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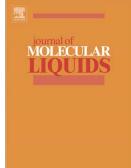
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ACCEPTED MANUSCRIPT

Imidazole based compounds as copper corrosion inhibitors in seawater

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Highlights:

- Inhibition efficiency at corrosion potential follows the order: imidazole < purine < adenine < 6-benzylaminopurine.
- Quantum chemical calculations show the same trend in the change of ΔE and IE.
- Adenine provided higher inhibition efficiency in the broader potential range.

Abstract: The effects of imidazole and its structural derivatives: purine, adenine and 6benzylaminopurine, on copper corrosion in seawater were investigated. Electrochemical methods were chosen for this purpose and the results show that they all act as mixed-type corrosion inhibitors under tested conditions. According to the potentiodynamic polarization results inhibition efficiency at corrosion potential increases in the following order imidazole < purine < adenine < 6-benzylaminopurine, which is in agreement with the expectation that the increase of molecular weight and number of heteroatoms in the molecule leads to the increase of inhibition efficiency degree. In the broader potential range, adenine is more efficient. The mechanism of inhibitor action includes adsorption on copper surface that fits the Langmuir adsorption isotherm. Quantum mechanical calculations indicate that there is a correlation between energy gap and inhibition efficiency.

Keywords: copper corrosion; imidazole; purine; adenine; 6-benzylaminopurine; seawater

1. Introduction

Copper is very important material in more than one aspect. It can be found, pure or in the form of an alloy, in the majority of modern electronic devices, plumbing, heat exchangers etc. However, the exposure to some media can induce the appearance of corrosion that either leads to dissolution or scales formation [1-5]. Either way the performance is in this way compromised. Very widespread and proved to be corrosive media is seawater [6,7]. According to the composition of seawater, the predominant ions are chloride ions that are well known for their ability to stimulate copper corrosion. According to the review published by Kear et al. [8], the mechanism of copper electro-dissolution in the presence of chloride ions can be proposed [8]:

(I)	$Cu + 2Cl^{-} \leftrightarrow CuCl_{2}^{-} + e^{-}$	(1)
(TT)	α α + \cdot	$\langle \mathbf{O} \rangle$

- (II) $Cu \leftrightarrow Cu^+ + e^-$ (2) $Cu^+ + 2Cl^- \leftrightarrow CuCl_2^-$ (3)
- (III) $Cu + Cl \leftrightarrow CuCl + e^{-1}$ (4) $CuCl + Cl \leftrightarrow CuCl_{2}^{-1}$ (5)

Mechanisms I and III present the direct formation of a cuprous chloride species from copper, and II presumes the dissolution to Cu^+ ion. It is believed that $CuCl_2$ controls the kinetics of anodic dissolution of copper in inhibitor free solutions. Obviously, in such cases there is a need for the use of copper corrosion inhibitors. Nowadays, there is a plenty of proved

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