On the HCl and DCl complexes of methylenecyclopropane in liquid argon.

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Streszczenie

The formation of weak molecular complexes between methylenecyclopropane (MeCP) and HCl or DCl dissolved in liquid argon and liquid nitrogen has been investigated using infrared spectroscopy. Evidence was found for the formation of a 1:1 complex in which the HCl molecule binds to the CC double bond. Weaker bands due to the two different 1: 2 complexes derived from the 1:1 complex were observed. From spectra recorded at different temperatures between 90 and 130 K, the complexation enthalpy for the 1:1 complex formed was determined to be −9.9(3) kJ mol^{-1}, while the corresponding value for the most stable 1:2 complex, MeCP·HCl·HCl, was determined to be −14.6(4) kJ mol^{-1}. Structural and spectral information for the 1:1 and the 1:2 complexes was obtained from DFT calculations at the B3LYP/6-311++G(d,p) level. Using free energy perturbation Monte Carlo simulations to calculate the solvent influences, and statistical thermodynamics to account for zero-point vibrational and thermal contributions, the complexation energies for the 1:1 complex and the 1:2 complex were estimated from the experimental complexation enthalpies to be −16.9(12) and −28.7(14) kJ mol^{-1}. These numbers are compared with single-point energies calculated at the MP2/aug-cc-PVTZ level.

Adres publiczny

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