

Photochemistry of formaldoxime–nitrous acid complexes in an argon matrix: identification of formaldoxime nitrite.

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Streszczenie

We have studied the structure and photochemistry of the formaldoxime–nitrous acid system ($\text{CH}_2\text{NOH-HONO}$) by help of FTIR matrix isolation spectroscopy and ab initio methods. The MP2/6-311++G(2d,2p) calculations show stability of six isomeric $\text{CH}_2\text{NOH}\cdots\text{HONO}$ complexes. The FTIR spectra evidence formation of two hydrogen bonded complexes in an argon matrix whose structures are determined by comparison of the experimental spectra with the calculated ones for the six stable complexes. In the matrix there is present the most stable cyclic complex with two $\text{O-H}\cdots\text{N}$ bonds; a strong bond is formed between the OH group of HONO and the N atom of CH_2NOH and the weaker one between the OH group of CH_2NOH and the N atom of HONO. In the other complex present in the matrix the OH group of formaldoxime is attached to the OH group of HONO forming an $\text{O-H}\cdots\text{O}$ bond. The irradiation of the $\text{CH}_2\text{NOH}\cdots\text{HONO}$ complexes with the filtered output of the mercury lamp ($\lambda > 345 \text{ nm}$) leads to the formation of formaldoxime nitrite, CH_2NONO , and its two isomeric complexes with water. The main product is the $\text{CH}_2\text{NONO}\cdots\text{H}_2\text{O}$ complex in which water is hydrogen bonded to the N atom of the C=N group. The identity of the photoproducts is confirmed by both FTIR spectroscopy and MP2 or QCISD(full) calculations with the 6-311++G(2d,2p) basis set. The intermediate in this reaction is iminoxyl radical that is formed by abstraction of hydrogen atom from formaldoxime OH group by an OH radical originating from HONO photolysis.

Adres publiczny

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

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