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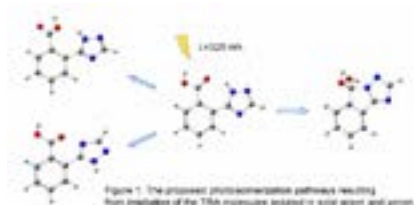
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Conformational changes in 2-(1,2,4-triazol-3-yl)benzoic acid induced by UV laser light

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The chemistry of five-membered N-heterocyclic compounds is an important and growing area of research. These compounds are significant structural fragments and show activity as biological factors, corrosion inhibitors, pesticides, dyes, acid-base indicators, and other industrial chemicals. Triazoles are also interesting molecules from a structural point of view. Hydrogen atoms directly bound to the triazole ring are labile and may give rise to different tautomers - their relative populations are dependent on the chemical environment. Furthermore, triazole derivatives exhibit a very rich photochemistry. The conformational/tautomeric properties and the photolysis behavior of the title compound 2-(1,2,4-triazol-3-yl)benzoic acid (TRA) were studied in argon and xenon matrices by infrared spectroscopy. Analysis of the experimental results was supported by extensive theoretical calculations carried out at the B3LYP/6-311++G(2d,2p) level of approximation. TRA can exist in several tautomeric forms depending on the position of the two hydrogens in the triazole ring. According to the theoretical prediction, the predominating form in the gas phase is the 1H-tautomer. A global minimum is the 2-TRA1c isomer stabilized by the N-H...O intramolecular hydrogen bond. This structure was identified in all two matrices. Photochemical transformations of matrix-isolated TRA were induced using UV-tunable laser radiation. The UV radiation in the 350-220 nm range induced conformationally selective transformations of 2-TRA1c form into less stable 2-TRA2c/2-TRA3c conformers and the back reactions. In addition to the conformational changes an interesting photoisomerization took place in the studied matrices leading to the annular H-atom shift 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.



Recent Publications:

1. Pagacz Kostrzewa M, Bil A and Wierzejewska M (2017) UV-induced proton transfer in 3-amino-1,2,4-triazole. J. Photochem. Photobiol. A 335(C):124-129.
2. Pagacz Kostrzewa M et al. (2016) Theoretical DFT and matrix isolation FTIR studies of 2-(1,2,4-triazolyl)phenol isomers. Chem. Phys. Lett. 657:156-161.
3. Pagacz Kostrzewa M, Krupa J and Wierzejewska M (2014) Carboxylic group and its tetrazolyl isostere in one molecule: matrix isolation FTIR and DFT studies on thermal decomposition and photochemistry of (tetrazol-5-yl)acetic acid. J. Phys. Chem. A. 118(11):2072-2082.
4. Pagacz Kostrzewa M, Krupa J and Wierzejewska M (2014) Photochemical transformations of 5-methyltetrazole: matrix isolation FTIR and DFT studies. J. Photochem. Photobiol. A. 277:37-44.
5. Pagacz Kostrzewa M et al. (2013) Conformational properties and photochemistry of new allyl tetrazoles: Matrix isolation FTIR and computational approach. J. Photochem. Photobiol. A. 251:118-127.

Biography

Magdalena Pagacz Kostrzewa has her expertise in low-temperature matrix studies on diverse molecular species and UV-induced photochemistry. In her PhD thesis she investigated widely the broadband UV photolysis of matrix isolated azoles. Recent studies concern narrowband photolysis of tetrazole and triazole derivatives. Her experimental work is supported by the high-level theoretical calculations. The main subjects of her scientific interests are: application of infrared spectroscopy coupled with matrix isolation technique to study structure and spectroscopic properties of diverse molecular species, theoretical and experimental conformational analysis of the molecules, their identification as well as structural and spectroscopic characteristics and analysis of photochemical processes in the molecular systems induced by UV-Vis and NIR radiation.

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