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Title:	Matrix isolation infrared spectroscopic and computational studies of azido derivatives of azoheteroarenes
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Abstract:	Aryl azides are highly reactive species which undergo an interesting and intricate photochemical and thermochemical reaction. Most of their reaction, along with their remarkable reactivity, arise from their capacity to produce nitrene intermediates following N <sub>2</sub> extrusion. Nitrenes, characterized by neutral, monovalent nitrogen atoms, are generally highly reactive and short-lived intermediates. Furthermore, in addition to this group, there is another division represented by azobenzenes, which are capable of undergoing both thermal and photochemical interconversion, exhibiting two perceptible configurations—trans (E) and cis (Z). In this study, we have considered the (E)-4-((4-azidophenyl)diazonyl)-3,5-dimethylisoxazole (E-Iso-p) and studied their photochemistry under cryogenic conditions using matrix isolation spectroscopy. The mechanistic studies are done computationally. Both functional groups, azo and azido, play significant roles in initiating and participating in photochemical processes. In this case, we have two possible photoconversions. First, under photodecomposition, the azide group has the potential to form nitrene, azirine, or ketenimine species. Concurrently, the azo group facilitates Z-E photoisomerization within the molecule, specifically upon exposure to UV light (Scheme 1). The evidence for the photodecomposition followed by the photoisomerization pathway has been proven by both experiments and computations. The preliminary results are presented in this work.
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