Title:	Phenylacetylene–water complex: Is it n···σ or H···π in the matrix?
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Keywords:	Matrix isolation Infrared spectroscopy Phenylacetylene Hydrogen bonds ab initio computations
Issue Date:	2016
Publisher:	Elsevier
Citation:	Journal of Molecular Structure, 1107, pp. 145-156
Abstract:	Hydrogen bonded complexes of phenylacetylene (PhAc) and water were studied using matrix isolation infrared spectroscopy and ab initio computations. In this work, we have for the first time identified the n···σ complex, in N2 and Ar matrixes. Earlier experiments on the PhAc-H2O system, using molecular beams, had observed only the H···π complex, where H2O was the proton donor to the acetylenic π cloud of PhAc, and which was indicated by computations, to be the global minimum. Computations also located two other minima on the PhAc-H2O potential surface. The technique of matrix isolation, which is known to trap local minima, was used to investigate the PhAc-H2O system, in an attempt to observe any of the local minima, which were not observed in the gas phase experiments. Our experiments, using both Ar and N2 matrixes, provided unambiguous evidence for the formation of the n···σ complex, a local minimum. Experiments with D2O and phenylacetylene deuterated at the acetylenic hydrogen (PhAcD) were also performed, to confirm the above observation, through the isotopic effect. Rather surprisingly, we were unable to observe any evidence for the global minimum in these experiments. The phenylacetylene-water system was theoretically investigated, employing MP2 and DFT (B3LYP, M06-2X, ωB97XD) methods, with 6-311++G** and aug/cc-pVDZ basis sets. AIM, EDA and NBO analysis were also performed to explore the nature, physical origin and the strength of noncovalent interactions.
URI:	https://www.sciencedirect.com/science/article/pii/S0022286015304348 (https://www.sciencedirect.com/science/article/pii/S0022286015304348) http://hdl.handle.net/123456789/2455 (http://hdl.handle.net/123456789/2455)
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