Computational study on the Rh-catalyzed chemodivergent oxidative annulation of benzamides and enynes

Jing Zhang[1], Qingli Zhang[2], Zhenyuan Zhu[1], and Bingkai Wang[1]

[1]Jining University
[2]China People's Police University

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Abstract

The mechanisms of Cp*Rh(OAc)2-catalyzed coupling reaction of N-methoxybenzamide with alkyl-terminated enyne have been investigated by density functional theory (DFT) calculations. With the addition of NaOAc and changing solvent, the product transforms from lactam P1 in reaction A to iminolactone P2 in reaction B, due to the formed stable OAc- coordinated intermediate. The electronic effect and steric effect account for the observed regioselectivity in reaction B collectively.

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