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Title:	Complexes of acetylene-fluoroform: A matrix isolation and computational study
Authors:	Viswanathan, K.S. (/jspui/browse?type=author&value=Viswanathan%2C+K.S.)
Keywords:	H-bonded complexes Acetylene Matrix isolation Fluoroform
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Citation:	Journal of Molecular Structure, 1049, pp.69-77.
Abstract:	<p>Hydrogen-bonded complexes of C₂H₂ and CHF₃ have been investigated using matrix isolation infrared spectroscopy and ab initio computations. The complexes were trapped in both solid argon and nitrogen matrices at 12 K. The structure of the complexes and the energies were computed at the B3LYP and MP2 levels of theory using a 6-311++G(d,p) basis set and at the MP2/aug-cc-pvdz level. Our computations indicated two minima for the 1:1 C₂H₂-CHF₃ complex, with the C-H...π complex being the global minimum, where CHF₃ is the proton donor. The second minimum corresponded to a relatively less exothermic C-H...F complex, in which C₂H₂ is the proton donor. Experimentally, we observed only the C-H...π complex in our matrix, which was evidenced by the shifts in the vibrational frequencies of the modes involving the C₂H₂ and CHF₃ sub-molecules. The increase in the blue shift of the C-H stretching frequency in going from CHCl₃-acetylene complex to CHF₃-acetylene complex with corresponding increase in the interaction energy helps to place these two complexes on the left hand end of the qualitative diagram (Fig. 1). We also performed computations to study the higher complexes of C₂H₂ and CHF₃. One minimum was found for the 1:2 C₂H₂-CHF₃ complexes and two minima for the 2:1 C₂H₂-CHF₃ complexes, at all levels of theory. Experimentally we observed the features corresponding to the 1:2 and 2:1 C₂H₂-CHF₃ complexes in the N₂ matrix. The computed vibrational frequencies of C₂H₂-CHF₃ complexes at B3LYP and MP2/6-311++G(d,p) level corroborated well with the experimental frequencies. Interestingly, no experimental evidence for the formation of higher complexes was observed in the Ar matrix.</p>
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