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QUANTUM CHEMICAL STUDY FOR AMINE DERIVATIVES

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Abstract: When a corrosion inhibitor is added to a liquid or gas, the corrosion rate of a metal or an alloy decreases. The efficiency of an organic inhibitor depends on the chemical structure so, electronic properties of the inhibitor. The organic acid inhibitor generally contains oxygen, nitrogen and/or sulfur and so they are adsorbed on the metallic surface blocking the active corrosion sites.

In this study, the correlation between inhibition efficiency and descriptor variables such as the highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), the energy gap between E_{HOMO} and E_{LUMO} , global hardness (η), softness (σ), chemical potential (μ), electronegativity (χ), Global Electrophilicity (ω), dipole moments (DM), molecular volume (MV), sum of the total negative charge (TNC), and sum of electronic and zero-point energies (SEZPE) obtained from the quantum chemical calculation using B3LYP/6-311++G(2d,2p), and CBS-APNO methods were evaluated and the result showed that the theoretical data obtained are in good agreement with the experimental inhibition.

Keywords: *Corrosion; Inhibitors; DFT; Band Gap.*

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