolated mass / yield	9 g / ca. 89–90%	Recalculated from stated reactant amounts
Melting range	185–188 °C	Experimental record; confirm reproducibility
FTIR C–H	2973 cm−1	Assignment needs spectrum-level inspection
FTIR band attributed to C=N	1590 cm−1	Can overlap aromatic or heterocyclic modes
Other reported FTIR bands	1312 and 850 cm−1	Assignments need comparison with precursor
FTIR 3245.09 cm−1	Originally marked N–H	Unexpected for proposed mono-imine; check residual starting material / moisture

The source provides aromatic resonances in the vicinity of δ 6.83–7.50 ppm, an azomethine-associated signal near δ 8.90 ppm and triazole proton signals near δ 9.00 ppm. However, descriptions of the isopropyl methyl region and signal integrations are inconsistent with the depicted structure. Moreover, an inserted predicted 1H spectrum cannot replace a measured spectrum. Full peak assignments, splitting patterns, integrations, solvent and experimental spectrum are therefore necessary before unequivocal structure confirmation. The mass-spectrometry section likewise lists incompatible purported molecular-ion values (including m/z 215 and 254.3); the precursor and product formulae should be cross-checked against the raw mass spectrum.

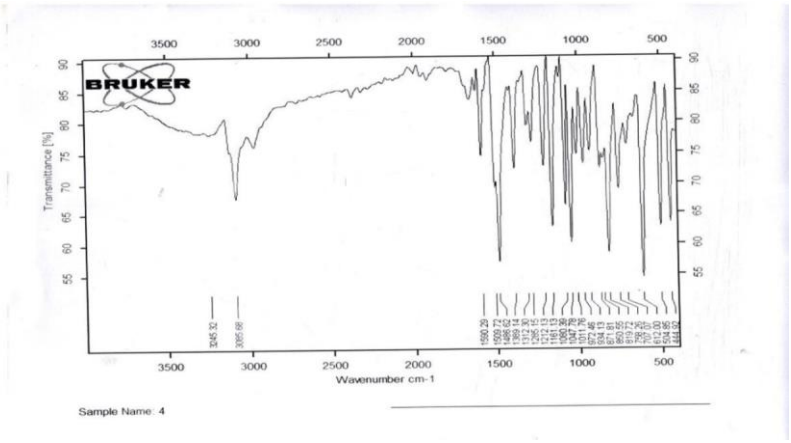


Figure 1. FTIR spectrum reproduced from the supplied manuscript. Peak assignments should be verified against the original digital spectral file.

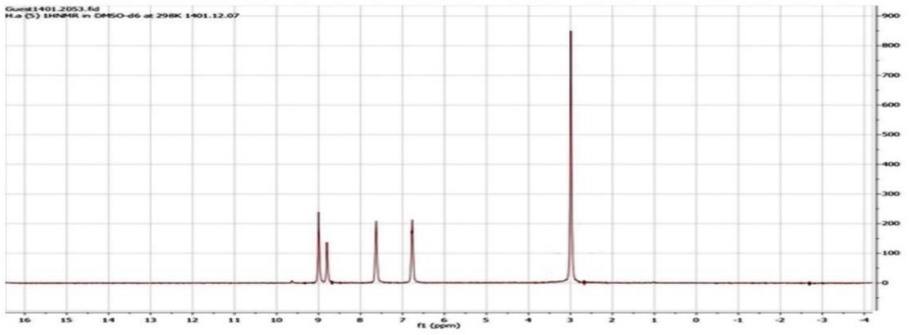


Figure 2. 1H NMR plot reproduced from the supplied manuscript. Original acquisition metadata and integrations are required; the separate ChemNMR prediction is not experimental proof.

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Electrochemical Corrosion Inhibition

The polarization data presented in the original manuscript indicate lower tabulated corrosion-current densities in the presence of the entry labeled "1" than in the uninhibited electrolyte. To make the numerical inference transparent, the inhibition efficiency was recalculated from IE (%) = 100 × (icorr,blank − icorr,inhibitor)/icorr,blank. The resulting values match two efficiencies reported in the source. Because the original table contains overlapping entries, the two paired conditions below are the only entries interpreted quantitatively here.

Temperature (K)	Blank icorr (mA cm−2)	With L icorr (mA cm−2)	Recalculated IE (%)
298	0.589	0.114	80.64
323	2.171	0.275	87.33

The apparent increase in calculated efficiency between these two temperatures should not be generalized as a temperature dependence without checking concentration, test conditions and replicate results. Some source rows list additional inhibitor entries and conflicting polarization parameters; these cannot reliably be assigned to the target ligand. The polarization traces and full Tafel fitting outputs must be re-exported at publication resolution. In the absence of verified anodic and cathodic slopes and shifts in Ecorr, assigning the inhibitor unambiguously as anodic, cathodic or mixed-type would be premature.

Adsorption and Thermodynamic Interpretation

For the inhibitor entry labeled "1", the original adsorption table reports surface coverage θ = 0.80 at 298 K and θ = 0.87 at 323 K, with Kads = 40 and 66.92 M−1, respectively. A further 323 K row (θ = 0.34) appears without a clearly matched inhibitor label and is excluded from interpretation. The adsorption model used to calculate Kads, concentration dependence, fitting statistics and standard-state convention are not provided. Accordingly, the reported free energies cannot independently establish a specific adsorption regime. The existing activation and thermodynamic tables also require full unit, sign and formula audits before they can support mechanistic claims.

3.4. DFT descriptors

The calculated descriptors supplied in the source include EHOMO = −6.511 eV, ELUMO = −2.180 eV and dipole moment μ = 3.793 D. The HOMO–LUMO gap must be defined as ELUMO − EHOMO and is therefore +4.331 eV, not −4.331 eV as originally printed. Under the conventional finite-difference orbital-energy approximations, the reported ionization potential is 6.511 eV, electron affinity 2.180 eV, electronegativity 4.3455 eV, hardness 2.1655 eV and softness approximately 0.4618 eV−1 (using S = 1/η). These quantities are approximate gas-phase molecular descriptors, not experimentally measured adsorption energies.

DFT parameter	Corrected/reported value	Units
EHOMO	−6.511	eV
ELUMO	−2.180	eV
ΔE = ELUMO − EHOMO	4.331	eV
Dipole moment (μ)	3.793	D
Ionization potential (I)	6.511	eV
Electron affinity (A)	2.18	eV
Electronegativity (χ)	4.3455	eV
Hardness (η)	2.1655	eV
Softness (1/η)	0.4618	eV−1

Taken together, the nitrogen-rich ring and azomethine group provide a chemically plausible framework for

interfacial interaction. However, an isolated-molecule frontier-orbital calculation cannot establish the adsorption geometry, surface coverage, binding energy or electrochemical mechanism on iron. Surface-sensitive measurements and/or explicit metal-surface simulations would substantially strengthen this interpretation [14–16].

CONCLUSIONS

The submitted experimental record describes the ethanol-based synthesis of a 1,2,4-triazole-derived mono-Schiff base, provisionally assigned the formula C12H14N4 and a melting range of 185–188 °C. Polarization current densities yield calculated inhibition efficiencies of 80.64% at 298 K and 87.33% at 323 K for the tabulated inhibitor entry. Reanalysis of the reported DFT frontier energies corrects the orbital gap to 4.331 eV. Nevertheless, contradictions between spectral assignments, incompletely documented electrochemical conditions and inconsistencies in selected tables prevent an unqualified claim of definitive molecular structure, high purity or a unique inhibition mechanism. Resolution of these points and verification of the raw measurements will be necessary before submission to a selective peer-reviewed journal.

Data Availability and Declarations

Data availability: The present redraft is based solely on the supplied manuscript; raw analytical, electrochemical and computational files were not provided. Before submission, include a genuine data-availability statement and any accessible supplementary files. Author contributions, funding, conflicts of interest, institutional affiliations and acknowledgments: to be completed and approved by the author(s), without invented declarations.

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Editorial Checklist — Required Before Submission

1. Check the actual starting reagent name and obtain unambiguous 1H/13C NMR and mass-spectral verification of molecular identity.
2. Check the original FTIR baseline and label assignments, particularly the unexplained 3245 cm−1 feature.
3. Reconstruct the full polarization dataset with steel composition, concentrations, units, cell setup, reference electrode, scan rate, replicates and error bars.
4. Verify which adsorption/activation-energy entries refer to the named compound and rederive their statistics and units.
5. Supply complete DFT input/output and identify the computed protonation state, phase and software; repeat calculations if necessary.
6. Produce high-resolution raw-data figures and assign final figures/schemes with consistent numbering; avoid presenting predicted NMR as measured.
7. Add verified affiliations, authorship roles, research ethics/funding declarations and journal-specific formatting.