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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.Scientist@gmail.com

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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 presented. Based on the graph theory, a new method for the prediction of topological, quantum chemical, physical and molecular spectroscopic properties and also other properties 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 Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies [11-22]. Also, this demonstrates strong correlations among quantum chemical, physical and molecular spectroscopic properties and one more topological indices. It should be noted that topological indices present a mathematical definition arising from the field of graph theory.

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, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6-31G*, 6-31+G*, 6-31G(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.

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