

Abstract Submitted
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Theoretical studies of the caged hydrocarbon, octahedrane ($C_{12}H_{12}$, D_{3d})¹ STEVEN RICHARDSON, Howard University, DANIEL FINKENSTADT, U. S. Naval Academy, MICHAEL MEHL, MARK PEDERSON, Naval Research Laboratory — Polyhedral hydrocarbon cages provide an interesting class of molecules for experimental and theoretical study because of their unique shapes. One such molecule is octahedrane ($C_{12}H_{12}$, D_{3d}) which was first synthesized by Lee *et al.* in 1993.² Octahedrane contains two fused three-membered rings and six five-membered rings. Theoretical work by de Meijere *et al.*³ using density-functional theory (DFT) has shown that octahedrane is more strained than the structurally related molecules decahedrane ($C_{16}H_{16}$, D_{4d}), which has two fused four-membered rings and eight five-membered rings, and dodecahedrane ($C_{20}H_{20}$, I_h), which has two fused-membered rings and ten five-membered rings. In this work we report the first DFT calculations of the infrared and Raman vibrational spectra for octahedrane which will be of importance for future efforts in characterizing this unique caged hydrocarbon.

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²C-H Lee, S. Liang, T. Haumann, R. Boese, and A. de Meijere, *Angew. Chem. Int. Ed. Engl.* **1993**, 32, 559.

³A. de Meijere, C-H Lee, M. A. Kuznetsov, D. V. Gusev, S. I. Kozhushkov, A. A. Fokin, and P. R. Schreiner, *Chem. Eur. J.* **2005**, 11, 6175.

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