HETERO-OLIGOMERS OF DIFLUOROMETHANE AND 1,1-DIFLUOROETHANE: CONFORMATIONAL EQUILIBRIA, MOLECULAR STRUCTURE AND WEAK HYDROGEN BONDS

TAO LU, JUNHA CHEN, QIAN GOU, GANG FENG, *School of Chemistry and Chemical Engineering, Chongqing University, Chongqing, China*.

The hetero-oligomers formed by difluoromethane (CH_2F_2) and 1,1-difluoroethane (CH_3CHF_2) were investigated by pulsed jet Fourier transform microwave spectroscopy and theoretical calculations. For the hetero-dimer of CH_2F_2-CH_3CHF_2, three most stable conformers predicted at MP2/6-311++G(d,p) level were observed. Experimental results, ab initio calculations and quantum theory of atoms in molecules (QTAIM) analyses indicate that all the observed conformers are stabilized through a net of three weak C-H···F-C interactions. Rotational measurements have also been extended to three ^{13}C isotopologues in natural abundance for each observed conformer, which allowed precisely structural determinations. The relative populations of these three conformers in the jet were estimated by relative intensity measurements. For the hetero-trimer of $(CH_2F_2)_2$-CH_3CHF_2, one conformer has been observed. The conformer is stabilized through eight C-H···F-C interactions.