Graph Theoretical Analysis of Zigzag Polyhexamethylene Biguanide, Polyhexamethylene Adipamide, Polyhexamethylene Biguanide Gauze and Polyhexamethylene Biguanide Hydrochloride (PHMB) Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a-BNNTs) and Hexagonal Boron Nitride Nanotubes (h-BNNTs)

Alireza Heidari
Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA

*Corresponding author: Alireza Heidari, Faculty of Chemistry, California South University (CSU), 14731 Comet St. Irvine, CA 92604, USA, Tel: 1-775-410-4974; E-mail: Scholar.Researcher.Scientists@gmail.com

Received date: October 06, 2016, Accepted date: October 06, 2016, Published date: October 16, 2016

Copyright: © 2016 Heidari A. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

Editorial

In this editorial, the relationship among energy, electric quadrupole and hexadecapole moments with a topological index has known Padmakar-Ivan (PI) index of some different types of zigzag polyhexamethylene biguanide, polyhexamethylene adipamide, polyhexamethylene biguanide gauze and polyhexamethylene biguanide hydrochloride (phmb) Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a-BNNTs) and Hexagonal Boron Nitride Nanotubes (h-BNNTs) is investigated [1-10]. Furthermore, graph theory has been extensively applied to predict the topological, quantum chemical, physical and molecular spectroscopic properties of small molecules such as Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a-BNNTs) and Hexagonal Boron Nitride Nanotubes (h-BNNTs) through Quantum Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies [11-22]. Also, study of Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) shows that energy, electric quadrupole and hexadecapole moments of these Nanotubes could be well predicted.

On the other hand, the energy, electric quadrupole and hexadecapole moments of these Nanotubes were performed using Hartree-Fock (HF) calculations and also Density Functional Theory (DFT) methods by performing HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, B3LYP, BLYP and B3LYP levels of theory using the standard 31G, 6-31G*, 6-311G*, 6-311G(3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09. Moreover, according to the extracted data from logarithmic values of Padmakar-Ivan (PI) index, by increasing the values of the logarithmic energy, electric quadrupole and hexadecapole moments of zigzag polyhexamethylene biguanide, polyhexamethylene adipamide, polyhexamethylene biguanide gauze and polyhexamethylene biguanide hydrochloride (phmb) Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a-BNNTs) and Hexagonal Boron Nitride Nanotubes (h-BNNTs), the values of the topological index will be increased with the number of Boron or Nanotubes circumference. In addition, dimensional diagrams are presented well-related of logarithmic values of Padmaker-Ivan (PI) index with logarithmic energy, electric quadrupole and hexadecapole moments of these Nanotubes. It can be concluded that the results of such studies were used to get into Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) subjects. Also, study of Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) shows that energy, electric quadrupole and hexadecapole moments of these Nanotubes could be well predicted.

References

Citation: Heidari A (2016) Graph Theoretical Analysis of Zigzag Polyhexamethylene Biguanide, Polyhexamethylene Adipamide, Polyhexamethylene Biguanide Gauze and Polyhexamethylene Biguanide Hydrochloride (PHMB) Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a-BNNTs) and Hexagonal Boron Nitride Nanotubes (h-BNNTs). J Appl Computat Math 5: e143. doi:10.4172/2168-9679.1000e143

vapor deposition at low temperature and their growth mechanism. Materials Chemistry and Physics 87: 31-38.


