**ABSTRACT**

Inhibition potential of synthesized pyrazoline derivatives on the corrosion inhibition of mild steel in 1M H2SO4 solution have been evaluated and studied by gravimetric, Tafel polarization, electrochemical impedance spectroscopy techniques and the quantum chemical studies using density functional theory (DFT). The results showed that the inhibition efficiency of the investigated compounds depend on the concentration and nature of the inhibitor. The effect of temperature on the corrosion behavior of mild steel in 1M H2SO4 without and with the inhibitors was studied in the temperature range 303 to 333 K. Some activated thermodynamic parameters were computed and discussed. Polarization studies showed that all the pyrazolines function as mixed inhibitor, but predominantly act as cathodic type. The surface morphology of inhibited mild steel was analyzed by scanning electron microscope technology with energy dispersive X-ray spectroscopy (SEM-EDX). FT-IR spectroscopic analysis was used to obtain information on bonding mechanism between the metallic surface and the inhibitors. Quantum chemical parameters such as highest occupied molecular orbital energy (EHOMO), lowest unoccupied molecular orbital energy (ELUMO), energy gap (∆E) and dipole moment (µ), the softness (σ), the fraction of the electrons transferred from the inhibitor to the metal surface (∆N) and the total energy (TE) have been calculated. It was found that theoretical data support the experimental results