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Supplementary Materials

Corrosion Mitigation of Carbon Steel using Pyrazole Derivative: Correlation of Gravimetric, Electrochemical, Surface Studies with Quantum Chemical Calculations

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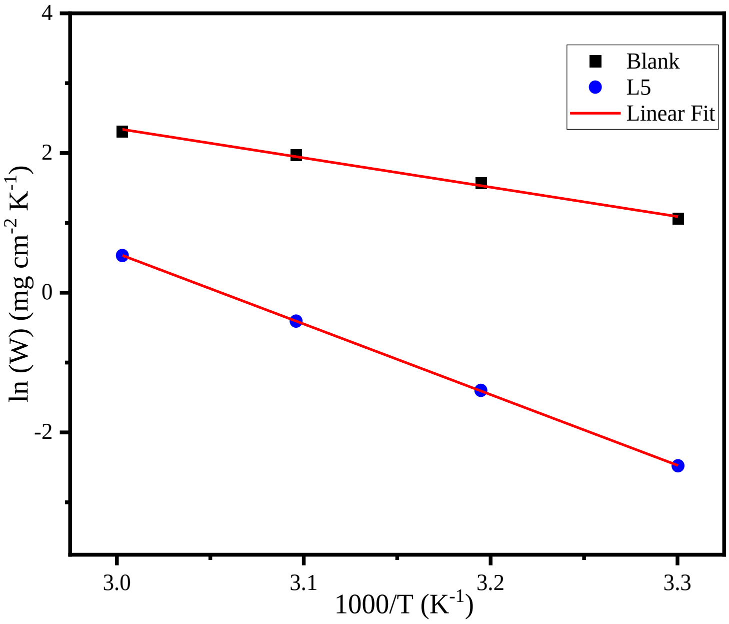

Figure S1. Arrhenius graphs for (CS/1MHCl) without and with 10^{-3} M of L5

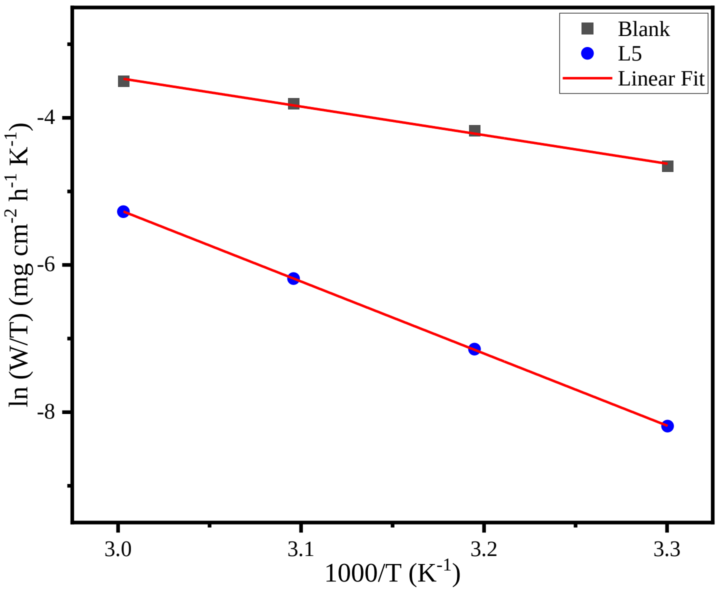

Figure S2. Transition state graphs for (CS/1MHCl) without and with 10^{-3} M of L5

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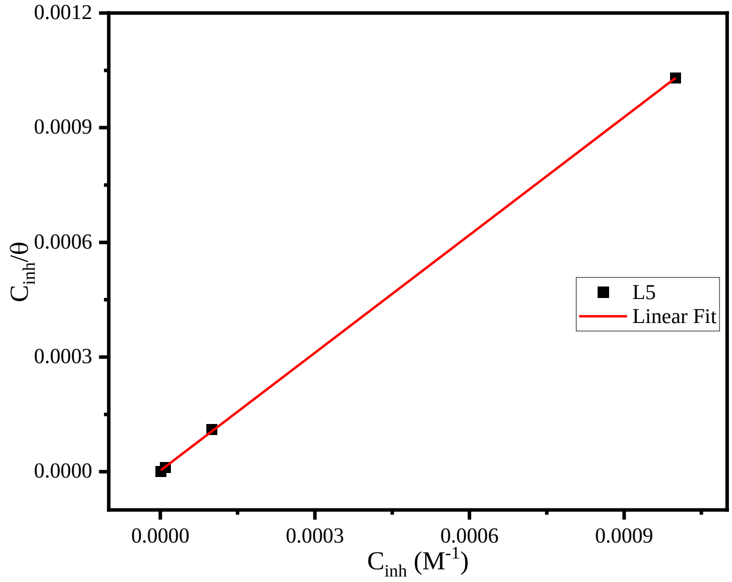

Figure S3. Langmuir isotherm for adsorption of L5 on CS surface in 1M HCl

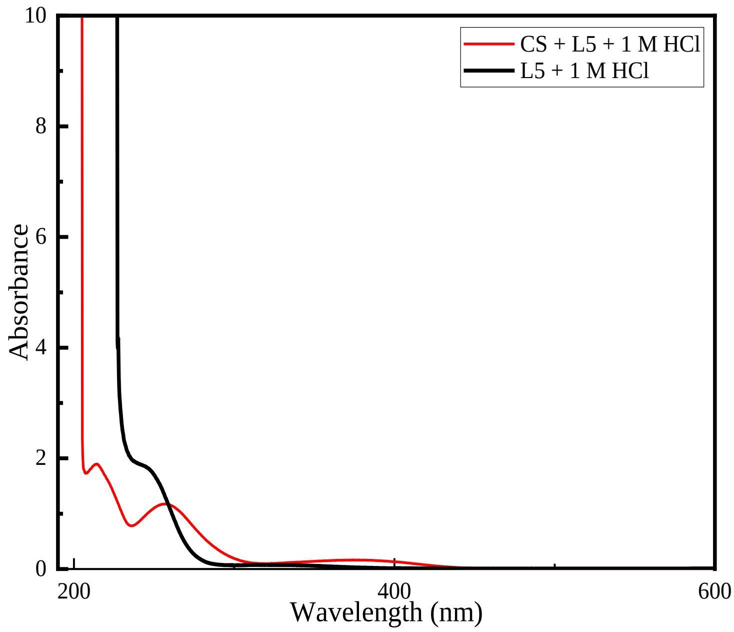

Figure S4. UV–visible spectra of 10^{-3} M L5 compound added to 1MHCl with and without carbon steel

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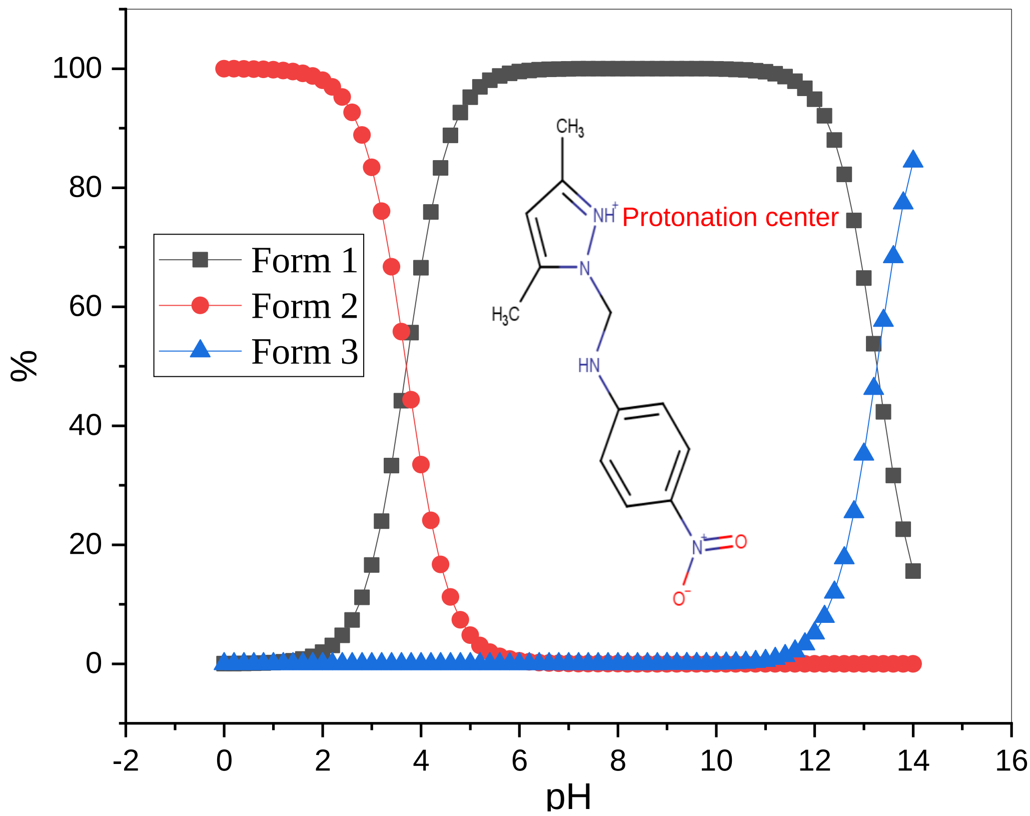


Figure S5. Protonation site defined by its percentage versus pH of L5

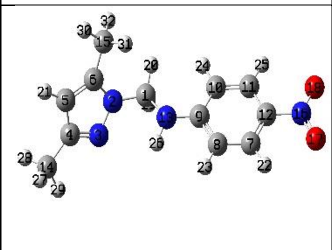
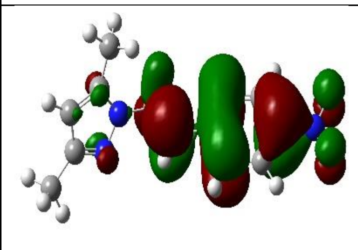
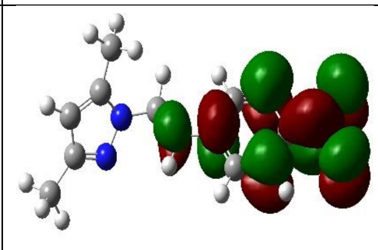
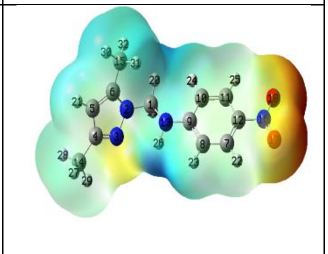
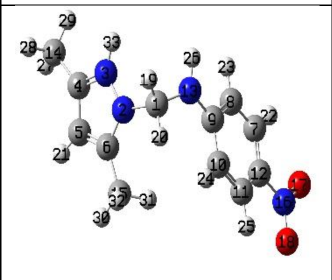
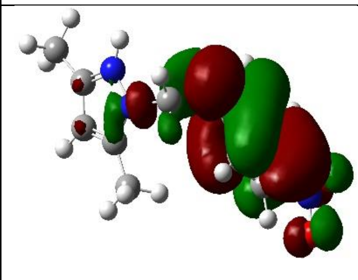
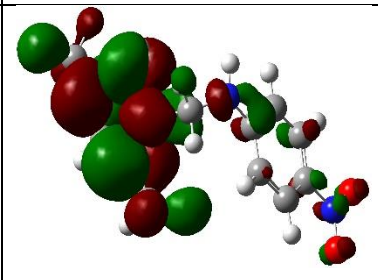
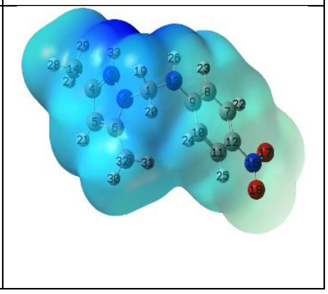
frs	**Optimized**	**HOMO**	**LUMO**	**MEP**
L5				
L5H$^+$				

Figure S6. Energy-minimized structures, FMOs, and MESPs of the two neutral and protonated forms for L5 and L5H$^+$

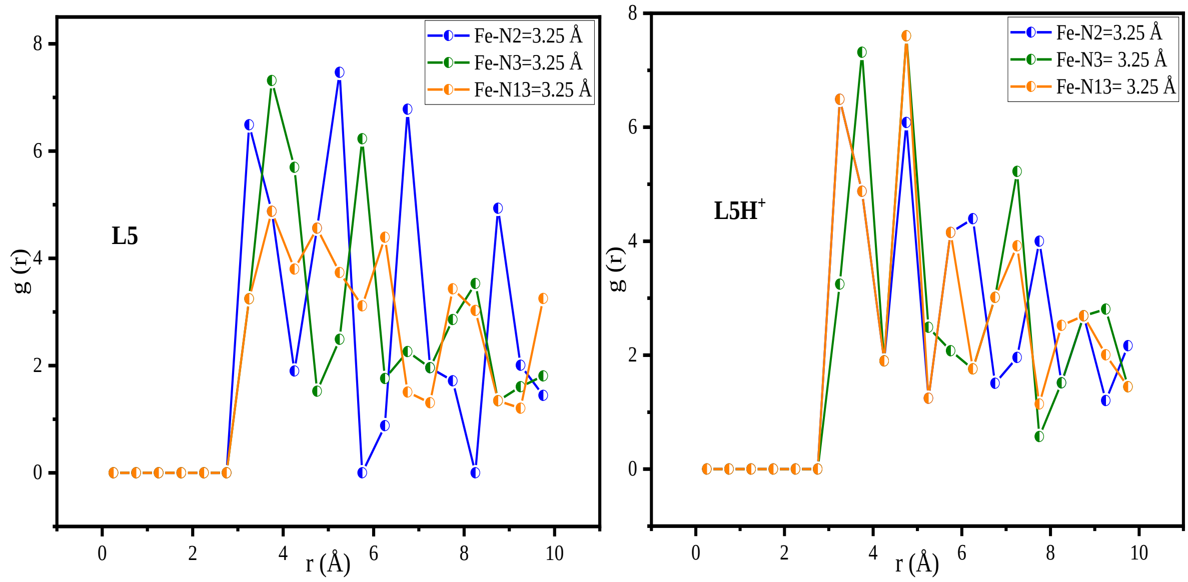


Figure S7. RDF of forms L5-Fe (110) and $L5H^+$-Fe (110)

Table S1. Evolution of W and the corresponding *IE*w% vs. various temperatures for CS immersed in 1M HCl with and without 10^{-3}M of L5

Medium	*T* (K)	*W* (mg/cm² h)	IE_w (%)	
Blank	303	2.880	----	----
	313	4.803	----	----
	323	7.187	----	----
	333	10.050	----	----
L5	303	0.084	97.1	0.971
	313	0.247	94.9	0.949
	323	0.665	90.7	0.907
	333	1.703	83.1	0.831

Table S2. Thermodynamic parameters were generated for 10^{-3} M of L5 in 1 M HCl

Conc(M)	R^2	E_a (kJ/mol)	ΔH_a^* (kJ/mol)	ΔS_a^* (J/mol K)	$E_a - \Delta H_a^*$ (kJ/mol)
Blank	0.99775	34.90	32.27	-129.50	2.63
10^{-3}M L5	0.99999	84.06	81.43	3.13	2.63

Table S3. Thermodynamic descriptors resulting from Langmuir isotherm plot for {L5/CS/1M HCl} system

Medium	Slope	R^2	K_{ads} (L/mol)	ΔG_{ads}^* (kJ/mol)
L5	1.03	0.9999	343299.31	-42.23

Table S4. EDX analysis of CS surface after 6h immersion in 1M HCl + 10^{-3} M of L5 at 303 K

Element	Weight %	Atom %
C	1.80	6.31
N	0.46	1.38
O	9.58	25.23
Al	0.22	0.34
S	0.11	0.14
Cl	0.70	0.84
Mn	0.83	0.64
Fe	86.30	65.12
Total	100.00	100.00

Table S5. E_{inter} for the systems L5/Fe(110) and $L5H^+$/Fe(110) (in kJ mol^{-1})

Systems	$\mathbf{E_{interaction}}$
L5/Fe(110)	-782.712
$L5H^+$/Fe(110)	-765.519

Table S6. Comparison of L5 results with other pyrazole derivatives

Inhibitors	Metallic alloys	Medium	Optimal concentration	IE (%)	Ref.
Ethyl 5-methyl-1-(((6-methyl-4-nitropyridin-3-yl)amino)methyl)-1H-pyrazole-3-carboxylate (EMPC)	Carbon steel	1 M HCl	10^{-3} M	92	[54]
3, 5-dimethyl-1H-pyrazol-1-yl) (4-((4-chlorobenzy-lidene) amino) phenyl) methanone) (DPCM)	Carbon steel	1 M HCl	400 ppm	89.5	[55]
N-((1H-pyrazol-1-yl)methyl)pyrimidin-2-amine (PPA)	Carbon steel	1 M HCl	10^{-3} M	94	[56]
2-(((1H-pyrazol-1-yl)methyl)amino)benzoic acid (PMB)	Carbon steel	1 M HCl	10^{-3} M	92	[56]
Ethyl 4-(5-acetyl-4-amino-3-(thiazol-2-ylcarbamoyl)-1H-pyrazol-1-yl)benzoate (EATPB)	Low carbon steel	0.5 M HCl	10^{-3} M	89	[12]
2,4-diamino-5-(5-amino-3-hydroxy-1H-pyrazole-1-carbonyl)thiophene-3-carbonitrile (I)	Carbon steel	1 M HCl	5 10^{-4} M	92	[13]
N-(2-aminophenyl)- 2-(5-methyl-1H-pyrazol-3-yl) acetamide (AMPA)	C38 steel	1 M HCl	5 mM	93	[57]
N,N-dimethyl-4-(((1-methyl-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)imino)methyl)-N-dodecyl benzenaminium bromide (APS-12)	Carbon steel	1 M HCl	5 10^{-3} M	94	[58]
N-((3,5 dimethyl-1H-pyrazol-1-yl)methyl)-4-nitroaniline (L5)	Carbon steel	1 M HCl	10^{-3} M	95.10	**Present work**