

## Infrared spectra and photochemistry of 2-(tetrazol-5-yl)benzoic acid isolated in nitrogen matrices.

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A combined FTIR matrix isolation and theoretical B3LYP/6-311++G(2d,2p) study of 2-(tetrazol-5-yl)benzoic acid isolated in solid nitrogen was performed. Out of fifteen stable isomers of this molecule located on the singlet potential energy surface the most stable one, comprising the intramolecular NH...O hydrogen bond, was detected experimentally in nitrogen matrices after deposition. Upon irradiation with  $\lambda = 305$  nm a new conformer of the precursor was generated and upon  $\lambda = 280$  nm radiation a reverse photorotamerization reaction was induced. Simultaneously with the photoisomerizations, a cleavage of the tetrazole ring with dinitrogen elimination was observed proceeding with a very small rate and leading to formation of a carbodiimide derivative.

### Słowa kluczowe

FTIR, matrix isolation, Potential energy surface, Isomers, azoles

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