THE FREE JET MICROWAVE SPECTRUM OF 2-PHENYLETHYLAMINE-WATER

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2-Phenylethylamine (PEA) is the parent structure for a variety of important compounds including dopamine, tyrosine, anphetamine and adrenaline. Due to the flexibility of the side chain, the conformational hypersurface of the isolated molecule contains several minima at relatively low energy. The conformational surface was studied by various spectroscopic and theoretical techniques and four of the five stable conformers were detected. [a]

The most stable conformers observed in isolated conditions are those in which the methylene side chain is folded into a *gauche* structure and the amino hydrogen is oriented towards the aromatic ring to form a weakly hydrogen bonded structure, while in the less stable conformers the amino group is in the *anti* position, thus the energy difference between the *gauche* and *anti* conformers (ca 4 kJ mol^{-1}) represents the energy associated with this weak interaction. Since bioactive molecules can be found in different environments including aqueous media and rotational spectroscopy coupled with high level *ab initio* calculations gives the most detailed structural picture, we studied the free jet microwave spectrum of the adducts formed between PEA and water in the region 60-78 GHz. The dominant spectrum is that of the 1:1 adduct of PEA and water where PEA is in its most stable *gauche* conformation and the water molecole is bound to the nitrogen lone pair. The orientation of the water molecole is such that the oxygen atom is closest (ca 2.5 Å) and equidistant from the ring and chain hydrogen atoms. The experimental data were complemented by *ab initio* calculations at the MP2/6311++G** level of theory; several stable conformations of the PEA-W have been characterized and the observed structure corresponds to the global minimum. The bonding of water seems to affect only slightly the structure of isolated PEA and the main structural parameters of the flexible amino side chain remain basically unaltered. Some lines still remain unassigned in the spectrum and we are hoping to assign them to a second conformational species of PEA-W.

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