FT-IR studies of CH...B interactions in fluoroform containing cryosolutions.

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Streszczenie

A transition from a blue shifted frequency of the _(CH) vibrations of CF3H to a conventional red frequency shift, accompanied by unusually varying integrated intensity of the corresponding _1 band, have been studied in CF3H/B systems, where B = Ar, N2, CO, CO2, O(CD3)2, NH3, and N(CD3)3. DFT/B3LYP and ab initio MP2 calculations, utilizing the 6-311++G(3df,3pd) basis set, predict a weakly H-bond-like linear F3CH…B complex formation in the series studied and reproduce experimentally observed variations of spectroscopic parameters. The results obtained are treated in the framework of induced dipole moment, taking into account opposite directions of the CH bond dipole moment and the dipole moment of the whole molecule. In the range of overtone and combination bands of fluoroform, new weak bands have been detected. They were attributed to simultaneous excitations of vibrations of interacting CF3HandB(=CO,CO2) molecular pairs.

Słowa kluczowe

fluoroform, CH...B interaction, hydrogen bond, vibrational spectra, blue shift