

PHOTOISOMERIZATION OF (CYANOMETHYLENE)CYCLOPROPANE (C_3H_3N) IN A LOW TEMPERATURE RARE GAS MATRIX

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The C_3H_3N potential energy surface is experimentally and computationally investigated through matrix isolation photolysis of 1-cyano-2-methylenecyclopropane, a pyridine isomer containing nitrile and methylenecyclopropane functional groups. Synthesis of the novel isomer 1-cyano-2-methylenecyclopropane, presented here for the first time, involves dehydration of the corresponding amide. 1-Cyano-2-methylenecyclopropane is also generated upon photoisomerization ($\lambda > 200$ nm) of (cyanomethylene)cyclopropane in argon at 19 K. Under these irradiation conditions, the photoisomerization favors the formation of 1-cyano-2-methylenecyclopropane, for which the UV absorption is blue-shifted, relative to (cyanomethylene)cyclopropane. The solution-phase UV-vis spectra and matrix-isolation IR spectra of both pure species are presented and compared to predicted spectra obtained using TD-DFT and anharmonic vibrational frequency calculations, respectively. Photoisomerization to pyridine was not observed.