

## **Pd<sup>II</sup>, and Pt<sup>II</sup> assisted 1,2-azaphosphole formation in a functionalized bisphosphine: Synthesis, mechanistic studies and catalytic *N*-alkylation reactions**

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The chemistry of phosphines, especially tertiary phosphines, is studied to an extent that the systematic fine-tuning of the steric and electronics attributes can now be achieved with certain degree of predictability. [1-3] Herein, we describe a novel bisphosphine with additional donor functionalities, *o*-Ph<sub>2</sub>PC<sub>6</sub>H<sub>4</sub>QC<sub>6</sub>H<sub>4</sub>PPh<sub>2</sub>-*o*, which showed unique reactivity towards Pd<sup>II</sup> and Pt<sup>II</sup> precursors. Reaction of bisphosphine with palladium afforded an 1,2-azaphosphole complex, whereas in a similar reaction with Pt<sup>II</sup>, a complex containing a Pt-Ph bond was isolated. By varying metal to ligand ratios and metal precursors, several interesting complexes including pincers were isolated and structurally characterized. Mechanistic studies for the formation of palladium complex were investigated using NMR spectroscopy, DFT calculations and by SCXRD analysis. It involves reductive elimination to form a phosphonium salt followed by the oxidative addition. The palladium complex showed exceptional catalytic activity towards *N*-alkylation of amines with alcohols with a very low catalyst loading (0.05 mol %). The details of reactions, synthesis, metal chemistry and catalytic aspects will be presented in detail.

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