CONFORMATION-SPECIFIC INSIGHTS INTO THE CHEMICAL DYNAMICS OF NO:CH_4 MOLECULAR COMPLEXES

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The photochemistry of flexible molecular complexes, such as a nitric oxide:methane (NO:CH_4), are defined by potential energy surfaces that depend on the chemical functionality and the relative orientation of conformational isomers. Experimental results are required to test and improve modern theoretical methods for accurate prediction of photoinitiated processes and chemical mechanisms. A thorough understanding of the intermolecular interactions and reaction mechanism outcomes can be obtained by elucidating the conformations adopted by NO:CH_4 molecular complexes. Moreover, by investigating the specific vibrational modes inherent to NO:CH_4 conformational isomers, we can assess their impact on energy transfer following fragmentation of the molecular complex isomers. We will leverage a synergy of laser-induced spectroscopy and chemical dynamics techniques, in particular conformation-specific infrared spectroscopy and velocity map imaging, to understand these fundamental mechanisms and dynamics at play within NO:CH_4 and NO:alkane complexes more broadly. Ultimately, we will gain insights into the mode-specific energy transfer pathways following fragmentation of NO:CH_4 molecular complex isomers. Furthermore, our experimental results will be compared to several theoretical approaches in order to reveal the multifaceted signatures of dynamical events using spectroscopy probes.