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Spectroscopic identification of bond strain and pi interactions in a series of saturated carbon-cage molecules: adamantane, twistane, octahedrane, and cubane TREVOR M. WILLEY, J.R.I. LEE, T. VAN BUUREN, LLNL, L. LANDT, TU Berlin, P.R. SCHREINER, A.A. FOKIN, B.A. TKACHENKO, N.A. FOKINA, JLU Giessen, D. BREHMER, SLAC — Novel nanocarbons such as fullerenes, nanotubes, graphene, and nanodiamond reside at the cutting edge of nanoscience and technology. Along with chemical functionalization, geometrical constraints such as extreme curvature or defects in crystallites can modify the electronic properties. This paper presents a fundamental study of how bond strain affects electronic structure in a benchmark series of novel saturated carbon cage compounds. Adamantane, the smallest diamondoid, has carbon atoms commensurate with the diamond lattice. Twistane has the same stoichiometry ($C_{10}H_{16}$), but introduces some bond strain into the cage. Octahedrane ($C_{12}H_{12}$) and cubane (C_8H_8) have increasing strain, culminating in cubane where C-C bonds lie either parallel, or orthogonal to one another. Using gas-phase NEXAFS spectroscopy, we observe the broad C-C σ^* splits into two more narrow and intense resonances with increasing strain. Also, LUMO states associated with tertiary C-H σ^* broaden and shift to lower energy, and are 3X more intense in cubane than octahedrane. The differences are entirely due to the shape rather than stoichiometry, and indicate, we believe, some π interaction between parallel C-C bonds in the cubane.

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