EXCITED STATE HYDROGEN ATOM DISLOCATION IN ANTHRANILIC ACID

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The electronic and infrared spectra of anthranilic acid and its dimer in a supersonic jet were measured. The fluorescence excitation spectrum of the monomer is extremely congested but results from a single rotamer, as determined by IR-UV hole-burning. Vibrational progressions in 252 cm^{-1} and 418 cm^{-1} modes are attributed to the in-plane bending motions of the amino and carboxyl groups of anthranilic acid. The presence of vibrational progressions in these modes suggests that the relative positions of the amino and carboxyl groups are different in the ground- and excited-electronic states of anthranilic acid. This observation is supported by the fluorescence-dip infrared spectra, which show a shift in the lower frequency NH stretch fundamental from 3394 to 2900 cm^{-1} upon electronic excitation, suggesting a dramatic strengthening of the intramolecular hydrogen bond in the excited state. The change in the hydrogen-bond strength does not lead to full excited-state intramolecular hydrogen-atom transfer, as the strongly red-shifted emission feature associated with this process is not observed. Instead, the excited-state behavior of anthranilic acid is best described as intramolecular hydrogen-atom dislocation, as has been postulated for the related molecule salicylic acid. The excited state infrared spectroscopy of anthranilic acid dimer suggests localization of the electronic excitation on one monomer unit. The effect of hydrogen atom dislocation on the anthranilic acid carbonyl stretch will also be discussed.