Toward Greater Understanding and Expanded Utility of the Palladium-Catalyzed Activation of Carbon-Carbon Single Bonds

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Methodology utilizing the controlled activation and functionalization of carbon-carbon single bonds has the potential to revolutionize chemical synthesis. Our approach to new methodology begins with the mechanistic understanding of existing transformations. Results of these studies have determined that electron withdrawing substitution promotes C-C bond cleavage during palladium-catalyzed β-aryl elimination from triarylmethanol, but that this propensity is greatly influenced by the electronic character of the Pd center.

**Parent Reaction**

\[
\text{Ph}_2\text{Ph} \text{-OH} + \text{Ph-Br} \xrightarrow{\text{Pd(OAc)}_2 (5 \text{ mol\%}), \text{PPh}_3 (20 \text{ mol\%}), \text{o-xylene, reflux, Cs}_2\text{CO}_3, 24 \text{ h}} \text{Ph}_2\text{CO} + \text{Ar-Ph}
\]

**Significant results:**

- Occurs via turnover limiting β-aryl elimination
- Electron deficient aryls undergo more facile β-aryl elimination
- Activation selectivity is greatly influenced by electronic character of Pd