



UV-induced proton transfer in 3-amino-1,2,4-triazole.

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Streszczenie

UV-induced proton transfer between two tautomeric forms of 3-amino-1,2,4-triazole (1-AT, 2-AT) was followed by FTIR spectroscopy coupled with matrix isolation technique. The 1-AT $\rightarrow$ 2-AT phototransformation was observed upon the 248 nm irradiation. State-averaged CASSCF(8,8)/6-311 ++G(2d,2p) approach was applied to study mechanism of the observed phototautomerization. The obtained results indicate that the S1/S0 conical intersection (CI) plays a crucial role in the mechanism under study. It was shown that the 1-AT(S1) $\rightarrow$ CI $\rightarrow$ 1-AT(S0)/2-AT(S0) path was responsible for the experimentally observed photo-induced tautomerization process.

Słowa kluczowe

matrix isolation, infrared spectroscopy, azoles, density functional theory, CASSCF, conical intersection

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