Title:	Structure-activity relationship under vibrational strong coupling
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Abstract:	Very recently, vibrational strong coupling was used as a tool to modify chemical reaction rates by coupling the reactant in the confined medium of a microfluidic cavity. This concept is called polaritonic chemistry. This is a novel and unconventional approach for controlling reaction rate and has better selectivity as the cavity modes can be tuned precisely to target a given vibrational band. Understanding the mechanism of polaritonic chemistry is a challenging task as it involves light and matter as components. Few experimental and theoretic studies are available in the literature that show the effect of ON resonance coupling of vibrational band to modify chemical reaction rates. However some of the reactions are accelerated and some others deaccelerated while coupling selected vibrational states. As of now, a clear microscopic picture is not yet available to understand the process of polaritonic chemistry. Achieving insight into the underlying concepts of the reaction mechanism of polaritonic chemistry can help to design experiments with high efficiency that can replace the conventional protocols of chemicals reaction control. In the current thesis, we focus on the effect of structure activity relationship to follow a simpler ester hydrolysis under VSC. Here, we used cooperative VSC, i:e coupling a solvent vibration that is overlapping with reactant vibrational state to modify the chemical reaction rate. The phenomenon of cavity catalysis is utilized by selecting different ester molecules with varying substitution and followed their linear free energy relationship under strong coupling condition. The current study is a small step towards understanding the unusual behavior of chemical reaction rates in strong coupling chemistry.
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