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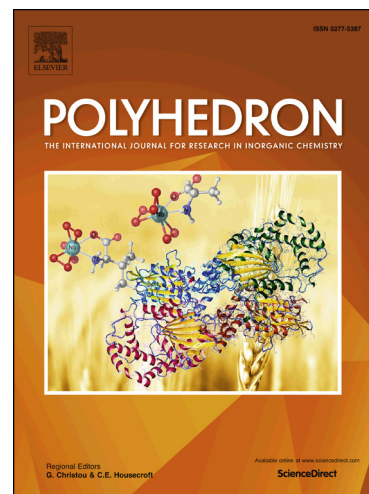
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Photocatalytic hydrogen production with alkylated nickel bis–dithiolene complexes

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ABSTRACT

Herein, we present the preparation and characterization of two nickel dithiolene complexes, namely $[\text{Ni}(\text{C}_3\{\text{S}_2\text{C}_2\text{Ph}_2\}_2)]$ (**1**) and $[\text{Ni}(\text{C}_3\{\text{p-OMe-C}_6\text{H}_4\}_2)]$ (**2**). X-ray diffraction data for **2** collected on single crystals reveal that the complex is a neutral mononuclear entity with symmetric square planar geometry around the metal center. Electrochemical, photophysical, and theoretical studies have been employed to characterize and to probe both compounds under study in photoinduced hydrogen evolution experiments. Catalyst (**2**) performs better than catalyst (**1**), reaching 73 TONs over a 5 h period with $[\text{Ru}(\text{bpy})_3]\text{Cl}_2$ as photosensitizer, in MeCN – water solvent mixture with ascorbate at pH = 4 as a sacrificial electron donor. The different catalytic activity between the two compounds is discussed based on their different electronic properties.

Keywords: Homogeneous, Photocatalysis, bridged-complex, Nickel, Hydrogen, Dithiolene

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