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Quantum Simulation of the Reaction Mechanism of Organocatalyses

Professor Chin-Hui Yu (*Department of Chemistry, National Tsing Hua University*)

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Organocatalysis has received remarkable attraction recently. For instances, organic molecules have been widely used as catalysts in the asymmetric synthesis of natural products. Two examples of computational study of organocatalysis will be presented. Our CRD method is employed to track reaction paths which are difficult to find by conventional methods. The cycloaddition of allenoates and enones yields [3+2] cyclopentenes in phosphine catalysis, and [2+4] dihydropyrans or pyrans in amine catalysis. The quantum calculation not only explains the different reactivity but also reveals a new path to the α-[2+4] product via an intermediate Rauhut-Currier reaction. In the second system, the computations show that nornicotine can catalyze the intermolecular Mannich reaction in wet solvents and water. The significant catalytic effect is owing to the elimination of the bottleneck of the enol-formation step.

問合せ先: 触媒化学研究センター・長谷川 淳也(hasegawa@cat.hokudai.ac.jp・011-706-9145)

B.S., Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, 1980.
M.S., Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, 1982.
Ph.D, Department of Chemistry, The Ohio State University, Columbus, OH, USA, 1987.
Postdoctoral Research Fellow, Department of Chemistry, University of Houston, Houston, TX, USA, 1987～1990.
Associated Professor, Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, 1990～1998.
Professor, Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, 1998～.