OLATION, CHARACTERISATION AND CORROSION INHIBITORY POTENTIALS OF EXTRACTS FROM THE SEEDS OF *Cola nitida* ON MILD STEEL IN HYDROCHLORIC ACID SOLUTION

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ABSTRACT

No background
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Mature seeds of *Cola nitida* were subjected to extraction using dichloromethane (DCM). The extract was concentrated and put through vacuum liquid, column and thin layer chromatographic processes. Three pure compounds were isolated, characterised using FT-IR, ^{1}H-NMR, ^{13}C-NMR and DEPT-135 and identified as 1, 3, 5-trimethoxymethylbenzene (TMMB), 1, 3-dimethyl-7H-purine-2, 6-dione (DMPD) and 1, 3, 7-trimethylpurine-2, 6-dione (TMPD). Two semi-pure compounds were also isolated and coded Mb4 and Mb5. Corrosion inhibition of mild steel in 1 M HCl with different concentrations of the isolates was investigated using weight loss and electrochemical methods. Computational studies and scanning electron microscopy were also carried out. Weight loss results revealed that corrosion inhibition efficiencies at 303 K and at 5.0 x10^{-4} gL^{-1} concentration of the inhibitors followed the order: Mb4 (80.82%) > TMPD (72.08%) > Mb5 (69.17%) > DMPD (65.83%) > TMMB (55.83%). Corrosion inhibition efficiencies obtained from electrochemical methods and computational studies had similar trend. Based on the values of ΔG_{ads} at 303 K and at 5.0 x 10^{-4} gL^{-1} [TMMB (-22.45 kJ mol^{-1}), DMPD (-17.74 kJ mol^{-1}), TMPD (17.46 kJ mol^{-1}), Mb4 (-22.47 kJ mol^{-1}) and Mb5 (-92.52 kJ mol^{-1})] and the values of ΔH_{ads} at 303 K and at 5.0 x 10^{-4} gL^{-1} [TMMB (38.47 kJ mol^{-1}), DMPD (36.84 kJ mol^{-1}), TMPD (36.69 kJ mol^{-1}), Mb4 (51.79 kJ mol^{-1}) and Mb5 (34.06 kJ mol^{-1})], the adsorption process of the inhibitors onto the surface of mild steel was spontaneous and endothermic. Adsorption of the inhibitors fitted to Temkin isotherm. Decrease in corrosion inhibition efficiencies with increase in temperature favoured physical adsorption phenomenon. Some of the quantum chemical parameters of the isolates obtained were E_{HOMO}: TMMB (-6.570 eV), DMPD (-6.079 eV) and TMPD (-6.033 eV), energy gap (ΔE): TMMB (6.248 eV), DMPD (5.181 eV) and TMPD (5.163 eV) and electronegativity (χ): TMMB (3.446 eV), DMPD (3.507 eV) and TMPD (3.545 eV). These values are lower than the work function of Fe(110) which is 4.82 eVand this implies that electrons migrate from inhibitors to the steel. E_{HOMO} projects corrosion inhibitory potential and high values reflect better inhibition. ΔE is a reactivity factor and its low value results in good inhibition. Interaction energy obtained from molecular dynamic simulation of the inhibitors on Fe(110) plane at 303 K were in the order: DMPD (-105.918 kcal mol^{-1}) > TMPD (-114.46 kcal mol^{-1}) > TMMB (-130.9 kcal mol^{-1}). Interaction energy represents the binding energy of the adsorbate on the adsorbent. Micrographs of scanning electron microscopy (SEM) revealed the formation of dense film on the surface of mild steel which retarded the activities of aggressive ions. Therefore, it is concluded that isolates from *C. nitida* are effective green corrosion inhibitors of mild steel in hydrochloric acid solution.

[392 words]