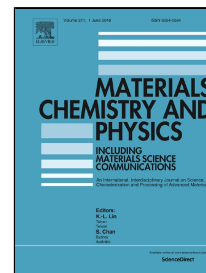


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Comparison of Inhibition Performance of Pyridine Derivatives Containing Hydroxyl and Sulfhydryl Groups: Experimental and Theoretical calculations

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Abstract: The inhibition performance of 2-hydroxypyridine (2HP), 4-hydroxypyridine (4HP), 2-mercaptopyridine (2MP) and 4-mercaptopyridine (4MP) on the corrosion of air hardening tool steel in 0.5 M HCl solution has been studied using electrochemical and weight loss method. Results indicated that the inhibition performance of these inhibitors follows the sequence: 4MP > 2MP > 4HP > 2HP. Theoretical calculation was employed to ascertain the effect of hydroxyl and sulfhydryl groups on the inhibition performance of these inhibitors. It was observed that 4MP molecule exhibits the best electrophilic attack ability, this could be attributed to the existence of sulfhydryl groups and also, its distribution position. The observed phenomenon favors the chemical adsorption of 4MP molecules onto the metal surface. Furthermore, scanning electron microscopy analysis revealed that the metal surface was more protected in the presence of 4MP compared to other inhibitors. This is in line with the electrochemical and weight loss results. The distribution position of sulfhydryl and hydroxyl groups have a significant effect on the electrophilic attack performance of the studied inhibitors, and the electrophilic attack ability decreases in the order 4MP > 2MP > 4HP > 2HP. 4MP gave the highest inhibition efficiency value of 98.9%.

Keywords: Carbon steel; EIS; Weight loss; Acid inhibition; Theoretical calculation

1. Introduction

Organic inhibitors containing heteroatoms (nitrogen, oxygen, and sulfur),

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