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

Magdalena Saldyka

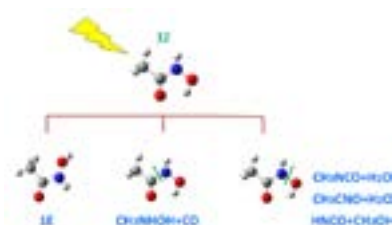
University of Wrocław, Poland

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 → 1E, and AHA photodissociation reactions. Four pairs of coproducts are experimentally found in the photolysis, they form the complexes: CH₃OH...HNCO (1), H₂O...CH₃NCO (2), H₂O...CH₃CNO (3) and CO...CH₃NHOH (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.



Recent Publications:

1. Kehl H (1982) Chemistry and Biology of Hydroxamic Acids. Karger.119-122.
2. Gupta S P (2013) Hydroxamic acids: A Unique Family of Chemicals with Multiple Biological Activities. Springer-Verlag. Doi:10.1007/978-3-642-38111-9.
3. Lipczynska Kochany E (1991) Photochemistry of hydroxamic acids and derivatives. Chemical Reviews. 91(4):477-491. Doi:101021/cr00004a002.
4. Saldyka M, Mielke Z (2007) Keto-iminol tautomerism in acetohydroxamic and formohydroxamic acids: experimental and theoretical studies. Vibrational Spectroscopy. 45(1):46-54. Doi:10.1016/j.vibspec.2007.06.003.

Biography

Magdalena Saldyka obtained her PhD from the University of Wrocław (Poland) under the supervision of Professor Zofia Mielke. She is continuing her work as an Assistant Professor at the same university Her research interests include: conformational analysis, photochemistry, inter- and intramolecular interactions – particularly in hydrogen bonded systems and theoretical modelling of molecular structure and vibrational spectra. She is an expert in low temperature matrix isolation technique combined with infrared spectroscopy. In the last years she has been developing studies on structural and spectroscopic properties of simple hydroxamic acids. Her academic teaching experience is related with methods of physicochemical analysis.

magdalena.saldyka@chem.uni.wroc.pl