

GAS PHASE CONFORMATIONS AND METHYL INTERNAL ROTATION FOR 2-PHENYLETHYL METHYL ETHER AND ITS ARGON VAN DER WAALS COMPLEX FROM FOURIER TRANSFORM MICROWAVE SPECTROSCOPY

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A mini-cavity microwave spectrometer was used to record the rotational spectra arising from 2-phenylethyl methyl ether and its weakly bonded argon complex in the frequency range of 10.5 – 22 GHz. Rotational spectra were found for two stable conformations of the monomer: anti-anti and gauche-anti, which are  $1.4 \text{ kJ mol}^{-1}$  apart in energy at wB97XD/6-311++G(d,p) level. Doubled rotational transitions, arising from internal motion of the methyl group, were observed for both conformers. The program XIAM was used to fit the rotational constants, centrifugal distortion constants, and barrier to internal rotation to the measured transition frequencies of the A and E internal rotation states. The best global fit values of the rotational constants for the anti-anti conformer are  $A = 3799.066(3) \text{ MHz}$ ,  $B = 577.95180(17) \text{ MHz}$ ,  $C = 544.7325(3) \text{ MHz}$  and the A state rotational constants of the gauche-anti conformer are  $A = 2676.1202(7) \text{ MHz}$ ,  $B = 760.77250(2) \text{ MHz}$ ,  $C = 684.78901(2) \text{ MHz}$ .

The rotational spectrum of 2-phenylethyl methyl ether – argon complex is consistent with the geometry where argon atom lies above the plane of the benzene moiety of gauche-anti conformer. Tunneling splittings were too small to resolve within experimental accuracy, likely due to an increase in three fold potential barrier when the argon complex is formed. Fitted rotational constants are  $A = 1061.23373(16) \text{ MHz}$ ,  $B = 699.81754(7) \text{ MHz}$ ,  $C = 518.33553(7) \text{ MHz}$ .

The lowest energy solvated ether - water complex with strong intermolecular hydrogen bonding has been identified theoretically. Progress on the assignment of the water complex will also be presented.