

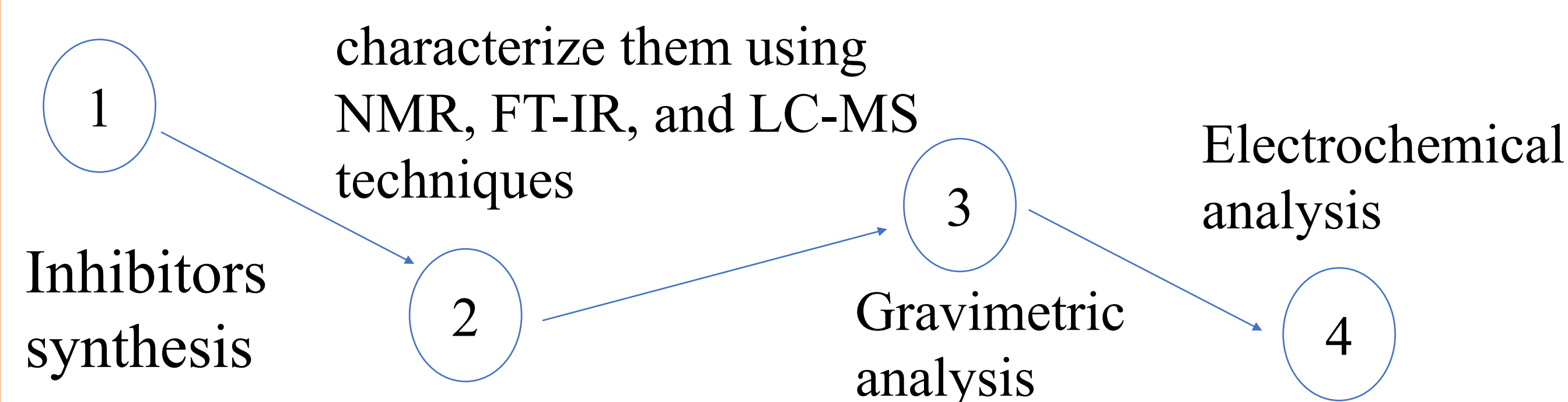
Synthesis of substituted triazines and their investigation as corrosion inhibitors on mild steel in 1M HCl: Practical and Computational Approach

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Introduction

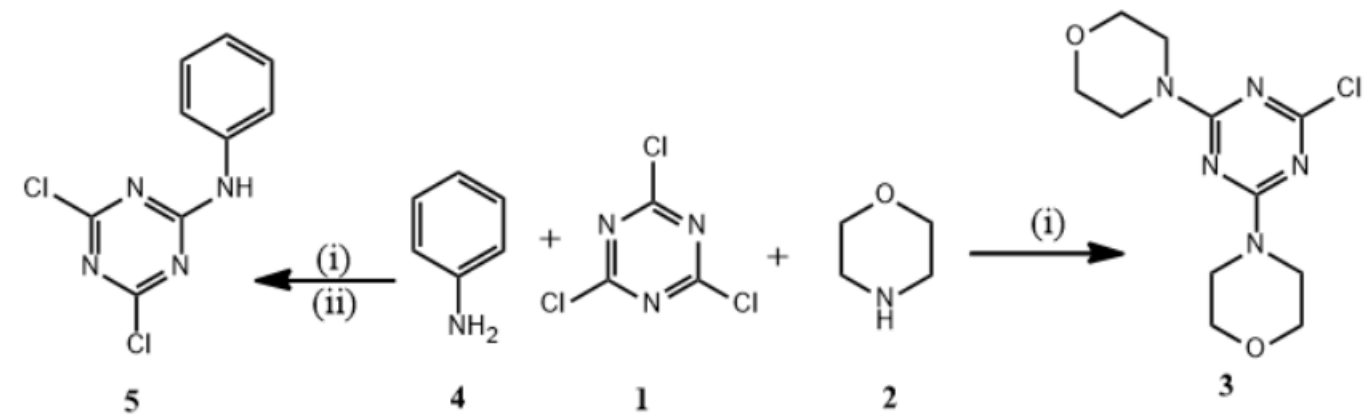
Corrosion is something that is happening in our daily lives that negatively affects the desirable properties of the materials. South Africa has one of the most aged infrastructures worldwide. Those infrastructures are being affected by corrosion resulting in the temporary closure of buildings to perform expensive maintenance and overdesign, bridges collapsing, oil pipelines breaking, chemical plants leaking, and putting human health at risk and this renders the process of technology in the country. It is important to study the corrosion of metals and methods to minimize corrosion due to the important role they play in industries. This study focuses more on synthesizing organic compounds namely 6-chloro-2,4-dimorpholino-1,3,5-triazine (DMT), 4,6-dichloro-N-phenyl-1,3,5-triazin-2-amine(DPT) and investigate their anti-corrosive effects on metal surface.

Experimental overview



Results and discussions

1. Organic synthesis



Scheme: Synthesis of DMT and DPT

Reagent and condition

i. DCM, ii) NaHCO₃, 4hrs stirring

1. Cyanuric chloride, 2. morpholine,

3.DMT, 4. Aniline, 5. DPT

2. Characterisation

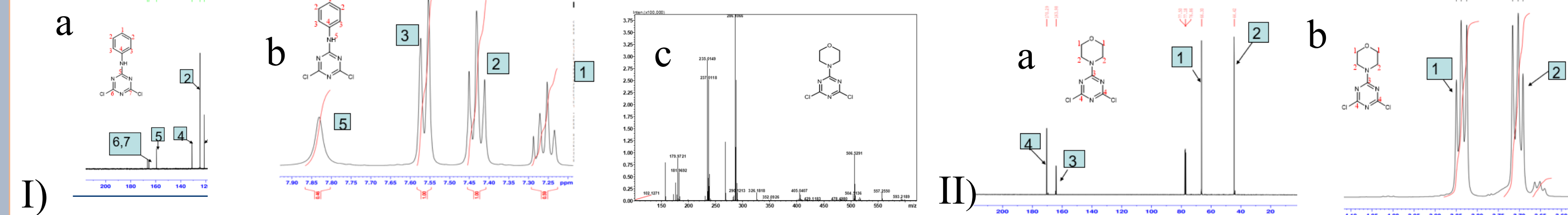


Figure 1: a) ¹³C NMR and b) ¹H NMR Spectra and c) MS. I) DMT and II) DPT.

- For the DMT(I) spectrum (a) revealed 4 peaks, 2CH₂ and 2C. Spectrum (b) revealed two peaks and further confirmation was done by MS (c) with the appearance of its molar mass.
- For DPT(II) there was an appearance of an N-H singlet peak at ~7.8ppm confirming the target product Figure 1:II) b)

3. Gravimetric analysis

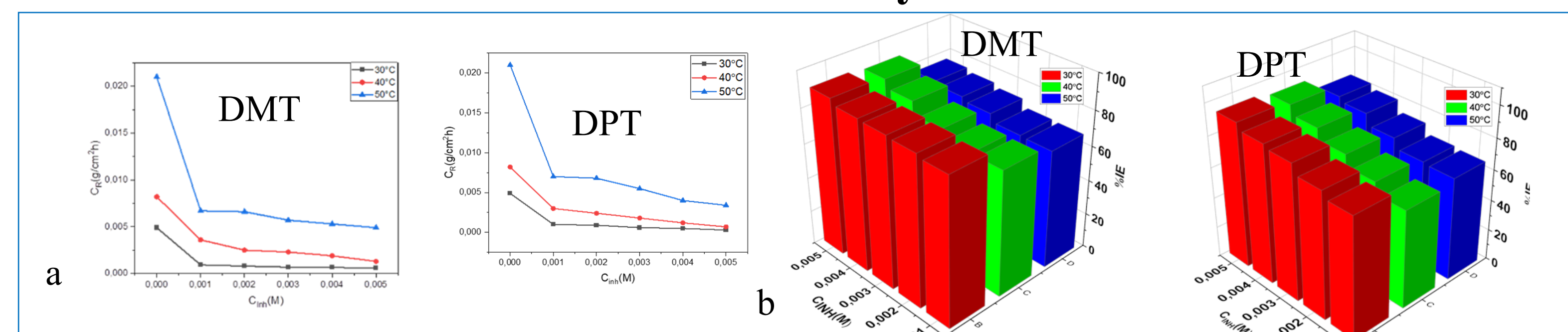


Figure 2: a) Rate of corrosion and b) inhibition efficiency with different concentrations.

This was done to determine what happens as the concentration of the inhibitor grows and at what temperature the inhibitor works the best.

Table1:Adsorption parameters from Langmuir Adsorption Isotherm

Inh	Temperature (°C)	R ²	K _{ads} (L/mol)	-ΔG ⁰ _{ads} (kJ/mol)
DCM	30	0.9682	609.756	26.27
	40	0.9828	182.815	24.01
	50	0.9516	78.003	22.49
DPT	30	0.9196	1018.3299	27.5652
	40	0.8897	253.1645	24.8529
	50	0.9613	90.6618	22.8892

The adsorption isotherm was done in order to describe the amount of inhibitor absorbed on the metal surface and the adsorption process in Table 1.

References

- Al-Moubaraki, A.H. and I.B. Obot, Corrosion challenges in petroleum refinery operations: Sources, mechanisms, mitigation, and future outlook. *Journal of Saudi Chemical Society*, 2021. 25(12): p. 101370
- Da Costa-Mattos, H.S., Bastos, I.N. and Gomes, J.A.C.P., 2008. A simple model for slow strain rate and constant load corrosion tests of austenitic stainless steel in acid aqueous solution containing sodium chloride. *Corrosion Science*, 50(10), pp.2858-2866.

Table 2: Arrhenius and transition parameters

Concentration(M)	E _a (KJ/mol)	ΔH (kJ/mol)	-ΔS (J/mol K)
Blank	60.5145	57.8530	98.9833
DMT			
0.001	76.9332	74.2813	56.3880
0.002	84.0847	81.4327	34.7574
0.003	92.1169	89.4554	11.5932
0.004	86.4589	97.4972	-10.7131
0.005	100.9441	98.2822	-10.7795
DPT			
0.001	90.4893	91.2552	4.1814
0.002	94.4911	91.8392	2.5577
0.003	90.2692	87.6747	17.0048
0.004	89.2161	86.5546	21.7910
0.005	96.5875	94.5294	-1.8824

This was done to understand the Energy change and structural rearrangement that take place during the reactions.

4. Electrochemical analysis

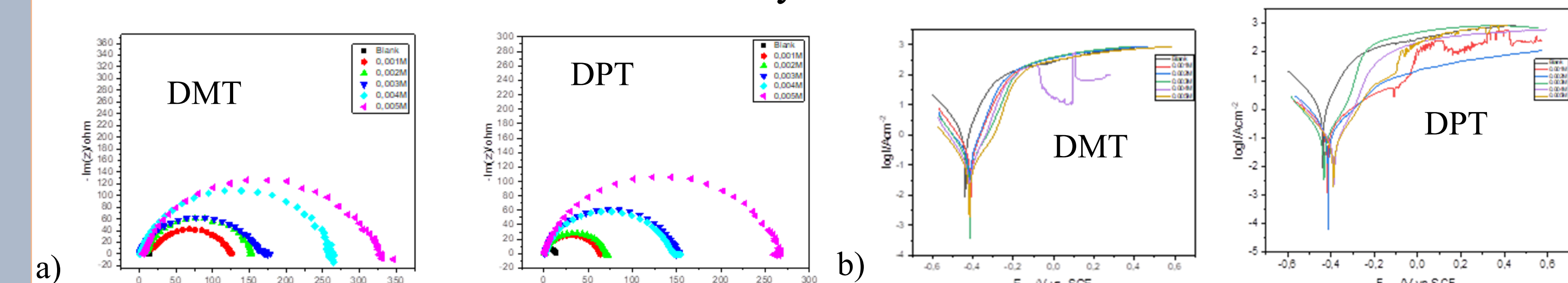


Figure 3: a) Nyquist plot and b) Tafel plots in the absence and presence of inhibitor.

To investigate the interaction of inhibitor and metal using Electrochemical Impedance (EIS) and Potentiodynamic Polarization (PD) .

Conclusion and future work

- The organic inhibitors were successfully synthesized.
- These inhibitors are effective in protecting MS at 30°C depending on inhibitor concentrations.
- The adsorption process of the inhibitor is a mixed-type process and it's a spontaneous reaction.

Future work

- To employ quantum chemical/theoretical techniques to evaluate molecular properties and behavior of corrosion inhibitors at the atomic level.
- To study the triazine derivatives effects with nanoparticle coating..
- Analyse the surface morphology and interaction between the triazines and metal surface using SEM and EDS.

Acknowledgments

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