A STUDY OF 2H- AND 2D-BENZOTRIAZOLE IN THEIR LOWEST ELECTRONIC STATES BY UV-LASER DOUBLE RESONANCE SPECTROSCOPY

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Hole burning spectra of *2H*-benzotriazole and *2D*- benzotriazole have been recorded in a range of 1250 cm^{-1} above the electronic origin to rule out the possibilty that the other tautomer (*1H*-benzotriazole) absorbs in this frequency range.[a]
The *1H*-conformer could be detected via FTIR in the region of the NH-stretch vibration and distinguished from the *2H*-conformer by its different band contour. The relative stabilities of both conformers have been determined from a simulation of the temperature dependent amount of each conformer and compared to the results of *ab initio* calculations.
After establishing the existence of only one absorbing species by spectral hole burning, dispersed fluorescence spectra taken through several low frequency vibronic bands of *2H*(*2D*)-benzotriazole have been recorded. The ground state vibrational frequencies are compared to the results of an *ab initio* MP2 based normal mode analysis. Assignments of S_1 vibrations to specific ground state vibrations were established by comparison to calculations. The rotational band contours of the vibronic *2H*-benzotriazole transitions have been determined to be pure *a*- or *b*-type, while rotationally resolved LIF showed the electronic origin of benzotriazole to be pure *b*-type.[b] This can be traced back to the existence of two close lying electronically excited states of *2H*-benzotriazole. While the electronic origin, investigated by Berden et al.[b] can be attributed to an $^1B_2(^1L_a) \leftarrow {}^1A_1$ transition, the *a*- type transitions end up in the ^1L_b state. The large number of vibronic levels and the possible mixing of states prevents a clear assignment of the observed transitions in the S_1- and S_2-state.

[a] W. Roth, Ch. Jacoby, A. Westphal and M. Schmitt accepted for publication in *J. Phys. Chem.* (1989)
[b] G. Berden, E. Jalviste and W.L. Meerts *Chem. Phys. Lett.* **226** (1994) 305-309