Photochemistry of acetohydroxamic acid in solid argon : FTIR and theoretical studies.

Autorzy

Magdalena Sałdyka

Zofia Mielke

Rok wydania

2018

Czasopismo

Journal of Physical Chemistry A

Numer woluminu

122

Strony

60-71

DOI

10.1021/acs.jpca.7b09461

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The products formed during exposure of the $CH_3CONHOH$/Ar (AHA/Ar) matrices to the full output of the Xe lamp and to 225 nm OPO radiation are studied. The irradiation promotes the isomerization, 1Z → 1E, and AHA photodissociation reactions. Four pairs of coproducts are experimentally found to appear in the photolysis, they form the complexes: $CH_3OH\cdots HNCO$ (1), $H_2O\cdots CH_3NCO$ (2), $H_2O\cdots CH_3CNO$ (3) and $CO\cdots CH_3NHOH$ (4). The structures of the complexes were optimized at the MP2 computational level with the 6-311++G(2d,2p) and aug-cc-pVTZ basis sets. Three local minima were predicted for the complex (1), two for the complexes (2) and (3) and four local minima were found for the complex (4). The comparison of the theoretical spectra with the experimental ones allowed us to determine the structures of the complexes formed in the matrix. The mechanisms of the reaction channels leading to formation of the four coproducts are proposed. It is concluded that the first step in formation of the (1), (2) and (3) complexes is the scission of the N-O bond whereas the creation of the complex (4) is due to the cleavage of the C-N bond.

Adres publiczny

http://pubs.acs.org/doi/10.1021/acs.jpca.7b09461

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html