HIGH RESOLUTION ELECTRONIC SPECTROSCOPY OF INDOLE AND INDOLE(H_2O) IN A MOLECULAR BEAM: EVIDENCE FOR ^1L_a- AND ^1L_b-STATE MIXING.[a]

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The electronic spectrum of indole and its sensitivity to the surrounding environment continues to attract much attention.[b] We report here studies of the rotationally resolved electronic spectra of several vibronic bands of indole and indole(H_2O) in a molecular beam, up to an energy of 990 cm^{-1} above the electronic origin of the ^1L_b state at 35231.525 cm^{-1} (≈284 nm). We find, as did Berden, et al.[c] for the 0_0^0 band, that the vibronic bands exhibit "anomalous" line intensities, evidencing axis tilting on S_1 excitation. The degree of tilt is different for different bands, showing that the $S_1 \longleftarrow S_0$ optical transition moment orientations are also different. We derive from careful analyses of these data information about ^1L_a–^1L_b state mixing in the isolated molecule and its dependence on displacements along different vibrational coordinates. We also show that complexation of indole with one water molecule significantly influences the degree of this mixing.

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[b] Y. Huang and M. Sulkes, *J. Phys. Chem.* 100(1996),16479 and references therein.

[c] G. Berden, W.L. Meerts, and E. Jalviste, *J. Chem. Phys.* 103(1995), 9596