ABSTRACT

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Title of the thesis: Studies in the synthesis and chemistry of aesthetically pleasing carbocyclic compounds

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This thesis deals with the synthesis of aesthetically pleasing carbocylic compounds derived from symmetrical trisannelated benzene derivatives such as trindane and dodecahydrotriphenylene. The scarcity of reports on the functionalization of these carbocycles suggests that it is a difficult challenge for synthetic chemists. We engaged on this challenge and used some simple synthetic methods to produce targeted molecules.

In the first chapter, the literature survey on the methodologies for the preparation of various BCTs having complex architectural beauty is discussed.

The second chapter of the thesis describes chemistry of ruthenium catalyzed oxidation of dodecahydrotriphenylene using $RuCl_3$–$NaIO_4$ system. The unusual behavior of dodecahydrotriphenylene under identical conditions to that of trindane has been studied and discussed. Density functional theory (DFT) calculations have also been carried out to support the experimental findings.

Third chapter describes the intriguing molecular architecture of the butterfly-shaped compound butterflyene, which was assembled by a series of reactions such as cyclocondensation, benzylic oxidation, McMurry coupling, and the Diels-Alder reaction, respectively. The beauty of the molecule was unveiled by envisioned, retrosynthetically planned and executed *via* a synthetic methodologies

without using complex or fancy reagents. DFT calculations have also been used to analyze the structural optimization and reaction energies.

Functionalization of the peripheral ring in trindane and dodecahydrotriphenylene has been explored and discussed in the fourth chapter. The synthesis of library of aesthetic carbocyclic derivatives of trindane and dodecahydrotriphenylene with diverse functionalities have been prepared under mild conditions and shorter reaction times with good to excellent yields.