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Title: Theoretical studies on the effect of substituents of the N-heterocyclic carbene ligand present in the Pd-PEPPSI complex on the formation mechanism of the Negishi cross-coupling reaction

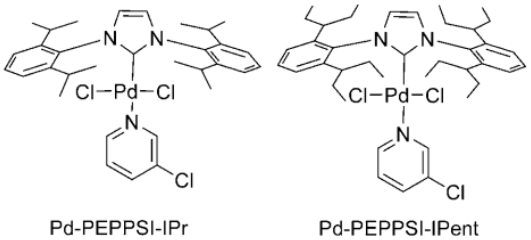
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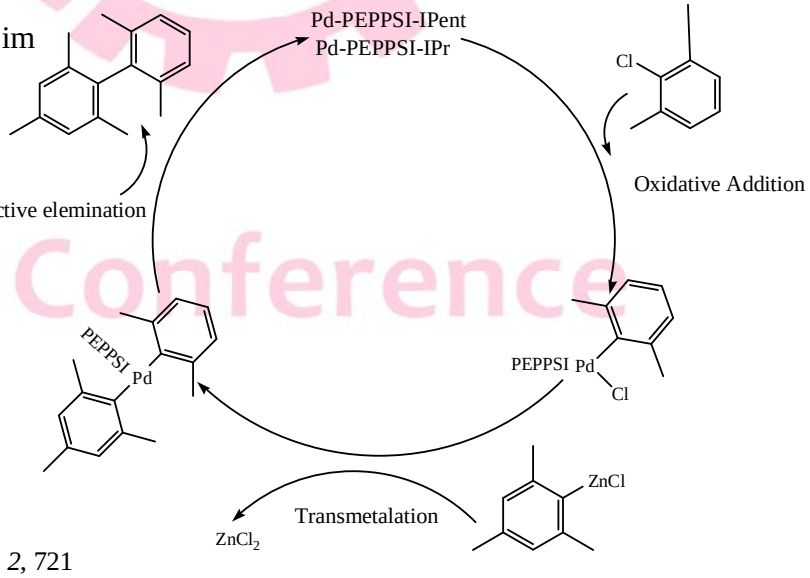
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Transition metal complexes bearing *N*-heterocyclic carbene ligands (NHCs) have gained a place of crucial importance in numerous areas of research such as medicinal chemistry, material sciences, and homogeneous/heterogeneous catalysis. [1]. Recently, several monoligated Pd–N-heterocyclic carbene (Pd–NHC) complexes have been prepared and have demonstrated high levels of activity in various Pd-catalyzed cross-coupling reactions, as reported [2]. The increased catalytic activity is attributed to the enhanced steric bulk of the NHC ligand. While oxidative addition does not seem to be significantly influenced by the sterics, both metal–metal exchange and reductive elimination appear to be affected [3]. The main focus of this project is to investigate the effect of NHC ligand side chains in Pd-PEPPSI complexes. Mechanistic studies on biaryl compounds using Pd-PEPPSI complexes as catalysts in Negishi cross-coupling reactions are being examined. The theoretical results obtained in this project demonstrate that the Pd-PEPPSI-iPent catalyst outperforms Pd-PEPPSI-iPr, which is consistent with experimental findings. Calculations were conducted using the Gaussian09 program with the CAM-B3LYP/DEF2-SVP method.

Keywords: Negishi, Cross-coupling, Mechanisim



Pd-PEPPSI-IPr Pd-PEPPSI-IPent



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