

Infrared matrix isolation and ab initio studies on isothiocyanic acid HNCS and its complexes with nitrogen and xenon.

Autorzy

Maria Wierzejewska

Robert Wieczorek

Rok wydania

2003

Czasopismo

Chemical Physics

Numer woluminu

287

Strony

169-181

DOI

10.1016/S0301-
0104(02)00989-8

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The isothiocyanic acid HNCS (DNCS) and its complexes with nitrogen and xenon have been studied experimentally by FTIR matrix isolation technique and computationally with the use of ab initio calculations at the MP2 level. The spectra show that HNCS (DNCS) interacts specifically with nitrogen forming 1:1 hydrogen bonded complex in argon matrix while non-hydrogen bonded structure is probably formed in solid xenon. Two stable minima were localized on the potential energy surface. One of them involves an almost linear hydrogen bond from NH group of the acid molecule to nitrogen molecule lone pair (structure I) and has an interaction energy ΔE^{CP} equal to -6.85 kJ/mol. The second structure (II) where the nitrogen molecule interacts with the sulfur atom of the HNCS was found to be weaker bound and is characterized by $\Delta E^{CP} = -1.99$ kJ/mol. A low energetic barrier of 5.86 kJ/mol between the structures I and II was found. Both experimental and theoretical results obtained for the $Xe \cdots HNCS$ system point to a structure with the NH group interacting with the xenon atom. An interaction energy ΔE^{CP} for this complex is equal to -3.64 kJ/mol.

Słowa kluczowe

Ab initio calculations, Hydrogen bond, Isothiocyanic acid, IR spectroscopy, Xenon

Adres publiczny

[https://doi.org/10.1016/S0301-0104\(02\)00989-8](https://doi.org/10.1016/S0301-0104(02)00989-8)

Strona internetowa wydawcy

<http://www.elsevier.com>