ROTATIONAL SPECTRUM AND STRUCTURE OF VAN DER WAALS COMPLEXES: $(CH_3)_2O\cdots CF_2{=}CH_2$ AND $(CH_3)_2O\cdots CF_2{=}CHF$

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The microwave spectra of van der Waals complexes of dimethy ether(DME) dimer[a] and dimethy ether$\cdots$Ar[b] have been studied. Following these investigations, the complexes of dimethyl ether and 1,2-difluoroethane(DFE)/ trifluoroethene(TFE) $(CH_3)_2O\cdots CF_2{=}CH_2$ and $(CH_3)_2O\cdots CF_2{=}CHF$ have been observed using a Fourie 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 super sonic 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) lebel have been made for these complexes, the structure obtained supported the experimental results and the bonding energies for these complexes were compared.

[a] Y. Tatamitani, B. Liu, J, Shimada, T. Ogata, P. Ottaviani, A. Maris, W. Caminati, and J. L, Alonso *J. Am. Chem. Soc.*, im press.
[b] P. Ottaviani, A. Maris, W. Caminati, Y. Tatamitani, Y. Suzuki, T. Ogata, and J. L, Alonso, *Chem. Phys. Lett.*, submitted.