

Catalytic Electrophilic Cyclopropanation without Diazo Compounds: De Novo Mechanistic Design and a Historical Twist

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We report mechanistic studies aimed at a catalytic, electrophilic cyclopropanation of unactivated olefins without diazo compounds, especially without diazomethane. The reaction would replace the Simmons-Smith cyclopropanation, which is super-stoichiometric in metal. Mass spectrometric experiments on electrosprayed organometallic complexes lays the groundwork for computational studies, using DFT methods, which then proceed to development of synthetic methodology under realistic solution-phase conditions. The new reactions designed and discovered in this work provide a further basis for mechanistic studies; we show an iterative cycle of discovery, investigation, and improvement of catalytic cycles.