MICROWAVE SPECTROSCOPY OF THE 2-METHYLAMINOETHANOL-WATER COMPLEX

DYLAN S VALENTE[a], *Department of Chemistry, University of Scranton, Scranton, PA, USA*; DINESH MARASINGHE, MICHAEL TUBERGEN, *Department of Chemistry and Biochemistry, Kent State University, Kent, OH, USA*.

The rotational spectrum of the 2-methylaminoethanol-water (2MAE-water) complex has been observed using a cavity based Fourier-transform microwave spectrometer in the range of 10-19 GHz. 2MAE exists in *trans* and *gauche* conformations[b,c,d]. We modeled 10 possible conformers of the 2MAE-water complex, five trans and five gauche conformers, using ab initio calculations (MP2/6-311++G(d,p)). 14 rotational transitions were fit to Watson's *A*-reduced Hamiltonian: A=3368.02 MHz, B=2282.60 MHz, and C=1538.00 MHz. ^{14}N nuclear quadrupole hyperfine splittings were resolved, and the 38 hyperfine components were fit to χ_{aa} = 1.543(7) MHz and χ_{bb} = -1.083(25) MHz. The measured spectrum is assigned to the lowest energy model structure of the complex, which has two intermolecular hydrogen bonds: from hydroxyl group to water and from water to the methylamino group. The structure of 2MAE-water is compared with 2-aminoethanol-water (2AE-water) and 2-methoxyethylamine-water (2MEA-water) complexes.

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[a]Summer 2019 REU student at Kent State University.

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