A JET-COOLED ROTATIONAL STUDY OF EPHEDRINE AND P-METOXYPHENYLAMINE

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The first gas phase rotational spectrum of ephedrine, a synthetic analog of the neurotransmitter adrenaline with similar effects on the cardiovascular system, has been observed using a molecular beam Fourier transform microwave spectrometer. Solid ephedrine (m.p. 36 °C) was vaporized by heating it in a reservoir located in pulsed valve. In these conditions the three lowest-energy conformers of ephedrine have been detected. Hyperfine structure due to the presence of a ^{14}N nucleus ($I = 1$) has been observed for all conformers, allowing the unambiguous assignment of their spectra.

Microwave spectroscopy in supersonic jets has been also applied to the conformational and structural analysis of the p-methoxiphenylethylamine molecule. The rotational spectra of the seven conformers previously observed by Pratt *et al*.[a] have been unambiguously assigned on the basis of the values of their rotational and nuclear quadrupole coupling constants. The predictions of *ab initio* calculations have been used as guidelines.

[a] J. T. Li, E. G. Robertson and D. W. Pratt, *Phys. Chem. Chem. Phys.*, **4**, 5244 (2002)