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Title: Synthesis of mononuclear Ni, Co and Zn complexes and study of electrolcatalyctic hydrogen evolution

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Abstract:

Electrocatalytic hydrogen evolution reaction (HER) is a promising strategy for the production of hydrogen as a sustainable and clean energy carrier, capable to substitute current fossil fuels. The electrocatalysts used in HER must possess high activity, stability, and selectivity towards proton reduction. The electrocatalyst play a crucial role in enhancing the efficiency of the reaction to proceed at a higher rate, reducing the overpotential required for hydrogen evolution, and providing stability. In recent years, significant efforts have been made to develop new electrocatalysts based on transition metal complexes, metal oxides, and metal sulfides. The design of these electrocatalysts involves the rational tuning of their electronic, geometric, and catalytic properties, which can be achieved through various synthetic and characterization methods. In this context, we have synthesized electrocatalysts using first row transition metals Ni, Co, Zn and non-innocent ligand 2,6-bis((E)-1-(2 - phenylhydrazineylidene)ethyl)pyridine which is also having  $\pi$ -accepting sites. These synthesized metal complexes were further characterized using NMR spectroscopy, UV- Visible spectroscopy, Infrared spectroscopy, ESI-Mass spectrometery, and single crystal X-ray diffraction. The electrochemical properties were then evaluated using cyclic voltammetry in presence of glacial acetic acid as proton source. The TOF of synthesized [Ni II (L 1) 2]Cl 2 and [Co II (L 1) 2]Cl 2 are 9.42 × 10 3 s -1 and 1.66 × 10 5 s -1 respectively at potential -2V. The higher TOF value of [Co II (L 1) 2]Cl 2 makes it comparatively better catalyst for hydrogen evolution reaction than corresponding [Ni II (L 1) 2]Cl 2.

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