FOURIER TRANSFORM MICROWAVE SPECTRUM OF N_2-$(CH_2)_2O$

YOSHIYUKI KAWASHIMA, *Department of Applied Chemistry, Faculty of Engineering, Kanagawa Institute of Technology, Atsugi, Kanagawa 243-0292, JAPAN*; EIZI HIROTA, *The Graduate University for Advanced Studies, Hayama, Kanagawa 240-0193, JAPAN*.

We have investigated the van der Waals complexes consisting of the one from each of the two groups: (Rg, CO, N_2 or CO_2) and (dimethyl ether, dimethyl sulfide, ethylene oxide or ethylene sulfide), by using Fourier transform microwave spectroscopy supplemented by ab initio MO calculations, in order to understand the dynamical behavior of van der Waals complexes and to obtain information on the potential function to internal motions in complexes[a]. One example of the N_2 complex was included: N_2-dimethyl ether, for which we reported a preliminary result[b]. In the present study we focused attention to the N_2-EO (ethylene oxide) complex. We have detected two sets of strong-weak pairs rotational spectra for the $^{15}N_2$-EO, and, because the complex was a very near prolate symmetric-top molecule with the asymmetric parameter ≈ -0.9998, have analyzed them using the asymmetric-rotor program of S-reduction, with the standard deviation of 20 kHz or so. The spectra of $^{14}N_2$-EO were similar, although they were split into hyperfine components due to the nuclear quadrupole coupling of the two nitrogen atoms. The relative intensities of the four sets of the spectra were consistent with the assignment that the four sets of the rotational spectra were due to the four eigenstates created by the exchange of the two nitrogen atoms of the N_2 and the two methylene groups of the EO. Two isomers were then expected to exist for ^{15}NN-EO, one with ^{15}N in the inner and the other in the outer position, and in fact the spectra of such isomers were observed, accompanied by one weaker set. We have observed an interesting correlation among some of the molecular parameters: A, D_{JK} and D_K, for the two pairs of the spectra. These perturbing effects cannot be ascribed to the first-order Coriolis interaction between the two states under consideration, but are probably caused by a combined effect of the two internal motions: exchanges of the equivalent atoms and/or groups in, or internal rotations of, N_2 and EO.

[a] Y. Kawashima, A. Sato, Y. Orita, and E. Hirota *J. Phys. Chem. A* **116**, 1224 2012.

[b] Y. Kawashima, Y. Tatamitani, Y. Morita, and E. Hirota *61st International Symposium on Molecular Spectroscopy*, TE10 2006.