Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Comparative studies of blue shifting and red shifting effects in fluoroform and acetylene cryogenic solutions.

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Rok wydania

2004

Czasopismo

Journal of Molecular Structure

Numer woluminu

705

Strony

49-61

DOI

10.1016/j.molstruc.2004.05.022

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The FTIR spectra of CF_3H and C_2H_2 have been studied in liquefied Ar, N_2, and CO. The frequency blue shift of the C–H stretching vibration accompanied by a decrease in the integrated intensity of the corresponding ν_1 band was found for CF_3H, whereas in the case of C_2H_2 the usual red shift and increasing integrated intensity of the C–H stretching ν_3 band was monitored in the studied series of solvents. Stronger CH···BY-type interactions (BY=CD_3CN, $(CD_3)_2CO$, C_5D_5N, $(CD_3)_3N$) show first increasing frequency blue shift and then result in the gradual transfer to the usual spectroscopic effect for fluoroform. The self-consistent reaction field approach (SCRF) in the frame of gaussian 98 program could be able to reproduce qualitatively the blue shift and decreasing intensity effects observed on the ν_1 band of CF_3H as well as the conventional red shift and increasing intensity effects only at non-realistically small value of the Onsager radius Å. Ab initio MP2 and density functional theory (DFT)/B3LYP calculations predict weak to medium CH···BY complex formation in the case of both CF_3H and C_2H_2 molecules, and suggest the crucial role of the features of the dipole moment function and the intermolecular potential in the observed unconventional effects. The substantial increasing induced dipole moment, accompanied by the predomination of attractive over repulsion forces between H atom of CH group and BY subunit predicted for stronger F_3CH···BY interactions result in the transfer from the blue shift and decreasing intensity to conventional spectroscopic effects in accordance with experimental observations.

Adres publiczny

https://doi.org/10.1016/j.molstruc.2004.05.022

Strona internetowa wydawcy

http://www.elsevier.com

Plik został wygenerowany dnia 2026-11-09 09:23:57

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/S0GFy1B.