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Short Communication

Theoretical Studies on Mild Steel Corrosion Inhibition by 5-Substituted 1H-Tetrazoles in Acidic Media

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In this theoretical study, calculations for the three types of the tetrazole which are 2-(1H-Tetrazole-5-yl)-3-phenylacrylonitrile, 2-(1H-Tetrazole-5-yl)-3-(4-nitrophenylacrylonitrile), and 2-(1H-Tetrazole-5-yl)-3-(4- hydroxyphenyl acrylonitrile) showing the corrosion inhibition efficiency on mild steel in 1M HCl were carried out with the Density Functional Theory (DFT) at the B3LYP functionals with the use of 6-311g (d, p) basis set. Calculated parameters such as E_{HOMO}, E_{LUMO}, energy gap, electronegativity (χ), chemical potential (μ), hardness (η), softness (S),electrophilicity, electrofugality, nucleofugality, Proton affinity, polarizability and hyperpolarizability. The correlation and regression analysis have been conducted to determine which descriptors have effect on inhibition efficiency. Both the theoretical results and experimental data are in accordance based on the inhibition efficiency.

Keywords: Theoretical study, inhibition efficiency, corrosion, DFT

FULL TEXT