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NIR and UV induced transformations of indazole-3-carboxylic acid isolated in low temperature matrices

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Streszczenie

The molecular structure and NIR and UV induced phototransformations of indazole-3-carboxylic acid were studied in low temperature argon and nitrogen matrices by FTIR spectroscopy and B3LYP/6–311++G(2d,2p) calculations. Eleven minima of IC were located on the S_0 potential energy surface. The three most stable structures were detected experimentally in both matrices after deposition. Upon NIR irradiation a dominant process was rotamerization within the carboxylic group leading to changes in the population of the *trans* 1HIC1 and *cis* 1HIC2 forms. In turn, at UV irradiation at λ = 260 nm two new tautomers (2HIC2 and 2HIC3) were generated indicating that the hydrogen atom transfer in pyrazole ring took place. Based on the obtained kinetic curves, differences in the phototransformation rates in different matrices were indicated.

Słowa kluczowe

Isomerization, Rotamerization, Photochemistry, Infrared spectra, DFT

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