# Structure, Spectra and Photochemistry of 2-Amino-4-Methylthiazole: FTIR Matrix Isolation and Theoretical Studies

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Rok wydania

2022

Czasopismo

Molecules

Numer woluminu

27

Strony

3897/1-3897/18

DOI

10.3390/molecules27123897

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The structure, tautomerization pathways, vibrational spectra, and photochemistry of 2-amino-4-methylthiazole (AMT) molecule were studied by matrix isolation FTIR spectroscopy and DFT calculations undertaken at the B3LYP/6-311++G(3df,3pd) level of theory. The most stable tautomer with the five-membered ring stabilized by two double C=C and C=N bonds, was detected in argon matrices after deposition. When the AMT/Ar matrices were exposed to 265 nm selective irradiation, three main photoproducts, N-(1-sulfanylprop-1-en-2-yl)carbodiimide (fp1), N-(1-thioxopropan-2-yl)carbodiimide (fp2) and N-(2-methylthiiran-2-yl)carbodiimide (fp3), were photoproduced by a cleavage of the CS–CN bond together with hydrogen atom migration. The minor photoreaction caused by the cleavage of the CS–CC bond and followed by hydrogen migration formed 2-methyl-1H-azirene-1-carbimidothioic acid (fp15). We have also found that cleavage of the CS–CN bond followed by disruption of the N–C bond produced cyanamide (fp11) and the ˙C(CH3)=CH–S˙ biradical that transformed into 2-methylthiirene (fp12) and further photoreactions produced 1-propyne-1-thiole (fp13) or methylthioketene (fp14). Cleavage of the CS–CC bond followed by disruption of the N–C bond produced propyne (fp22) and the ˙S–C($NH_2$)=N˙ biradical that transformed into 3-aminethiazirene (fp23); further photoreactions produced N-sulfanylcarbodiimide (fp25). As a result of these transformations, several molecular complexes were identified as photoproducts besides new molecules in the AMT photolysis process.

Słowa kluczowe

thiazole, argon matrices, DFT

Adres publiczny

http://dx.doi.org/10.3390/molecules27123897

Strona internetowa wydawcy

http://www.mdpi.com/journal/metals