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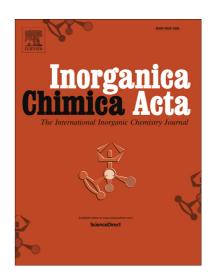
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Interaction of Benzene-1,2-diamines with Isocyanide Complexes of Palladium(II): Insight into the Mechanism

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Abstract

Reactivity of 4-toluidine (2) and 4,5-dimethylbenzene-1,2-diamine (3) were compared in coupling with the palladium-bis(isocyanide) complex cis-[PdCl₂(CNXyl)₂] (Xyl = 2,6-Me₂C₆H₃, 1), mixed isocyanide/diaminocarbene species cis-[PdCl₂(CNXyl){C(NHXyl)=NH(4-C₆H₄CH₃)}] (4), and cis-[PdCl(CNXyl){C(NHXyl)=NHC₆H₂(Me)₂NH₂}]Cl (5). In these Pd(II)-mediated reactions, 4,5-dimethylbenzene-1,2-diamine (3) was significantly more reactive than 4-toluidine (2),leading to the first *bis*(diaminocarbene) mixed complex cis- $[PdCl\{\underline{C}(NHR)=NHC_6H_2X_2\underline{N}H_2\}\{C(NHXyl)=NH(4-C_6H_4CH_3)\}]Cl$ (6) containing two different diaminocarbene ligands. Complex 6 was isolated and characterized by elemental analyses (C, H, N), HRESI⁺-MS, IR, ¹H and ¹³C{¹H} NMR spectroscopies, and single-crystal X-ray diffraction.

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