Title:	Multiple Hydrogen Bond Tethers for Grazing Formic Acid in Its Complexes with Phenylacetylene
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Abstract:	Complexes of phenylacetylene (PhAc) and formic acid (FA) present an interesting picture, where the two submolecules are tethered, sometimes multiply, by hydrogen bonds. The multiple tentacles adopted by PhAc–FA complexes stem from the fact that both submolecules can, in the same complex, serve as proton acceptors and/or proton donors. The acetylenic and phenyl π systems of PhAc can serve as proton acceptors, while the ≡C–H or −C–H of the phenyl ring can act as a proton donor. Likewise, FA also is amphiprotic. Hence, more than 10 hydrogen-bonded structures, involving O–H···π, C–H···π, and C–H···O contacts, were indicated by our computations, some with multiple tentacles. Interestingly, despite the multiple contacts in the complexes, the barrier between some of the structures is small, and hence, FA grazes around PhAc, even while being tethered to it, with hydrogen bonds. We used matrix isolation infrared spectroscopy to experimentally study the PhAc–FA complexes, with which we located global and a few local minima, involving primarily an O–H···π interaction. Experiments were corroborated by ab initio computations, which were performed using MP2 and M06-2X methods, with 6-311++G (d,p) and aug-cc-pVDZ basis sets. Single-point energy calculations were also done at MP2/CBS and CCSD(T)/CBS levels. The nature, strength, and origin of these noncovalent interactions were studied using AIM, NBO, and LMO-EDA analysis.
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