

Abstract Submitted
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Theoretical Confirmation of the Experimental Raman Spectra of the Diamondoid Molecule: Cyclohexamantane (C₂₆H₃₀)¹ STEVEN L. RICHARDSON, Howard University, Washington, DC 20059, TUNNA BARUAH, MICHAEL J. MEHL, MARK R. PEDERSON, Naval Research Laboratory, Washington, DC 20375 — Diamondoids (C_{4n+6}H_{4n+12}) are rigid, cage-like hydrocarbon molecules which are superimposable upon the diamond crystal structure. For n=1, we have the simplest diamondoid, adamantane C₁₀H₁₆. While most of the diamondoids for n≤3 have been synthesized in the lab, routes for preparing larger diamondoids for n>4 have not yet been realized. The diamondoid, cyclohexamantane (C₂₆H₃₀), has recently been isolated from distilled Gulf Coast petroleum.[1] While its structure has been confirmed through x-ray diffraction, mass spectroscopy, and ¹H/¹³C NMR spectroscopy, its vibrational Raman spectra has only been identified through an indirect comparison with the experimental Raman spectra for adamantane and diamond. We have used density-functional theory (DFT) to calculate a Raman spectra which is in excellent agreement with the experimental Raman spectra for C₂₆H₃₀, thus providing direct vibrational proof of its existence.[2] ¹J. E. P. Dahl *et al.*, *Angew. Chem. Int. Ed.* **42**, 2040 (2003). ²S. L. Richardson, T. Baruah, M. J. Mehl, and M. R. Pederson, accepted for publication in *Chem. Phys. Lett.*

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