Title:	Hydrogen-Bonded Complexes of Phenylacetylene-Acetylene: Who is the Proton Donor
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Keywords:	oncovalent interactions Hydrocarbons Interaction energies Isolation
Issue Date:	2015
Publisher:	American Chemical Society
Citation:	Journal of Physical Chemistry A, 119(51)
Abstract:	Hydrogen-bonded complexes of C2H2 and phenylacetylene (PhAc) were studied using matrix isolation infrared spectroscopy and quantum chemical computations. Both C2H2 and PhAc, being potential proton donors, the question arises as to which of the two species would be the proton donor in the PhAc-C2H2 complex; a question that this work primarily addresses. The molecular structures, vibrational frequencies, and interaction energies of the PhAc-C2H2 complexes were calculated at the M06-2X and MP2 levels of theory, employing both 6-311++G(d,p) and aug-cc-pVDZ basis sets. At the M06-2X/aug-cc-pVDZ level, two nearly isoenergetic complexes (BSSE corrected) were indicated to be the global minima; one a C-H···π complex, where C2H2 served as a proton donor to the phenyl π-system in PhAc, and the other a C-H···π complex, where C2H2 served as a proton donor to the acetylene π-system in PhAc. Of the two, only the second complex was identified in the matrix, evidenced by a characteristic large shift in the ≡C-H stretch of C2H2. Experiments were also performed using PhAc deuterated at the acetylene hydrogen (PhAcD) to study the isotopic effects on the vibrational spectra of complexes. The isotopic studies further confirmed the structure of the complex trapped in the matrix, thereby presenting unambiguous evidence that C2H2 served as the proton donor to the acetylene π-system of PhAc. The theory of atoms-in-molecules (AIM), energy decomposition (EDA), and natural bond orbital (NBO) analysis were performed to understand the nature of the interactions involved in the complexes.
URI:	https://pubs.acs.org/doi/abs/10.1021/acs.jpca.5b08559?src=recsys (https://pubs.acs.org/doi/abs/10.1021/acs.jpca.5b08559?src=recsys) http://hdl.handle.net/123456789/2714 (http://hdl.handle.net/123456789/2714)
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