ROTATIONAL SPECTRA, CONFORMATIONAL STRUCTURES AND DIPOLE MOMENTS FOR N-METHYL (AND N-ETHYL)-DIETHANOL-AMINE BY JET COOLED FTMW SPECTROSCOPY AND AB INITIO CALCULATION

LI-HONG XU, QIANG KEVIN LIU, *Department of Physical Sciences, University of New Brunswick, Saint John, NB, Canada E2L 4L5*; R.D. SUENRAM, F.J. LOVAS, *Optical Technology Division, National Institute of Standards and Technology, MD, U.S.A. 20899-8441*; J.O. JENSEN and A.C. SAMUELS, *Standoff Detection, Edgewood Chemical and Biology Center, Edgewood Area, Aberdeen Proving Ground, MD*.

The rotational spectra have been measured for N-methyl-diethanol-amine and N-ethyl-diethanol-amine in a molecular beam using a pulsed-nozzle Fourier-transform microwave spectrometer (FTMW). In each case, FTMW measurements consist of broad-band scans ranging from 10 - 20 GHz and 12 - 20 GHz for N-methyl and N-ethyl, respectively, and numerous spot scans with fully resolved N-quadrupole hyperfine components. Analyses based on asymmetric rotor Hamiltonian analysis have led to the identification of two conformers for N-methly-diethanol-amine and three conformers for N-ethyl-diethanol-amine. Conformational structures of assigned conformers have been obtained by ab initio calculations at the MP2=Full/6-311G** level and ab initio results agree nicely with experimentally determined rotational constants and observed relative conformer spectral intensities. Where nuclear quadrupole splittings were observed, hyperfine components have been fitted to obtain χ_{aa}, χ_{bb}, and χ_{cc} nuclear quadrupole coupling constants and the determined center frequencies were used in subsequently refined rotational analyses.