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Title: The elusive $\equiv\text{C-H}\cdots\text{O}$ complex in the hydrogen bonded systems of Phenylacetylene: A Matrix Isolation Infrared and Ab Initio Study

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Keywords: Methanol
Phenylacetylene
Hydrogen-bonded complexes

Issue Date: 2016

Publisher: Springer Link

Citation: Journal of Chemical Sciences, 128(10),pp. 1557-1569.

Abstract: Hydrogen-bonded complexes of phenylacetylene (PhAc) with methanol (MeOH) and diethylether (DEE) were studied using matrix isolation infrared spectroscopy. This study specifically searched for the $\equiv\text{C-H}\cdots\text{O}$ hydrogen bonded complex in these systems, which manifest a $n\text{-}\sigma^*$ interaction and which is a local minimum on the PhAc-MeOH potential surface, as in the case of PhAc-H₂O heterodimer. This $n\text{-}\sigma^*$ local minimum eluded observation in gas phase studies and it was therefore thought interesting to look for this isomer in cryogenic matrices. While MeOH can interact with PhAc as both a proton donor ($\text{O-H}\cdots\pi$ complex) or a proton acceptor ($n\text{-}\sigma^*$ complex), DEE can only manifest the $n\text{-}\sigma^*$ isomer. A comparison of the spectral shifts observed in the features of PhAc-MeOH and PhAc-DEE would therefore independently confirm the existence or not of $n\text{-}\sigma^*$ complex in both these systems. In addition to the $n\text{-}\sigma^*$ complex observed in both the above systems, the $\text{O-H}\cdots\pi$ complex was also discerned in the PhAc-MeOH system. These complexes have stabilization energy in the range of 8-25 kJ/mol. The experimental results were corroborated by computations performed at MP2 and M06-2X, levels of theory, using 6-311 ++G(d,p) and aug-cc-pVDZ basis sets. Single point calculations at the CCSD level of theory were also performed. Atoms-in-molecules (AIM), NBO and LMOEDA analysis were also performed to understand the nature of the intermolecular interactions in these complexes.

URI: <https://link.springer.com/article/10.1007/s12039-016-1166-1>
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