DISPERSED FLUORESCENCE AND HOLE BURNING SPECTRA OF BENZOTRIAZOLE

MICHAEL SCHMITT, W. ROTH, CH. JACOBY and K. KLEINERMANNS , *Institut für Physikalische Chemie und Elektrochemie I, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany.*

The 1+1 resonance ionization (REMPI) spectra of benzotriazole (BT) and its deuterated isotopomer have been measured in a molecular beam between 34919 cm^{-1} and 36100 cm^{-1} together with the corresponding hole burning spectra (SHB), analyzed via different vibronic bands. The existence of another conformer which absorbs in the region between 34000 and 37000 cm^{-1} could be ruled out by SHB. Stability and vibrational frequencies of the two possible tautomers (1H and 2H) of BT have been calculated by ab initio calculations on the Hartree-Fock level using the 6-31G(d,p) basis. To give an assignment of the S_1 vibrations to S_0 vibrational frequencies, dispersed fluorescence (DF) spectra have been taken through most of the prominent vibronic transitions. Guided by the propensity rule and the comparison of calculated and measured vibrational frequencies for both isotopomers in the S_0-state a vibrational assignment will be presented.