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| Title: | Steric effect of NHC ligands in Pd(II)–NHC-catalyzed non-directed C–H acetoxylation of simple arenes |
| Authors: | Yadav, Sudha (/jspui/browse?type=author&value=Yadav%2C+Sudha) |
| Keywords: | Palladium N-heterocyclic carbene (NHC) Non-directed C–H functionalization Acetoxylation Arene Site-selectivity |
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| Abstract: | <p>Although there has been a lot of progress in oxidative arene C–H functionalization reactions catalyzed by Pd(II/IV) system, the non-directed, site-selective functionalization of arene molecules is still challenging. It has been established that ligands play a pivotal role in controlling rate- as well as selectivity-determining step in a catalytic cycle involving well-defined metal-ligand bonding. N-heterocyclic carbene (NHC) ligands have had a tremendous contribution in the recent extraordinary success of achieving high reactivity and excellent selectivity in many catalytic processes including cross-coupling and olefin-metathesis reactions. However, the immense potential of these NHC ligands in improving site-selectivity of non-directed catalytic C–H functionalization reactions of simple arenes is yet to be realized, where overriding the electronic bias on deciding selectivity is a burdensome task. The presented work demonstrated an initiative step in this regard. Herein, a series of well-defined discrete [Pd(η³-py)₂] complexes with systematically varied degree of spatial congestion at the Pd centre, exerted through the R and R' substituents on the NHC ligand, were explored in controlling the activity as well as the site-selectivity of non-directed acetoxylation of representative monosubstituted and disubstituted simple arenes (such as toluene, iodobenzene and bromobenzene, naphthalene and 1,2-dichlorobenzene). The resulting best yields were found to be 75% for toluene and 65% for bromobenzene with [Pd(η³-py)₂], 75% for iodobenzene and 79% for naphthalene with [Pd(η³-py)₂], and 41% for 1,2-dichlorobenzene with [Pd(η³-py)₂]. Most importantly, with increasing the bulkiness of the NHC ligand in the complexes, the selectivity of the distal C-acetoxylation products in comparison to the proximal ones, was enhanced to a great extent in all cases. Considering the vast library of NHC ligands, this study underscores the future opportunity to develop more strategies to improve the activity and the crucial site-selectivity of C–H functionalization reactions in simple as well as complex organic molecules.</p> |
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