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Title:	Computational and Matrix Isolation Infrared Spectroscopic Studies of Hydroxypyridyl and Pyridyloxy Radicals
Authors:	Gupta, Divanshu (/jspui/browse?type=author&value=Gupta%2C+Divanshu)
Issue Date:	10-Oct-2019
Abstract:	<p>Phenoxy radical is one of the interesting transient and reactive species involved in various environmental and biological processes. It has also been reported as a key intermediate in the combustion processes of aromatic compounds. Moreover, simple and substituted phenoxy radical as metal-complexes play crucial roles in biocatalysis, redox reactions of proteins and electron-transfer reactions involving carotenoids. They also play a significant role in lignin biosynthesis, phenol-inhibited oxidation of hydrocarbons, and green plant photosynthesis. Despite the importance of phenoxy radical, direct observation and experimental studies on the heterocyclic analogues of them are scarce. In this regard, we adopted a strategy developed by Radziszewski and performed the photochemistry of 2-iodo-3-hydroxypyridine in argon matrices at 4 K in achieving the elusive 3-pyridyloxy radical. In line with the same literature report, instead of the expected target radical, we observed a ketene, arising due to the abstraction of the hydrogen by the iodine atom followed by Wolff rearrangement step. Now the situation is exciting because of the possibility of photogeneration of the prototypical N- heterocyclic carbene (NHC) with one heteroatom that has no substituent. So far, no reports are available with respect to the NHC without any substituent at the nitrogen centers. Considering the importance of NHC in variety of fields, such as catalysis, where the NHCs can either is used as an organocatalyst or as a ligand in making transition metal complexes. Through this work, matrix isolation infrared spectroscopic studies on 2-Iodo-3-hydroxy pyridine and relevant photochemistry and computational investigations on the isomeric pyridyloxy and hydroxypyridyl radicals are done.</p>
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