# Infrared spectra and relative stability of the $F_3CH/NH_3$ H-bonded complex in liquefied Xe.

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Streszczenie

FTIR spectra of mixtures of fluoroform (F3CH) and ammonia (NH3), have been studied in liquid xenon between 5400 and 500 cm-1. Spectroscopic evidence for the formation of a hydrogen bonded complex has been found and the complexation enthalpy Delta(LXe)H degrees in the temperature interval between 173 and 215 K, was determined to be 14.4 (7) kJ mol-1. The parallel fundamentals nu1 and nu2 of ammonia reveal a strong narrowing effect upon complex formation, whereas the perpendicular fundamentals nu3 and nu4 show a modest decrease of their width. CP corrected ab initio calculations at the MP2(FULL)/6-311++G(3df,2pd) level predict a linear geometry for the complex, characterized by a small red shift of the CH stretch frequency of fluoroform. The ab initio interaction energy was found to be compatible with the isolated molecule complexation energy extrapolated from the experimental Delta(LXe)H degrees .

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