CONFORMATIONAL CHANGES UPON COMPLEXATION: THE MICROWAVE SPECTRA AND STRUCTURES OF 2-AMINOETHANOL VAN DER WAALS COMPLEXES

RICHARD J. LAVRICH, CHARLES R. TOROK, and MICHAEL J. TUBERGEN, *Department of Chemistry, Kent State University, Kent, OH 44242*.

Rotational spectra of the van der Waals complexes of 2-aminoethanol-water and 2-aminoethanol-argon have been recorded using a Fourier-transform microwave spectrometer. Eleven a- and b-type transitions were fit to the Watson A-reduction Hamiltonian for 2-aminoethanol-water yielding A = 4886.29 (7) MHz, B = 3355.93 (8) MHz, and C = 2311.66 (4) MHz, and twelve a-, b-, and c-type transitions for 2-aminoethanol-argon were fit to A = 4986.16 (12) MHz, B = 1330.190 (7) MHz, and C = 1143.831 (6) MHz. The spectra are identified with ab initio structures of the two complexes. The 2-aminoethanol monomer has an intramolecular hydrogen bond from the hydroxyl group to the amine;[a] the O - C - C - N torsional angle is 58° and the O - N distance is 2.83 Å. The argon complex is based on the 2-aminoethanol monomer conformation, and the argon sits 3.91 Å from the nitrogen and 3.49 Å from the oxygen. The 2-aminoethanol-water complex is stabilized by hydrogen bonds from the hydroxyl to the water oxygen and from water to the amino nitrogen. Formation of the intermolecular hydrogen bonds requires the O - C - C - N torsional angle to increase to 71°, and the O - N distance increases to 3.04 Å. Rotational spectra of the ^{13}C isotopomers of the 2-aminoethanol monomer have been recorded and enable a substitution structure of the heavy atoms to be determined.

[a] R. E. Penn, R. F. Curl, Jr. *J. Chem. Phys.* **55**, 651 (1971)