Blue shifted $F_3CH\cdots FCD_3$ and $Cl_3CH\cdots FCD_3$ weakly H-bound complexes. Cryospectroscopic and ab initio study.

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Streszczenie

The FTIR spectra of F_3CH/FCD_3 and Cl_3CH/FCD_3 mixtures have been studied in liquefied Kr in the range of frequencies ~500–10 000 cm^{-1}. Spectroscopic evidence of a weak H-bonded complex formation in the solutions studied have been found. The blue frequency shift of the ν_1C–H stretching vibration and of the majority of the combination and overtone bands, with the ν_1 vibration being excited, were revealed for both F_3CH/FCD_3 and Cl_3CH/FCD_3 complexes characterized by the opposite change in the integrated intensity of the ν_1 band. The effects observed are treated in the frame of features of the dipole moment function of molecules studied. In the case of both systems, ab initio MP2(Full)/6-31+G(d,p) CP corrected calculations predict a linear structure and 2 non-linear stable structures with spectroscopic features being in qualitative agreement with experimental observations. Contributions of the components of the interaction energy in the frequency shift have been analysed by using the SAPT decomposition scheme. The NBO analysis performed suggests, that the competition between rehybridization/repolarization effect and hyperconjugation CT interaction might result in a transfer from the blue to red shift in the case of stronger H bonds.

Słowa kluczowe

Blue shift, H-bond, CH···B interactions, Fluoroform, Chloroform, Methyl fluoride, Liquid phase, SAPT decomposition

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