QUANTUM CHEMICAL CALCULATION FOR THE INHIBITORY EFFECT OF COMPOUNDS

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The effects of the molecular structure on the corrosion inhibition efficiency are investigated by nine methodsof calculations. The selected thio compounds were previously identified as corrosion inhibitors for mild steel in the 1.0 M HCl solution. The electronic properties such as highest occupied molecular orbital (EHOMO) energy, lowest unoccupied molecular orbital (ELUMO) energy, dipole moment (μ), and Fukui indices are calculated and discussed. Results show that the corrosion inhibition efficiency increase with the increase in both EHOMO and μ values, respectively, and decrease in ELUMO. QSAR approach is utilized in this study; a good relationship is found between the experimental corrosion inhibition efficiency (IE_{exp}, %) and the theoretical corrosion inhibition efficiency (IE_{theor}, %). The calculated inhibition efficiency is found closer to the experimental inhibition efficiency with a coefficient of correlation (R^2) of 0.875.

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