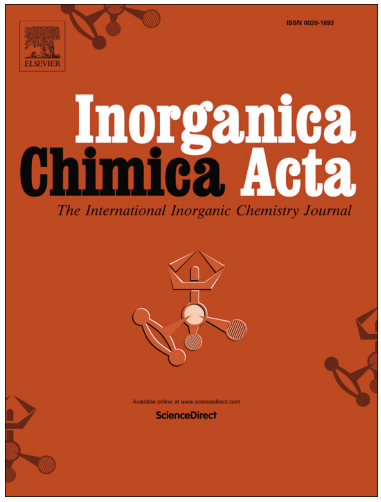


Research paper

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# Synthesis, Characterization and Electrocatalytic $H_2$ Production of Base-containing Fe/S and Fe/Se Clusters

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**Abstract:** Reaction of base-containing diphosphine ligand $NP^S_2$ ($NP_2$ = $(Ph_2PCH_2)_2NCH_3$) with $[Fe_3(CO)_{12}]$ in THF at room temperature forms $[\{Fe_2(CO)_6(\mu\text{-}PPh_2)\}_2(\mu_4\text{-}S_2)]$ (**1**) and $[Fe_3(CO)_8(\mu_3\text{-}S)_2\{kP\text{-}PPh_2CH_2N(CH_3)CH_2P(=S)Ph_2\}]$ (**2**) resulting from P=S bond cleavage and P-Fe bond formation. Similarly, $NP_2^{Se}{}_2$ reacts with $Fe_3(CO)_{12}$ to provide $[\{Fe_2(CO)_6(\mu\text{-}PPh_2)\}_2(\mu_4\text{-}Se_2)]$ (**3**) and $[Fe_3(CO)_7(\mu_3\text{-}Se)_2\{k^2P,P\text{-}(PPh_2CH_2)_2NCH_3\}]$ (**4**). All the compounds have been completely characterized by elemental analyses, IR, $^1H$ NMR, $^{13}C$ NMR and $^{31}P$ NMR spectroscopy and structurally determined by X-ray crystallography. Electrochemical studies reveal that when using HOAc or TFA as a proton source, **2** and **4** exhibit catalytic $H_2$ production.

**Keywords:** Fe/S Cluster; Fe/Se Cluster; Cyclic voltammetry; $H_2$ production

## 1. Introduction

The development of renewable energy is nowadays one of the most important challenges as global energy consumption is rising significantly. Molecular hydrogen is a carbon-free fuel that could become the energy carrier of the future, thus making the reversible interconversion of protons to molecular hydrogen a key process for future energy schemes. Nature is able to catalyze this process by a class of