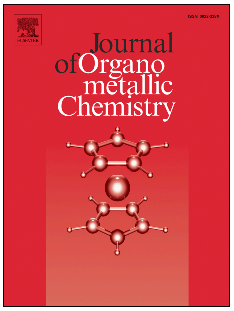

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Synthesis of *N*-Heterocyclic Carbene-Palladium-PEPPSI Complexes and Their Catalytic Activity in The Direct C-H Bond Activation

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ABSTRACT: A series of benzimidazolium salts having their two nitrogen atoms substituted by bulky groups have been synthesized. The benzimidazolium salts were readily converted into the corresponding palladium-NHC-PEPPSI complexes with general formula [$PdBr_2$(NHC)(Py)], (NHC = *N*-heterocyclic carbene; PEPPSI = pyridine-enhanced precatalyst preparation, stabilisation, and initiation). The structures of all new compounds were characterised by NMR, IR spectroscopy and microanalysis techniques, which support the proposed structures. The molecular structure of complex **2g** was determined by single-crystal X-ray diffraction study. Next, the palladium-NHC-PEPPSI complexes were used as catalysts in the direct C5-arylation of 1-methylpyrrole-2-carboxaldehyde by aryl halides. These complexes exhibited moderate to high catalytic activities and gave C-H activation selectively at the C5-position of 1-methylpyrrole-2-carboxaldehyde. Both electron-donating and electron-withdrawing substituents were well tolerated with catalytic systems based on these complexes, even non-activated aryl chlorides such as chlorobenzene or 4-chlorotoluene were coupled with pyrrole in moderate yields.

Keywords: *N*-heterocyclic carbene, benzimidazolium salts, PEPPSI-type palladium-NHC complexes, pyrroles, direct arylation.

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