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| ABSTRACTThe inhibition effect of some azole derivatives for the corrosion of mild steel in 1 M H2SO4 has been studied by gravimetric, electrochemical polarization and electrochemical impedance spectroscopy measurements. The results obtained reveal that these compounds are efficient inhibitors. Polarization studies showed that all the azoles function as a mixed inhibitor, but predominantly act as cathodic type. The inhibitors were adsorbed on the steel surface according to the Langmuir adsorption isotherm model. Quantum chemical parameters such as energy of highest occupied molecular orbitals, energy gap and dipole moment, softness, the fraction of electrons transferred from the inhibitor to the metal surface and the total energy have been calculated. Results reveal that theoretical data support the experimental results. |  |  |