MICROSOLVATION OF CARBENES IN SUPERFLUID HELIUM NANODROPLETS

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Carbenes are classified as an important reactive intermediate in chemical reactions owing to their multiple spin states. Recent studies in matrix isolation technique (3 K) demonstrated that a single water molecule is able to switch the spin state of diphenylcarbene[1] (triplet to singlet) and furthermore confirmed the formation of the carbenium ion in the LDA ice matrix[2]. In this line helium nanodroplet spectroscopy provides an ideal environment to study such solvation processes at ultracold temperature (0.37 K) by successive addition of water molecules. Here, we aim to determine the minimum number of water molecules required for the formation of the carbenium ion from its parent carbene molecule.

To understand the solvation process of diphenylcarbene, it is crucial to investigate the initial hydration framework of the precursor molecule, diazodiphenylmethane. Therefore, the present study elucidated the IR spectroscopic investigation of diazodiphenylmethane ($C_{13}H_8N_2$)-water (D_2O) complexes in helium nanodroplets. To assign the observed bands corresponding to $C_{13}H_8N_2$-D_2O complex, we also performed ab-initio calculation at B3LYP-D3/def2-TZVP level.

References: 1. Costa, P.; Sander, Angew. Chem. 2014, 126, 5222– 5225. 2. Costa, P.; Fernandez-Oliva, M; Sanchez-Gracia, E;Sander, W., J.Am. Chem. Soc. 2014, 136, 15625-30.