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Pd^{II} square planar complexes of the type $[IL]_2[PdX_4]$ as catalyst precursors for the Suzuki-Miyaura cross-coupling reaction. The first*in situ* ESI-MS evidence of $[(IL)_xPd_3]$ clusters formation.

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Streszczenie

Pd^{II} anionic, square planar complexes of the type $[IL]_2[PdX_4]$, where IL = imidazolium cations, X = Cl, Br, have been applied for the first time as catalyst precursors for the Suzuki–Miyaura (S–M) reaction carried out in alcohols at 40 °C. Depending on the structure of the catalyst precursor used, different yields of 2-methylbiphenyl (2-MePh–Ph) were obtained in a test reaction of 2-bromotoluene (2-MePhBr) with phenyl boronic acid ($PhB(OH)_2$). The highest yield, *ca.* 95%, was obtained for $[dmiop]_2[PdCl_4]$ (dmiop-1,2-dimethyl-3-propoxymethylene imidazolium cation) in methanol in the presence of KOH as a base. It was found that during the reaction Pd^0 nanoparticles of 4–7 nm have been formed *in situ* from the palladium(II) precursor. In the first stage of this process, $[(IL)_3Pd(OH)_2]^+$-type species have been formed from $[IL]_2[PdX_4]$ precursors. Small Pd^0 clusters, $[(IL)_5Pd_3(H_2O)]^+$ and $[(IL)_3Pd_3(H_2O)_7]^+$, were also identified by ESI-MS. These species reacted with $ArB(OH)_2$ forming palladium aryl complexes of the type $[(IL)_2PdAr]^+$, key intermediates in the catalytic process. The first experimental evidence of the IL stabilized Pd^0 species in S–M reaction is presented.

Słowa kluczowe

Palladium complexes, N-Heterocyclic carbenes, palladium nanoparticles, ESI-MS, Suzuki-Miyaura

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