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QUINOLINE CARBONITRILES AS NOVEL INHIBITORS FOR N80 STEEL CORROSION IN OIL-WELL ACIDIZING: EXPERIMENTAL AND COMPUTATIONAL INSIGHTS

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Abstract—Three quinoline derivatives as corrosion inhibitors for N80 steel 15% HCl solutions. Influence of the $-H$, $-OCH_3$ groups and the introduction of π bonding are reported in the present report. Experimental studies were performed using gravimetric tests, electroanalytical methods, and surface analysis. The cinnamaldehyde derivative displayed the maximum inhibition efficiency of 95% at 300 mg L^{-1}, followed by the $-OCH_3$ and the $-H$ derivatives. The inhibitor adsorption on the metal surface obeyed the Langmuir isotherm with a mixed mode of physical and chemical adsorption. Impedance measurements revealed an increase in the charge transfer resistance with the addition of increasing inhibitor dosage, which supported the inhibitor adsorption. Frequency modulations displayed a lowering in the corrosion current density upon the addition of the corrosion inhibitors. Polarization studies revealed that all the three inhibitors showed a mixed-type inhibition behavior with cathodic prevalence. SEM and FTIR of the inhibitor-adsorbed steel surface affirmed the adsorption of inhibitor and improvement in the surface smoothness of the N80 steel. The p*K*a analysis revealed that all the three inhibitors undergo protonation at the pyridine Nitrogen at the experimental pH. The DFT studies showed that the protonated form of the inhibitors is more active compared to the neutral form.

Keywords: oil-well acidizing, corrosion inhibitor, quinolines, impedance spectroscopy, p*K*a analysis

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CONCLUSIONS

Three quinoline derivatives, namely AHQ-1, AHQ-2, and AHQ-3, were synthesized following a simple microwave irradiation method and characterized using spectroscopic methods. The inhibition performance of the three molecules was studied on the N80 steel in 15% HCl following gravimetric measurements, electrochemical studies, and surface analysis. The major conclusions are as follows:

(1) The inhibition efficiency increased with temperature and attained 97% at a concentration as low as 300 mg L^{-1}. The inhibition efficiency followed the trend AHQ-3 > AHQ-2 > AHQ-1.

(2) The inhibitor adsorption followed the Langmuir isotherm and showed a high value of the ΔG^0_{ads} supporting chemical adsorption. The inhibition efficiency increased with an increase in the temperature, supporting the strong adsorption of the three inhibitors.

(3) The EIS studies showed that the inhibitors acted by adsorbing on the steel surface, and the charge transfer resistance increased with an increase in the added concentrations of the inhibitors.

(4) Polarization measurements showed that the inhibitors showed mixed type adsorption with a cathodic prevalence, and the adsorption of the inhibitors on the metal did not alter the mechanism of corrosion.

(5) Surface analysis using the SEM measurements showed that the inhibitors exhibited improved surface smoothness of the steel surface in their presence. FTIR measurements showed the existence of the characteristic functional groups of the inhibitors on the metallic surface and the formation of a protective inhibitor film.

(6) The p*K*a analysis showed that the inhibitor molecules show a strong tendency of protonation at the pyridine nitrogen atom at the experimental pH range. The DFT based quantum chemical parameters supported the above observations and supported that the trend in the inhibition efficiency for in the order AHQ-3 > AHQ-2 > AHQ-1. Monte Carlo simulations revealed higher adsorption energy in the protonated AHQ-3 compared to the neutral molecule supporting the primary action of the inhibitor in the protonated state.

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