

Phototransformations of 2-(1,2,4-triazol-3-yl)benzoic acid in low temperature matrices.

Autorzy

Magdalena Pagacz-Kostrzewa
Magdalena Sałdyka
Andrzej Bil
Wioletta Gul
Maria Wierzejewska
Dmytro M. Khomenko
Roman O. Doroschuk

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Streszczenie

Phototransformations of 2-(1,2,4-triazol-3-yl)benzoic acid induced by tunable UV laser were studied in low temperature matrices by FTIR spectroscopy. Out of 36 possible isomers of this molecule the most stable one, comprising the intramolecular N–H...O hydrogen bond, was detected experimentally in argon and xenon matrices after deposition. Upon irradiation with $\lambda = 325$ nm, two new conformers of the precursor were formed. The corresponding reverse photorotamerizations were also detected at 250 nm partly reproducing the initial molecules. In addition to the conformational changes, an interesting photoisomerization took place in the studied matrices leading to a proton transfer from N atom of the triazole ring to the carbonyl oxygen of the carboxylic group. As a result of this reaction, a new product with two OH groups was identified for the first time. The experimental studies were supported by DFT calculations in both ground and excited electronic states.

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