

ROTATIONAL SPECTRUM AND STRUCTURE OF VAN DER WAALS COMPLEXES: $(\text{CH}_3)_2\text{O} \cdots \text{CF}_2=\text{CH}_2$ AND $(\text{CH}_3)_2\text{O} \cdots \text{CF}_2=\text{CHF}$

YOSHIO TATAMITANI, YASUFUMI SUZUKI, TERUHIKO OGATA, *Department of Chemistry, Faculty of Science, Shizuoka University, Shizuoka, Japan 422-8529.*

The microwave spectra of van der Waals complexes of dimethyl ether(DME) dimer^a and dimethyl ether $\cdots \text{Ar}^b$ have been studied. Following these investigations, the complexes of dimethyl ether and 1,2-difluoroethane(DFE)/ trifluoroethene(TFE) $(\text{CH}_3)_2\text{O} \cdots \text{CF}_2=\text{CH}_2$ and $(\text{CH}_3)_2\text{O} \cdots \text{CF}_2=\text{CHF}$ have been observed using a Fourier transform microwave spectrometer from 5 to 19 GHz. The samples of 1% DME/DME-*d*₆ and DFE/TFE in Ar were used to form the complexes in a supersonic expansion. For normal DME \cdots DFE, 37 *a*-type transitions were assigned and 87 *a*- and *b*-type transitions were assigned for normal DME \cdots TFE. Rotational and centrifugal distortion constants have been determined for these complexes of normal and -*d*₆ species, leading to molecular structures. Both complexes were found to be C_s symmetry and bound with triple hydrogen bonds: One is the strong O \cdots HC type and two are the weaker CH \cdots F type. The structures of both complexes are similar, however, the hydrogen bond lengths and bond angles are different. Ab initio MO calculations of MP2/6-311+G(d,p) level have been made for these complexes, the structure obtained supported the experimental results and the bonding energies for these complexes were compared.

^aY. Tatamitani, B. Liu, J. Shimada, T. Ogata, P. Ottaviani, A. Maris, W. Caminati, and J. L. Alonso *J. Am. Chem. Soc.*, in press.

^bP. Ottaviani, A. Maris, W. Caminati, Y. Tatamitani, Y. Suzuki, T. Ogata, and J. L. Alonso, *Chem. Phys. Lett.*, submitted.