Photodecomposition of formohydroxamic acid. Matrix isolation FTIR and DFT studies.

Autorzy

Magdalena Sałdyka

Zofia Mielke

Rok wydania

2003

Czasopismo

Physical Chemistry Chemical Physics

Numer woluminu

5

Strony

4790-4797

DOI

10.1039/B306785H

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Primary dissociation pathways of formohydroxamic acid have been investigated in argon and xenon matrices. The irradiation of the HCONHOH/Ar(Xe) matrices with full output of an Xe arc lamp leads to the formation of hydrogen bonded HNCO–H_2O and NH_2OH–CO complexes. Two structures were identified for the isocyanic acid–water complex, in the first one HNCO is hydrogen bonded to an oxygen atom of the water molecule and in the second, water serves as a proton donor toward the nitrogen atom of HNCO. For the hydroxylamine–carbon monoxide complex the spectra prove the existence of the structure with the OH group attached to the carbon atom and also suggest the existence of the structure with the NH_2 group interacting with the carbon atom. The identification of the products is confirmed by ^{15}N isotopic substitution and by DFT calculations (at the B3LYP level of the theory with 6-311++G(2d,2p) basis set) of the structure and vibrational frequencies of the identified complexes.

Adres publiczny

https://doi.org/10.1039/B306785H

Strona internetowa wydawcy

https://www.rsc.org/