CONFORMATIONAL EFFECTS ON RESOLVED EMISSION SPECTRA OF FLOPPY AROMATIC MOLECULES

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Conformations of a flexible polyatomic molecule represent the energetically favorable arrangements of its constituent atoms and groups. The resolved emission spectra of flexible molecules have been found to be sensitive to its conformations and bear the signatures of conformation dependent interactions among the different groups. We have used laser-induced fluorescence spectroscopy in combination with quantum chemistry calculations to investigate the effects of conformations in electronic spectra of selected substituted benzenes. In the talk, I shall present the results of our recent investigations on allylbenzene, n-propylbenzene, 2-phenylethanol and 4-fluoro-2-phenylethanol. In allylbenzene it has been found that the symmetry breaking substitution effect in the electronic spectra of the phenyl chromophore is very sensitive to the conformation of the allyl group. In the case of n-propylbenzene, the relative inert propyl group has also been found to have significant effect to alter the emission spectra of its $anti$ and $gauche$ conformers. Similar conformation-specific vibronic signatures are found also in the emission spectra of the other two molecules. The effect of fluorine substitution on conformational preferences of 2-phenylethanol will be discussed in the talk.