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Theoretical Studies on the Configurations of Benzhomobarrelene Derivatives

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Abstract: Reaction of 7-carbomethoxy-cycloheptatriene with benzyne resulted in the formation of only one benzhomobarrelene isomer, {\bf 5A}. Theoretically, four addition products, {\bf 5A-D}, can be formed from this reaction. Certain molecular mechanic calculations (MM2 force field) have been undertaken on these isomers. It has been shown that the isomers {\bf 5A} and {\bf 5C} have the lowest energies. The non-existence of {\bf 5C} has been discussed in terms of a benzyne approach to a norcaradiene structure. Furthermore, MM2 calculations on two different conformers of {\bf 5A} have revealed that the bisected conformer {\bf 5AE} has the highest strain energy. However, AM1 semiempirical calculations of those conformers have shown that the conformer {\bf 5AE} possesses a lower heat of formation than the isomer {\bf 5AA}.

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