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Title:	CH···π and π···π interaction in benzene–acetylene clusters
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Abstract:	Ab initio calculations at the MP2/aug-cc-pVXZ (where, X = D, T and Q) and CCSD(T)/aug-cc-pVDZ levels of theory and certain density functional theoretic calculations were carried out for different configurations of benzene–acetylene clusters. The interaction energy was estimated at the CCSD(T)/CBS limit. For the 1:1 complex, the T-shaped geometry (C6v symmetry) was found to be the most stable (−2.72 kcal/mol) and the π···π stacked structure was the least stable (−0.58 kcal/mol). For the 1:2 complex, the ring-shaped (−5.87 kcal/mol) and the double T-shaped (−5.23 kcal/mol) geometries were found to be the most stable and the second most stable, respectively.
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