# PREFACE

Corrosion is a naturally occurring phenomenon commonly defined as the deterioration of a material that results from a chemical or electrochemical interaction with its environment. It is a major problem in several industries. It causes enormous economic wastage of metallic materials, which leads to heavy economic losses all over the world. The direct cost of corrosion includes the replacement of corroded components, the use of corrosion resistant alloys and the use of coating and inhibitors etc. The indirect costs of corrosion includes the loss of production during downtime, loss of products due to leakage, loss of efficiency, contaminations and sometimes it causes loss of human lives due to explosion/fire. The annual global cost of corrosion was estimated to be around $ US 2.5 trillion which constitute about 3% of the world GDP.

In industries mild steel (MS) is mostly used alloy due to its low cost, high mechanical strength, and easy of availability. It is widely used as a construction material in petroleum refineries. Mild steel is used for the construction of components in fractionation tower,

separator drums, heat exchangers shell and tubes, reactor cladding, tubes in furnaces, piping and reboiler tubes etc. The mild steel is severely attacked in acid solutions by hydrochloric acid, sulphuric acid, formic acid, hydrogen sulphide, hydrofluoric acid, acetic acid and caustic in oil sector during processes related to drilling and distillation. However, the cost of mild steel corrosion can be reduced about 20-25% by applying recently available methods of corrosion prevention. There are various corrosion control techniques. These are proper design, materials selection, electrochemical protection and the use of inhibitors and paints/coatings. Among these methods, inhibitors are used in a wide range of applications, such as oil pipelines, domestic central heating systems, industrial water-cooling systems and metal extraction plants. The advantage of corrosion inhibitor is that it can be implemented or charged in situ without disrupting a process and is also a cost effective method. The major industries using corrosion inhibitors are the oil and gas exploration and production industry, the petroleum refining industry, the chemical industry, heavy industrial manufacturing industry, water treatment facilities, and the product additive industries. Due to ease of application and cost effectiveness, the use of inhibitors has increased manifold during the past several years.

Nowadays, the corrosion inhibitors is being used as the most popular and effective technique for combating corrosion. As the title itself reflects, the thesis highlights the attempts made in developing heterocyclic compounds such as pyrano-pyrazole derivatives (EPPs), pyrazolo-pyridine derivatives (PPs), imidazole derivatives( IMs) and Schiff bases derived from 2, 6 diaminopyridine (DAPs) as corrosion inhibitors.

The thesis starts with introduction highlighting the technological and economic significance of the problems associated with corrosion. The various forms and theories of

corrosion have been described in order to explain the mechanism of corrosion. In the later part of the introduction, different measures of metallic corrosion inhibition with particular emphasis of heterocyclic compounds as corrosion inhibitors in acid solution have been described. The literature on the metallic corrosion inhibition by heterocyclic compounds as corrosion inhibitors has been surveyed. The results obtained from the gravimetric and electrochemical techniques have been discussed section wise in terms of several commonly used corrosion parameters such as percentage inhibition efficiency ($\eta$%), corrosion rate ($C_R$), charge transfer resistance ($R_{ct}$), corrosion current ($i_{corr)}$ and corrosion potential ($E_{corr}$). The activation and thermodynamic parameters have also been calculated in order to find mechanistic information about the adsorption of inhibitor molecules on the metallic surface. The effects of inhibitors concentration and solution temperature on inhibition efficiency of the heterocyclic compounds have also been discussed. The SEM and AFM studies have been employed to confirm the presence of protective film of inhibitors on the mild steel surface. The DFT based quantum chemical calculations and molecular dynamics simulations have been carried out in order to correlate experimentally determined inhibition efficiencies with several computed parameters such as energy of highest occupied and lowest unoccupied molecular orbitals, $E_{HOMO}$ and $E_{LUMO}$, respectively, energy band gap ($\Delta E$), dipole moment ($\mu$), electronegativity ($\chi$), global hardness ($\eta$) and softness ($\rho$) and fraction of electron transfer ($\Delta N$). A possible mechanism of corrosion has been proposed on the basis of experimental and computational analysis.

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