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Inhibitive performance of dapoxetine drug for corrosion of aluminum alloy (AA6063) in acidic and alkaline solutions: experimental and theoretical studies using Materials Studio v7.0

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ABSTRACT

The inhibiting effect of the dapoxetine drug towards corrosion of aluminum alloy (AA6063) in 1.0 M HCl and 1.0 M NaOH solutions using weight loss, potentiodynamic polarization, and theoretical calculation. The results demonstrated that the inhibition efficiency (IE%) was increased with increasing the concentration of dapoxetine and lowering the temperature. IE% of dapoxetine is higher in 1.0 M HCl than in 1.0 M NaOH solution. The activation parameters of the corrosion process are endothermic, and the formation of the activated compound includes an association process. Inhibition was demonstrated in light of the horizontal adsorption of the complex formed between dapoxetine and the alloy surface on AA6063 according to the Langmuir absorption isotherm. The inhibition performance of Dapxitine on AA6063 was investigated using materials Studio v7.0. The quantum chemical descriptors are found to suitable to explain the performance of title molecule as corrosion inhibitors. Additionally, adsorption of dapoxetine on an aluminum alloy (Al) (111) has been investigated. The results of the current theoretical approach comply with that obtained experimentally.

Keywords: Corrosion inhibitor; Dapoxetine; Adsorption; Frontier molecular orbital; Fukui function

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