CONFORMATION STUDY OF EPHEDRINE AND 2-PHENYLETHANOL AND THEIR HYDRATED CLUSTERS BY MASS SELECTIVE HIGH-RESOLUTION UV SPECTROSCOPY AND AB INITIO CALCULATIONS

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A promising approach to the understanding of the interaction mechanisms and intrinsic properties of biological systems is the spectroscopic investigation of their conformational structures and dynamics at molecular level in the gas phase. Recently we measured the first resonance-enhanced two-photon ionization (R2PI) spectra with rotational resolution (70 MHz FWHM laser bandwidth) and mass selection of almost all vibronic bands of the $S_1 \longleftarrow S_0$ electronic transition in the range between 37500 cm^{-1} and 37650 cm^{-1} for two biologically relevant molecules, ephedrine ($C_{10}H_{15}NO$)[a], and 2-phenylethanol ($C_8H_{10}O$), in a cold molecular beam. Employing a computer-assisted fit based on genetic algorithms for the analysis of the experimental rotational structures we determined the rotational constants for the ground S_0 and the first excited S_1 electronic states, respectively, and the transition moment ratios. To aid the unambiguous determination of the discussed conformations[b] of the observed species we performed *ab initio* calculations on their structures and energies. The experiment corroborates the predictions that the most abundant conformers of ephedrine and 2-phenylethanol are the *gauche* ones, stabilized by the intramolecular hydrogen-bonding interaction of their side-chains with the π electrons of the aromatic ring. As a further step towards the investigation of these species in a biologically more realistic environment we started high-resolution experiments of the water complexes of ephedrine and 2-phenylethanol. The new results avail to a better insight into the intra- and intermolecular hydrogen bond formation and the influence of the solvent upon the conformational structure of these molecules.

[a] S. Chervenkov, P. Q. Wang, J. E. Braun, and H. J. Neusser *J. Chem. Phys.* **121**, 7169 (2004).
[b] P. Butz, R. T. Kroemer, N. A. Macleod, and J. P. Simons *J. Phys. Chem. A* **105**, 544 (2001).