

Photo-transformations of 2-aminothiazole-4-carboxylic acid in low-temperature matrices

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Streszczenie

The structure, spectroscopic properties and photo-induced conformational changes of 2-aminothiazole-4-carboxylic acid (ACA) isolated in argon and nitrogen matrices were studied using matrix-isolation FTIR spectroscopy and DFT calculations undertaken at the B3LYPD3/6–311++G(3df,3pd) level of theory. Out of 18 stable isomers, the three most stable structures with the five-membered ring stabilized by two C=C and C=N double bonds and with different arrangement of the carboxyl group were identified in both matrices after deposition. Conformer ACA1 has *trans* and conformers ACA2 and ACA3 have *cis* conformation of the COOH group and the calculated abundance of 69.5%, 18.2% and 12.2%, respectively. Following irradiation at 285 nm, a rotation of the OH group around the C–O bond in ACA1 was detected leading to increase of ACA2. The corresponding reverse photo-rotamerization was detected at 296 nm, resulting in the recovery of the initial isomer ACA1. Upon NIR irradiation a dominant process was rotamerization within the carboxylic group leading to changes in the population of the ACA1 *trans* and ACA2 *cis* forms.

Słowa kluczowe

Thiazole, FTIR, Matrix isolation, Isomerization, Photochemistry, DFT

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