Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Complexation of formaldoxime with water. Infrared matrix isolation and theoretical studies.

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Rok wydania

2012

Czasopismo

Spectrochimica Acta Part A-Molecular and Biomolecular Spectroscopy

Numer woluminu

86

Strony

461-466

DOI

10.1016/j.saa.2011.10.069

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The 1:1, 1:2 and 2:1 formaldoxime-water complexes isolated in the argon matrices have been studied by help of FTIR spectroscopy and MP2/6-311++G(2d,2p) method. The calculations predicted the stability of the three $CH_2NOH\cdots H_2O$ isomeric complexes, three $CH_2NOH\cdots(H_2O)_2$ ones and one $(CH_2NOH)_2\cdots H_2O$ complex. The analysis of the experimental spectra and their comparison with theoretical ones indicated that both the 1:1 and 1:2 complexes trapped in solid argon have the most stable cyclic structures stabilized by the O–H···O and O–H···N bonds between the formaldoxime and water molecules. In the 1:2 complex formaldoxime interacts with the water dimer, one H_2O molecule acts as a proton acceptor for the OH group of formaldoxime whereas the second H_2O molecule acts as a proton donor toward the nitrogen atom of the formaldoxime molecule. In the $(CH_2NOH)_2\cdots H_2O$ complex the OH group of the water molecule acts as a proton donor toward one of the oxygen atoms of the formaldoxime cyclic dimer.

Słowa kluczowe

Matrix isolation, hydrogen bonding, Formaldoxime, Ab initio calculations, Water complexes

Adres publiczny

https://doi.org/10.1016/j.saa.2011.10.069

Strona internetowa wydawcy

http://www.elsevier.com

Plik został wygenerowany dnia 2026-08-24 08:17:19

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/P0h2qw_.