

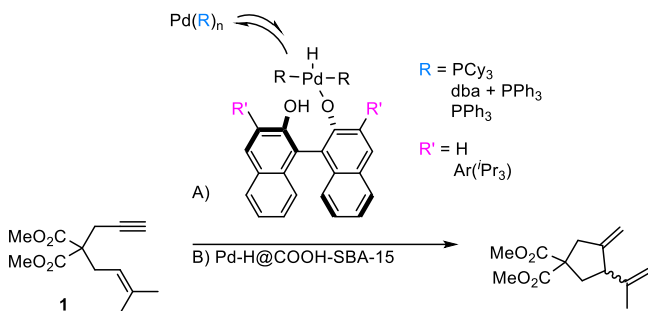
# Palladium and Platinum hydrides as catalysts for enyne cycloisomerization reaction and advanced solid state nmr spectroscopy

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In this study, we investigated the use of Pd(PCy<sub>3</sub>)<sub>2</sub> in combination with chiral alcohols such as BINOL and its derivative phosphoric acid as pre-catalyst components. We measured the equilibrium constants of the oxidative addition to produce the active Pd-H species for various BINOL derivatives using solution NMR measurements. These catalyst systems are capable of enantioselective cyclization<sup>[1]</sup> of substrate **1** which are measured as a function of sterics, acidity, solvent, concentration, and temperatures. The catalytic activity of these systems increases with increasing acid/alcohol concentration.<sup>[2]</sup> Additionally, COOH functionalized SBA-15 (varying pore sizes) are synthesized and tested as heterogenous acid. The equilibrium constants and the catalytic activity are compared to the homogenous system. Furthermore, surface immobilized Platinum hydrides<sup>[3]</sup> on metal oxides are investigated using <sup>195</sup>Pt NMR spectroscopy.<sup>[4]</sup>



**Figure 1:** Scheme of Precatalyst equilibrium for enyne cycloisomerization homogenous (A) and heterogenous (B).

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[2] Erik J. Wimmer, Deven P. Estes, *Organometallics*, 2024, 43, 9, 1068–1075.

[3] S. Maier, D. P. Estes, *Organometallics* **2021**, 40, 11, 1751–1757.

[4] Benjamin A. Atterberry, Erik Wimmer, Deven P. Estes, Aaron J. Rossini, *J. of Magn. Res.*, Volume 352, **2023**, 107457.