NITROGEN MOLECULE-ETHYLENE SULFIDE COMPLEX INVESTIGATED BY FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND AB INITIO CALCULATION

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We have systematically 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] Two examples of the N_2 complex were investigated: N_2-DME (dimethyl ether), for which we reported a preliminary result[b] and N_2-EO (ethylene oxide).[c] In the present study we focused attention to the N_2-ES (ethylene sulfide) complex. We have detected two sets of the b-type transitions for the $^{15}N_2$-ES in ortho and para states, and have analyzed them by using the asymmetric-rotor program of A-reduction. In contrast with the N_2-EO, for which each of the ortho and para states were found split into a strong/weak pair, only some transitions of the $^{15}N_2$-ES were accompanied by two or three components. The observed spectra of the $^{14}N_2$-ES were complicated because of hyperfine splittings due to the nuclear quadrupole coupling of the two nitrogen atoms. We concluded that the N_2 moiety was located in the plane perpendicular to the C-S-C plane and bisecting the CSC angle of the ES. Two isomers were expected to exist for ^{15}NN-ES, one with ^{15}N in the inner and the other in the outer position, and in fact two sets of the spectra were detected. We have carried out ab initio molecular orbital calculations at the level of MP2 with basis sets 6-311++G(d, p), aug-cc-pVDZ, and aug-cc-pVTZ, to complement the information on the intracomplex motions obtained from the observed rotational spectra.

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

[b] Y. Kawashima, Y. Tatamitani, Y. Morita, and E. Hirota, $61stInternationalSymposiumonMolecularSpectroscopy$, TE10 (2006)

[c] Y. Kawashima and E. Hirota, $J.Phys.Chem.A$ **2013** *117* 13855