**ABSTRACT**

The inhibition ability of mild steel in 1 M H2SO4 by bis-pyrimidine derivatives was investigated using chemical and electrochemical techniques. Results obtained indicate that bis-derivatives inhibited the corrosion of mild steel in the acid medium. The inhibition efficiency increases with increase in concentration of bis-derivatives but decrease with rise in temperature. Adsorption of bis-derivatives on the steel surface in 1 M H2SO4 follows the Langmuir adsorption model. Kinetic and thermodynamic parameters such as activation energy, enthalpy, entropy and free energy of activation and adsorption were calculated. Gibbs free energy indicated that the adsorption process is spontaneous. Scanning electron microscopy and atomic force microscopy were used to study morphology of the steel surface. Results obtained from quantum chemical studies show excellent correlations between quantum chemical parameters and experimental inhibition efficiencies using density functional theory (DFT).