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QUANTUM CHEMICAL CALCULATION FOR THE INHIBITORY EFFECT OF COMPOUNDS

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The effects of the molecular structure on the corrosion inhibition efficiency are investigated by nine methods of calculations. The selected thio compounds were previously identified as corrosion inhibitors for mild steel in the 1.0 M HCl solution. The electronic properties such as highest occupied molecular orbital (EHOMO) energy, lowest unoccupied molecular orbital (ELUMO) energy, dipole moment (μ), and Fukui indices are calculated and discussed. Results show that the corrosion inhibition efficiency increase with the increase in both EHOMO and μ values, respectively, and decrease in ELUMO. QSAR approach is utilized in this study; a good relationship is found between the experimental corrosion inhibition efficiency (IE_{Exp}%) and the theoretical corrosion inhibition efficiency (IE_{Theo}%). The calculated inhibition efficiency is found closer to the experimental inhibition efficiency with a coefficient of correlation (R^2) of 0.875.

K e y w o r d s: corrosion inhibition, quantum chemical parameter, thio, QSAR.

Corrosion is the destructive attack of metal or alloy chemically or electrochemically against its environment which leads to the loss of useful properties of materials. The protection of metals against corrosion can be achieved by adding inhibitors in small concentrations to its environment [1]. Corrosion inhibitor can effectively reduce the corrosion rate of metallic materials in acid solution and has been widely applied in acidic cleanout, crude oil refiner, electrochemical and chemical etching [2]. Organic compounds, mainly containing oxygen, nitrogen and sulfur atoms and having multiple bonds, are recognized as effective inhibitors of the corrosion of many metals and alloys [3]. The protection of metal surfaces against corrosion is an important industrial and scientific issue. Inhibitors are one of the practical means of preventing corrosion, particularly in acidic media. Inhibitors can adhere to a metal surface to form a protective barrier against corrosive agents in contact with metal [4]. The effectiveness of an inhibitor to provide corrosion protection depends to a large extent on the interaction between the inhibitor and the metal surface.

The most efficient corrosion inhibitors are organic compounds containing electronegative functional groups and π electrons in their triple or conjugated double bonds [5]. Some thio compounds have been found to be good inhibitors for mild steel in acid [6—8]. Recently theoretical chemistry, such as quantum chemical calculations [9, 10], has been used to explain the mechanism of corrosion inhibition. Quantum chemical calculations are proved to be a very powerful tool for studying the inhibition mechanism [11, 12].

The objective of this study is to determine the relationship between the corrosion inhibition efficiency and the molecular structures of the nine previously studied thio compounds (contains double