

En Route to Cyclacenes: A Diels-Alder Strategy for the Synthesis of Molecular Belts

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Abstract

The aim of this project is to complete the first laboratory synthesis of cyclacenes. Cyclacenes are belt shaped molecules composed of repeating six-membered benzene rings. To date, only a few cyclacene-like structures have been synthesized. These structures are the thinnest possible analogue of a carbon nanotube. The synthetic design of this project involves the generation of two connected, flexible molecular halves with complementary reactive ends. These halves will snap together head-to-tail and form the closed belt. Molecular modeling indicates that this reaction should be a favorable, exothermic process that can result in the formation of the stable precursors needed to reach a fully aromatic cyclacene. The chemical and structural features of cyclacenes can then be explored by researchers. Cyclacenes are expected to have diradical character, a novel electronic characteristic. Additionally, the composition of cyclacenes can be feasibly used for the precise, bottom-up synthesis of carbon nanotubes. This study proposes a new synthesis of cyclacenes in order to further these scientific endeavors.