

Spectroscopic evidence of weak complex formation between *N,N*-dimethylformamide and fluoroform in the gas phase.

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Streszczenie

The interactions between *N,N*-dimethylformamide (DMF) and fluoroform (CHF₃) in the gas phase are studied with the help of FTIR spectroscopy. Temperature changes observed in the region of the CO stretching mode of DMF suggest a weak complex formation that results in a red wavenumber shift of the $\nu(\text{CO})$ band. Series of van Hoff plots obtained by means of temperature and concentration spectroscopic measurements give the energy of the complex formation $\Delta E \sim -19.6$ kJ/mol. Ab initio calculations performed at the MP2/6-311++G(df,pd) level are in good agreement with the experimental results.

Słowa kluczowe

FTIR spectroscopy, *N,N*-dimethylformamide, Fluoroform, Gas phase, Relative stability, ab initio calculations

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