

# New Palladium(II)-N-Heterocyclic Dicarbene Complexes: Synthesis, Characterization and Catalytic Applications

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## Summary

The main aim of the project was to design and produce new homogeneous and water soluble palladium(II)-NHC complexes that should be applied as catalysts in cross coupling reactions. This project was funded by KFUPM within KFUPM-NUS research agreement.

## Introduction

Coupling reactions are well-established and important tools for carbon-carbon bond formation and for the synthesis of new interesting monomers, intermediates and materials for petrochemical and polymer industries. New Pd(II)-NHC catalysts are synthesized and applied to Suzuki-Miyaura and Heck-Mizoroki cross coupling reactions.

## Synthesis of palladium(II) bis-(1,2,4-triazolin-5-ylidene) complexes

New palladium(II) bis-(1,2,4-triazolin-5-ylidene) complexes (Pd-NHC) were synthesized and fully characterized by NMR, ESI, EA, and single crystal X-ray diffraction.

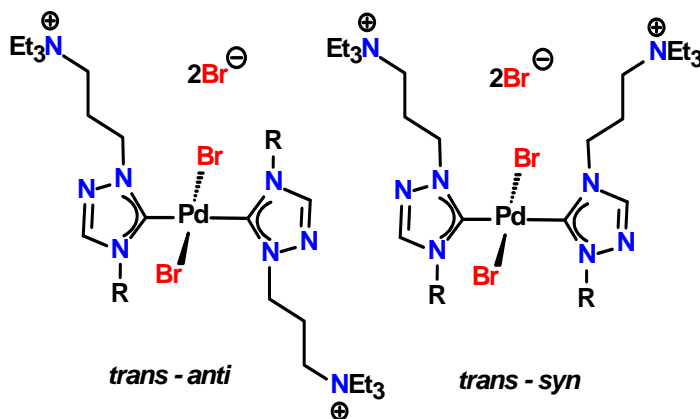


Figure 1. New palladium(II) bis(1,2,4-triazolin-5-ylidene) complexes.

Pd-NHC-1: R=mes; Pd-NHC-2: R=Cy;  
Pd-NHC-3: R=Dipp; Pd-NHC-4: R=Ph.

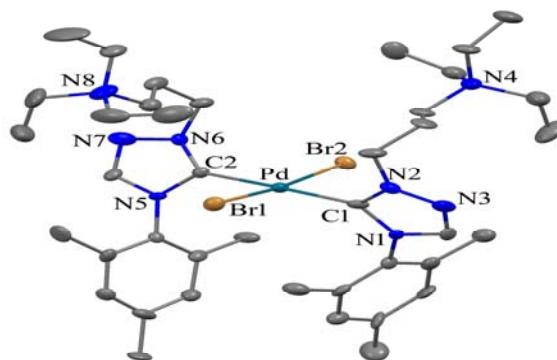
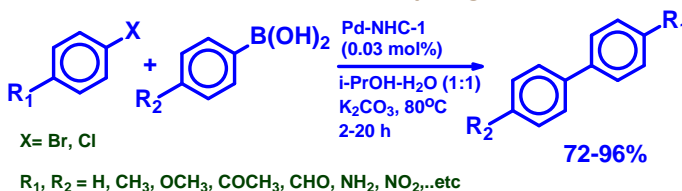


Figure 2. Molecular structure in solid state of Pd-NHC-1.

## Suzuki-Miyaura coupling reactions by Pd-NHC-1

Suzuki-Miyaura coupling reaction of arylboronic acids and aryl halides is a dominant method for the synthesis of biaryls. Pd-NHC-1 catalyzed successfully the coupling reactions of arylboronic acids with various aryl bromides and aryl chlorides. The other Pd-NHC complexes were also active in these coupling reactions.



## Mizoroki-Heck coupling reactions by Pd-NHC-1

Mizoroki-Heck reaction is a widely used method for the regioselective synthesis of unsaturated compounds. The catalytic activity of Pd-NHC-1 complex was also evaluated in Mizoroki-Heck coupling reaction of styrene derivatives with different aryl bromides. The other Pd-NHC complexes were also active in Heck coupling reactions.

