## Investigation of corrosion inhibition of mild steel in 1M HCl by 3-methyl-4-(3-methyl-isoxazol-5-yl)isoxazol-5(2H)-one monohydrate using experimental and theoretical approaches

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## Abstract

The inhibition effect of 3-methyl-4-(3-methylisoxazol-5-yl)isoxazol-5(2H)one monohydrate (P1) on the corrosion of carbon steel in 1 M HCl was studied by weight loss, electrochemical impedance spectroscopy (EIS) techniques and potentiodynamic polarization methods. The results showed that isoxazole P1 was a good inhibitor in 1 M HCl and inhibition efficiency increases with isoxazole P1 was oncentration to attain 93% at 10-3M at 308 K. E(%) values obtained from various methods used are reasonably good agreement. The adsorption of isoxazole P1 obeyed the Langmuir adsorption isotherm. Polarization curves showed that isoxazole P1 acted as a mixed-type inhibitor in HCl. The effect of the temperature on the corrosion behavior with addition of 10-3M of the inhibitor was studied in the temperature range 313-343 K, and the thermodynamic parameters were determined and discussed. In addition, a quantum chemical study suggests isoxazole P1 inhibitor is structurally essential for the protection of metal surface



Scheme 1: Characterization of 3-methyl-4-(3-methylisoxazol-5-yl)isoxazol-5(2H)one monohydrate (P1).

**Key words:** Mild Steel, EIS, Polarization, Weight loss, Acid inhibition, adsorption isotherm, DFT.