THE SHAPE OF NEUROTRANSMITTERS: JET COOLED ROTATIONAL STUDIES

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Solid samples of ephedrine (m.p. 36 °C), pseudoephedrine (m.p. 120 °C) and norephedrine (m.p. 54 °C) vaporized by heating are seeded in Ne and expanded supersonically into an evacuated Fabry-Perot resonator where they are probed using Fourier Transform microwave spectroscopy (MB-FTMW). Laser ablation was used to vaporize solid adrenaline (m.p. 215 °C). In all cases the three lowest-energy conformers have been observed and their rotational and ^{14}N-nuclear quadrupole coupling constants determined. Ab initio calculations at the MP2/6-311++G(d,p) level of theory predicted rotational and quadrupole coupling constants which helped us to identify the different conformations unequivocally. The relative energies of the various species are estimated from the relative intensities of the spectra.