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Abstract:

Polaritonic chemistry is a very promising research topic in the field of physical chemistry. In Polaritonic chemistry, selected vibrational band of a molecule gets strongly coupled to an infrared cavity mode, thereby modifying its energy-reaction co- ordinate. Strong coupling happens when a particular vibrational transition comes in resonance with an optical cavity mode and that exchange energy back and forth, creating hybrid vibro-polaritonic states. These vibro-polaritonic states possess very interesting properties: (1) their energy can be tuned depending upon the coupling strength and (2) are half-molecule like and half-photon like. This results in interesting chemical changes with respect to a reaction co-ordinate. So far, three examples are shown in the literature: vibrational strong coupling (VSC) of a desilination reaction, Prins cyclisation and an ester hydrolysis. In the earlier two cases the activation free energy increases, whereas in the later, activation free energy decreases. In the current work, we look into the effect of VSC of first order kinetics of adduct formation between phenylisocynate and a phenol derivative by coupling the isocyanate stretching mode to an infrared cavity mode.

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