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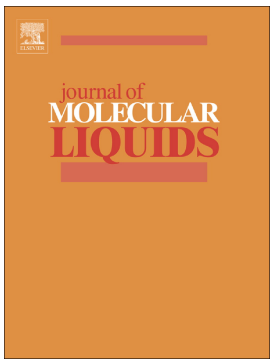

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Understanding Corrosion Inhibition of Mild Steel in Acid Medium by new Benzonitriles: Insights from Experimental and Computational Studies

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ABSTRACT

Two benzonitrilederivatives, namely 4-(isopentylamino)-3-nitrobenzonitrile(PANB) and 3-amino-4-(isopentylamino)benzonitrile(APAB) have been synthesized and evaluated as corrosion inhibitors for mild steel (MS) in 1 M HCl solution at 303K by gravimetric, potentiodynamic polarization (PDP) curves, and electrochemical impedance spectroscopy (EIS) methods, as well as Density Functional Theory (DFT) and Molecular Dynamic (MD) simulations. The results suggest that tested compounds are excellent corrosion inhibitors for mild steel with PANB showing superior performance. Polarization measurements revealed that PANB and APAB behaved as mixed type inhibitors. The polarization resistance, according to EIS studies, found to be dependent on the inhibitor's concentration. The adsorption of PANB

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