LASER PROBES OF THE POTENTIAL ENERGY SURFACES OF FLEXIBLE MOLECULES AND WATER-CONTAINING COMPLEXES

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Molecular reaction dynamics has typically focused its attention on small molecules, in which state-to-state studies provide detailed information about the potential energy surface on which reaction takes place and the energy redistribution that necessarily accompanies reaction. In large molecules with several flexible coordinates, conformational isomerization occurs on a multidimensional potential energy surface involving many minima and transition states. This makes it necessary to employ different experimental methods to probe key aspects of the potential energy surface on which isomerization occurs. This talk will describe one such method developed in our group that enables the study of isomerization between specific $X \rightarrow Y$ reactant-product pairs free from interference from other conformations present. Both infrared and stimulated emission pumping have been used to initiate isomerization. Studies on isolated flexible molecules will include a series of isolated molecules of varying complexity, including bichromophores in which the close proximity of excited states provides fascinating vibronic dynamics. The talk will also describe recent work on water-containing complexes, in which a single water molecule shuttles between remote sites on a solute or undergoes photodissociation in competition with isomerization in a flexible solute-water complex.