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Title: Solvolysis of benzal chloride under vibrational strong coupling

Authors: Gupta, Yashika.

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Abstract:

Over the last few years, theoretical and experimental studies observed that the moulding of the chemical reaction landscape had been made possible by selective vibrational strong coupling (VSC) of the reactant molecules. In VSC, the excited vibrational state undergoes strong coupling with the photon in an infrared cavity, leading to the formation of new vibro- polaritonic states. In the current project, our motive is to study the effects of VSC on controlling the reaction rate. For this purpose, we chose the solvolysis reaction of benzal chloride with water, leading to the formation of benzaldehyde as the final product. This reaction follows an S N 1 mechanism in which the cleavage of the C-Cl bond is the rate- determining step. So we tried to couple C-Cl stretch frequency inside an optical cavity. Due to poor oscillator strength and lower concentration of C-Cl, we barely managed to get direct coupling in the system, whereas the rate control was little due to weak interactions. As a next step, we also tried the coupling of the O-H stretching mode of water molecules, which can trigger the reaction rate control by co-operative interaction or by directly involving in the solvolysis process. In this thesis, we optimized the conditions for kinetic experiments in both non-cavity and cavity conditions and further suggested the option of doing the experiments in base-catalyzed and buffer mediated conditions. Further studies are required to completely understand the effect of VSC on these classes of molecular reactions.

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