Short Communication

Quantum Chemical Studies on the Corrosion Inhibition of Fe₇₈B₁₃Si₉ glassy alloy in Na₂SO₄ Solution of Some Thiosemicarbazone Derivatives

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In this study, the density functional theory (DFT) at the gradient-corrected correlation functional of Lee-Yang-Parr (B3LYP) functional with 6-311++G(2d,2p), correlation-consistent, polarized valence, X-zeta (cc-pVTZ) basis sets, BP86 functional with/6-311++G(2d,2p) basis set and ab initio calculations using the Hartree-Fock (HF)/6-311++G(2d,2p) methods in gas and water phase of neutral and protonated forms of molecules were performed on six thiosemicarbazone derivatives, namely 4-methyl acetophenone thiosemicarbazone (Inh 1), 4-methoxy acetophenone thiosemicarbazone (Inh 2), Benzaldehyde thiosemicarbazone (Inh 3), 4-methoxy benzaldehyde thiosemicarbazone (Inh 4), 4-ethyl benzaldehyde thiosemicarbazone (Inh 5) and 4-bromo benzaldehyde thiosemicarbazone (Inh 6). The quantum chemical parameters/descriptors, namely, dipole moment (D), highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), HOMO-LUMO energy gap (ΔE), absolute electronegativity (χ), absolute hardness (η), softness (σ), proton affinity (PA), electrophilicity (ω) and nucleophilicity (ε) were calculated and correlated with the experimental inhibition efficiencies (%IE). It was observed that the theoretical and experimental results were in good agreement.

Keywords: Corrosion; Inhibitors; organic molecules; Fe₇₈B₁₃Si₉ glassy alloy; theoretical study.

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