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Theoretical study of the corrosion inhibition of some bipyrazolic derivatives: a conceptual DFT investigation

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Abstract

Corrosion inhibition of copper through six bipyrazolic compounds has been elucidated by means of density functional theory (DFT)-derived reactivity indexes. The DFT calculated parameters and experimental corrosion inhibition efficiency (IE%) indicate that their inhibition effect is closely related to the frontier orbital energies, polarizability, electronic chemical potential and global nucleophilicity. The quantum chemistry calculations were performed at the B3LYP/6-31G (d) level. The theoretical results, predicted using DFT-based reactivity indexes, are in good agreement with experimental outcomes.