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### Quantum Study of Synthesized 4-(Pyridin-2yl)-N-P-TolylPiperazine-1-Carboxamide as Corrosion inhibitor for Mild steel in Acidic medium

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**Abstract :** Corrosion inhibition of mild steel in 1 M HCl was investigated in the absence and presence 4-(pyridin-2yl)-N-p-tolylpiperazine-1-carboxamide (PTC) has been characterized using LC-MS. Simultaneous thermogravimetry and differential scanning calorimetry ( TG-DSC), were used to characterize and to study the thermal behaviour of PTC. The results led to information about thermal stability and thermal decomposition of PTC. The UV-visible absorption spectra indicate the formation of a PTC-Fe complex. Surface analysis by AFM and XRD confirmed the formation of protective coating on the mild steel surface. Quantum chemical calculation were also performed using density functional theory. The quantum chemical parameters such as  $E_{HOMO}$  (highest occupied molecular orbital energy),  $E_{LUMO}$  (lowest unoccupied molecular orbital energy), energy gap ( $\Delta E$ ), dipole moment ( $\mu$ ), absolute electronegativity ( $\chi$ ), global electrophilicity ( $\omega$ ), polarizability and hyperpolarizability were obtained for the PTC to predict their activity towards metal surface.

**Keywords:** TG-DSC, UV-visible, DFT, HCl, Mild steel, corrosion.

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