

MATRIX-ISOLATION FTIR SPECTROSCOPY OF THE DEHYDRO-PYRAZINE RADICAL

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Photochemistry of nitrogen-based heterocyclic radicals plays a vital role in our understanding of the fundamental chemical processes in multiple fields including combustion, and atmospheric/troposphere chemistry^a. Photochemical studies provide insights about the mechanistic pathways and the origin of various interstellar molecules. Radical and biradical species containing heteroatoms play a significant role as intermediates in photochemical processes. The photolysis and pyrolysis studies of one such heterocycle, pyrazine have been done using various spectroscopic and computational techniques^b. However, the photochemical investigations of the pyrazine radical have not been reported so far. In this work, we have explored the electronic structures of the radicals corresponding to all the possible diazines- pyrimidine, pyridazine, and pyrazine, at various levels of theories. Investigations for 3c-5e interactions between the two nitrogen lone pairs and the radical center have also been carried out^c. This has been coupled with an experimental study; the photochemical generation and characterization of the pyrazine radical using Matrix Isolation FT-Infrared spectroscopy. Isolated pyrazine radical photochemistry in solid nitrogen and argon matrices at 4 K using strong UV irradiation leads to the formation of numerous products via ring opening and fragmentation channels, which were identified by comparing the experimental spectrum with the computationally obtained spectrum.

^aPeeters, Z. et al., *A&A* **2005**, 433, 583-590.

^bWilhelm, M. J. et al., *J. Phys. Chem. A* **2018**, 122, 9001-9013.

^cSaraswat, M. et al., *Phys. Chem. Chem. Phys.* **2018**, 20, 4386-4395.