Short Communication

A Quantum Chemical Study on Some Schiff Bases as Inhibitors of Mild Steel Corrosion in HCl Solution

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A quantum chemical study using a DFT/6-31+G(d) method has been performed on three types of Schiff base compound that are used as corrosion inhibitors for mild steel to determine the relationship between their molecular structures and their inhibition efficiency (*IE*). HOMO orbital (E_{HOMO}) and LUMO orbital (E_{LUMO}) energies and other physical properties have been calculated, with these results showing that *IE* had a good linear relationship to ΔE , η , σ and Q_N charge (imino nitrogen). These theoretical results were in accord with previously reported experimental results and have been used to identify some new homologous Schiff base compounds that are predicted to exhibit better corrosion inhibition performance.

Keywords: modeling studies; corrosion inhibition; Schiff base; prediction of inhibition performance

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