Title:	How different is the borazineâ€“acetylene dimer from the benzeneâ€“acetylene dimer? A matrix isolation infrared and ab initio quantum chemical study
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Abstract:	The 1:1 dimer of borazine–acetylene has been studied for the first time, both experimentally and computationally. The borazine–acetylene dimer was trapped in Ar and N2 matrices, and studied using infrared spectroscopy. Our experiments clearly revealed two isomers of the borazine–acetylene complex, one in which the N–H of borazine interacted with the carbon of acetylene, and another in which the C–H of acetylene formed a hydrogen bond with a nitrogen atom of borazine. The formation of both isomers in the matrix was evidenced by shifts in the vibrational frequencies of the appropriate modes. Reassuringly, the experimental observations were corroborated by our computations using the second-order Møller–Plesset perturbation theoretic method and coupled-cluster singles, doubles and perturbative triples method in conjunction with different Dunning basis sets, which indicated both these isomers to be stable minima, with the N–H···C complex being the global minimum. Atoms-in-molecules and energy decomposition analysis were also carried out for the different isomers of the dimer. These studies reveal that replacing the three C–C linkages in benzene with three B–N linkages in borazine modifies the interaction in the dimer sufficiently, to result in a different potential energy landscape for the borazine–acetylene system when compared with the benzene–acetylene system.
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