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Title: Matrix Isolation Infrared and ab-initio Study of Hydrogen Bonded Complexes of N-Heterocyclic Carbene and Water

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Keywords: Chemistry
Carbenes
N-Heterocyclic Carbenes
Hydrogen bonds

Issue Date: 13-Jul-2017

Publisher: IISER-M

Abstract: Carbenes are neutral species having six electron in valence shell. Their incomplete octet and coordinative unsaturation, it makes unstable and they have only traditionally studied as highly reactive species. But after the emergence of N-Heterocyclic Carbenes (NHC's) in 1991 it opened a new class of research in organic chemistry and in transition metal chemistry, with numerous applications. Many experimental techniques are available to study carbenes. Matrix isolation infrared spectroscopy is one such technique in which carbenes can be trapped at very low temperature and provide long life time to study. This technique has advantage of small line width, which is efficient to study weak bonded complexes like hydrogen bond and various conformations. Very recently, hydrogen bonding interaction studied between carbene and proton donor solvent as $R_2C \cdots H-X$. The nucleophilic nature of NHC provides strong hydrogen bonding site with the proton donor solvents like H_2O , $MeOH$. I am currently working on the conformational analysis and the weak interaction study of the "N-heterocyclic carbene" using Matrix Isolation FTIR Spectroscopy supported by ab-initio calculations. In this work, the hydrogen bonded complexes of N-heterocyclic carbene with water have been studied. The main aim of this work is to investigate the structure of the various hydrogen bonded complexes between the precursor molecules. The computational work has been performed at R-B3LYP, M06-2X and MP2 level of theories using 6-311++G (d,p) basis set. The interaction between N-heterocyclic carbene carbon and hydrogen of proton donor solvent ($NHC \cdots H-OH$) 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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