Methylenecyclopropane-boron trifluoride van der Waals complexes; an infrared and DFT study.

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Streszczenie

The formation of weakly bound molecular complexes between methylenecyclopropane (MeCP) and BF_3 dissolved in liquid argon has been investigated using FTIR spectroscopy. Experimental evidence was found for the formation of a 1:1 complex in which the BF_3 moiety binds to the exocyclic CC double bond, whereas at higher concentrations of BF_3, weak absorption bands due to MeCP·$(BF_3)_2$ were also observed. Using spectra recorded at different temperatures between 105 and 129 K, the complexation enthalpy for the 1:1 complex in liquid argon was determined to be −10.7(3) kJ mol^{-1}. Structural and spectral information on the complexes was obtained from density functional calculations at the B3LYP/6-311++G(d,p) level. Applying Free Energy Perturbation Monte Carlo calculations to account for the solvent influences and statistical thermodynamics to calculate the zero-point vibrational and thermal influences, the complexation energy for the 1:1 complex was estimated, from the experimental complexation enthalpy, to be −16.0(10) kJ mol^{-1}. This value is compared with the B3LYP/6-311++G(d,p) complexation energies and with single point energies calculated at the MP2 = full/aug-cc-PVTZ level.

Słowa kluczowe

Complexation, Energy, Liquids, Molecular structure, Monomers

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