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Title:	Stabilizing influence of silicon substitution on dibenzene and its isomers
Authors:	Koner, A. (/jspui/browse?type=author&value=Koner%2C+A.) Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
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Abstract:	The stabilizing effect of silicon substitution on sixteen different isomers of dibenzene (C ₁₂ H ₁₂) has been investigated using second-order Møller-Plesset perturbation (MP2) theory and the cc-pVDZ basis set. While the most stable isomers of Si ₁₂ H ₁₂ have only Si-Si bonds, some of the stable isomers have isolated Si=Si bonds and may be amenable to experimental observation. Vibrational frequencies were calculated for the optimized geometries at the Hartree-Fock level of theory to ensure that they corresponded to true minima on the potential energy landscape. Natural bonding orbital analysis confirms the existence of isolated Si=Si double bonds in some of the isomers. Dipole moment values were determined to check for the presence of centre of symmetry in certain geometries.
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