



Library Indian Institute of Science Education and Research Mohali



DSpace@IISERMohali / Thesis & Dissertation / Master of Science / MS-15

Please use this identifier to cite or link to this item: <http://hdl.handle.net/123456789/1403>

Title:	Effect of Vibrational Strong Coupling on Concerted Reactions
Authors:	V C, Athul Vijay
Keywords:	Vacuum fluctuations Vibrational Strong Coupling Quantum description of strong coupling regime Cyclisation of Citronellal to Isopulegol
Issue Date:	May-2020
Publisher:	IISER Mohali
Abstract:	Formation of new hybrid light matter states-called as polaritonic states-by interaction of molecular transitions and resonant optical cavity mode is a novel research field in the area of physical chemistry. Strong coupling between molecular transition and cavity mode gives us the possibility for altering the physical and chemical properties of a system. It can also apply in the ground state molecular vibrations which is called as vibrational strong coupling that helps to perturb a given bond and thus changes the rate of a reaction. In the current thesis we focus on understanding the effect of vibrational strong coupling on concerted reactions. For that purpose, we choose cyclisation of citronellal to isopulegol as a model reaction under study. Isopulegol is the starting material for the production of menthol, which is a commercially important product. In the current thesis, we try to follow a concerted reaction by either directly coupling the reactant state or co operatively coupling a solvent in which their vibrational energy overlaps. Preliminary studies suggest that the reaction rate get decelerated by approximately 1.5 times compared to the non-cavity conditions. These studies prove that how VSC can influence rate of a reaction that varies with nature of the reactant and the transition state as their free energy variation are purely depend upon the coupling conditions. Further studies are required to understand the effect of VSC on controlling the potential energy surface of a chemical reaction.
URI:	http://hdl.handle.net/123456789/1403
Appears in Collections:	MS-15

Files in This Item:

File	Size	Format	
MS15117.pdf	1.82 MB	Adobe PDF	View/Open

Show full item record



Items in DSpace are protected by copyright, with all rights reserved, unless otherwise indicated.