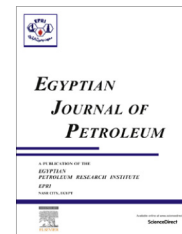


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## FULL LENGTH ARTICLE

# Corrosion protection of mild steel in hydrochloric acid solution through the synergistic of alkylbenzimidazoles and semicarbazide pair – Electroanalytical and computational studies

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## KEYWORDS

Adsorption;  
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**Abstract** Hydrogen bonded interaction and synergistic effect on the corrosion protection properties of alkyl benzimidazoles and semicarbazide pair on mild steel in hydrochloric acid at 303, 308 and 313 K have been studied by polarization, electrochemical impedance spectroscopy, adsorption, surface studies and basic computational calculations. The inhibition efficiencies and the global chemical reactivity relate to total energy,  $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$  and gap energy ( $\Delta E$ ). Semicarbazide interacts with alkyl benzimidazoles up to an average bond length of 1.9296 Å. This interaction may be due to the formation of a hydrogen bond between semicarbazide and alkyl benzimidazoles. This synergistic interaction offer extended inhibition efficiency toward mild steel in hydrochloric acid. The corrosion inhibition efficiencies and the global chemical reactivity relate to total energy,  $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$  and gap energy ( $\Delta E$ ).

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## 1. Introduction

Superior properties such as structural and mechanical strengths of mild steel make it as a very crucial material in various industrial and engineering applications [1–3]. Acid solutions are widely used in industrial fields of application being acid pickling of steel, chemical cleaning and processing, ore

production and oil well acidification [4]. Hydrochloric acid and sulfuric acid are commonly used for this purpose. However, these acids attack the metal and initiate corrosion. This corrosion can cause serious damages to the metal and degrade its properties, thereby limiting its applications [5–7]. That is, corrosion causes economic loss and even serious operational problems [8,9]. The use of inhibitor is the most important method for protecting metals from corrosion, and many scientists are conducting research on this topic. New inhibitors are discovered every day. In principle, inhibitors prevent the corrosion of metals by interacting with the metal surface via adsorption through the donor atoms,  $\pi$  orbitals, electron density and the electronic structure of the molecule [10–15].

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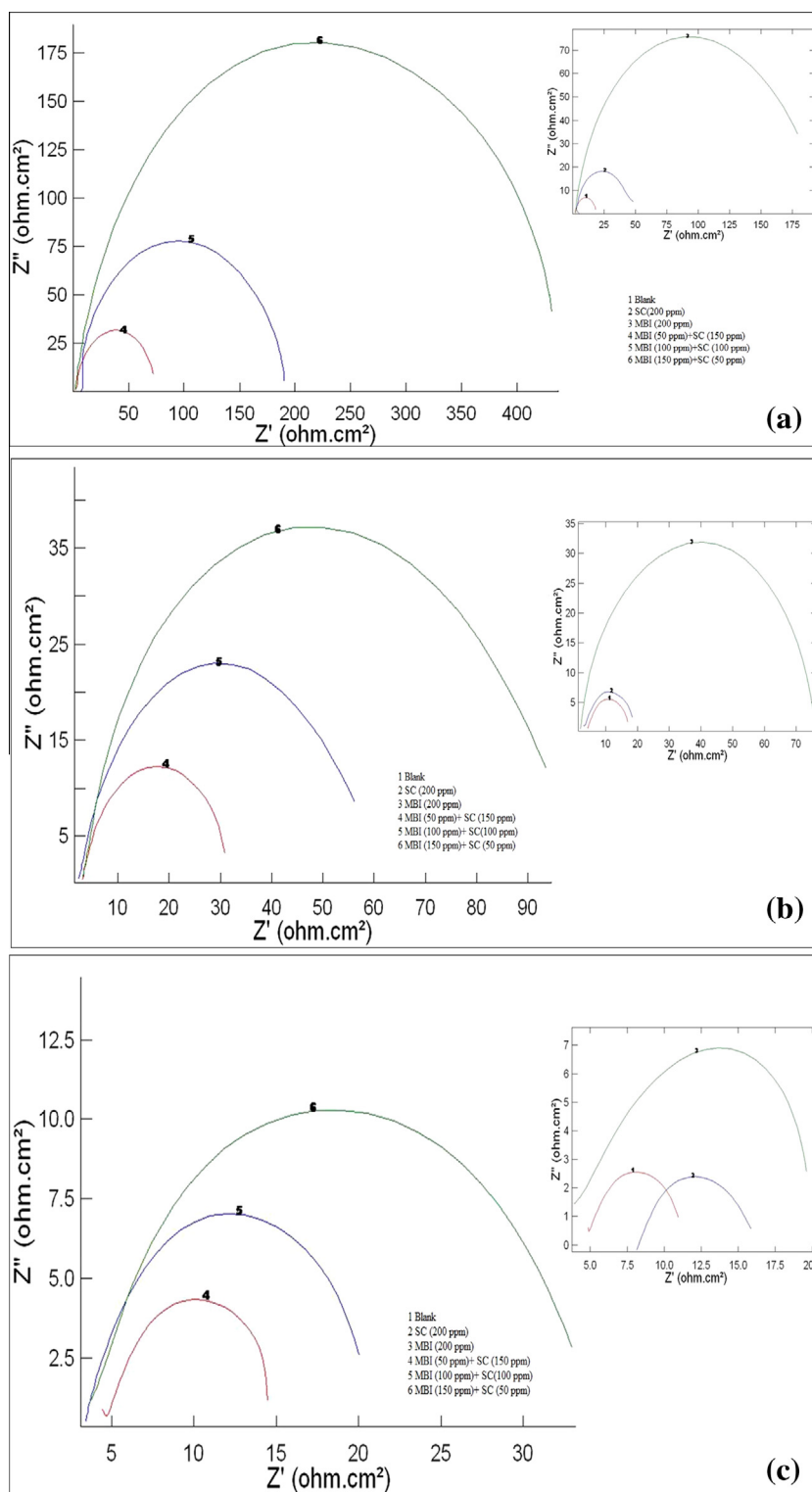
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**Figure 1** Nyquist plot for mild steel in 1 M HCl in the presence of MBI and SC at different temperatures (a) 303 K, (b) 308 K and (c) 313 K. [Inset: Nyquist plot for blank and in the presence of individual inhibitor MBI and SC].

That is, the inhibitor molecules adsorb on the metal surface by displacing water molecules on the surface and forming a protective film [16–19]. Regarding the adsorption of inhibitor on the metal surface, two types of interactions are responsible. One is physical adsorption, which involves electrostatic forces

between ionic charges or dipoles of the adsorbed species and the electric charge at the metal/solution interface. The other is chemical adsorption, which involves charge sharing or charge transfer from inhibitor molecules to the metal surface to form coordinate type of bond [20,21].

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