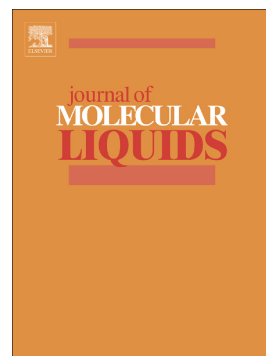


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Amino acid Based Imidazolium Zwitterions as Novel and Green Corrosion Inhibitors for Mild Steel: Experimental, DFT and MD Studies

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Abstract

Three novel amino acids based corrosion inhibitors namely 2-(3-(carboxymethyl)-1H-imidazol-3-ium-1-yl)acetate (AIZ-1), 2-(3-(1-carboxyethyl)-1H-imidazol-3-ium-1-yl)propanoate (AIZ-2) and 2-(3-(1-carboxy-2-phenylethyl)-1H-imidazol-3-ium-1-yl)-3-phenylpropanoate (AIZ-3) were synthesized by condensing glyoxal, formaldehyde and amino acids, and characterized. The corrosion inhibition performance of synthesized inhibitors was studied by electrochemical impedance (EIS) and potentiodynamic polarization (PDP) methods. Among the studied inhibitors, AIZ-3 showed the maximum inhibition efficiency (IE) of 96.08% at a concentration as low as 0.55 mM (200 ppm). The results of potentiodynamic study reveal that AIZ-1 acts as cathodic inhibitor while AIZ-2 and AIZ-3 act as mixed type inhibitors. The results of EIS studies showed that in the presence of inhibitors, polarization resistance increased and C_{dl}

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