ROTATIONAL SPECTRA OF ADRENALINE AND NORADRENALINE

V. CORTIJO, J. C. LÓPEZ, and J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47005 Valladolid, Spain*.

The emergence of Laser Ablation Molecular Beam Fourier Transform Microwave (LA-MB-FTMW) spectroscopy has rendered accessible the gas-phase study of solid biomolecules with high melting points. Among the biomolecules to benefit from this technique, neurotransmitters have received special attention due to the lack of experimental information and their biological relevance. As a continuation of the work on norephedrine, ephedrine and pseudoephedrine[a] we present the study of adrenaline and noradrenaline. The comparison between the experimental rotational and ^{14}N nuclear quadrupole coupling constants and those calculated *ab initio* provide a definitive test for molecular structures and confirm unambiguously the identification of four conformers of adrenaline and three conformers of noradrenaline. Their relative population in the jet has been evaluated by relative intensity measurements of selected rotational transitions. The most abundant conformer in both neurotransmitters present an extended *AG* configuration with a O−H· · ·N hydrogen bond in the side chain.

[a] J.L. Alonso, M.E. Sanz, J.C. López and V. Cortijo, *J. Am. Chem. Soc.* (in press), 2009