ROTATIONAL SPECTRUM AND STRUCTURE OF VAN DER WAALS COMPLEXES: (CH₃)O···CF₂=CH₂ AND (CH₃)₂O···CF₂=CHF

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The microwave spectra of van der Waals complexes of dimethy ether(DME) dimer and dimethy ether···Ar have been studied. Following these investigations, the complexes of dimethyl ether and 1,2-difluoroethane(DFE)/ trifluoroethene(TFE) (CH₃)₂O···CF₂=CH₂ and (CH₃)₂O···CF₂=CHF have been observed using a Fourier transform microwave spectrometer from 5 to 19 GHz. The samples of 1% DME/DME-d₆ and DFE/TFE in Ar were used to form the complexes in a super sonic expansion. For normal DME···DFE, 37 α-type transitions were assigned and 87 α- and β-type transitions were assigned for normal DME···TFE. Rotational and centrifugal distortion constants have been determined for these complexes of normal and -d₆ species, leading to molecular structures. Both complexes were found to be C₂v symmetry and bound with triple hydrogen bonds: One is the strong O···HC type and two are the weaker CH···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.