

Palladium(II) complexes with small N-heterocyclic carbene ligands as highly active catalysts for the Suzuki-Miyaura cross-coupling reaction.

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Streszczenie

Four new palladium(II) complexes of the type $[Pd(NHC)_2X_2]$ with N-heterocyclic carbene (NHC) ligands of relatively small steric hindrance were prepared and characterized by using spectroscopic and X-ray methods. For $[Pd(bmim-y)_2Br_2]$ ($bmim-y=1$ -butyl-3-methylimidazol-2-ylidene), crystals of both *cis* and *trans* isomers were obtained. All the studied complexes demonstrated very high activity in Suzuki–Miyaura cross-coupling in ethylene glycol, which yielded turnover numbers of up to 760 000. High activity was also observed if $NaBPh_4$ was used instead of $PhB(OH)_2$, and the best results (turnover number=580 000) were obtained with $[Pd(emim-y)_2Cl_2]$ ($emim-y=1$ -ethyl-3-methylimidazol-2-ylidene). In the reaction mixture, different forms containing $[Pd_x(NHC)_y]^+$ fragments ($x=1-4$, $y=2-5$) were identified by using ESI-MS. In the presence of Suzuki–Miyaura reaction substrates, catalytic palladium intermediates with aryl groups— $[Pd(NHC)_2Ph]^+$ and $[Pd_3(NHC)_4Ph]^+$ —were detected. Additional mechanistic investigations, such as TEM observations and mercury poisoning experiments, substantiated the formation of nanoparticles as a catalyst resting state. These heterogeneous particles serve as a reservoir for soluble palladium species—atoms or clusters that function as homogeneous catalysts for the Suzuki–Miyaura reaction.

Słowa kluczowe

carbene compounds, cross-coupling reactions, Heterogeneous catalysis, homogeneous catalysis, palladium

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