M. POMPEO, R. D. J. FROESE, N. HADEI, M. G. ORGAN* (YORK UNIVERSITY, TORONTO, CANADA)

Pd-PEPPSI-IPent^{Cl}: A Highly Effective Catalyst for the Selective Cross-Coupling of Secondary Organozinc Reagents
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Pd-PEPPSI-IPent^{Cl} – Selective Coupling of Secondary Organozinc Nucleophiles

Selected examples:

Significance: The authors report the new catalyst Pd-PEPPSI-IPent^{Cl}, which highly efficiently couples secondary alkylzinc reagents to (hetero)aryl bromides, chlorides and triflates. The corresponding alkylated aromatics are obtained in excellent yield and with high regioselectivity.

Comment: β-Hydride elimination (BHE) constitutes one of the main drawbacks for the cross-coupling of secondary alkyl reagents, especially if they react with electron-rich coupling partners. These problems are overcome by the new palladium-catalyst, which bears bulkier substituents and additionally, is characterized by a decreased electron density, thus favoring reductive elimination instead of BHE. Density functional theory (DFT) calculations support the theoretical selectivities.

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