Section A-Research paper
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On Computation of Multiplicative Indices for Borophene Nanosheet

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Abstract: Nanomaterials have unique superlative properties with potential applications in electronics, medical and other fields. Borophene, a two dimensional nanomaterial, have a variety of intriguing characteristics. They left an indelible influence on the fields of chemistry, material science, nanotechnology and condensed matter physics with their astounding physical and chemical properties. They can also be used to support immunotherapy, medication delivery systems, biosensors, electronic devices, etc. A breakthrough was made in the fields of mathematics and chemistry with the concept of modelling the structure of a molecule to a chemical graph and then quantitatively analysing the related graph with the aid of topological indices. The topological index is a purely mathematical representation of a molecular structure, which can be utilised as a forecasting tool in QSPR/QSAR studies. These indices could be used in the fields of pharmaceutical, biological and chemical sciences. New indices that more precisely connect with the structural characteristics of a chemical structure are being developed by researchers working on this idea. The multiplicative degree based indices for theβ_{12}-Borophene nanosheet are determined in this study.

Keywords: Multiplicative degree based indices, Nanosheet, β_{12}-Borophene nanosheet.

1 Introduction

Graph theory is a branch of discrete mathematics concerned with the study of relationships between entities. The graph theory research was expanded to include chemical networks and structures, giving rise to the idea of chemical graph theory. Chemical graph theory, a sub-branch that utilised the concept of graph theory to characterise molecular structures, was therefore created by fusing graph theory and chemistry [1]. Here, the objective is to use topological indices to quantitatively assess the structure of a chemical substance or network using a chemical graph model. Topological indices are essential in the study of structural attributes with several applications in structural chemistry. "A topological index is a numerical value which is associated with the chemical constitution and is used for correlation of chemical structure with various physical properties, chemical reactivity, or biological activity", according to the definition provided by the IUPAC [2]. Topological descriptors make it relatively easy to determine a chemical structure’s physical, chemical, biological or medicinal capabilities [1,3-7]. It has applications in a diverse range of disciplines including chemistry, informatics, biology, quantitative structure-acticity-property relationships, etc. The Wiener index, which Harnold Wiener introduced in 1947 [3], was the first topological index. Gutman [8, 9] worked on the multiplicative degree based indices for tree graphs, and Kwunet et al. [10] investigated the multiplicative degree based indices for silicon carbides. Some

Zagreb indices are quite similar to the Wiener index [11] and some Zagreb indices are also very near to the Wiener index. More topological indices, particularly numerous degree-based indices, are present in chemical graph theory. Researchers working on this notion are developing new descriptors that more precisely correlate with the structural features of a chemical structure and their applications in a variety of industries are astounding [12].

The discovery of the two-dimensional nanomaterial known as graphene has sparked an incredible amount of research in the area of two-dimensional materials. The applications of two dimensional materials in numerous industries have improved noticeably as a result, and there has been a tremendous response in the material field. Scientists have paid close attention to these materials due to their exceptional and one-of-a-kind characteristics, exceptional performances, and possible applications. The majority of the atoms in two-dimensional nanosheets are exposed to the surface and are ultrathin compared to bulk materials, allowing for larger surface areas, increased chemical and physical activity, and the onset of quantum confinement phenomena [13]. They are endowed by their natural state with unique photonic, electrical, catalytic, and magnetic capabilities. These nanoparticles have also found extensive use in bio-like materials, drug carriers, biosensors, electronic devices, etc. Borophene is one of the two-dimensional allotropes of boron and has a number of unique properties. Borophene possesses exceptional mechanical rigidity and superconducting properties due to its low weight. Additionally, it has a number of outstanding therapeutic properties that broaden the range of its potential applications in the technological and medical fields. A significant immunological function and catalytic activity are predicted for borophene, which has the potential to be exploited as a channel for drug distribution in immunotherapy due to its exceptional structural endurance and high reliability [13]. These nanoparticles are perfect for a variety of scientific and technological applications, including higher energy fuel, enhanced temperature devices, coatings, atomic engineering, and atmospheric emissions, due to their exceptional physical and chemical properties. Borophene has steadily grown in importance in the fields of chemistry, bioengineering, nanoelectronics and quantum physics. Graphene has a hexagonal framework throughout, but borophene has a triangular framework with hexagonal cavities (HH), and the distribution of these cavities varies throughout the structure. The most studied borophene nanostructures, according to borophene, are β_{12}, χ^3, 2-Pmmn and honeycomb [14].

The multiplicative degree based indices of the β_{12}-Borophene nanosheet [14] is analysed in this research. The analysis uses the degree counting and edge partition approach. Researchers have examined various topological indices of borophene nanosheets and borophene nanotubes of other varieties, specifically 2-Pmmn, χ^3 and honeycomb [15-17]. The degree based indices of β_{12}-Borophene nanosheet was recently studied in [18]. The β_{12}-Borophene nanosheet is designated in this study as $\beta(j,k)$, where $'j'$ is the number of rows and $'k'$ is the number of columns that repeat hexagons with the centre vertex. Figure 1 presents the molecular graph of $\beta(3,4)$. See [10,19-25] for more papers based on multiplicative degree based indices.

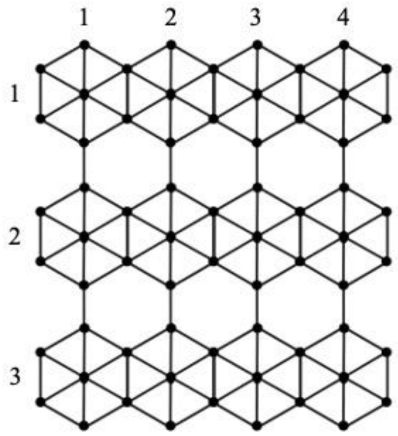

Figure 1: β_{12}-Borophene nanosheet, $\beta(3,4)$.

2 Mathematical Concepts

The concepts and notations used for the study are summarized in this section. Consider a connected simple graph $\Psi = (\partial(\Psi), \mathcal{E}(\Psi))$, where $\partial(\Psi)$ stands for the vertex set and $\mathcal{E}(\Psi)$ stands for the edge set. A vertex $\nu \in \partial(\Psi)$ has degree, $d(\nu)$, which is the number of edges incident to the vertex. The mathematical expressions for the multiplicative degree based indices are given in Table 1.

Table 1: The multiplicative degree based indices of graph Ψ.

S. No.	**Multiplicative Index**	**Mathematical Expression**
1	Generalised Multiplicative Zagreb Indices [26]	$II_1^{\sigma}(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \big(d(\nu)+d(\omega)\big)^{\sigma}$ $II_2^{\sigma}(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \big(d(\nu)\times d(\omega)\big)^{\sigma}$
2	Multiplicative Zagreb Indices [27]	$II_1(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \big(d(\nu)+d(\omega)\big)$ $II_2(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \big(d(\nu)\times d(\omega)\big)$
3	Multiplicative Hyper Zagreb Indices [28]	$HII_1(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \big(d(\nu)+d(\omega)\big)^{2}$ $HII_2(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \big(d(\nu)\times d(\omega)\big)^{2}$
4	Multiplicative Connectivity Indices [29]	$SCII(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \big(d(\nu)+d(\omega)\big)^{\frac{-1}{2}}$ $PCII(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \big(d(\nu)\times d(\omega)\big)^{\frac{-1}{2}}$

5	Multiplicative Harmonic Index [30]	$HII(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \frac{2}{(d(\nu)+d(\omega))}$
6	Multiplicative Atom Bond Connectivity Index [31]	$ABCII(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \frac{\sqrt{(d(\nu)+d(\omega)-2)}}{\sqrt{(d(\nu)\times d(\omega))}}$
7	Multiplicative Geometric Arithmetic Index [31]	$GAII(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\Psi)} \frac{2\times\sqrt{(d(\nu)\times d(\omega))}}{(d(\nu)+d(\omega))}$

3 Multiplicative Degree based Indices for β_{12}-Borophene Nanosheet

3.1 Methods and Methodology

The degree counting and edge partition approach is utilized to compute the multiplicative indices for the β_{12}-Borophene nanosheet, $\beta(j,k); j,k \geq 1$.

$\beta(j,k)$ has 5jk + 2j vertices and (12jk − k) + j edges. The vertex degree's of $\beta(j,k)$ are 3, 4, 5 and 6. Based on the vertex degree, the edge set $\mathcal{E}(\beta(j,k))$ of $\beta(j,k)$ can be partitioned into sets $\mathfrak{E}_{(p,q)} = \{(\upsilon,\omega) \in \mathcal{E}(\Psi): d(\upsilon) = p, d(\omega) = q\}$. The number of edges in each partition of $\beta(j,k)$ is generalizable and there are nine types of edge partitions, say $\mathfrak{E}_{(3,3)}$, $\mathfrak{E}_{(3,4)}$, $\mathfrak{E}_{(3,5)}$, $\mathfrak{E}_{(3,6)}$, $\mathfrak{E}_{(4,4)}$, $\mathfrak{E}_{(4,5)}$, $\mathfrak{E}_{(4,6)}$, $\mathfrak{E}_{(5,5)}$ and $\mathfrak{E}_{(5,6)}$. The cardinality of the corresponding edge partition set is given by $|\mathfrak{E}_{(p,q)}|$. Table 2 contains the edge partition sets for $\beta(j,k)$ with their corresponding cardinality. The edge partition for $\beta(3,4)$ is demonstrated in Figure 2.

Table 2: The edge partitions, $\mathfrak{E}_{(p,q)}$ for $\beta(j,k)$ and their corresponding cardinality.

Edge Partition, $\mathfrak{E}_{(p,q)}$	**Cardinality, $\lvert\mathfrak{E}_{(p,q)}\rvert$**
$\mathfrak{E}_{(3,3)}$	$2j+4$
$\mathfrak{E}_{(3,4)}$	$4j-4$
$\mathfrak{E}_{(3,5)}$	$4k-4$
$\mathfrak{E}_{(3,6)}$	$4j+2$
$\mathfrak{E}_{(4,4)}$	$jk-k$
$\mathfrak{E}_{(4,5)}$	$4(j-1)(k-1)$
$\mathfrak{E}_{(4,6)}$	$2jk-2k$
$\mathfrak{E}_{(5,5)}$	$jk-j$
$\mathfrak{E}_{(5,6)}$	$4jk-4j$

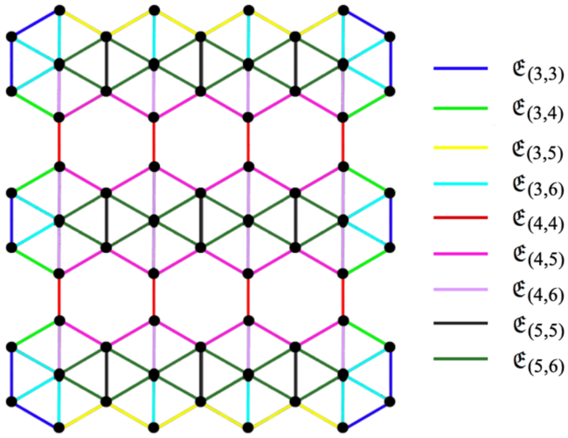

Figure 2: Edge partition for β(3, 4)

Further, the analytical expressions for the multiplicative indices of $\beta(j,k); j,k \geq 1$ are derived from the mathematical expressions of the corresponding multiplicative degree based indices using the data in Table 2.

3.2 Results

Theorems based on the computation of multiplicative degree based indices for β_{12}-Borophene nanosheet, $\beta(j,k); j,k \geq 1$ are presented in this section.

3.2.1 Generalised Multiplicative Zagreb Indices

***Theorem 1**: For $\beta(j,k); j,k \geq 1$*

$$II_1^\sigma(\beta) = 2^{3\sigma(3k+jk-4)} \times 3^{2\sigma(4jk-2k+4)} \times 6^{\sigma(2j+4)} \times 7^{\sigma(4j-4)} \times 10^{\sigma(3jk-j-2k)} \times 11^{4\sigma j(k-1)}$$

$$II_2^\sigma(\beta) = 2^{4\sigma(jk-k)} \times 3^{2\sigma(2j+4)} \times 5^{2\sigma(jk-j)} \times 12^{\sigma(4j-4)} \times 15^{\sigma(4k-4)} \times 18^{\sigma(4j+2k)} \times 20^{\sigma(4j-4)(k-1)} \times 24^{2\sigma k(j-1)} \times 30^{4\sigma j(k-1)}$$

***Proof**:* Using the mathematical expressions given in Table 1 and the data from Table 2,

$$II_1^\sigma(\Psi) = \prod_{\nu\omega \in \mathcal{E}(\beta)} \big(d(\nu) + d(\omega)\big)^\sigma$$

$$= (3+3)^{\sigma|\mathfrak{E}_{(3,3)}|} \times (3+4)^{\sigma|\mathfrak{E}_{(3,4)}|} \times (3+5)^{\sigma|\mathfrak{E}_{(3,5)}|} \times (3+6)^{\sigma|\mathfrak{E}_{(3,6)}|} \times (4+4)^{\sigma|\mathfrak{E}_{(4,4)}|} \times (4+5)^{\sigma|\mathfrak{E}_{(4,5)}|} \times (4+6)^{\sigma|\mathfrak{E}_{(4,6)}|} \times (5+5)^{\sigma|\mathfrak{E}_{(5,5)}|} \times (5+6)^{\sigma|\mathfrak{E}_{(5,6)}|}$$

$$= 2^{3\sigma(3k+jk-4)} \times 3^{2\sigma(4jk-2k+4)} \times 6^{\sigma(2j+4)} \times 7^{\sigma(4j-4)} \times 10^{\sigma(3jk-j-2k)} \times 11^{4\sigma j(k-1)}.$$

Also,

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$$II_2^{\sigma}(\Psi) = \prod_{\nu\omega\in\mathcal{E}(\beta)} \left(d(\nu)\times d(\omega)\right)^{\sigma}$$

$$\begin{aligned} &= (3\times 3)^{\sigma|\mathfrak{E}_{(3,3)}|} \times (3\times 4)^{\sigma|\mathfrak{E}_{(3,4)}|} \times (3\times 5)^{\sigma|\mathfrak{E}_{(3,5)}|} \times (3\times 6)^{\sigma|\mathfrak{E}_{(3,6)}|} \\ &\quad \times (4\times 4)^{\sigma|\mathfrak{E}_{(4,4)}|} \times (4\times 5)^{\sigma|\mathfrak{E}_{(4,5)}|} \times (4\times 6)^{\sigma|\mathfrak{E}_{(4,6)}|} \times (5\times 5)^{\sigma|\mathfrak{E}_{(5,5)}|} \\ &\quad \times (5\times 6)^{\sigma|\mathfrak{E}_{(5,6)}|} \end{aligned}$$

$$\begin{aligned} &= 2^{4\sigma(jk-k)} \times 3^{2\sigma(2j+4)} \times 5^{2\sigma(jk-j)} \times 12^{\sigma(4j-4)} \times 15^{\sigma(4k-4)} \times 18^{\sigma(4j+2k)} \\ &\quad \times 20^{\sigma(4j-4)(k-1)} \times 24^{2\sigma k(j-1)} \times 30^{4\sigma j(k-1)}. \end{aligned}$$

3.2.2 Multiplicative Zagreb Indices

Theorem 2: *For* $\beta(j,k); j,k \geq 1$

$$II_1(\beta) = \frac{1}{614656}\left(2^{(7k+j+6jk)} \times 3^{(2j-4k+8jk+12)} \times 5^{(3jk-j-2k)} \times 7^{(4j)} \times 11^{4j(k-1)}\right)$$

$$II_2(\beta) = 2^{2k(11j-8)} \times 3^{(6jk+12j+6k)} \times 5^{10j(k-1)}$$

Proof: The multiplicative Zagreb indices can be generated by substituting $\sigma = 1$ in the mathematical expressions given for generalised multiplicative Zagreb indices in Table 1. Hence, substituting $\sigma = 1$ in the results of Theorem 1, the multiplicative Zagreb indices can be calculated and the obtained results are as follows.

$$II_1(\beta) = \frac{1}{614656}\left(2^{(7k+j+6jk)} \times 3^{(2j-4k+8jk+12)} \times 5^{(3jk-j-2k)} \times 7^{(4j)} \times 11^{4j(k-1)}\right).$$

$$II_2(\beta) = 2^{2k(11j-8)} \times 3^{(6jk+12j+6k)} \times 5^{10j(k-1)}.$$

3.2.3 Multiplicative Hyper Zagreb Indices

Theorem 3: *For* $\beta(j,k); j,k \geq 1$

$$HII_1(\beta) = 2^{(12jk+2j+14k-16)} \times 3^{(16jk+4j-8k+24)} \times 5^{(6jk-2j-4k)} \times 7^{(8j-8)} \times 11^{8j(k-1)}$$

$$HII_2(\beta) = 2^{4k(11j-8)} \times 3^{(12jk+24j+12k)} \times 5^{20j(k-1)}$$

Proof: The multiplicative hyper Zagreb indices can be obtained by substituting σ = 2 in the mathematical expressions given for generalised multiplicative Zagreb indices in Table 1. As a result of substituting σ = 1 in the results of Theorem 1, the multiplicative hyper Zagreb indices can be deduced as follows.

$$HII_1(\beta) = 2^{(12jk+2j+14k-16)} \times 3^{(16jk+4j-8k+24)} \times 5^{(6jk-2j-4k)} \times 7^{(8j-8)} \times 11^{8j(k-1)}.$$

$$HII_2(\beta) = 2^{4k(11j-8)} \times 3^{(12jk+24j+12k)} \times 5^{20j(k-1)}.$$

3.2.4 Multiplicative Connectivity Indices

Theorem 4: *For* $\beta(j,k); j,k \geq 1$

$$SCII(\beta) = 2^{(12jk+2j+14k-16)} \times 3^{(16jk+4j-8k+24)} \times 5^{(6jk-2j-4k)} \times 7^{(8j-8)} \times 11^{8j(k-1)}$$

$$PCII(\beta) = 2^{4k(11j-8)} \times 3^{(12jk+24j+12k)} \times 5^{20j(k-1)}$$

Proof: The multiplicative hyper Zagreb indices can be obtained by substituting σ = 2 in the mathematical expressions given for generalised multiplicative Zagreb indices in Table 1. As a result of substituting σ = 1 in the results of Theorem 1, the multiplicative hyper Zagreb indices can be deduced as follows.

$$SCII(\beta) = 2^{(12jk+2j+14k-16)} \times 3^{(16jk+4j-8k+24)} \times 5^{(6jk-2j-4k)} \times 7^{(8j-8)} \times 11^{8j(k-1)}.$$

$$PCII(\beta) = 2^{4k(11j-8)} \times 3^{(12jk+24j+12k)} \times 5^{20j(k-1)}.$$

3.2.5 Multiplicative Harmonic Index

Theorem 5: *For* $\beta(j,k); j,k \geq 1$

$$HII(\beta) = 28^4 \times \left(\frac{2}{11}\right)^{4jk-4j} \times \left(\frac{1}{5}\right)^{3jk-j-2k} \times \left(\frac{2}{9}\right)^{4jk-2k} \times \left(\frac{1}{4}\right)^{jk+3k} \times \left(\frac{2}{7}\right)^{4j} \times \left(\frac{1}{3}\right)^{2j+12}$$

Proof: Using the mathematical expressions from Table 1 and the data from Table 2,

$$\begin{aligned} HII(\beta) &= \prod_{\nu\omega\in\mathcal{E}(\beta)} \frac{2}{(d(\nu)+d(\omega))} \\ &= 28^4 \times \left(\frac{2}{11}\right)^{4jk-4j} \times \left(\frac{1}{5}\right)^{3jk-j-2k} \times \left(\frac{2}{9}\right)^{4jk-2k} \times \left(\frac{1}{4}\right)^{jk+3k} \times \left(\frac{2}{7}\right)^{4j} \times \left(\frac{1}{3}\right)^{2j+12}. \end{aligned}$$

3.2.6 Multiplicative Atom Bond Connectivity Index

Theorem 6: *For* $\beta(j,k); j,k \geq 1$

$$ABCII(\beta) = \frac{196 \times 2^{\left(\frac{13k}{2}+\frac{j}{2}-6jk\right)} \times 3^{\left(\frac{3jk}{2}-\frac{3k}{2}-10j\right)} \times 7^{(2jk-k)}}{225 \times 5^{(5jk-7j)}}$$

Proof: Using the mathematical expressions from Table 1 and the data from Table 2,

$$ABCII(\beta) = \prod\nolimits_{\nu\omega\in\mathcal{E}(\beta)} \frac{\sqrt{(d(\nu)+d(\omega)-2)}}{\sqrt{(d(\nu)\times d(\omega))}} = \frac{196\times 2^{\left(\frac{13k}{2}+\frac{j}{2}-6jk\right)}\times 3^{\left(\frac{3jk}{2}-\frac{3k}{2}-10j\right)}\times 7^{(2jk-k)}}{225\times 5^{(5jk-7j)}}.$$

3.2.7 Multiplicative Geometric Arithmetic Index

Theorem 7*: For* $\beta(j,k); j,k \geq 1$

$$GAII(\beta) = \left(\frac{4\sqrt{3}}{7}\right)^{4j-4} \times \left(\frac{\sqrt{15}}{4}\right)^{4k-4} \times \left(\frac{2\sqrt{2}}{3}\right)^{4j+2k} \times \left(\frac{4\sqrt{5}}{9}\right)^{4(j-1)(k-1)} \times \left(\frac{2\sqrt{6}}{5}\right)^{2jk-2k} \times \left(\frac{2\sqrt{30}}{11}\right)^{4jk-4j}$$

Proof*:* Using the mathematical expressions from Table 1 and the data from Table 2,

$$GAII(\beta) = \prod_{\nu\omega\in\mathcal{E}(\beta)} \frac{2 \times \sqrt{\left(d(\nu) \times d(\omega)\right)}}{\left(d(\nu) + d(\omega)\right)}$$

$$= \left(\tfrac{4\sqrt{3}}{7}\right)^{4j-4} \times \left(\tfrac{\sqrt{15}}{4}\right)^{4k-4} \times \left(\tfrac{2\sqrt{2}}{3}\right)^{4j+2k} \times \left(\tfrac{4\sqrt{5}}{9}\right)^{4(j-1)(k-1)} \times \left(\tfrac{2\sqrt{6}}{5}\right)^{2jk-2k} \times \left(\tfrac{2\sqrt{30}}{11}\right)^{4jk-4j}.$$

5 Conclusion

The edge partition approach was adopted to compute the multiplicative degree based indices of β_{12}-Borophene nanosheets in this study. These descriptors have applications in a variety of fields, making the study timely. The derived analytic expressions may aid researchers and scientists in future innovations in the field of nanomaterials, as well as in investigating the nature and behaviour of the β_{12}-Borophene nanosheet without any experimental research. The determined results can also be used to compare the multiplicative indices with other topological indices that are already derived for the nanosheet.

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