Pd(η^3-1-Ph-C_3H_4)(η^5-C_5H_5), a preferred precatalyst for cross-coupling reactions catalyzed by bis-phosphine palladium(0) compounds
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Little attention has been given to the formation of the putative PdL_2 species required for Pd-catalyzed cross-coupling reactions. Active species are generally difficult to store due to air-sensitivity and are therefore formed in situ at unknown rates and in unknown yields via a variety of palladium precatalysts. We have noted previously (Mitchell, E. A.; Baird, M. C. Organometallics 2007, 26, 5230) that commonly employed Pd(0) and Pd(II) precatalysts are often relatively ineffective because they generate only low concentrations of the bis(phosphine) species PdL_2 under most reaction conditions. Our group has recently demonstrated that the easily synthesized and easily handled Pd(η^3-1-Ph-C_3H_4)(η^5-C_5H_5) (I) is a superior precursor for the in situ quantitative formation of PdL_2 than any other documented system (Fraser, A. W.; Baird, M. C. Organometallics 2012, 31, 2470). These findings allow us to demonstrate that I is also the best precatalyst known for PdL_2-catalyzed cross-coupling reactions. We will discuss the Suzuki-Miyaura reaction of 4-bromoanisole with phenylboronic acid and demonstrate that, under mild reaction conditions, higher initial rates and higher conversions with (I) can be obtained compared with other common precatalysts containing a variety of phosphine ligands. We will also demonstrate that this finding holds true with other Suzuki-Miyaura reactions, in addition to Heck arylation and Buchwald-Hartwig aminations.