

Theoretical characterization of linear [n]-ladderanes and some isomers

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The electronic structure of the first members of the ladderane family has been theoretically studied.

The compounds are predicted to be highly symmetric and stable. Their geometries, heat of formation, vibrational frequencies and NMR spectra have been calculated and analyzed. The

reported theoretical results can be useful for the experimental detection of this interesting family of molecules. © 2003 Elsevier B.V. All rights reserved.