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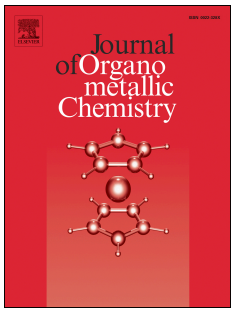

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Synthesis, Characterization and Electrocatalytic H_2 Production of Diiron Complexes Containing SeNC Donors

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Abstract: The three-component reactions of $ArNHC(=Se)OCH_3$, Et_3N and $Fe_3(CO)_{12}$ afford the $[Et_3NH]^+$ salt of the $(\mu\text{-}ArN{=}COCH_3)Fe_2(CO)_6(\mu\text{-}Se^-)$ cluster anion. The Se-centered cluster anion reacts with CH_3I to give two pairs of isomers $(\mu\text{-}k^2N,C\text{-}ArN{=}COR)Fe_2(CO)_6(\mu\text{-}SeCH_3)$ (**1**-e, **1**-a, Ar = C_6H_5) and $(\mu\text{-}k^2N,C\text{-}ArN{=}COR)Fe_2(CO)_6(\mu\text{-}SeCH_3)$ (**2**-e, **2**-a, Ar = 4-ClC_6H_4). Furthermore, trapping the Se-centered cluster anion $(\mu\text{-}ArN{=}COR)Fe_2(CO)_6(\mu\text{-}Se^-)$ with PPh_2Cl offers $(\mu\text{-}k^2N,C\text{-}ArN{=}COR)Fe_2(CO)_6(\mu\text{-}k^2Se,P\text{-}SePPh_2)$ (**3**, Ar = C_6H_5, **5**, Ar = 4-ClC_6H_4, R = CH_3; **4**, Ar = C_6H_5, **6**, Ar = 4-ClC_6H_4, R = CH_2Ph). Reactions of **1** with monophosphine L lead to the corresponding substituted complexes $(\mu\text{-}k^2N,C\text{-}PhN{=}COCH_3)Fe_2(CO)_5(L)(\mu\text{-}SeCH_3)$ (**7**-e, **7**-a, L = PPh_3; **8**-e, L = PPh_2Py). All the new complexes 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, all of the complexes can catalyze H_2 production.

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