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Title:	Stabilisation of the [6]-prismane structure by silicon substitution
Authors:	Equbal, Asif (/jspui/browse?type=author&value=Equbal%2C+Asif) Srinivasan, S. (/jspui/browse?type=author&value=Srinivasan%2C+S.) Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	[6]-prismane silicon Møller–Plesset perturbation (MP2)
Issue Date:	2017
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Citation:	Journal of Chemical Sciences, 129 (7)
Abstract:	Using the second-order Møller–Plesset perturbation (MP2) theoretic method and the cc-pVDZ basis set, it is shown that with an increase in the number of carbon atoms substituted by silicon, the [6]-prismane structure becomes increasingly more stable, relative to the two isolated benzene (like) structures. A similar trend is observed for germanium substituted prismanes as well. Extending this investigation, the stability of benzene-capped fullerene (C60 fused with benzene) is also investigated.
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