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Synthesis and transition metal chemistry of ferrocenylbis(benzo-oxazaphosphininone)

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ABSTRACT: The new ferrocenylbis(oxazaphosphininone), $[\text{Fe}\{\text{C}_5\text{H}_4\text{P}(\text{OC}_6\text{H}_4)(\text{CO})\text{N}(\text{C}_2\text{H}_4\text{Cl})\}_2]$ (**1**) was synthesized by the reaction of bis(dichlorophosphino)ferrocene with two equivalents of 2(2'-hydroxy)phenyloxazoline in the presence of triethylamine in 83% yield. The reactions of **1** with aq. H_2O_2 or elemental sulfur afforded bis-chalcogenides $[\text{Fe}\{\text{C}_5\text{H}_4\text{P}(\text{E})(\text{OC}_6\text{H}_4)(\text{CO})\text{N}(\text{C}_2\text{H}_4\text{Cl})\}_2]$ (**2** E = O, **3** E = S). Treatment of **1** with $[\text{M}(\text{CO})_4(\text{C}_5\text{H}_{11}\text{N})_2]$ (M = Mo, W), $[\text{RuCp}(\text{PPh}_3)_2\text{Cl}]$ and $[\text{M}(\text{COD})\text{Cl}_2]$ (M = Pd, Pt) afforded the chelate complexes $[\text{Fe}\{\text{C}_5\text{H}_4\text{P}(\text{OC}_6\text{H}_4)(\text{CO})\text{N}(\text{C}_2\text{H}_4\text{Cl})\}_2\{\text{M}(\text{CO})_4\}]$ (**4** M = Mo, **5** M = W), $[\text{Fe}\{\text{C}_5\text{H}_4\text{P}(\text{OC}_6\text{H}_4)(\text{CO})\text{N}(\text{C}_2\text{H}_4\text{Cl})\}_2\{\text{RuCp}(\text{Cl})\}]$ (**7**) and $[\text{Fe}\{\text{C}_5\text{H}_4\text{P}(\text{OC}_6\text{H}_4)(\text{CO})\text{N}(\text{C}_2\text{H}_4\text{Cl})\}_2\{\text{MCl}_2\}]$ (**8** M = Pd, **9** M = Pt), whereas the reaction of **1** with $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}_2]_2$, yielded a bimetallic complex $[\text{Fe}\{\text{C}_5\text{H}_4\text{P}(\text{OC}_6\text{H}_4)(\text{CO})\text{N}(\text{C}_2\text{H}_4\text{Cl})\}_2\{\text{RuCl}_2(\eta^6\text{-p-cymene})\}_2]$ (**6**). The reaction between **1** and CuX in equimolar ratio also yielded binuclear complexes, $[\text{Fe}\{\text{C}_5\text{H}_4\text{P}(\text{OC}_6\text{H}_4)(\text{CO})\text{N}(\text{C}_2\text{H}_4\text{Cl})\}_2\{\text{CuX}\}_2]$ (**10** X = Cl, **11** X = Br, **12** X = I). All the compounds are characterized by spectroscopic methods and the structures of complexes **3**, **7**, **9** and **10** were confirmed by single crystal X-ray diffraction studies. The electrochemistry of **1**, **3**, **8**, **9** and **12** is also reported.

Keywords: ferrocene; X-ray structure; dppf; phosphininone; diastereomer

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1. Introduction

The *1,1'*-bis(phosphino)ferrocene ligands have spotted a continuous growth since the discovery of dppf.[1] Dppf and analogues ferrocenylbisphosphines have been used in several catalytic applications [2-6]; whereas the chiral counterparts have been employed in

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