NON-COVALENT INTERACTIONS AND INTERNAL DYNAMICS IN PYRIDINE-AMMONIA: A COMBINED QUANTUM-CHEMICAL AND MICROWAVE SPECTROSCOPY STUDY

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The 1:1 complex of ammonia with pyridine has been characterized by using state-of-the-art quantum-chemical computations combined with pulsed-jet Fourier-Transform microwave spectroscopy. The computed potential energy landscape pointed out the formation of a stable σ-type complex, which has been confirmed experimentally: the analysis of the rotational spectrum showed the presence of only one 1:1 pyridine – ammonia adduct. Each rotational transition is split into several components due to the internal rotation of NH_3 around its C_3 axis and to the hyperfine structure of both ^{14}N quadrupolar nuclei, thus providing the unequivocal proof that the two molecules form a σ-type complex involving both a N-H$\cdots$N and a C-H$\cdots$N hydrogen bond. The dissociation energy (BSSE and ZPE corrected) has been estimated to be 11.5 kJ$\cdot$mol^{-1}. This work represents the first application of an accurate, yet efficient computational scheme, designed for the investigation of small biomolecules, to a molecular cluster.