

Theoretical and matrix isolation FTIR studies of 3-amino-1,2,4-triazole and its isomers.

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The structure, isomerization pathways and vibrational spectra of the important heterocyclic 3-amino-1,2,4-triazole (AT) molecule were studied by MP2 and B3LYP methods. Among 11 minima located on PES, 3-amino-1,2,4-*1H*-triazole (1-AT) and 3-amino-1,2,4-*2H*-triazole (2-AT) are the most stable with the calculated abundance at 298 K of 79.4% and 20.6%, respectively. The presented FTIR results allow unequivocal identification and characterization of two AT tautomers isolated in an argon matrix. The performed studies reveal that conformational cooling does not take place in the studied matrices. This observation is consistent with the predicted high energy barrier of ca. 45 kcal/mol for a direct 1,2-hydrogen transfer between 1-AT and 2-AT species.

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