



Preparation, Spectral Characterization, and Corrosion Inhibition Studies of (*E*)-*N*-{(thiophene-2-yl)methylene}pyrazine-2-carboxamide Schiff Base Ligand

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ABSTRACT

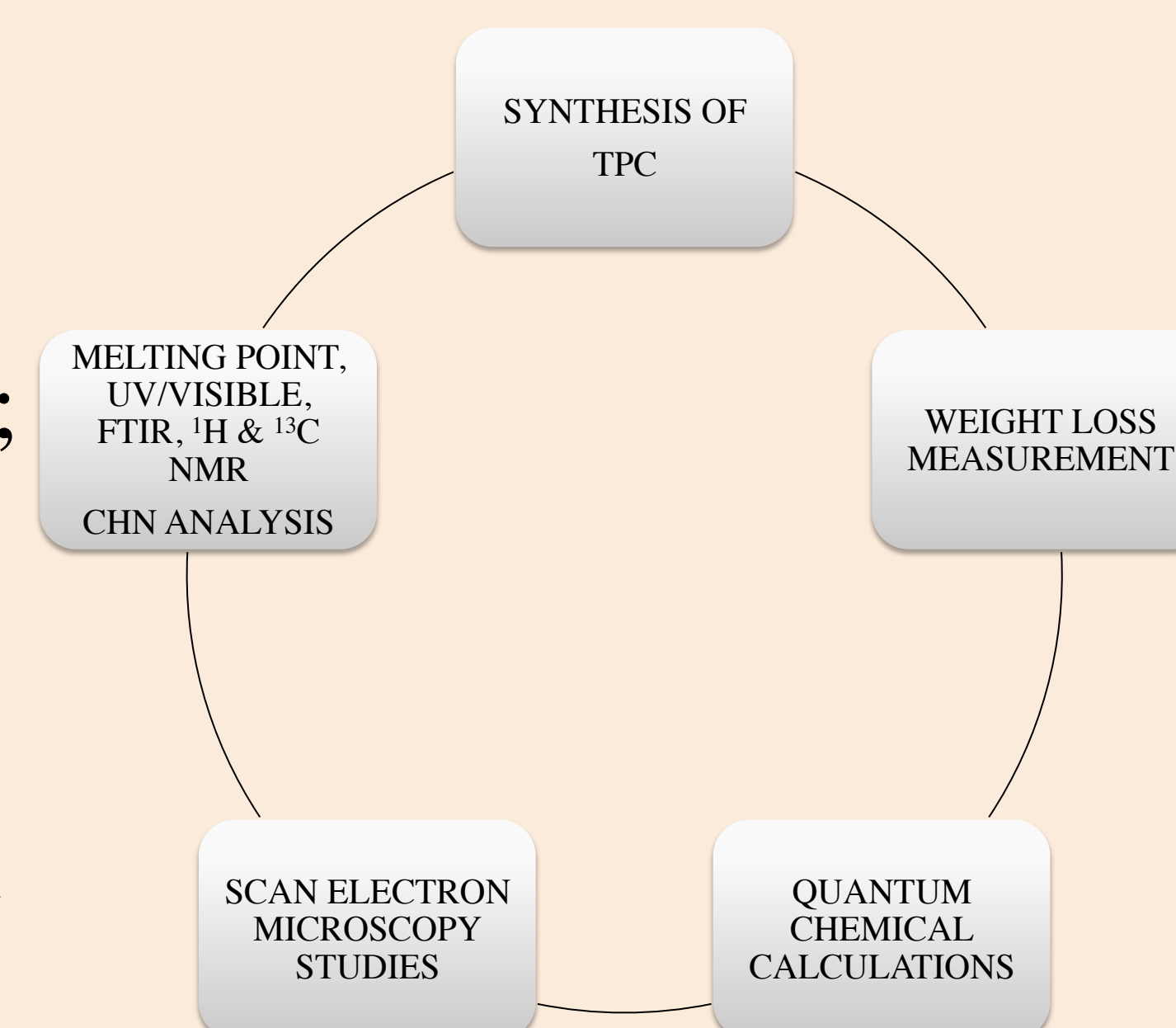
The study shows the preparation and characterisation of thiophene/pyrazine Schiff base, (*E*)-*N*-{(thiophene-2-yl)methylene}pyrazine-2-carboxamide (TPC) via melting point, micro (CHN) analysis; vibrational, nuclear magnetic resonance (¹H- and ¹³C-NMR) and electronic spectroscopies. Theoretical and experimental studies on TPC were also carried out for its adsorption and corrosion inhibitive properties. The spectral data showed tridentate bonding nature and enolimine tautomeric arrangement. The Density functional theory calculations correlated the experimental data.

INTRODUCTION

Mild steel (ms), is expansively adopted in chemical as well as allied industries owing to its accessibility, low cost and unfussy assemblage[1]. Research has shown that steels and their byproducts, which are vulnerable to bout in destructive media, are the frequently exposed species in manufacturing environments. For prevention of metallic dissolution in addition to reduction of acid intake, corrosion inhibitors are normally adopted. Derivatives of heterocyclic assemblages have stood as the utmost operative inhibitors due to the presence of N, O, S, Se and P for forming coordinate-covalent bonds with metallic ions; a consequence of free electron pairs residing on the heteroatoms. In an attempt to broaden the existence of economical and environmentally friendly inhibitors, this present study reports the preparation of a new thiophene/pyrazine Schiff base ligand, TPC as a probable corrosion inhibitor.

METHODOLOGY

The percentage composition of ms sample (wt%) used were C-0.21; Mn-0.9; P-0.022; Si-0.03; S-0.030; Cr-0.11; Ni-0.12; Mo-0.022; Al-0.07; Cu-0.15 and Fe as the balance.



RESULTS AND DISCUSSION

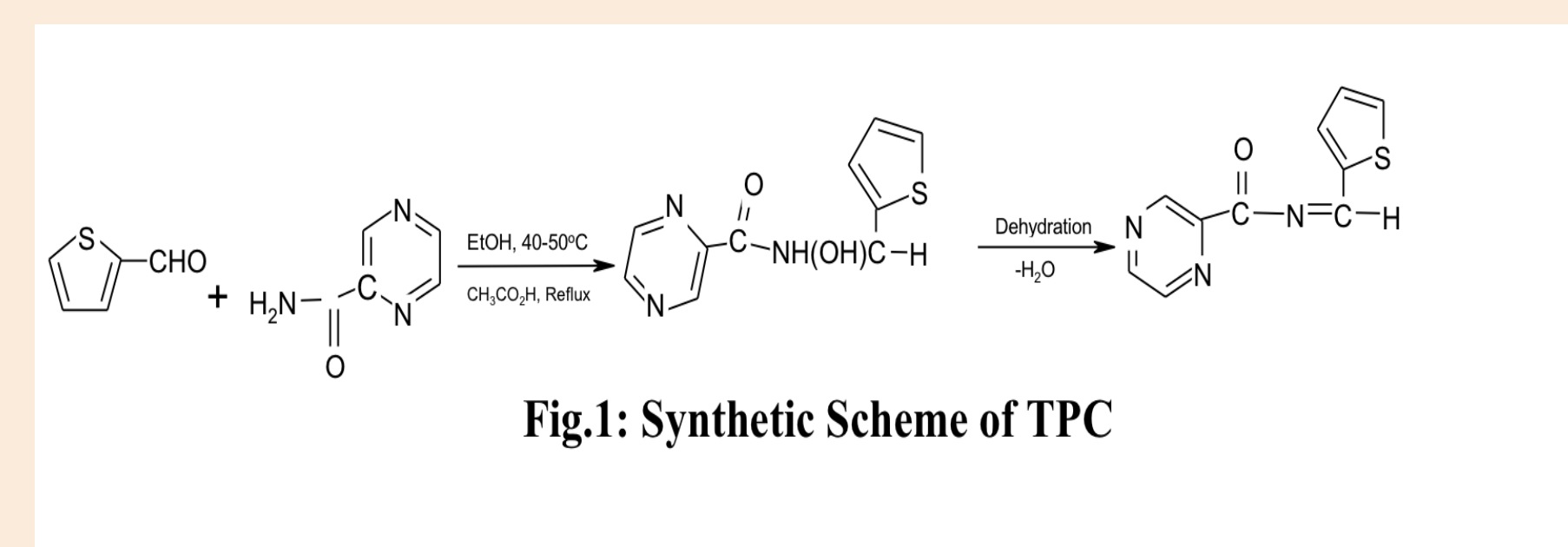
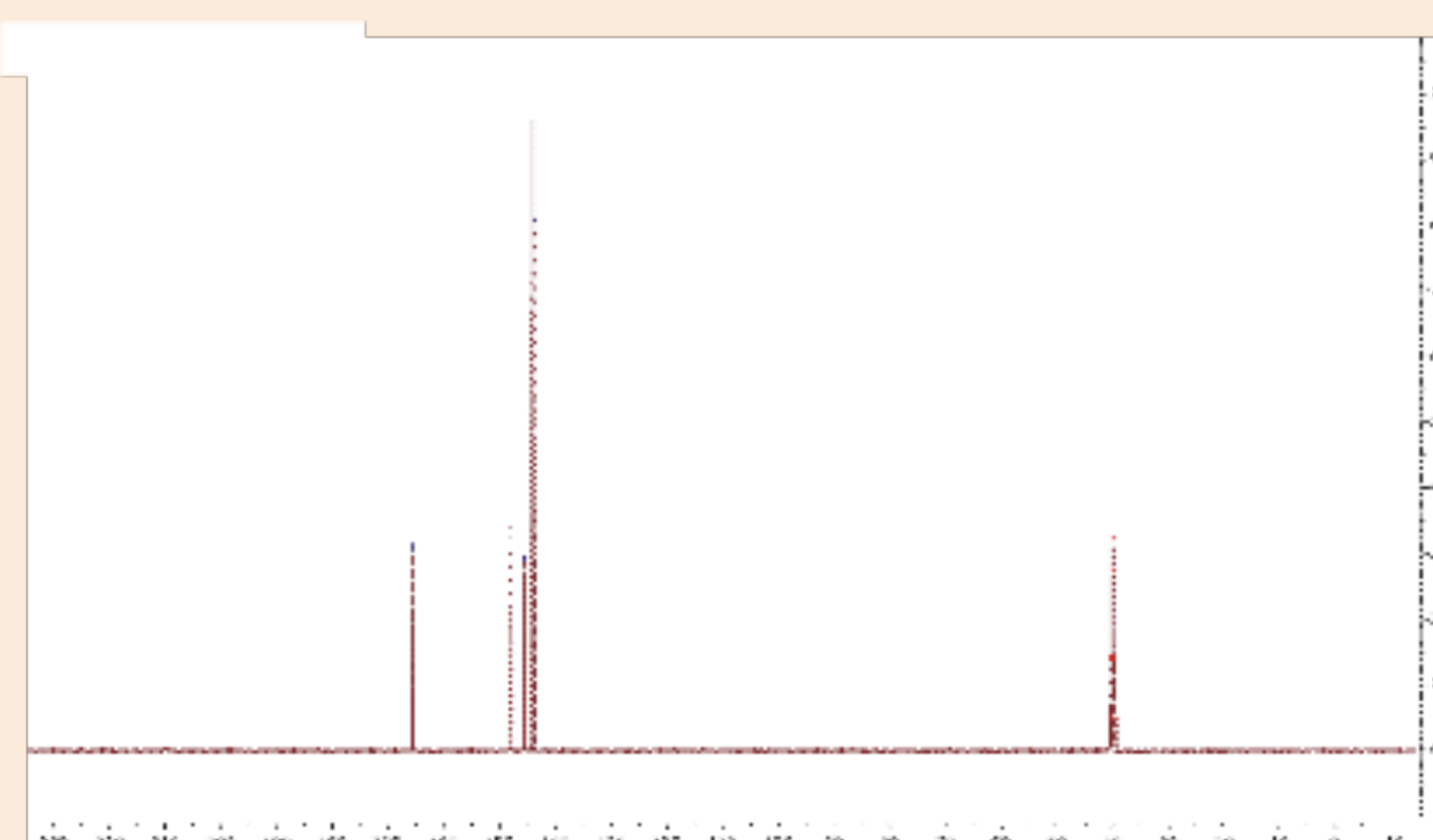


Fig. 2: ¹³C NMR Spectrum of TPC

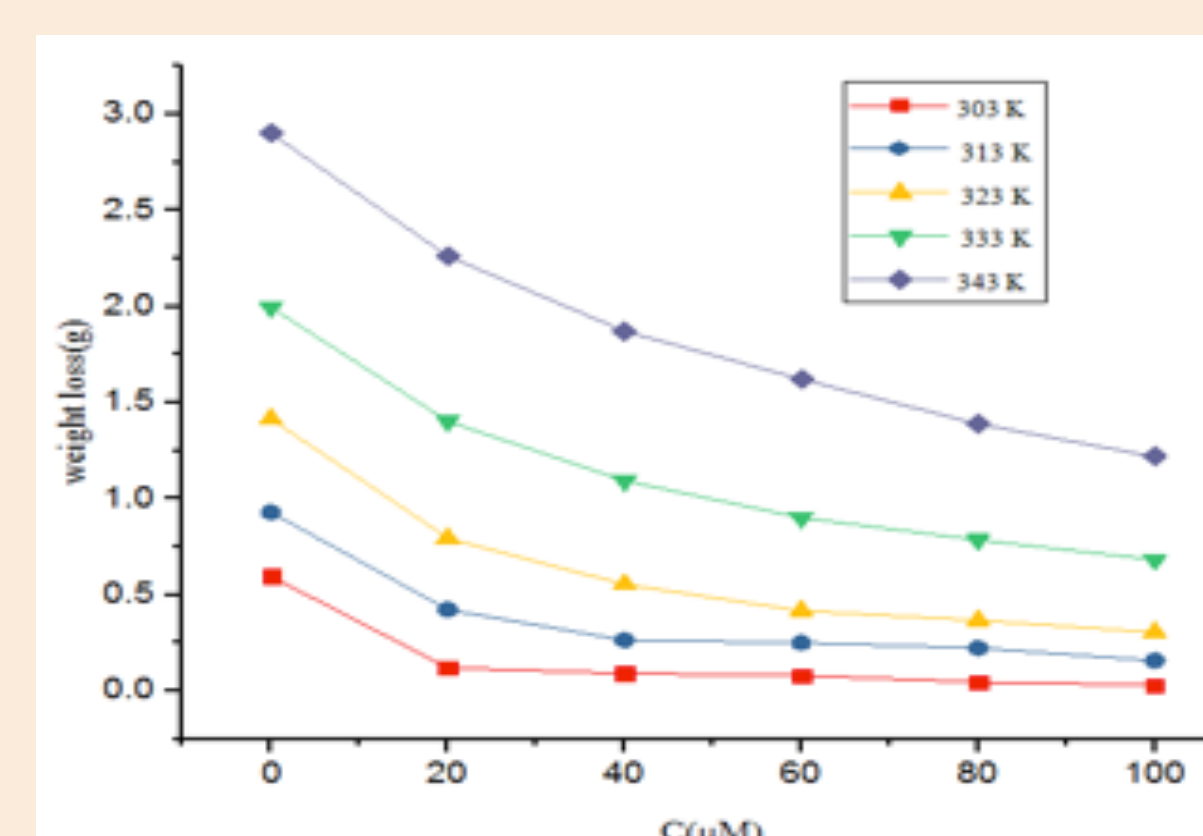


Fig. 3: Wt. loss vs C at different temperatures

- 1:1 mole ratio reaction of thiophene-2-carbaldehyde and pyrazine-2-carboxamide in ethyl alcohol solution afforded the pyrazine Schiff base, TPC.

Table 1: Various corrosion parameters obtained from weight loss measurements for mild steel in 1 M HCl with and without inhibitor at studied temperatures

Temp. (K)	Conc. of Inhibitor (μM)	Weight Loss (g)	C _r (g cm ⁻² h ⁻¹)	%IE	θ
303	0.0	0.5968	74.60	-	-
	20	0.1217	15.21	79.61	0.796
	40	0.0925	11.56	84.50	0.845
	60	0.0818	10.23	86.29	0.863
	80	0.0476	5.95	92.02	0.920
313	100	0.0320	4.00	94.64	0.946
	0.0	0.9298	116.23	-	-
	20	0.4239	52.99	54.41	0.544
	40	0.2650	33.13	71.50	0.715
	60	0.2520	31.50	72.90	0.729
323	80	0.2241	28.01	75.90	0.759
	100	0.1589	19.86	82.91	0.829
	0.0	1.4144	176.80	-	-
	20	0.7951	99.39	43.79	0.438
	40	0.5550	69.38	60.76	0.608
333	60	0.4172	52.15	70.50	0.705
	80	0.3677	45.96	74.00	0.740
	100	0.3053	38.16	78.41	0.784
	0.0	1.9952	249.40	-	-
	20	1.4026	175.33	29.70	0.297
343	40	1.0944	136.80	45.15	0.452
	60	0.9018	112.73	54.80	0.548
	80	0.7861	98.26	60.68	0.606
	100	0.6828	85.35	65.78	0.658
	0.0	2.8993	362.40	-	-
	20	2.2615	282.70	22.00	0.220
	40	1.8711	233.89	35.46	0.355
	60	1.6221	202.76	44.05	0.441
	80	1.3890	173.63	52.09	0.521
	100	1.2152	152.40	57.95	0.580

C_r = Corrosion rate, %IE = Inhibition efficiency, θ = Surface coverage

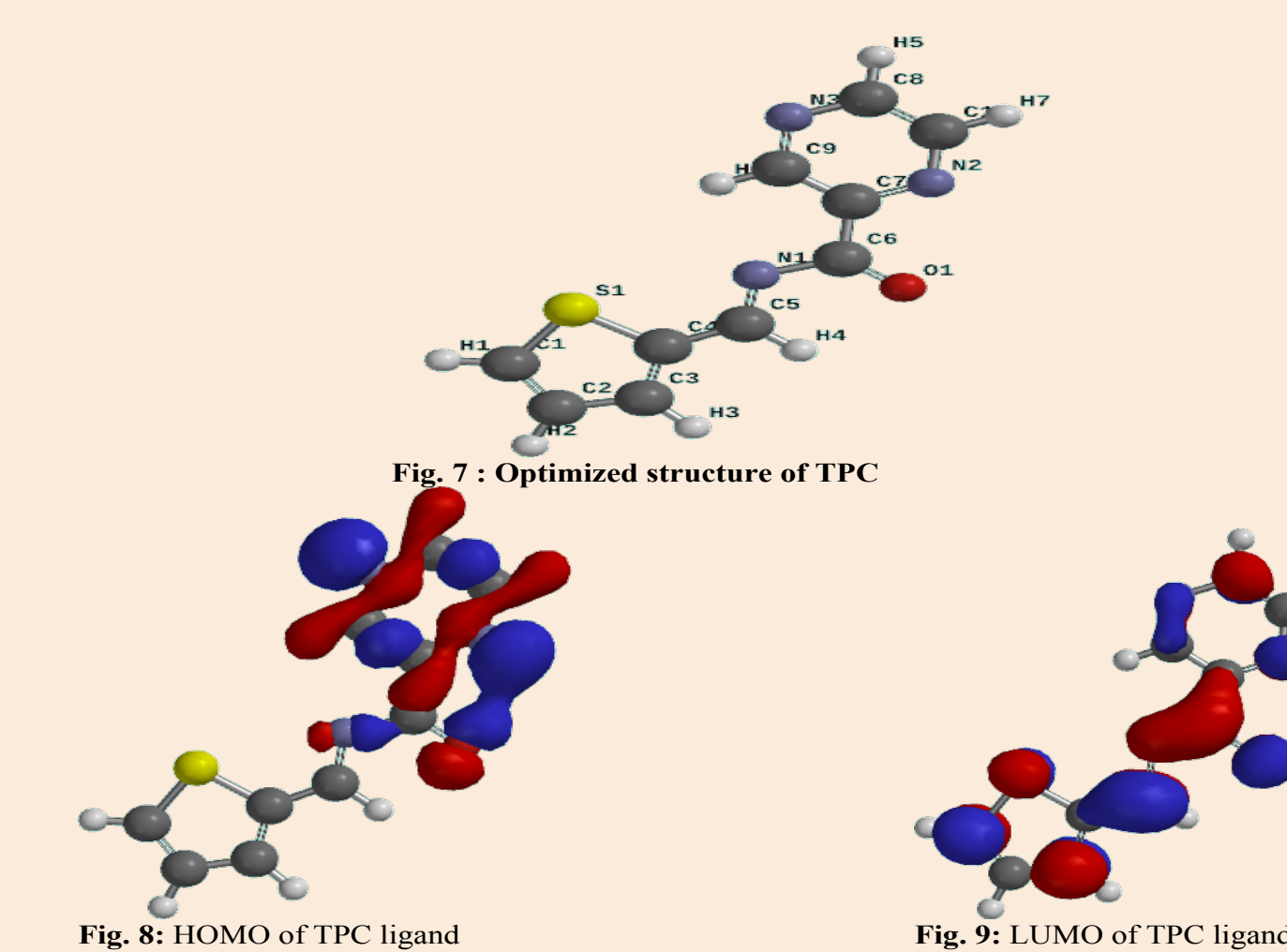


Fig. 8: HOMO of TPC ligand

Fig. 9: LUMO of TPC ligand

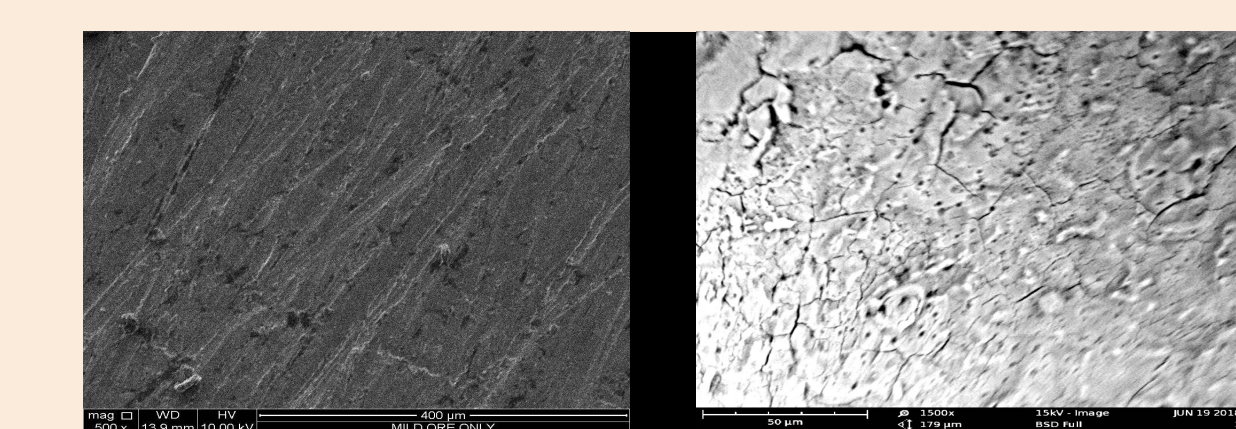


Fig. 5: SEM image for mild steel in 1 M HCl solution in the absence of TPC ligand

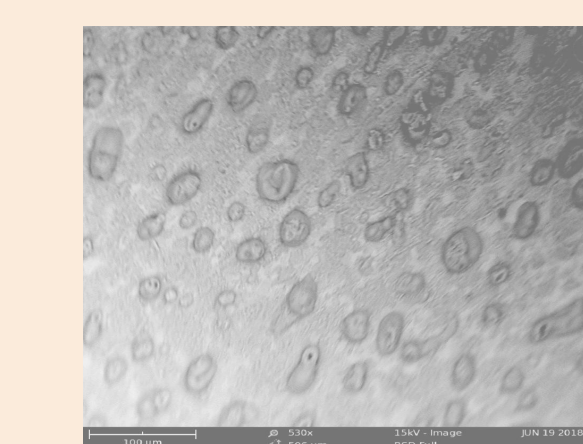


Fig. 6: SEM image for ms in 1 M HCl solution in the presence of TPC ligand

Surface morphology by SEM

corroborated the high protective effect of TPC due to the inhibitor film on the metal surface that limits the corrosion rate in the acid media

- The acquired analytical and spectral data corroborated the structures of the synthesized Schiff base ligand.

- Table 1 revealed that the high inhibition efficiency (94.64%) exhibited by TPC at optimum concentration (100 μM) and room temperature suggests more coverage of the ms surface by the inhibitor molecule [2]

- Theoretical calculations suggests that oxygen and nitrogen atoms could serve as the adsorption sites connecting the molecule and the ms surface.

CONCLUSION

- The spectral data confirmed the synthesis and the structure of the TPC ligand

- This study establishes the feasibility and potential of TPC ligand to inhibit ms corrosion in 1M HCl solution

- Theoretical calculations were in good agreement with experimental results.

REFERENCES

- [1] Singh, A., Ebenso, E. E. and Quraishi, M. A., 2012. *Int. J. Electchem. Sci.* 7: 4766-4789.
- [2] Singh, P., Srivastava, V., and Quraishi, M. A. 2016. *Journal of Molecular Liquids* 216: 164–173.