## 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  $\sigma$ -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<sub>3</sub> around its  $C_3$  axis and to the hyperfine structure of both <sup>14</sup>N quadrupolar nuclei, thus providing the unequivocal proof that the two molecules form a  $\sigma$ -type complex involving both a N-H···N and a C-H···N hydrogen bond. The dissociation energy (BSSE and ZPE corrected) has been estimated to be 11.5 kJ·mol<sup>-1</sup>. This work represents the first application of an accurate, yet efficient computational scheme, designed for the investigation of small biomolecules, to a molecular cluster.