Abstract Submitted
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**Golcondane (C20H24): Theoretical studies of a novel strained, caged hydrocarbon molecule**[1] 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 $C_{20}$ polyhedrane, which they named golcondane ($C_{20}H_{24}$, $D_{2d}$) in honor of the $400^{th}$ 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 Its chemical structure was determined by $^{13}C$ NMR spectroscopy and unpublished X-ray crystal diffraction studies.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 *sila*-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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