

Title	Theoretical and Experimental Investigation of the Synergistic Influence of Tricine and Iodide Ions on the Corrosion Control of Carbon Steel in Sulfuric Acid Electrolyte
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### Abstract

The combination of experimental and theoretical investigations of the adsorption/inhibition effect of tricine [*N*-(Tri(hydroxymethyl)methyl)glycine] as newly green corrosion inhibitor for the carbon steel has been investigated in aqueous H<sub>2</sub>SO<sub>4</sub> electrolyte. The synergistic inhibition effect of tricine molecules and iodide ions on the corrosion of carbon steel in H<sub>2</sub>SO<sub>4</sub> solution was scrutinized. Potentiodynamic polarization, electrochemical impedance spectroscopy, scanning electron microscope, and energy dispersive X-ray analysis techniques have been exploited to examine the influence of tricine and iodide on the corrosion of carbon steel in 0.1 M H<sub>2</sub>SO<sub>4</sub> solution. SEM analysis shows the adsorbed layer inhibitors on carbon steel surface composed of tricine and iodide ions offering the long time protection for carbon steel in 0.1 M H<sub>2</sub>SO<sub>4</sub> solution. Computational quantum and molecular dynamic simulation studies have been further used to calculate the electronic properties of tricine molecule to clarify the tricine molecular structure and inhibitive effect of the corrosion. Total energy (TE),  $E_{LUMO}$ ,  $E_{HOMO}$ , dipole moment ( $D$ ), energy gap ( $\Delta E$ ), softness ( $\delta$ ), and the change of the total energy (DET) have been calculated. The electrochemical and microstructure techniques display that the tricine is the greatly efficient inhibitor of mixed type with inhibition efficiency up to 87.4% and the adsorption of tricine adheres to Langmuir isotherm. The tricine inhibition efficiency increases via addition of iodide ions owing to synergistic effect.