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Title: A Matrix Isolation Infrared and ab-initio Study of N-Heterocyclic Carbene and Proton Donor Solvents

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Abstract: Weak interactions, particularly hydrogen bonding interactions, play a crucial role in many biological and chemical systems. Most of the bio-molecular conformations are maintained by the hydrogen bonding. Many experimental techniques have been used to study weak interactions. Matrix isolation infrared spectroscopy is one such a technique, which has proved to be efficient to study weak interactions and various conformations. The technique offers the advantage of small linewidths, which has made this technique a powerful tool to study weakly bound complexes and conformations of molecules. This technique also provides a long lifetime for reactive species and hence such species can be easily studied. Hydrogen bonding has been extensively studied in last two decades. Very recently, hydrogen bonding interaction between carbene and proton donors such as $R_2C \cdots H-X$ has drawn considerable attention. Electron density at carbene carbon offers hydrogen bonding site. The nucleophilic nature of N-heterocyclic carbene carbon provides an opportunity to investigate hydrogen bonding interactions. In this work, the hydrogen bonded complexes of N-heterocyclic carbene with water and methanol have been studied. Water and methanol both can act as very good proton donors. The main aim of this work is to investigate the structures of the various hydrogen bonded complexes between the precursor molecules. The computational work has been performed at R-B3LYP level of theory using 6-311++G (d, p) basis set. Two different geometries at the R-B3LYP were obtained in each case, N-heterocyclic carbene – water and N-Heterocyclic carbene – methanol. The interaction between N-heterocyclic carbene carbon and hydrogen of proton donor solvent ($NHC \cdots H-X$) has been observed as a dominating interaction in the optimized ground state. To study these complexes experimentally, the matrix isolation experimental facility has been used.


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