**ABSTRACT**

The inhibition potential of four Quinoxaline derivatives namely 1,4-dihydroquinoxaline-2,3-dione, (3E)-3-hydrazinylidene-3,4-dihydroquinoxalin-2(1H)-one, 1-[(2E)-3-oxo-3,4-dihydroquinoxalin-2(1H)-ylidene]urea and 1-[(2E)-3-oxo-3,4-dihydroquinoxalin-2(1H)-ylidene]thiourea have been investigated against mild steel in 1M H2SO4 solution using conventional weight loss, electrochemical impedance spectroscopy, potentiodynamic polarization and atomic absorption spectroscopy. The percentage inhibition efficiency was found to increase with increase in the inhibitor concentration due to the adsorption of the inhibitor molecules on the metal surface. In addition, it was established that the adsorption follows Langmuir adsorption isotherm. Moreover, some thermodynamic data were calculated and discussed. The density functional theory at the B3LYP/6-311G (d,p) basis set level was performed for two inhibitors namely 1,4-dihydroquinoxaline-2,3-dione and (3E)-3-hydrazinylidene-3,4-dihydroquinoxalin-2(1H)-one. The quantum chemical parameters such as highest occupied molecular orbital energy (EHOMO), lowest unoccupied molecular orbital energy (ELUMO), energy gap (∆E), dipole moment (µ), softness (σ), hardness (η), electronegativity (χ), Mulliken atomic charges, the fraction of electrons transferred from the inhibitor to the metal surface (∆N) and the total energy (TE) have been calculated for these compounds. It was found that theoretical data support the experimental results.