

THE USE OF POLYHEDRAL BORANE DERIVATIVES AS MOLECULAR ELECTRONIC SCAFFOLDS

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ABSTRACT

When functionalized, the highly symmetrical, three-dimensional aromatic cluster, *closo* – dodecahydrododecaborate, or dodecaborate, has a two, one – electron oxidation pathway available to it. The framework of dodecaborate is constructed from 26 delocalized electrons. Upon oxidation, electron density from the substituents is needed to allow for a stable oxidation pathway. This work examines the oxidation pathway of a large variety of dodecaborate derivatives via Density Functional Theory (BPV86 / cc-pVTZ) towards the elucidation of dodecaborate as a scaffold for molecular electronics.

In this work it was observed that π -back bonding from the substituents to the framework of dodecaborate occurred in the oxidized product. It was also observed that the substituents are able to become conjugated with the framework of dodecaborate, suggesting that it could become coupled with an electronic component. Additionally, a variety of realistic, functionalized ethers were examined to highlight the versatility of functionalizing the cage. Both the use of the cage as a scaffold for a molecular transistor and molecular rotor were examined.

To test the molecular transistor, it was observed that a chemical source, NH_2 , and drain, NO_2 , could serve similar to an actual circuitry source and drain. The molecular rotor was examined through the use of transition metal bisdicarbollide sandwich complexes. Here, it was observed that Palladium, a second – row metal, was found to have energy barriers of such high as to be amenable to a molecular rotor.