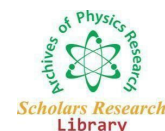




Extended Abstract

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

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Statement of the Problem: Hydroxamic acids exhibit a wide spectrum of biological activities that stimulated progress in the chemistry of this class of compounds. They are known to be involved in iron transport phenomena and are active as antibiotics, antitumor and antifungal agents, and specific enzyme inhibitors. Extensive work has been carried out on the formation of hydroxamic acids, their reactions and structure in the ground state. However, the photochemical properties of hydroxamic acids are still not well recognized. Methodology & Theoretical Orientation: The acetohydroxamic acid (AHA)/Ar matrices, prepared by co-deposition of AHA vapor coming out of the oven assembled inside the cryostat with a large excess of argon onto the cold CsI window, were exposed to 225 nm OPO radiation and to full output of the Xe lamp. The experimental studies were supported by ab initio calculations at the MP2/aug-cc-pVTZ level of theory. Findings: The performed irradiation of acetohydroxamic acid isolated in Ar matrices promotes the isomerization,  $1Z \rightarrow 1E$ , and AHA photodissociation reactions. Four pairs of coproducts are experimentally found in the photolysis, they form the complexes:  $\text{CH}_3\text{OH}\cdots\text{HNCO}$  (1),  $\text{H}_2\text{O}\cdots\text{CH}_3\text{NCO}$  (2),  $\text{H}_2\text{O}\cdots\text{CH}_3\text{CNO}$  (3) and  $\text{CO}\cdots\text{CH}_3\text{NHOH}$  (4). The comparison of the theoretical spectra with the experimental ones allowed to determine the structures of the complexes formed in the matrix. Conclusion & Significance: The importance of the AHA molecule for biological and pharmaceutical applications triggers questions about the influence of UV-VIS irradiation on the photochemical properties of AHA. The mechanisms of the photodecomposition reaction channels leading to formation of the four co-products 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. Statement of the Problem: Hydroxamic acids exhibit a wide spectrum of biological activities that stimulated progress in the chemistry of this class of compounds. They are known to be involved in iron transport phenomena and are active as antibiotics, antitumor and antifungal agents, and specific enzyme inhibitors. Extensive work has been carried out on the formation of hydroxamic acids, their reactions and structure in the ground state. However, the photochemical properties of hydroxamic acids are still not well recognized.

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**Bottom Note:** *This work is partly presented at 5th International Conference on Physical and Theoretical Chemistry October 11-13, 2018, Edinburgh, Scotland*