

Infrared spectra and photodecomposition of benzohydroxamic acid isolated in argon matrices.

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Streszczenie

The structure and spectra of the benzohydroxamic acid (BHA) molecule were studied by matrix isolation FT-IR spectroscopy and molecular orbital calculations undertaken at the MP2/6–311++G(2d,2p) level of theory. In consonance with theoretical predictions, 1Z represents the most stable keto tautomer in the gas phase, being the dominant species trapped in argon matrices, while the 2Z tautomer also contributes to the spectrum of the isolated BHA. The abundances calculated at the temperature of evaporation of BHA are equal to 80.6% and 19.2% for 1Z and 2Z tautomers of BHA, respectively, which is in consonance with the experimental relative abundance values (74.4% for 1Z and 25.6% for 2Z). The irradiation of the C₆H₅CONHOH/Ar matrices with the full output of the Xe arc lamp leads to the formation of the C₆H₅NHOH⋯CO (1) and C₆H₅NCO⋯H₂O (2) complexes. The comparison of the theoretical spectra with the experimental ones allowed to determine the structures of the complexes formed in the matrix. The mechanisms of the reaction channels leading to formation of the photoproducts are proposed. It is concluded that the first step in formation of the complex (1) is the cleavage of the C–N bond, whereas the creation of the complex (2) is due to the scission of the N–O bond.

Adres publiczny

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