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C–X···O halogen bonding: interactions of trifluoromethyl halides with dimethyl ether.

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Streszczenie

he formation of weakly bound molecular complexes between dimethyl ether (DME) and the trifluoromethyl halides CF_3Cl, CF_3Br *and* CF_3I *dissolved in liquid argon and in liquid krypton is investigated, using Raman and FTIR spectroscopy. For all halides evidence is found for the formation of C□X···O halogen-bonded 1:1 complexes. At higher concentrations of* CF_3Br*, a weak absorption due to a 1:2 complex is also observed. Using spectra recorded at temperatures between 87 and 125 K, the complexation enthalpies for the complexes are determined to be* $-6.8(3)$ *kJ* mol^{-1} *(DME·*CF_3Cl*),* $-10.2(1)$ *kJ* mol^{-1} *(DME·*CF_3Br*),* $-15.5(1)$ *kJ* mol^{-1} *(DME·*CF_3I*), and* $-17.8(5)$ *kJ* mol^{-1} *[DME(·*CF_3Br*)*$_2$*]. Structural and spectral information on the complexes is obtained from ab initio calculations at the MP2/ 6-311++G(d,p) and MP2/6-311++G(d,p)+LanL2DZ* levels. By applying Monte Carlo free energy perturbation calculations to account for the solvent influences, and statistical thermodynamics to estimate the zero-point vibrational and thermal influences, the ab initio complexation energies are converted into complexation enthalpies for the solutions in liquid argon. The resulting values are compared with the experimental data deduced from the cryosolutions.*

Słowa kluczowe

ab initio calculations, halogen bonding, Raman spectroscopy, van der Waals molecules, vibrational spectroscopy

Adres publiczny

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