

Modified Polyacenes as Monomers of Mobius Molecules

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This is an interdisciplinary investigation of the efficacy of patterns of 5-, 6-, and 7-membered carbon rings as subunits of linear, cylindrical, and Mobius-topology molecules. Carbon rings with odd numbers of atoms allow for patterns to have increased variety in shape and increased flexibility. These patterns also allow the comparison of structures with $4n$ and $4n + 2$ pi electrons with regard to aromaticity. Molecular mechanics (OPLS-2005) and quantum mechanics (B3LYP/6-31G*) geometry optimization calculations have been performed on various structures. Data and techniques from the mathematical field of differential geometry guide the selection of favored patterns.