PURE ROTATIONAL AND ULTRAVIOLET-MICROWAVE DOUBLE RESONANCE SPECTROSCOPY OF TWO WATER COMPLEXES OF PARA-METHOXYPHENYLETHYLAMINE

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The neurotransmitter p-methoxyphenylethylamine (pMPEA) has been well-studied by ultraviolet and microwave spectroscopy. Seven conformers of this molecule have been assigned in total, showing good agreement with *ab intio* rotational constants, relative dipole moments, ^{14}N quadrupole coupling constants, and relative energies. In this talk, we present the assignment of two conformations of the water complex of pMPEA by chirped pulse Fourier transform microwave spectroscopy. These two structures are the two lowest energy conformations of the pMPEA monomer, with a water molecule donating a hydrogen bond to the nitrogen atom. Good agreement between *ab initio* and experimental parameters is observed. In addition, ultraviolet-microwave double resonance spectra have been collected on a Balle-Flygare type cavity to determine the electronic band origins of these complexes, confirming that these water clusters are the same as those previously observed by Unamuno *et al*.[a]

[a] I.Unamuno, J.A.Fernández, C.Landajo, A.Longarte, F.Castaño, *Chem. Phys.* **271** (2001) 55-69.