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| **ABSTRACT**  Quantum chemical calculations based on density functional theory (DFT) method were performed on heterocyclic azole derivatives as corrosion inhibitors for mild steel in acid media to investigate the relationship between molecular structure of the inhibitors and the corresponding inhibition efficiencies (%). Quantum chemical parameters most relevant to their potential action as corrosion inhibitors have been calculated in the non-protonated and protonated forms in aqueous phase for comparison. Results obtained in this study indicate thatin acidic media, both the protonated and non-protonated forms of the azoles represent the better actual experimental situation. |  |