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EXPERIMENTAL AND THEORETICAL STUDY OF NEW TRIAZOLE-BASED SCHIFF BASE LIGAND AS AN EFFECTIVE CORROSION INHIBITOR FOR XC40 CARBON STEEL IN 1.0 M HYDROCHLORIC ACID SOLUTION

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INTRODUCTION

Corrosion, as an inevitable natural phenomenon, is an important destructive factor in industrial production and causes serious economic losses. Among anti-corrosion technology, adding inhibitors is a convenient, economic and effective way to inhibit the corrosion of metal materials in corrosive solution, which is widely used in acid pickling, oil and gas exploitation processing, cooling system, and so on [1]. carbon steel is one of the most widely used engineering materials owing to its outstanding mechanical properties, low cost, and ready availability. Its high vulnerability to corrosion attack, however, limits some of its applications [2].

RESULTS AND DISCUSSION

It could be observed from the figure that The OCP shifted positively with time until reach a relatively steady state is attained after approximately 500s to reach near stable OCP values both in the absence and presence of the inhibitor except in the presence of 5.10^{-4} M where the OCP stabilization is longer [3].

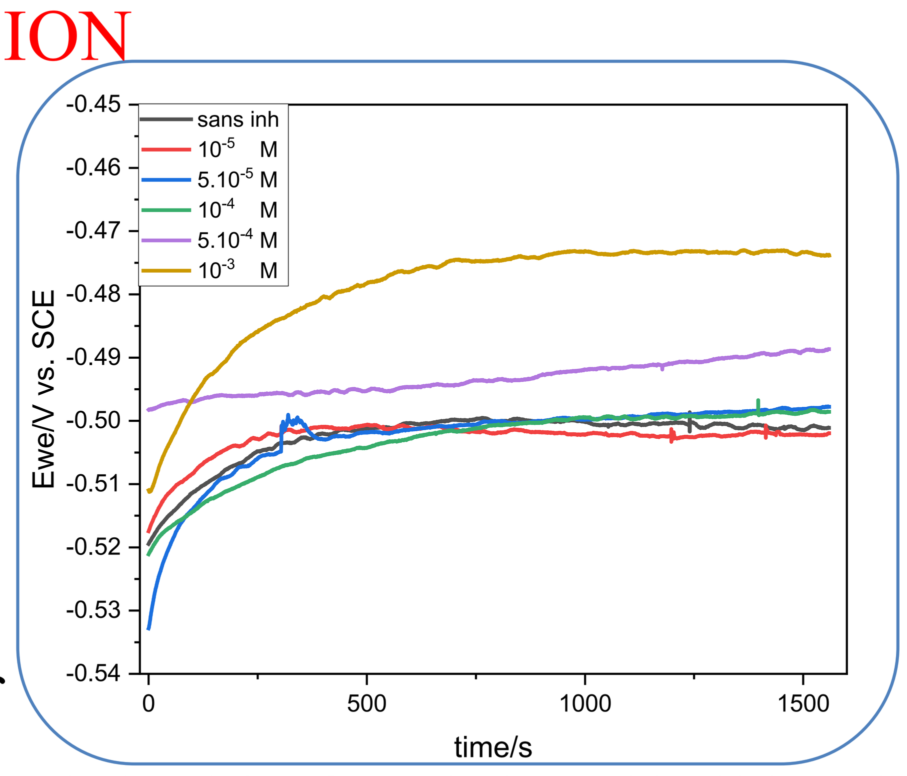


Fig. 1. Variation of open circuit potentials with immersion time for XC40 carbon steel in 1.0 M HCl in the presence and absence of different concentrations of *inhibitor* at 25 ºC

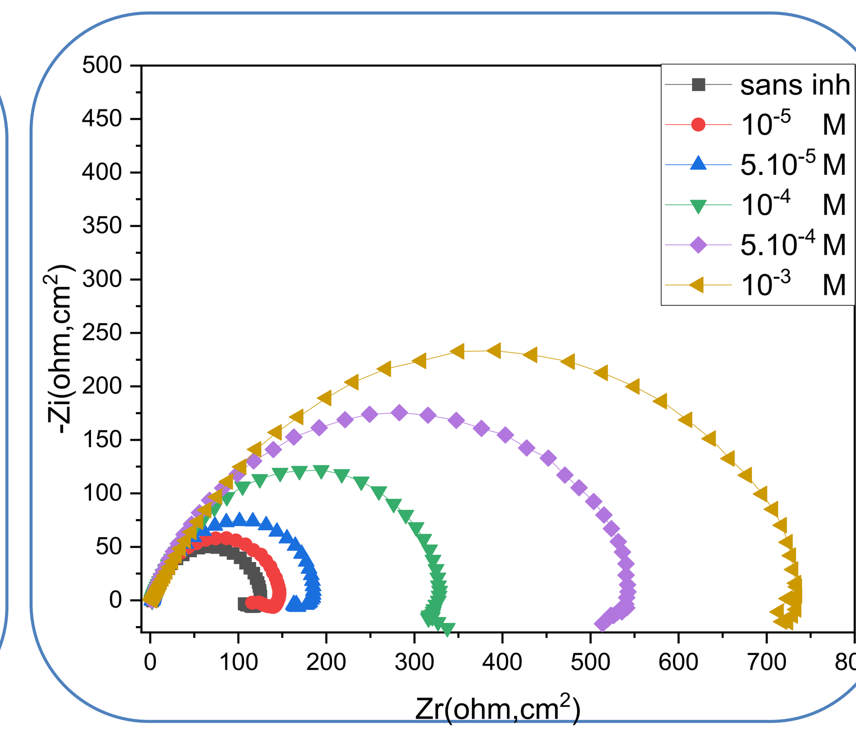


Fig. 3. Nyquist diagrams of XC40 steel in 1 M HCl solution without and with various concentrations of inhibitor at 25 ºC.

Table 2. Electrochemical parameters obtained from EIS for XC40 steel in 1 M HCl solution without and with different concentrations of inhibitor at 25 C

	C (M)	$-E_{ocp}$ (mV/SCE)	R_s (Ω)	R_{ct} (Ω)	C_{dl} (F)	η (%)	θ
HCl	1	0.501	2.579	123.5	0.243	-	-
Inhibiteur	10^{-5}	0.502	2.63	144.3	0.216	14.41	0.1441
	5×10^{-5}	0.498	2.548	181.9	0.193	32.11	0.3211
	10^{-4}	0.497	2.255	330.4	0.186	62.62	0.6262
	5×10^{-4}	0.488	1.905	548.6	0.132	77.49	0.7749
	10^{-3}	0.473	2.168	745.5	0.120	83.43	0.8343

the impedance spectra shown in Fig. 3 comprised of two loops, one large depressed capacitive loop at high and intermediate frequency regions, followed by one small inductive loop at low frequencies region for the blank solution and inhibitor concentrations lower than 10^{-4} M.

The potentiodynamic polarization plots demonstrated that triazole compound can reduce the corrosion current density as a function of the concentration, indicating the mixed type protection character [4].

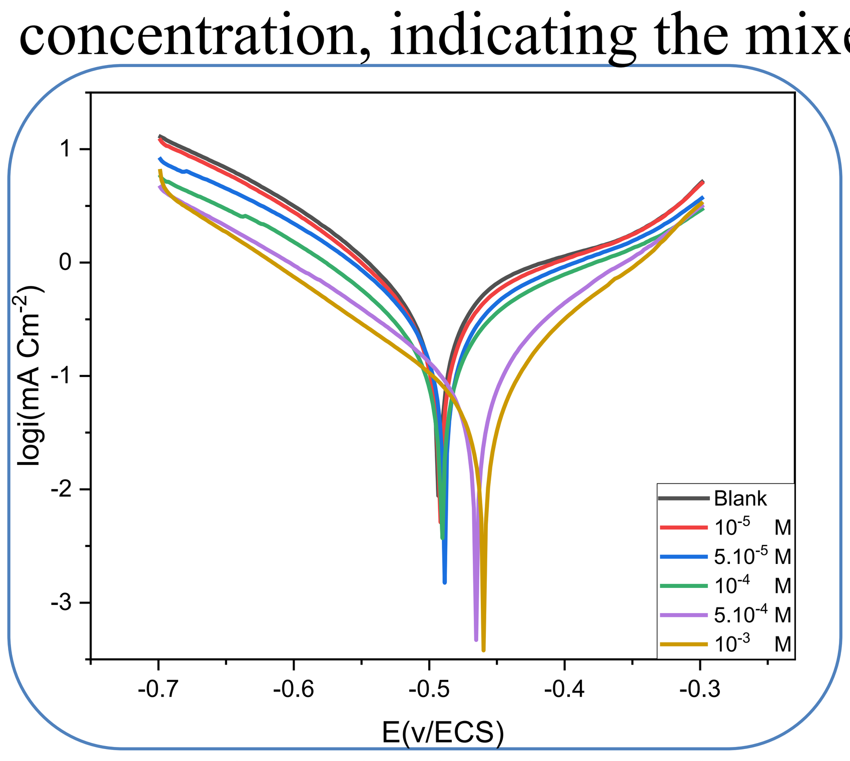
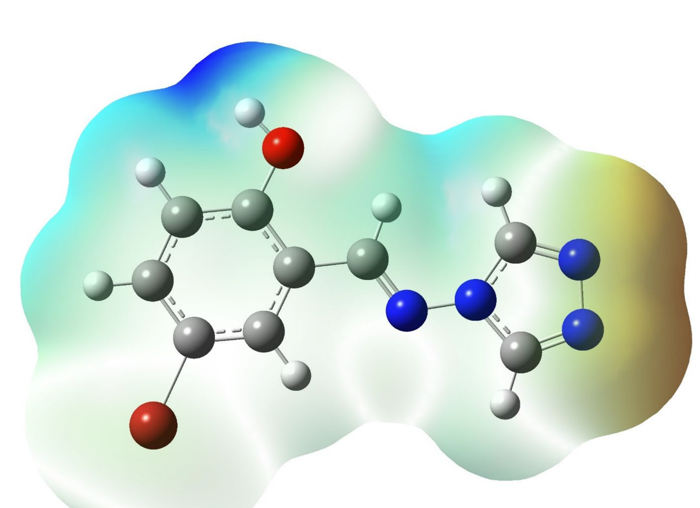


Fig. 2. Potentiodynamic polarization curves for XC40 steel in 1.0 M HCl solution without and with different concentrations of inhibitor at 25 ºC

Table 1. Potentiodynamic polarization parameters obtained for XC40 carbon steel in a 1 M HCl solution without and with different concentrations of inhibitor at 25 ºC.

	C (M)	-Ecorr (mV/ECS)	i corr (µA.cm⁻²)	β a (mV)	β c (mV)	EI (%)	Θ
HCl	1	493.264	439.373	214.3	124.3	-	-
Inh	10^{-5}	491.812	354.532	184.0	120.4	19.30	0.1930
	5×10^{-5}	488.715	275.110	161.5	120.4	37.39	0.3739
	10^{-4}	490.735	195.931	140.8	121.2	55.40	0.5540
	5×10^{-4}	465.135	76.998	82.9	120.0	82.48	0.8248
	10^{-3}	459.814	52.611	75.0	121.7	88.03	0.8803



Theoretical calculations imply that Nitrogen atoms may serve as adsorption sites linking the molecule and the iron.

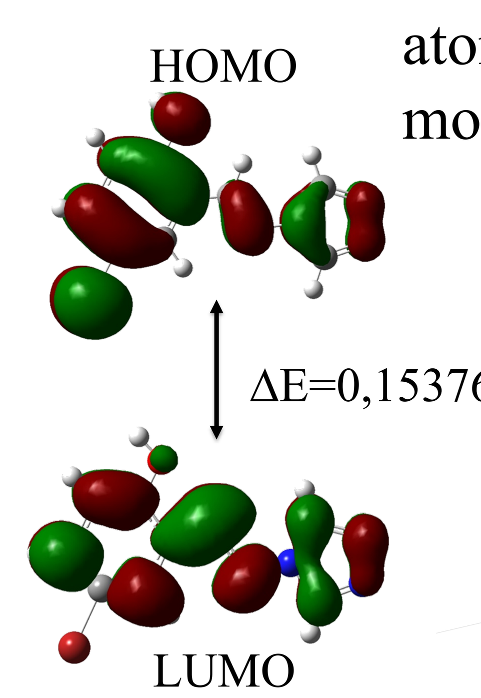
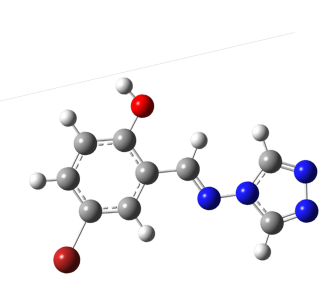


Table 3. Quantum chemical parameters of protonated form of Trz inhibitor derived from the B3LYP/6-311G(d,p) method in aqueous phase.

E_{HOMO}	E_{LUMO}	I	A	χ	η	σ	ΔN
-0,252	-0,098	0,252	0,098	0,175	0,076	13,007	44,383



2-(((4H-1,2,4-triazol-4-yl)imino)methyl)-4-bromophenol

Conclusion

The main conclusions drawn from this study are:

- ✓Potentiodynamic polarization results revealed that the triazole compound performed as a mixed inhibitor, controlling both anodic and cathodic reactions.
- ✓EIS exhibit a large capacitive loop at high frequencies (HF) followed by a small inductive loop at low frequencies (LF) in 1.0 M HCl.
- ✓The quantum calculations of this molecule using DFT methods gave a good indication of the reactivity against the corrosion of mild steel and confirmed the obtained results

References

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