STRUCTURE DETERMINATION, CONFORMATIONAL EQUILIBRIA AND WEAK HYDROGEN BONDS IN HETERODIMERS OF FREONS: THE ROTATIONAL STUDY OF CH_2F_2-CF_3CH_2F

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The rotational spectra of the 1:1 heterodimer of difluoromethane and 1,1,1,2-tetrafluoroethane has been investigated by pulsed jet Fourier transform microwave spectroscopy and quantum chemical calculations. 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.The measurements have also been extended to three or two ^{13}C isotopologues in natural abundance for the conformers II and III, respectively, which allowed precisely structural determinations of these two conformers. The relative populations of these three conformers in the jet estimated to be 50/7/1.