Toward a Theoretical Understanding of the Corrosion Inhibitive Performance on Iron Surface by Some Macrocyclic Polyether Compounds Containing 1, 3, 4-thiadiazole Entity

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The corrosion inhibitive performance, in acidic medium, of macrocyclic polyether compounds: 1-MCTH, 2-MCTH and their protonated forms, was studied on the basis of their degree of planarity, global and local electronic proprieties as well as their deformation capacity to adhere the metal surface, by using DFT calculations and Dynamic Monte Carlo simulations. The proton affinity evaluation locates the most favourable site of protonation. 2-MCTH was found more reactive in vacuo and aqueous phase. Moreover, the Fe-(N9N10)-like interaction involving 2-MCTH is the strongest, as the interaction with iron obeys the following order: 2-MCTH > 2-MCTH (NH⁺)₂ > 1-MCTH > 1-MCTH(NH⁺)₂ in accordance with electrochemical results.

Keywords: Acid solution; Iron surface; DFT calculations; Dynamic Monte Carlo calculations; Corrosion inhibitive performance.

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