Pyridoxal (thio) Semicarbazone Ligands and Their Fe(III) Complexes as Potential Electrocatalysts for Hydrogen Evolution Reaction

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A significant requirement for a future hydrogen economy and easily accessible renewable energy is efficient production of hydrogen from aqueous protons by direct solar energy conversion. The synthesis of a catalyst that can facilitate the reaction of hydrogen evolution (HER) is of paramount importance to achieve this overall objective. This study focuses on catalytic activity of pyridoxal-semi (H₂-PLSC) and pyridoxal-thiosemi (H₂-PLTSC) carbazone molecules and their iron complexes Fe(H-PLTSC)(PLTSC)]·4H₂O and [Fe(H₂-PLSC)Cl₂ (H₂O)]Cl, for electrochemical proton reduction into hydrogen. The free ligands (H₂-PLSC and H₂-PLTSC) were able to electrocatalyze the reduction of proton into hydrogen. Even though, the studied complexes were more catalytically active than the free ligand, this observation provided crucial evidence for the proposed mechanism that involved protonation of the ligand.

Keywords: Pyridoxal-semicarbazone, Pyridoxal-thiosemicarbazone, Iron complexes, electrocatalysis

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