Unusual spectroscopic properties of CF_3H dissolved in liquified Ar, N_2, CO, and CO_2.

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Streszczenie

The FTIR spectra of CF_3H have been studied in liquefied Ar, N_2, CO, and CO_2. The effect of a blue shift of frequency of the *C–H* stretching vibration accompanied by a decrease in the integral intensity of the corresponding ν_1 band was found in the studied series of solvents. The combination bands ascribed to simultaneous excitation of vibrations of interacted molecular partners have been revealed in CO and CO_2 solutions. DFT/B3LYP and ab initio MP2 calculations utilizing the 6-311++G(3df,3pd) basis set suggest weak linear $F_3CH\cdots B$ complex formation, reproduce the experimentally observed unusual trends for , CO, CO_2, and predict the conventional red frequency shift of the ν_1 band for B=NH_3.

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