**ABSTRACT**

The inhibition ability of mild steel in 1 M H2SO4 by bis-pyrimidine derivativeswas 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 weren used to studymorphologyofthesteelsurface.Resultsobtainedfromquantumchemicalstudiesshowexcellentcorrelations between quantum chemical parameters and experimental inhibition efﬁciencies using density functional theory (DFT).