Poly(pyrazol-1-ylmethyl)benzene Palladium Complexes: Synthesis, Characterisation and Evaluation as Heck Coupling Catalysts

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The poly(pyrazol-1-ylmethyl)benzenes **L1** – **L5** react with $[PdCl_2(NCMe)_2]$ or [PdClMe(COD)] to form dinuclear palladium complexes $[\{PdClX(3,5\text{-}Me_2pzCH_2)_2\text{-}1,2\text{-}C_6H_4\}_2]$ (X = Cl (**1**), Me (**2**)), $[\{PdCl_2(3,5\text{-}Me_2pzCH_2)_2\text{-}1,3\text{-}C_6H_4\}_2]$ (**3**), palladium complexes $[\{Pd_2(\mu\text{-}Cl)_2Me_2(3,5\text{-}Me_2pzCH_2)_2\text{-}1,3\text{-}C_6H_4\}]$ (**4**), $[\{Pd_2(\mu\text{-}Cl)_2X_2(3,5\text{-}Me_2pzCH_2)_2\text{-}1,4\text{-}C_6H_4\}]$ (X = Cl (**5**), Me (**6**)), $[\{Pd_2(\mu\text{-}Cl)_2Cl_2(3,5\text{-}{}^tBu_2pzCH_2)_2\text{-}1,4\text{-}C_6H_4\}]$ (**7**), and tetranuclear $[\{Pd_2(\mu\text{-}Cl)_2Cl_2(3,5\text{-}Me_2pzCH_2)_2\}_2\text{-}1,4\text{-}C_6H_4]$ (**8**). The structures of **1**, **2** and **8** were confirmed by X-ray structure analysis. The complexes efficiently catalyse the coupling reaction of iodobenzene and butylacrylate at 80 °C.

Key words: Poly(pyrazol-1-ylmethyl)benzene Ligands, Palladium Complexes, Crystal Structures, Heck Coupling, Catalysts