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Theoretical study for several synthesized compound as a corrosion inhibitors

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Abstract : Semi-empirical method (PM3) using Gaussian03and Gaussian view03and (MOPAC) computational packages was carried out to achievedQuantum chemistry calculations for geometrical complete optimization of number synthesized inhibitors.The calculated quantum parameters were:(E_{HOMO}) the energy of highest occupied molecular orbital,(E_{LUMO})the energy, oflowest,unoccupied,molecular orbital,, (ΔE) = (E_{LUMO}) – (E_{HOMO}) is Energy gap,(X) is ,the Electronegativity, (μ) is the dipole moment, (δ)=1/(γ) is Softness, (γ) is hardness, ,(π) = - X is chemical potential,,ΔN= No. of electron transferand(M_g) is molecularvolume.The research study the effect of synthesis organic inhibitors:[N – Phenyl-N\-(4-aminobenzene)thiourea], N – Phenyl-N\-(4-methyl benzene)thiourea, N-Phenyl-N\-(4 -amino-5-methyl benzene)thiourea, N-Phenyl-N\-(3-aceto benzene) thiourea, N-Phenyl-N\-(2,3-Dimethyl benzene)thiourea, N-Phenyl-N\-(4-bromo benzene)thiourea, N-Phenyl-N\-(4-Cloro benzene)thiourea, N,N\-Diphenylthiourea and thiourea as acorrosion inhibitors. The inhibition efficiency P% of these compounds wereexamined by Semi–empirical method and the experimental P% results were compared with variation of (ΔE), (E_{HOMO}) , (μ) , (E_{LUMO}), ΔN and the nature of the inhibitor. It is clear from the results that P% increased with the increase of inhibitor (I) ionization potential and (A) electron affinity,from Polarization measurement, the inhibition type by these inhibitors were like mixed type inhibitors because corrosion potential stays the same before and after adding these inhibitors. Theaction of studied organic compounds wasanalyzed through PM3 Quantum chemical methods, to compare the P% of compounds with experimental P%.There is excellentconsistency between theoretical and experimental data, where the correlation factor (R^2)reach to 0.9950 for relationbetween the highest occupied molecular orbital (E_{HOMO}), (μ) the dipole moment, (I) is inhibitor ionization potentialandexperimental P% for synthesize compound that used in the study.

Keywords : Gaussian program package,Corrosion inhibitors,Optimization,Inhibition efficiency, PM3.

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