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Structural and Vibrational Properties of Boron Nitride Analogues of Diamondoids STEVEN L. RICHARDSON, Howard University, KYUNGWHA PARK, Virginia Polytechnic Institute and State University, TUNNA BARUAH, MARK R. PEDERSON, Naval Research Laboratory — Diamondoids are stable cage-like hydrocabon molecules that possess a structure that is superimposable upon the diamond crystal. These highly symmetric structures have a generic structural formula $C_{4n+6}H_{4n+12}$, and they have been isolated from petroleum oil. Because of their various shapes and sizes, there has been speculation in the literature that diamondoids might be suitable building blocks for possible applications in nanotechnology. One could ask whether boron nitride (BN) analogues of diamondoids might exist. It is known experimentally that cyclotriborazane ($B_3N_3H_{12}$), the BN-analogue of the smallest diamondoid molecule adamantane exists, but there is no experimental evidence for the existence of higher-order BN-diamondoids at the present time. In this work we perform accurate all-electron density-functional theory (DFT) calculations to study the structural and vibrational properties of a small set of lower order BN-diamondoids (e.g. BN-adamantane ($B_6N_4H_{16}$), BN-diamantane ($B_7N_7H_{20}$), BN-triamantane ($B_{10}N_8H_{24}$), and BN-*anti*-tetramantane ($B_{11}N_{11}H_{24}$)). We discuss the relative stability of each of these representative BN-diamondoid molecules and provide theoretical infrared and Raman spectra for future identification of this novel class of molecules.

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