**ABSTRACT**

In the present study, four imidazoline (IDZ) and four isoxazolines (ISO) heterocyclics differing in the nature of methoxy (‐OCH3) and aromatic (phenyl and naphthyl) moieties are synthesized, characterized and evaluated as corrosion inhibitors for mild steel in acidic solution of 1 M HCl. Results showed that imidazoline based heterocyclic compounds are better corrosion inhibitors than isoxazoline based heterocyclics and both classes of compounds showed inhibition efficiency of more than 85% at 20 mgL−1 concentration. Results further showed that inhibitors containing methoxy, phenyl, and naphthyl moieties showed higher protection efficiency as compared to the inhibitors without these moieties. PDP Study revealed that investigated IDZs and ISOs acted as mixed type inhibitors and their adsorption on the metallic surface followed the Langmuir adsorption isotherm model.All the experimental results were corroboratedby density function theory (DFT) based quantum chemical calculations.Numerous DFT based indices calculated for neutral as well asprotonated forms of the IDZs and ISOs in order to get better insight aboutmetal-IDZs/ISOs interactions. Outcomes of the DFT analysis showed that protonated(cationic) form of the all the inhibitors are more strongly adsorbed onthe metallic surface as compared to their neutral form.