

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

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The microwave spectra of van der Waals complexes of difluoromethane (DFM) and 1,1-difluoroethene (DFE)/trifluoroethene (TFE)  $\text{CH}_2\text{F}_2 \cdots \text{CF}_2=\text{CH}_2$  and  $\text{CH}_2\text{F}_2 \cdots \text{CF}_2=\text{CHF}$  have been observed using a Fourier transform microwave spectrometer from 5 to 19 GHz. The samples of 1% DFM and DFE/TFE in Ar were used to form the complexes in a supersonic expansion. For  $\text{DFM} \cdots \text{DFE}$ , 48 *a*-type transitions were assigned and 72 *a*- and *b*-type transitions were assigned for  $\text{DFM} \cdots \text{TFE}$ . The rotational and centrifugal distortion constants have been determined, leading to the molecular structures of  $\text{DFM} \cdots \text{DFE}$  and  $\text{DFM} \cdots \text{TFE}$  complexes. Both complexes were found to be  $C_s$  symmetry and bound with triple hydrogen bonds: One is the strong F  $\cdots$  HC type and two are the weaker CH  $\cdots$  F type. Molecular structures of these complexes are, however, quite different from each other. For  $\text{DFM} \cdots \text{DFE}$ , the out of plane atoms are two hydrogens which are bonded to a fluorine in DFE and a fluorine in DFM is bonded to a hydrogen in DFE. For  $\text{DFM} \cdots \text{TFE}$ , the out of plane atoms are two fluorines which attach to a hydrogen in DFE and a fluorine in DFM is bonded to the hydrogen in the same carbon of DFE. Ab initio MO calculations of MP2/6-311+G(d,p) level have supported these experimental results.