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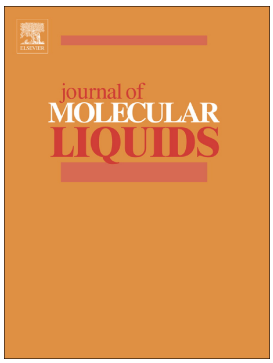

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High performance corrosion inhibition of novel tricationic surfactants on carbon steel in formation water: Electrochemical and computational evaluations

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Abstract

Three tricationic surfactants were prepared from quaternization of pentamethyl diethylene triamine. Their chemical structures were characterized using FTIR and ^{1}H-NMR spectroscopy. Their surface activities were determined using surface tension, critical micelle concentration, interfacial tension and emulsification power measurements. The results revealed that the surface activity was increased by increasing the hydrophobic chain length of the different surfactants. Increasing the hydrophobic chain length decreased the critical micelle concentrations, effectiveness and area at interface. Electrochemical polarization and impedance spectroscopy were used to investigate their molecular action as efficient corrosion inhibitors. The different inhibitors showed high inhibition efficiencies in protection of carbon steel in formation water, which was increased by increasing their concentration in the medium. Quantum chemical studies were correlated the inhibition efficiencies including: highest occupied molecular orbital (*HOMO*), lowest unoccupied molecular orbital (*LUMO*), energy gap (ΔE), dipole moment (DM), softness (σ), hardness (η), total negative charge (ΔN), molecular volume (*MV*), chemical potential (μ) and electronegativity (χ). The computational study supported the electrochemical studies and gave a clear sight on the mechanism of the surfactants during their inhibition process of carbon steel corrosion.

Keywords

Cationic surfactant; surface activity; corrosion inhibition; computational study

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