Revisiting the Mechanism of Metal Catalyzed Carbene Insertion Reactions

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Abstract

Metal catalyzed carbene insertion reactions have provided an elegant set up to construct various C-X bonds.¹ While there is no dearth of metals (Fe, Cu, Rh, Au, Pd, etc.) to carry out the transformations, the control of stereoselectivity in many reactions remains a challenge. The major problem lies with the ambiguous and incomplete mechanistic understanding.² In the talk, I will discuss our recent efforts to study the mechanism and develop stereochemical models for Cu, Fe, and Rh catalyzed reactions. During our study, we stumbled upon a few interesting deviations from the currently accepted mechanistic paradigms.^{3,4} Importantly, using on our DFT studies, we re-examine the occurrence of some key intermediates such as terminal carbene species and metal-enolates that have been invoked to explain several experimental observations. Our initial investigation reveals that such intermediates may not be applicable across all carbene transfer reactions.



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