



Azo Schiff Base as Antiscaling Agent for Mild Steel in Hydrochloric Acid: Electrochemical, Non-electrochemical, and DFT Studies

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Abstract

Anticorrosive behavior of Azo Schiff base ligand comprising 4-[5-((4-chlorophenyl) diazenyl)-2-hydroxybenzylideneamino]-1,5-dimethyl-2-phenyl-1H-pyrazole-3-(2H)-one (CDHBAP) on mild steel in 1 M HCl was investigated by Gravimetric method, AC Impedance measurements, and Tafel polarization techniques. The corrosion rate of mild steel in 1 M HCl solutions increased with increasing temperature (308–328 K). When increasing the concentration of CDHBAP (15–100 ppm), the corrosion rate of mild steel in 1 M HCl solutions decreases and inhibition efficiency is increased. Nyquist plot shows that charge resistance value increased with increasing concentration of CDHBAP. Polarization studies confirm that CDHBAP acts as mixed type inhibitor with predominant anodic effect. The Fourier transform-infrared spectroscopy (FT-IR) and UV-visible (UV-Vis) studies confirm the existence of an absorbed film on mild steel surface. Thermodynamic and adsorption studies reveal that adsorption of CDHBAP abide Langmuir adsorption isotherm. Quantum chemical calculations are further employed to enumerate the relation between quantum chemical parameters (E_{HOMO} , E_{LUMO} , ΔN) and corrosion inhibition efficiency.

Keywords Mild steel · Weight loss · Adsorption · Langmuir · DFT studies

1 Introduction

Corrosion problem is one of the major economic concerns in the gas and petrochemical industry. Therefore, protection of metallic structures against corrosion is regarded as a very important subject. Oil well acidizing, industrial acid cleaning, acid pickling, and acid descaling are processes in which iron alloys are subjected to acid solutions like hydrochloric acid and sulphuric acid. In these environments, inhibitors are necessary in order to minimize the acid dissolution of iron alloys via adsorption at the metal/solution interface [1]. Most of the accepted acid inhibitors are organic compounds containing oxygen, nitrogen, and/or sulfur atoms. Organic inhibitors often work by adsorbing themselves on the iron surface, protecting it by forming a film [2]. The strength of

the adsorption bond is the main factor for organic inhibitors and its effectiveness depends on the chemical structure, their chemical composition, and their affinity. Unfortunately, some of the organic inhibitors used are quite expensive and potentially harmful to the environment because the use of toxic and hazardous chemicals is responsible for various biological risks [3, 4]. Their toxic properties limit the area of application. Therefore, it remains an important goal to find cost-effective inhibitors of the harmless type to protect metals against corrosion. Pyrazole compounds satisfy these requirements [5]. These compounds have a large number of functional adsorption centers (e.g., -OH group, -CH₃ group, -C=O, -N=N- group, O and N heteroatoms, and aromatic rings). They are strongly basic, and hence they can be readily soluble in the acid medium. Recently, a few modern procedures are associated to check corrosion inhibitors [6]. The theoretical approach to the present issue continues to be foremost half standard and unbroken to quantum chemical calculations together with confined inhibitor molecules [7] and to few degree to the interaction of inhibitor particles with surface particles through semi-empirical and ab initio strategies [8]. In this way within the field of theoretical examination of corrosion inhibitors, improvement of

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