Pd–PEPPSI N-Heterocyclic Carbene Complexes from Caffeine: Application in Suzuki, Heck, and Sonogashira Reactions

Autorzy

Md. Mahbubur Rahman

Jin Zhang

Qun Zhao

Jessica Feliciano

Elwira Bisz

Błażej Dziuk

Roger Lalancette

Roman Szostak

Michal Szostak

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The first synthesis of Pd–PEPPSI *N*-heterocyclic carbene complexes derived from the abundant and renewable natural product caffeine is reported. The catalysts bearing 3-chloropyridine, pyridine, and *N*-methylimidazole ancillary ligands were readily prepared from the corresponding N9-Me caffeine imidazolium salt by direct deprotonation and coordination to PdX_2 in the presence of *N*-heterocycles or by ligand displacement of $PdX_2(Het)_2$. The model Pd–PEPPSI–caffeine complex has been characterized by X-ray crystallography. The complexes were successfully employed in the Suzuki cross-coupling of aryl bromides, Suzuki cross-coupling of amides, Heck cross-coupling, and Sonogashira cross-coupling. Computational studies were employed to determine frontier molecular orbitals and bond order analysis of caffeine-derived Pd–PEPPSI complexes. This class of catalysts offers an entry to utilize benign and sustainable biomass-derived xanthine NHC ligands in the popular Pd–PEPPSI systems in organic synthesis and catalysis.

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