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DFT and QSAR-ANN studies of ionic liquids used as green corrosion inhibitors for mild steel dissolution in 1 M HCl

Nowadays, ionic liquids have gained wide usage as green corrosion inhibitors due to their effectiveness, eco-friendliness and outstanding physiochemical characteristics. The present study investigates the computational analysis of thirty ionic liquids used as green corrosion inhibitors of metallic dissolution in molar HCl environment. Density functional theory was employed to study the electronic parameters of the inhibitor molecules in relation to their inhibitive effect. Dragon 7 software was utilized to calculate high dimensional structural parameters. Five significant molecular descriptors were selected from the screening of DFT and Dragon-generated descriptors using standardization technique. Quantitative structure activity relationship (QSAR) models using multiple linear regression (MLR) and artificial neural network (ANN) were developed to elucidate the corrosion inhibition mechanism of studied ionic liquids. Using the selected five molecular descriptors alongside with the inhibitor concentration, MLR model showed a fair prediction. Robust statistical parameters such as MSE, RMSE, MAD and MAPE were used to characterize the ANN model. The best ANN model yielded low error estimates which suggests the strong reliability and predictive capacity of the developed model. In addition, the developed models were further used to forecast the inhibition efficiencies of five non-synthesized ionic liquids. The predicted excellent inhibition efficiencies suggest that QSAR models could offer a quick, reliable and cheap approach to determining the inhibition efficiencies of organic compounds.

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