Cryospectroscopic and ab initio anharmonic studies of acetylene-trimethylamine H-bonded complex.

Autorzy

K. S. Rutkowski

S. M. Melikova

Jerzy Jański

Aleksander Koll

Rok wydania

2010

Czasopismo

Chemical Physics

Numer woluminu

375

Strony

92-100

DOI

10.1016/j.chemphys.2010.07.028

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The FTIR spectra of C_2H_2 in mixtures with trimethylamine (TMA) have been studied in liquefied Kr in the frequency range of ~800–7000 cm^{-1}. The data obtained for C_2H_2 subunit suggest the formation of 1:1 complexes stabilized by a moderate strength conventional H-bond. CH and CN stretching vibrations, related to the vicinal bonds of proton acceptor, were found to shift in opposite directions – blue in the former and red in the latter case. New weak bands, revealed in the range of ~6000–7000 cm^{-1}, were ascribed to the overtone and combination bands of CH stretching vibrations of acetylene which participates in the H-bond formation. The relative stability of the complex has been determined in a series of temperature (T = 118–157 K) measurements of integrated intensities of vibrational bands ascribed to monomer and complex species. Ab initio MP2/6-311++G(2d,2p) a priory counterpoise corrected calculations, made for acetylene, TMA, and the complex reproduce the main spectroscopic observations. They suggest that the most stable non-linear structure of the complex is very floppy. Evaluations of anharmonic effects on position and integrated intensity of selected bands of CH stretching modes of C_2H_2 subunit have been made within perturbation theory on the basis of single point potential energy surface (PES) and dipole moment function calculations.

Słowa kluczowe

Hydrogen bond, Anharmonicity, CH⋯B interactions, Trimethylamine, Acetylene, Liquefied Kr

Adres publiczny

https://doi.org/10.1016/j.chemphys.2010.07.028

Strona internetowa wydawcy

http://www.elsevier.com