Highly strained nonclassical nanotube end-caps. A single-step solution synthesis from strain-free, non-macrocyclic precursors.

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Streszczenie

Nonclassical nanotube end-caps have been constructed from strain-free heterocyclic precursors using a one-step synthetic procedure, involving multiple nickel-mediated Ullmann couplings. These systems consist of tubular macrocyclic sections that are tightly capped on one side with a bridging benzene ring, forming deep, chemically accessible cavities. The end-caps are characterized by exceptionally high internal strain energies reaching 144 kcal/mol. The optical absorption and emission properties of these molecules show a marked dependence on conjugation length and geometrical factors. The mechanism of end-cap formation, investigated using DFT calculations, relies on precise timing of transmetalation and reductive elimination events.

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https://www.acs.org/content/acs/en.html