UNFOLDING THE QUANTUM NATURE OF PROTON BOUND SYMMETRIC DIMERS OF $(MeOH)_2H^+$ AND $(Me_2O)_2H^+$: A THEORETICAL STUDY

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A proton under a tug of war between two competing Lewis bases is a common motif in biological systems and proton transfer processes[a – b]. Over the past decades, model compounds for such motifs can be prepared by delicate stoichiometric control of salt solutions [c]. Unfortunately, condensed phase studies, which aims to identify the key vibrational signatures are complicated to analyze. As a result, gas-phase studies do provide promising insights on the behavior of the shared proton. This study attempts to understand the quantum nature of the shared proton under theoretical paradigms. Proton bound symmetric dimers of $(MeOH)_2H^+$ and $(Me_2O)_2H^+$ are chosen as the model compounds. The simulation is performed using Density Functional Theory (DFT) at the B3LYP level with 6-311+G(d,p) as the basis set. It was found out that stretching mode of shared proton couples with several other normal modes and its corresponding oscillator strength do distribute to other normal modes.

[a] J.R. Roscioli, L.R. McCunn and M.A. Johnson. Science 2007, 316, 249

[b] T.E. DeCoursey. Physiol. Rev., 2003, 83, 475

[c] E.S. Stoyanov. Psys. Chem. Phys., 2000,2,1137