Strong and weak effects caused by non covalent interactions between chloroform and selected electron donor molecules.

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The FTIR spectra of chloroform (Cl(3)CH) in mixtures with various electron donors (B = CH(3)CCH, HCCH, NCCD(3), ClCD(3) and CO) have been studied in liquefied Kr. Spectroscopic evidence of weak H-bond formation has been found. The relative stability of some complexes has been evaluated from temperature studies of integrated intensities of vibrational bands attributed to monomer and complex species. A weak red shift of the stretching vibration of chloroform involved in H-bonding with CH(3)CCH and HCCH having π-electron area was observed. However, in the case of interactions with NCCD(3) and CO, a weak blue shift was detected. In most of the cases, a noticeable increase in the integrated intensity of the CH stretching band was found. Ab initio MP2/6-311++G(2d,2p) a priori counterpoise corrected calculations have been performed for a series of Cl(3)CH and B. Stationary points at the potential energy surface were examined and the structures related to the real minima have been found. The calculations reproduce the majority of experimental results. It has been found that the commonly used correlation between the frequency shift of the CH stretching vibration of the proton donor subunit and the change in CH bond length can fail in the case of the complexes characterized by a weak frequency shift effect.

Adres publiczny

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