

演題：“Designing a catalyst from first principals for C-C and C-X Bond formation”

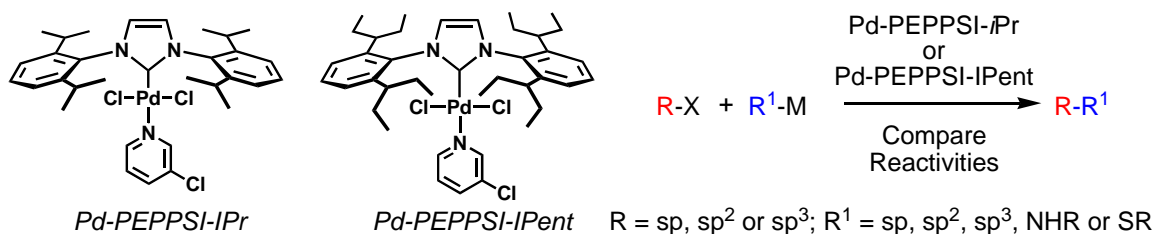
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日時：2010年10月29日(金) 16:00-17:30

場所：北海道大学創成科学研究棟 5階 大会議室

共催：触媒化学研究センターコロキウム（談話会）

要旨： The Pd N-Heterocyclic carbene (NHC)-based pre-catalyst based on bis N,N-(2,6-diisopropylphenyl) imidazolium (Pd PEPPSI-*i*Pr) has shown to be highly reactive in a wide variety of cross-coupling procedures. The catalyst has been examined in Suzuki-Miyaura, Negishi, Kumada-Tamao-Corriu, Sonagashira, and Hiyama couplings, in addition to enolate arylation and Buchwald-Hartwig-Yagupol'skii amination. PEPPSI-*i*Pr shows great reactivity in every case, in particular for the synthesis of complex, heteroatom-containing molecules (e.g., heterocycles) of biological interest; the coupling of intensely hindered oxidative addition and organometallic centres is routinely obtained. Within all of these families of reactions, couplings involving sp , sp^2 and sp^3 centers have been examined and all possible combinations yield good to excellent conversions.



In an attempt to gain understanding on the reactivity of NHC-based catalysts, an aggressive mechanistic study has been undertaken comprised of NMR spectroscopy, computational methods, and rate studies. Clearly the size of the groups on the flanking N-phenyl substituents plays a key role in the reactivity of the Pd-NHC complex. Attempts have been made to construct a catalytic cycle for Pd-NHC complexes and to subsequently dissect it to see where sterics plays its biggest part. This physical and structural analysis has led to the creation of second generation NHC catalyst, bis N,N-(2,6-di(3-pentyl)phenyl) imidazolium (Pd PEPPSI-*i*Pent), whose activity has surpassed all previously reported N-phenyl imidazolium-based Pd catalysts.

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