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Reactivity of Iron Complexes containing Monodentate Aminophosphine Ligands - Formation of Four-Membered Carboxamido-Phospha-Metallacycles

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Abstract

Treatment of $[FeCp(CO)_2Cl]$ with 1 equiv of the amidophosphine ligands $Li[R_2PNR']$ (R = Ph, *i*Pr, R' = *i*Pr, *t*Bu, Cy) afforded complexes of the type $[FeCp(CO)(\kappa^2(C,P)\text{-}(C{=}O)\text{-}N\textit{i}Pr\text{-}PPh_2)]$ (**1a**), $[FeCp(CO)(\kappa^2(C,P)\text{-}(C{=}O)\text{-}N\textit{t}Bu\text{-}PPh_2)]$ (**1b**), and $[FeCp(CO)(\kappa^2(C,P)\text{-}(C{=}O)\text{-}NCy\text{-}P\textit{i}Pr_2)]$ (**1c**) in 40-50% yields. Complex **1a** was also formed when $[FeCp(CO)_2(PPh_2NH\textit{i}Pr)]^+$ (**2**) was reacted with 1 equiv of KO*t*Bu. These complexes feature a four-membered carboxamido-phospha-ferracycle as a result of an intramolecular nucleophilic attack of the amidophosphine ligand on coordinated CO. Upon treatment of **1a** with the electrophile $[Me_3O]BF_4$ the aminocarbene complex $[FeCp(CO)(\kappa^2(C,P)\text{=}C(OMe)\text{-}N\textit{i}Pr\text{-}PPh_2)]^+$ (**3**) was obtained bearing an aza-phospha-carbene moiety. Upon treatment of *cis,trans,cis*-$[Fe(CO)_2(Ph_2PNH\textit{i}Pr)_2(Br)_2]$ (**4a**) and *cis,trans,cis*-$[Fe(CO)_2(Ph_2PNH\textit{t}Bu)_2(Br)_2]$ (**4b**) with KO*t*Bu the carboxamido-phospha-ferracycles *trans*-$[Fe(CO)_2(\kappa^2(C,P)\text{-}(C{=}O)\text{-}N\textit{i}Pr\text{-}PPh_2)(Ph_2PNH\textit{i}Pr)Br]$ (**5a**) and *trans*-$[Fe(CO)_2(\kappa^2(C,P)\text{-}(C{=}O)\text{-}N\textit{t}Bu\text{-}PPh_2)(Ph_2PNH\textit{t}Bu)Br]$ (**5b**) were formed in moderate yield. Finally, representative structures were determined by X-ray crystallography.

Keywords: Iron, cyclopentadienyl, carbon monoxide, aminophosphines, nucleophilic attack, ferracycles

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