

Accepted Manuscript

Alkyl-Functionalized and Methyldiyne-Doped Boron Nitride Fullerene Polymer Precursors

Ryan C. Fortenberry

PII: S2210-271X(17)30089-0

DOI: <http://dx.doi.org/10.1016/j.comptc.2017.02.022>

Reference: COMPTC 2418

To appear in: *Computational & Theoretical Chemistry*

Received Date: 4 January 2017

Accepted Date: 22 February 2017

Please cite this article as: R.C. Fortenberry, Alkyl-Functionalized and Methyldiyne-Doped Boron Nitride Fullerene Polymer Precursors, *Computational & Theoretical Chemistry* (2017), doi: <http://dx.doi.org/10.1016/j.comptc.2017.02.022>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Alkyl-Functionalized and Methylidyne-Doped Boron Nitride Fullerene Polymer Precursors

Ryan C. Fortenberry*

Georgia Southern University, Department of Chemistry & Biochemistry, Statesboro, GA 30460, U.S.A.

Abstract

Boron nitride fullerenes are stabilized by including methylidyne (CH) groups in place of some of the nitrogen atoms. Such a process also produces carbon atoms in the cage that can subsequently be functionalized. The present work shows that attaching ethyl groups to these carbons destabilizes the fullerene cages somewhat. However, replacing other nitrogen atoms with CH groups returns to a path of stabilization. In fact, the energy minima for inclusion of an ethyl substituted carbon and five CH groups can be lower than simply replacing six nitrogens with six methylidyne. Consequently, it is shown that $B_{12}N_{12}$ dimers linked with ethyl groups are further stabilized with CH replacements of nitrogens. This result indicates that polymers containing these nanoparticles can be made into strong materials. Replacing nitrogens is only favorable within four-membered rings keeping the likely size of the included carborated boron nitride fullerene molecules themselves small as they reside within polymers. Additionally, these materials are promising for aerospace applications where the presence of boron and hydrogen nuclei will shield against cosmic rays and neutron radiation.

Keywords: Boron nitride nanoparticles; fullerenes; hydrogen storage; radiation shielding; wave function theory

1. Introduction

Replacing nitrogen atoms with methylidyne (CH) groups in boron nitride fullerenes strengthens the cage [1]. Additionally, the inclusion of the carbons opens the possibility for the attachment of strongly-bound ligands. These ligands could even be linked to other fullerenes of similar construction allowing for some type of potential polymerization.

Inorganic fullerenes composed of boron and nitrogen were originally suggested as far back as the early days of fullerene chemistry itself [2] and were detected shortly thereafter [3–6]. Since the C_2 base units of C_{60} contain twelve electrons and B–N units are isoelectronic, replacement of C_2 with B–N in part or totality produces the boron-nitride fullerenes [7, 3]. In fact, some boron nitride nanoparticles are known to be more stable and of higher strength than their carbon counterparts [8, 9], especially in the

*Corresponding author

Email address: rfortenberry@georgiasouthern.edu (Ryan C. Fortenberry)

Preprint submitted to Elsevier

January 4, 2017

Download English Version:

<https://daneshyari.com/en/article/5392453>

Download Persian Version:

<https://daneshyari.com/article/5392453>

[Daneshyari.com](https://daneshyari.com)