

# A Theoretical Study on The Structures of Monosila[5.7]<sub>n</sub>cyclacenes

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Cyclacenes are currently a major topic of interest because of their remarkable structural similarity to carbon nanotubes [1] and the possible utility of their cylindrical cavities in host–guest chemistry [2]. Hence, many of the theoretical and experimental chemists have studied the cyclacenes and the silacyclacenes to gain an insight into the physical and chemical properties of these interesting molecular systems or to find out some synthetic routes to obtain hitherto unknown compounds [3-6].



Hence, we have been keen on investigating a novel family of [n]silacyclacene isomers; the [5.7]<sub>n</sub> silacyclacenes (Figure are depicted above). The nomenclature presented herein is as follows: “n” for [n]silacyclacenes refers to the number of fused benzene rings, whereas “n” for [5.7]<sub>n</sub> silacyclacenes refers to the number of fused azulene ring systems. In this work, we report several theoretically predicted properties of this new family of molecules using Density Functional Theory (DFT) with the B3LYP functional and the 6-31G(d) basis set.

As the [5.7]<sub>n</sub> silacyclacenes increase in size, the bond length alternation along the top edge decreases suggesting greater delocalization of the  $\pi$ -system with increasing size. The [5.7]<sub>n</sub> silacyclacene optimized geometries show  $C_{nv}$  symmetry. NICS may be considered as a useful indicator of the aromatic character of a system and usually correlates well with the other energetic, structural, and magnetic criteria for aromaticity [7]. For n=3, the NICS values are close to zero, indicating the molecule is nonaromatic, whereas for n>4, the NICS values become more negative with increasing size and the negative NICS values denote aromaticity.

[1] R. Gleiter, B. Esser, S.C. Kornmayer, *Acc. Chem. Res.*, **2009**, *42*, 1108-1116.

[2] R. M. Cory, C. L. McPhail, *Tetrahedron Lett.*, **1996**, *37*, 1987-1990.

[3] K. N. Houk, P.S. Lee, M. Nendel, *J. Org. Chem.*, **2001**, *66*, 5517-5521.

[4] A. Azizoglu, *Struct. Chem.*, **2003**, *14*, 575-580.

[5] L. Turker, I. Bayer, *J. Phys. Chem. Solids*, **2000**, *61*, 1041–1045.

[6] E. S. Hirst, F. Wang, R. Jasti, *Org. Lett.*, **2011**, *13*, 6220-6223.

[7] P.v.R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao, N.J.R.E. Hommes, *J. Am. Chem. Soc.*, **1996**, *118*, 6317-6318.