Title:	"A Tale of Two Structures": The Stacks and Ts of Borazine and Benzene Hetero and Homo Dimers
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Abstract:	The heterodimers of borazine and benzene were studied using matrix isolation infrared spectroscopy and ab initio calculations, for an eventual comparison with the corresponding homodimers of the submolecules. The homo and hetero dimers are expected to show the stacked and T-shaped structures as a general class of geometries; a study which promises to present an interesting comparison of the landscape of the homo and the heterodimers. Computations on the heterodimers were performed at the MP2 and M06-2X levels of theory using aug-cc-pVDZ basis set. The heterodimer manifested both the T-shaped and stacked structures, with the former being the global minimum. The T-shaped structure itself showed two isoenergetic variations: one was the T-NH structure, where the N−H of borazine pointed towards the center of the benzene ring and the second was the NH…C structure, where the N−H pointed towards a carbon atom of benzene; in short, the borazine formed the stem and the benzene formed cap of the T. We were able to discern both the T-shaped structures in our matrix isolation experiments. A third geometry, the parallel displaced stacked structure, was indicated to be a local minimum, which however was not observed in our experiments. AIM, LMO-EDA and NBO analysis was carried out to explore the nature of interactions in the various structures.
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