

Quantum Chemical Calculations Synthesis and Corrosion Inhibition Efficiency of Nonionic Surfactants on API X65 Steel Surface under H₂S Environment

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Abstract : Inhibition effect of four novel nonionic surfactants based on sulphonamide, of linear alkyl benzene sulphonic acid (LABS), was reacted with 1 mole triethylenetetramine, tetraethylenepentamine then Ethoxylation of amide X 65 type carbon steel in oil wells formation water under H₂S environment was investigated by electrochemical measurements. Scanning electron microscopy (SEM) and energy dispersion X-ray (EDX) were used to characterize the steel surface. The results showed that these surfactants act as a corrosion inhibitor in and their inhibition efficiencies depend on the ethylene oxide content in the system. The obtained results showed that the percentage inhibition efficiency ($\eta\%$) was increased by increasing the inhibitor concentration until the critical micelle concentration (CMC) reached. The quantum chemistry calculations were carried out to study the molecular geometry and electronic structure of obtained derivatives. The energy gap between the highest occupied molecular orbital and lowest unoccupied molecular orbital has been calculated using the theoretical computations to reflect the chemical reactivity and kinetic stability of compounds.

Keywords : corrosion, surfactants, steel surface, quantum

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