

Phototransformations of 2-aminonicotinic acid resolved with matrix isolation infrared spectroscopy and *ab initio* calculations.

Autorzy

Magdalena Pagacz-
Kostrzewa

Michał Andrzej Kochman

Wioletta Gul

Maria Wierzejewska

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Streszczenie

The structure and phototransformations of 2-aminonicotinic acid (ANA) induced by tunable UV laser were studied in low-temperature argon matrices with the use of Fourier-transform infrared (FTIR) spectroscopy. After the deposition of the argon matrix, two amino isomers (ANA-1 and ANA-2) were detected, with populations of 96 % and 4 %, respectively. Electronic structure calculations confirm these to be the two most stable isomers of ANA. The irradiation of the amino isomers gives rise to an intricate system of photoinduced reactions, which involves amino-imino phototautomerism, and rotations of the carboxylic group. Following irradiation at 350nm, a rotation of the carboxylic group of ANA-1 was detected leading to increase of the ANA-2 form. In turn, at 310nm two new imino forms (INA-1 and INA-2) of 2-aminonicotinic acid were generated indicating that UV-induced hydrogen atom transfer between ANA and INA tautomeric forms took place. The corresponding reverse photorotamerizations were also detected at 390nm, resulting in the recovery of the initial ANA-1 and ANA-2 isomers. On the basis of electronic structure calculations, we hypothesize that ANA-INA phototautomerization takes place in the vibrationally hot electronic ground state. Its occurrence appears to be contingent on the molecule being able to access a conical intersection between the lowest singlet excited state and the ground state.

Słowa kluczowe

2-aminopyridine-3-carboxylic acid, Photoisomerization, Photochemistry, UV laser-induced processes, Potential energy surfaces

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