

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 possibility 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 S₁ 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 ¹B₂(¹L_a) ← ¹A₁ 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 S₁- and S₂-state.

^aW. Roth, Ch. Jacoby, A. Westphal and M. Schmitt accepted for publication in *J. Phys. Chem.* (1989)

^bG. Berden, E. Jalviste and W.L. Meerts *Chem. Phys. Lett.* **226** (1994) 305-309