**ABSTRACT**

The aim of this work is to obtain deeper insight into the mechanism of the protective action of the imidazole-based corrosion inhibitor, 2-(4’-N, N-Dimethylaminophenyl)-imidazoline (DMAP2I). Investigations were performed on mild steel in 0.5 M H2SO4 by electrochemical methods and non - electrochemical methods. Maximum protection efficiency reaches about 85% for DMAP2I at 200 ppm concentration level. The adsorption of the imidazoline derivative on mild steel surface follows Langmuir and Tempkin isotherm. The adsorption free energy on mild steel (20 – 30 kJ/mol) reveals a comprehensive (physical and chemical) adsorption of the inhibitors on the metal surface. Polarization curves reveal that DMAP2I act as a mixed-type inhibitor. Results obtained from potentiodynamic polarization and impedance measurements are in good agreement. Quantum chemical method is used to explore the relationship between the inhibitor molecular properties and its inhibition efficiency. The density function theory (DFT) is also used to study the structural properties of the inhibitor. It is found that when the imidazole derivative adsorbs on the mild steel surface, molecular structure influences their interaction mechanism. The inhibition efficiencies of the compound showed a certain relationship to highest occupied molecular orbital (HOMO) energy and Mulliken atomic charges.