Title:	Computational and Spectroscopic Studies of Bimolecular Complexes of Pyridine-N-oxide with Water and Attempts Towards 2-Dehydrothiazole Radical
Authors:	Singh, Amandeep (/jspui/browse?type=author&value=Singh%2C+Amandeep)
Issue Date:	10-Oct-2019
Abstract:	Intermolecular interactions of reactive intermediates derived from biomolecules with water are very important in the understanding of many biochemical channels. Pyridine-N-oxide (1) is a heterocyclic compound with different types of hydrogen bonding donor/acceptor sites, which can be considered as a model system for studying such interactions with water. If a radical center is created in pyridine-N-oxide (1) by homolytic cleavage of C-H bond, the intermolecular interactions is getting very interesting that can now be influenced by the position of the radical center and the type of interactions. In this regard, we investigated the interactions of water with the pyridine-N-oxide (1) and their three isomeric radicals (α, β and γ-radicals) (Scheme A1). For understanding such interactions, computational studies have been carried out. In this regard, the above mentioned complexes have been optimized at different levels of theory (B3LYP/cc-pVTZ and M06-2X/cc-pVTZ and CBS-QB3). Followed by, thermochemistry studies, spin density, electrostatic potential surface, singly occupied molecular orbital (SOMO), NBO analysis and AIM analysis have also been carried out in understanding the electronic structural and stability aspects. Scheme A1 : Pyridine-N-oxide (1), and three isomeric radicals (1α, 1β and 1γ) respectively. Thiazole is a biologically and pharmaceutically important heterocyclic moiety. The generation and catalysis of bio-inspired N-heterocyclic carbene based on thiamine molecule is well known in the literature. However, rather simpler radical molecule of thiazole is unknown. Based on a recent Miyazaki J. et al. photo fragmentation study of thiazole using FTIR matrix isolation spectroscopy has demonstrated that C-S in thiazole can be cleaved easily that can lead to multiple photoproducts. If an additional photo labile iodine atom is attached to the same carbon, the resulting 2-iodothiazole (2) system will be interesting with respect to the photochemistry.
URI:	http://hdl.handle.net/123456789/1259 (http://hdl.handle.net/123456789/1259)
Appears in Collections:	MS-14 (/jspui/handle/123456789/1078)

Files in This Item:

File	Size	Format	
MS14001.pdf (/jspui/bitstream/123456789/1259/1/MS14001.pdf)	4.35 MB	Adobe PDF	View/Open (/jspui/bitstream/123456789/1259/1/MS140(

Show full item record (/jspui/handle/123456789/1259?mode=full)

(/jspui/handle/123456789/1259/statistics)