

Cryosolution infrared study of hydrogen bonded halothane acetylene complex.

Autorzy

S. M. Melikova

K. S. Rutkowski

Maria Rospenk

Rok wydania

2018

Czasopismo

Journal of Molecular
Structure

Numer woluminu

1160

Strony

434-439

DOI

10.1016/j.molstruc.2018.02.006

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The interactions between halothane (2-bromo-2-chloro-1,1,1-trifluoroethane) and acetylene (C₂H₂) are studied by FTIR spectroscopy. Results obtained in liquid cryosolutions in Kr suggest weak complex formation stabilized by H – bond. The complexation enthalpy (~11kJ/mol) is evaluated in a series of temperature measurements (T ~ 120–160 K) of integrated intensity of selected bands performed in liquefied Kr. The quantum chemical MP2/6-311++G(2d,2p) calculations predict four different structures of the complex. The most stable and populated (94% at T~120 K) structure corresponds to the H – bond between H atom of halothane and pi-electron of triple bond between C atoms of acetylene. Wave numbers of vibrational bands of the most stable structure are calculated in anharmonic approximation implemented in Gaussian program.

Słowa kluczowe

FTIR cryospectroscopy, Halothane, Acetylene, H - bond, Ab initio calculations, Anharmonicity

Adres publiczny

<https://doi.org/10.1016/j.molstruc.2018.02.006>

Strona internetowa wydawcy

<http://www.elsevier.com>