Golcondane (C20H24): Theoretical studies of a novel strained, caged hydrocarbon molecule

DANIEL FINKENSTADT, U.S. Naval Academy, MICHAEL MEHL, MARK PEDERSON, U.S. Naval Research Laboratory, STEVEN RICHARDSON, Howard University — In 1993 Mehta and Reddy reported the synthesis of a new C20 polyhedrane, which they named golcondane (C20H24, D2d) in honor of the 400th anniversary of the founding of the Indian city of Hyderabad, whose original name was Golconda. Golcondane is a caged, nonacyclic hydrocarbon that has two fused four-membered rings, four fused five-membered rings, and two fused seven-membered rings. Its chemical structure was determined by 13C NMR spectroscopy and unpublished X-ray crystal diffraction studies. Motivated by our previous success in using density-functional theory (DFT) to compute the structural, electronic, and vibrational properties of other hydrocarbons such as cubane, octanitrocubane, the medium-sized diamondoid molecule cyclohexamantane, as well as the novel class of materials known as silica-diamondoids, we have used DFT and tight-binding molecular dynamics (TBMD) to compute from first-principles similar properties for golcondane. Our work is especially significant with the lack of other theoretical or experimental studies on this interesting molecule in the published literature.

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