THE ROTATIONAL SPECTRUM OF BENZAMIDE: MICROWAVE FOURIER TRANSFORM SPECTROSCOPY AND AB INITIO CALCULATIONS.

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The ground state rotational spectra of two isotopologues $C_7H_7{}^{14}NO$ and $C_7H_7{}^{15}NO$ of benzamide have been observed in the gas phase by using a pulsed-jet microwave Fourier transform spectrometer. Each spectrum was analyzed and fitted to obtain principal rotational constants A_0, B_0 and C_0, centrifugal distortion constants and hyperfine components of the nitrogen nuclear quadrupole coupling tensor. A detailed analysis of the molecular parameters evidenced the torsion motion of the (NH_2)-C=O radical with respect to the phenyl ring, as well as a large amplitude motion of NH_2 along the C-N bond, in part hindered by a hydrogen bonding on one side and by the steric repulsion on the other side. *Ab initio* calculations performed at the MP2 and B3LYP levels of the theory refined the molecular structure obtained by electron diffraction (H. Takeuchi M. Sato, T. Tsuji, H. Takashima, T. Egawa, S. Konaka, J. Mol. Struct. 485-486, 1999, 175-176). The structural parameters obtained in the present study confirm the non planarity of benzamide, the (NH2)-C=O radical being tilted by α_e=23 degrees relatively to the phenyl group. The potential energy function along the α angle was calculated in order to model the effects of the torsion motion observed on the spectra.