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Octaselenododecane ($C_4H_8Se_8$): a novel polyselenoether crown macrocycle[1] STEVEN RICHARDSON, Howard Universiy, MICHAEL MEHL, MARK PEDERSON, Naval Research Laboratory — In this work we have used density-functional theory (DFT/GGA-PBE) to calculate the structural, electronic, and vibrational properties of octaselenododecane ($C_4H_8Se_8$), a novel twelve-membered crown-shaped heterocycle which contains four diselenide groups.[2] Our all-electron DFT calculations have yielded results that are in excellent agreement with the observed experimental x-ray diffraction data and infrared and Raman vibrational spectra for the solid state phase of octaselenododecane. In addition to obtaining good general agreement with the selected IR and Raman frequencies reported to lie within the range of 282-2925 cm^{-1}, we have obtained other vibrational modes which have not been reported in the literature. In particular, we have computed a Raman active mode at 267 cm^{-1} which is in good agreement with the experimental band at 282 cm^{-1} and have determined that it represents significant asynchronous stretches of diselenide groups within the heterocycle. Our gas phase calculations also show the presence of strong low frequency distortions that are supressed in the crystal due to close Se-Se intramolecular interactions.

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[2]G. Hua, J. M. Griffin, S. E. Ashbrook, A. M. Z. Slawin, and J. D. Wollins, *Angew Che. Int. Ed.* **2011,** 50, 4123-4126.

Steven Richardson
Howard Universiy

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