Infrared spectroscopy and ab initio study of hydrogen bonded $Cl_3CD{\cdot}N(CH_3)_3$ complex in the gas phase.

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Streszczenie

FTIR spectra of the gas phase Cl3CD+TMA mixture have been studied at room temperature in ~800-4000 cm(-1) frequency domain. The formation of the H-bonded Cl3CD…TMA complex has been detected. Spectroscopic parameters of the band ascribed to the complex were evaluated. MP2 frozen core ab initio calculations have been carried out with the Pople-type 6-311++G(d,p) basis set. The equilibrium geometries and harmonic vibrational frequencies of the complex were obtained using CP-corrected gradient techniques. The "freq=anharm" option has been tested for Cl3CD monomer and Cl3CD…TMA complex to examine possible anharmonic effects on the vibrations localized on the proton donor. The effects of Darling-Dennison and Fermi resonances on the frequency of the stretching vibration of the CH proton donor were analyzed.

Słowa kluczowe

FTIR spectroscopy, Gas phase, Chloroform, H-bond, Fermi resonance, Anharmonisity

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