

ROTATIONALLY RESOLVED $S_1 \leftarrow S_0$ ORIGIN BANDS OF DIFFERENT METHYLINDOLES AND THEIR INTERNAL ROTATION EFFECTS

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We determined the electronic nature, the dipole moments and the torsional barriers in the ground and electronically lowest excited singlet state of substituted indoles using rotationally resolved laser induced fluorescence Stark spectroscopy. The electronic origin bands of 1-, 3- and 5-methylindole have been investigated before *via* high resolution spectroscopy and the perturbation by the hindered internal rotation of the methyl group was discussed in detail by the groups of Pratt and Meerts [1,2]. In general each spectrum consists of two overlapping subbands due to the $0a_1 \leftarrow 0a_1$ and $1e \leftarrow 1e$ torsional transitions. In 6-methylindole the difference of the torsional level splitting between the $0a_1$ and $1e$ levels in the ground and excited state is large enough, to have the two origins of the subbands shifted more than 90 GHz, i.e. completely separated. Both resulting spectra were evaluated *via* evolutionary algorithms and compared to the results of *ab initio* calculations. The rotational constants, the orientation of the transition dipole moment, the size and orientation of the permanent dipole moment, the torsional barrier heights and the orientation of the internal rotor axis in the ground and electronically excited states along with the fluorescence lifetime could be determined. Finally a comparison with the torsional barriers of other methylindoles is given in this presentation.

[1] T. M. Korter and D. W. Pratt, *J. Phys. Chem. B* **105**, 4010 (2001)

[2] K. Remmers, E. Jalviste, I. Mistrík, G. Berden, and W. L. Meerts, *J. Chem. Phys.* **108**, 8436 (1998)