DECIPHERING THE COMPLETE NUCLEAR QUADRUPOLE COUPLING TENSOR OF IODINE WITH THE ROTATIONAL SPECTRUM OF 2-IODOETHANOL

MICHAEL J. CARRILLO, LINDSEY ANN SPEARE, DINESH MARASINGHE, MICHAEL TUBERGEN, *Department of Chemistry and Biochemistry, Kent State University, Kent, OH, USA*.

High level ab initio calculations at the CCSD(T)//MP2/6-311++ level were used to model the rotational constants and hyperfine constants of 2-iodoethanol. A potential energy surface scan was performed at the B3LYP/6-311G++ level of theory to obtain a better understanding of the conformational landscape and possible conformations. The B3LYP/6-311G++ level of theory was also used to calculate centrifugal distortion constants and zero-point vibrational corrections. We report for the first time the rotational spectroscopic observation on the gauche hydrogen bonding conformer of 2-iodoethanol using a molecular beam, cavity-based Fourier transform microwave spectrometer in the frequency range of 9.4-18.0 GHz. A semi-rigid rotor Hamiltonian perturbed by nuclear quadrupole hyperfine interactions was used to fit the spectrum. 20 rotational transitions split into 104 hyperfine components by the 5/2 nuclear spin of iodine have been measured. A least-squares fit of 3.9 kHz provided the fitted rotational constants which are A = 11369.8531(10), B = 1833.107(5), C = 1654.322 (5) MHz, and the nuclear quadrupole coupling constants which are χ_{aa} = -1476.693(9) MHz, χ_{bb}-χ_{cc} = -189.0537(2) MHz, χ_{ab} = -1180.354(12) MHz, χ_{ac} = 332.17(6) MHz, and χ_{bc} = 243.862(24) MHz. The spectrum of 2-iodoethanol is consistent with the theoretical model structure which predicts a 2.91Å intramolecular hydrogen bond.