DETERMINATION OF THE STRUCTURE OF 7-AZAINDOLE IN THE ELECTRONIC GROUND AND EXCITED STATE USING HIGH RESOLUTION ULTRAVIOLET SPECTROSCOPY AND AN AUTOMATED ASSIGNMENT BASED ON A GENETIC ALGORITHM.

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7-Azaindole (1H-Pyrrolo(2,3-b)pyridine) (7AI) has been subject to numerous experimental and theoretical studies in the last decades, mainly because the 7-azaindole dimer serves as a model system for tautomeric processes in DNA base pairs. Furthermore, 7-azaindole is the chromophore of amino acid analog 7-azatryptophan, that is used to replace tryptophan in proteins. Absorption and emission of 7AI are redshifted, compared to tryptophan and show a single exponential decay, which makes 7AI a good alterative in optical probing of proteins.

The rotationally resolved electronic spectra of four different isotopomers of 7-azaindole (1H-Pyrrolo(2,3-b)pyridine) have been measured in order to obtain the geometric structure in the electronic ground and excited state. The electronic origins of the rotationally resolved UV spectra overlap strongly and an assigned fit to single rovibronic lines is hardly possible. We performed an automatized fit based on the genetic algorithm[a] to assign all four spectral components simultaneously and extract the molecular constants.

The resulting inertial parameters were used to determine the structure of 7-azaindole in the ground and electronically excited state. It was found, that the pyridine moiety expands on electronic excitation, while the pyrrole ring showed only minor geometry changes.

From the hybrid type of the spectra of three isotopomers, the direction of the $\widetilde{A}\,^1A'(\pi\pi^*) - \widetilde{X}\,^1A'$ transition dipole moment for the transition is found to be –21°. The evaluation of the individual lineshapes yielded an excited state lifetime of 7-azaindole of 2.55 ns.

[a] J.A. Hageman, R. Wehrens, R. de Gelder, W.L. Meerts and L.M.C. Buydens. J. Chem. Phys. 113 (2000) 7955-7962.
W. L. Meerts, M. Schmitt and G. C. Groenenboom. accepted Can. J. Chem. (2004)