

Structure, spectra and photochemistry of 2-amino-4-methylthiazole: FTIR matrix isolation and theoretical studies

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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.

Out of eight optimized isomers of this molecule located on the singlet potential energy surface the most stable one, the amine tautomer with the five-membered ring stabilized by two double C=C and C=N bonds, was detected experimentally in argon matrices after deposition.

When the AMT/Ar matrices were exposed to 265 nm irradiation emitted by a tunable laser beam, 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 produced by a cleavage of the CS-CN bond 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) molecule. We have also found that cleavage of the CS-CN bond followed by disruption of the N-C bond produced cyanamide (fp11) and the $\cdot\text{C}(\text{CH}_3)=\text{CH}\cdot\text{S}$ 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 $\cdot\text{S}-\text{C}(\text{NH}_2)=\text{N}$ 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. The molecular complexes presented in this paper may have potential significance for astrophysics, astrochemistry or astrobiology.