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HEXAGONAL BORON NITRIDE NETWORKS: CLOSED-FORM EXPRESSIONS AND COMPARATIVE ANALYSIS OF MOSTAR, PI, AND SZEGED-TYPE INDICES

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Abstract
In the study of molecular structures, topological indices are crucial, especially in mathematical chemistry where they are employed to describe the physicochemical characteristics of compounds. In this work, we examine various topological indices of the hexagonal boron nitride network based on degree and distance. In particular, we use the cut method to calculate the vertex, edge, and total variants of the Mostar, PI, and Szeged indices. The number of horizontal rings in the network, denoted by the structural parameter ρ, is used to derive closed-form expressions for these indices. The results show that the Szeged index has hexic growth behavior, whereas the Mostar and PI indices grow quadratically. Additionally, to show how these indices vary for various values of ρ and to compare them with corresponding values for carbon nanotube structures, numerical calculations and graphical comparisons are provided. The findings show these indices' structural sensitivity and discriminating power, which could be helpful in researching the chemical stability, reactivity, and other molecular characteristics of boron nitride-based nanomaterials.

INTRODUCTION

The branch of Mathematical chemistry that is used to discuss and forecast the behaviour of mathematical structures is known as theoretical chemistry [13, 14]. Many studies have been conducted in this field over the last few decades. In the field of chemistry, this principle has been extremely useful. There are different topological indices [20, 21, 22]. The degree and distance based topological indices are mainly applicator in the fields of pharmacy, theoretical chemistry, and, in particular, $QSPR/QSAR$ research [5]. Let $\mathcal{H} = (V_{\mathcal{H}}, E_{\mathcal{H}})$ be a graph with the vertex set $V_{\mathcal{H}}$ and the edge set $E_{\mathcal{H}}$, where $|V_{\mathcal{H}}|$ and $|E_{\mathcal{H}}|$ represents the order and size of H, respectively. The bond-additive topological invariants are largely employed to recognize the characteristics of chemical graphs. The Wiener invariant [28] is a

first notable bond-additive invariant. Inspired by the miscellaneous productive invariants, such as Zagreb [10], irregularity [1], Szeged [11], and revised-Szeged [19, 24, 25]. Padmakar-Ivan a bond additive invariant was proposed by Khadikar et al [23]. They abbreviated this new topological index as PI. For an edge $e = rz \in E_{\mathcal{H}}$, there are two kinds of weights regarding degrees of end vertices.

$$W^*(e = rs) = deg_{\mathcal{H}}(r)deg_{\mathcal{H}}(s), W^+(e = rs) = deg_{\mathcal{H}}(r) + deg_{\mathcal{H}}(s).$$

Now, by using the above edge weights we can interpret the weighted PI invariants for $\mathcal{H}$ as:

$$\begin{aligned}
W^+PI_v(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^+(e=rs)(\mathrm{n}_r(e|\mathcal{H}) + \mathrm{n}_s(e|\mathcal{H})),\\
W^+PI_e(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^+(e=rs)(\mathrm{m}_r(e|\mathcal{H}) + \mathrm{m}_s(e|\mathcal{H})),\\
W^+PI_t(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^+(e=rs)(\mathrm{t}_r(e|\mathcal{H}) + \mathrm{t}_s(e|\mathcal{H})),\\
W^*PI_v(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^*(e=rs)(\mathrm{n}_r(e|\mathcal{H}) + \mathrm{n}_s(e|\mathcal{H})),\\
W^*PI_e(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^*(e=rs)(\mathrm{m}_r(e|\mathcal{H}) + \mathrm{m}_s(e|\mathcal{H})),\\
W^*PI_t(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^*(e=rs)(\mathrm{t}_r(e|\mathcal{H}) + \mathrm{t}_s(e|\mathcal{H})).
\end{aligned} \quad (1)$$

where $\mathrm{n}_r(e|\mathcal{H})$ (or $\mathrm{n}_s(e|\mathcal{H})$) is the cardinality of vertices closer to r (or s) than s (or r), $\mathrm{m}_r(e|\mathcal{H})$ (or $\mathrm{m}_s(e|\mathcal{H})$) is the cardinality of edges closer to r (or s) than s (or r), and $\mathrm{t}_r(e|\mathcal{H})$ (or $\mathrm{t}_s(e|\mathcal{H})$) is the cardinality of vertices and edges closer to r (or s) than s (or r). Farahani [9] computed a closed formula for $PI_e(\mathcal{H})$ and $PI_v(\mathcal{H})$ of the structure of the circumcoronene series of benzenoid H_k by the use of cut method. Farahani et al. [8] computed the vertex PI index of Titania carbon Nanotubes $TiO_2[m,n]$. Zheng et al. [30] computed the edge PI index of Titania carbon Nanotubes $TiO_2[m,n]$. In 1994, Gutman introduced Szeged Index [12] for any connected graph $\mathcal{H}$ by:

$$Sz_v(\mathcal{H}) = \sum_{rs\in E(\mathcal{H})} \mathrm{n}_r(e|\mathcal{H})\mathrm{n}_s(e|\mathcal{H}) \qquad Sz_e(\mathcal{H}) = \sum_{rs\in E(\mathcal{H})} \mathrm{m}_r(e|\mathcal{H})\mathrm{m}_s(e|\mathcal{H})$$
$$Sz_t(\mathcal{H}) = \sum_{rs\in E(\mathcal{H})} \mathrm{t}_r(e|\mathcal{H})\mathrm{t}_s(e|\mathcal{H}) \quad (2)$$

Now, by using the above edge weights we can interpret the weighted Szeged invariants for $\mathcal{H}$ as:

$$\begin{aligned}
W^{+}Sz_{v}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{+}(e=rs)\mathrm{n}_{r}(e|\mathcal{H})\mathrm{n}_{s}(e|\mathcal{H}),\\
W^{+}Sz_{e}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{+}(e=rs)\mathrm{m}_{r}(e|\mathcal{H})\mathrm{m}_{s}(e|\mathcal{H}),\\
W^{+}Sz_{t}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{+}(e=rs)\mathrm{t}_{r}(e|\mathcal{H})\mathrm{t}_{s}(e|\mathcal{H}),\\
W^{*}Sz_{v}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{*}(e=rs)\mathrm{n}_{r}(e|\mathcal{H})\mathrm{n}_{s}(e|\mathcal{H}),\\
W^{*}Sz_{e}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{*}(e=rs)\mathrm{m}_{r}(e|\mathcal{H})\mathrm{m}_{s}(e|\mathcal{H}),\\
W^{*}Mo_{t}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{*}(e=rs)\mathrm{t}_{r}(e|\mathcal{H})\mathrm{t}_{s}(e|\mathcal{H}).
\end{aligned} \tag{3}$$

The Szeged index has various critical applications in network theory and chemistry. Due to importance of Szeged index, several variations of this index including edge-Szeged index and the PI index were defined. In 2017, Doslić et al. [6] introduced the Moster index to acquire the peripherality measure of any given molecular structure and it was defined as follows:

$$Mo_{v}(\mathcal{H}) = \sum_{rs\in E(\mathcal{H})} |\mathrm{n}_{r}(e|\mathcal{H}) - \mathrm{n}_{s}(e|\mathcal{H})|. \tag{4}$$

Deng et al. [7] determined the Mostar invariant of benzenoid system. Further they found its extremal Mostar invariant for trees and unicyclic graphs. Later the expression for the Mostar invariant of bicyclic graphs was derived in [26]. Tratnik [27] proved that the Mostar invariant of the weighted graph can be deduced in the form of Mostar invariant of quotient graphs. Recently, other versions of Mostar invariant, named as edge Mostar and total Mostar invariants, were presented by Arockiaraj et al. [2].

$$Mo_{e}(\mathcal{H}) = \sum_{rs\in E(\mathcal{H})} |\mathrm{m}_{r}(e|\mathcal{H}) - \mathrm{m}_{s}(e|\mathcal{H})|. \; Mo_{t}(\mathcal{H}) = \sum_{rs\in E(\mathcal{H})} |\mathrm{t}_{r}(e|\mathcal{H}) - \mathrm{n}_{s}(e|\mathcal{H})|. \tag{5}$$

Now, by using the above edge weights we can interpret the weighted Mostar invariants for $\mathcal{H}$ as:

$$
\begin{aligned}
W^{+}Mo_{v}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{+}(e=rz)|\mathrm{n}_{r}(e|\mathcal{H})-\mathrm{n}_{s}(e|\mathcal{H})|,\\
W^{+}Mo_{e}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{+}(e=rz)|\mathrm{m}_{r}(e|\mathcal{H})-\mathrm{m}_{s}(e|\mathcal{H})|,\\
W^{+}Mo_{t}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{+}(e=rz)|\mathrm{t}_{r}(e|\mathcal{H})-\mathrm{t}_{s}(e|\mathcal{H})|,\\
W^{*}Mo_{v}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{*}(e=rz)|\mathrm{n}_{r}(e|\mathcal{H})-\mathrm{n}_{s}(e|\mathcal{H})|, \qquad (6)\\
W^{*}Mo_{e}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{*}(e=rz)|\mathrm{m}_{r}(e|\mathcal{H})-\mathrm{m}_{s}(e|\mathcal{H})|,\\
W^{*}Mo_{t}(\mathcal{H}) &= \sum_{e=rs\in E_{\mathcal{H}}} W^{*}(e=rz)|\mathrm{t}_{r}(e|\mathcal{H})-\mathrm{t}_{s}(e|\mathcal{H})|.
\end{aligned}
$$

For more results related to Mostar invariants, see [3, 4, 15, 16, 29]. In the late $1950s$, they employ the cut method proposed in [17], which they used to determine the Wiener index of graphs. This approach was extended for general graphs by establishing a connection between the graph's canonical metric representation and its Wiener index in [18]. For a graph H the edges $e=rs$ and $f=r's'$ of H represents the the Djokovic-Winkler Θ relation if $d_H(rr')+d_H(ss')\neq d_H(rs)+d_H(r's')$. It is important to revise the substantial preliminaries of the Cut method which is critical to our computations. For any connected graph H, the edges $h=pq$ and $e=rs$ are in Djokovic-Winkler relation, whenever $d_H(p,r)+d_H(q,s)\neq d_H(p,s)+d_H(q,r)$.

Hexagonal Boron nitride graph

In Section 2, we provide a methodical way to use the cut method to calculate the Mostar, PI, and Szeged invariants of the hexagonal boron nitride graph. The numerical results and graphical comparisons for these topological indices for the hexagonal boron nitride structure are presented in Section 2. $\mathbb{BN}$ represents the hexagonal boron nitride graph, which is a straightforward, connected planar graph. Figure 1 shows how its rings are arranged both horizontally and vertically. $\rho\times\rho$ is the total number of rings in the structure, where ρ is the number of horizontal rings. The order of $\mathbb{BN}$ is $2\rho^2+4\rho$, and its size is $3\rho^2+4\rho-1$. The two-dimensional covalent network found in hexagonal boron nitride can be found in both cubic and hexagonal structural forms. Atoms of nitrogen and boron alternate in the hexagonal arrangement to create a regular honeycomb-like pattern. There are an equal number of nitrogen and boron atoms in each hexagon. The formation of boron nitride nanotubes frequently exhibits the single-layered hexagonal $\mathbb{BN}$ structure. All cuts for Hexagonal boron nitride graph are depicted in Figure 1.

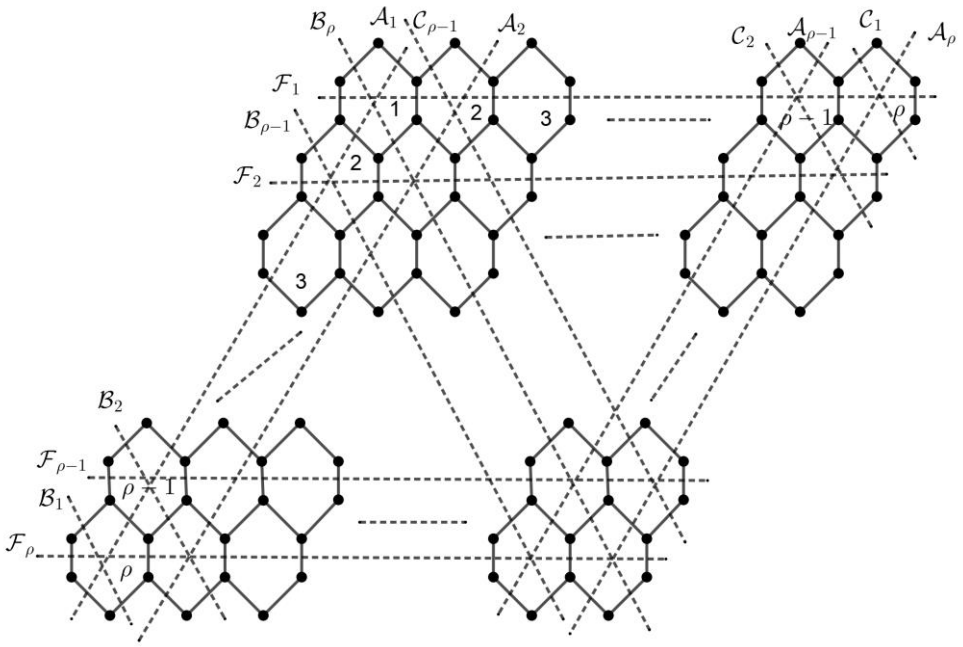


Figure 1: Hexagonal boron nitride graph with edge cuts.

The cuts $\mathcal{A}_\eta$ and $\mathcal{F}_\eta$, where $1 \le \eta \le \rho$, are symmetric and $|\mathcal{A}_\eta| = |\mathcal{F}_\eta| = \rho + 1$. Their specifications are provided by

$$ccn_{\mathcal{A}_\eta}(r) = n_{\mathcal{F}_\eta}(r) = 2(\rho+1)\eta - 1, n_{\mathcal{A}_\eta}(s) = n_{\mathcal{F}_\eta}(s) = 2\rho(\rho+2) - 2(\rho+1)\eta + 1, \quad (7)$$

$$m_{\mathcal{A}_\eta}(r) = m_{\mathcal{F}_\eta}(r) = (3\rho+2)\eta - (\rho+2), m_{\mathcal{A}_\eta}(s) = m_{\mathcal{F}_\eta}(s) = 3\rho^2 + 4\rho - (3\rho+2)\eta. \quad (8)$$

The pairs of degrees for these cuts are

$$\left(d_{\mathcal{A}_\eta}(r), d_{\mathcal{A}_\eta}(s)\right) = \begin{cases} (2,3), & if\ 2 \le \eta \le \rho - 1\ and\ size\ is\ 2; \\ (3,3), & if\ 1 \le \eta \le \rho\ and\ size\ is\ \rho - 1; \\ (2,3), & if\ \eta = 1\ or\ \eta = \rho\ and\ size\ is\ 1; \\ (2,2), & if\ \eta = 1\ or\ \eta = \rho\ and\ size\ is\ 1. \end{cases} \quad (9)$$

Similarly, the cuts $\mathcal{B}_\eta$ for $1 \le \eta \le \rho$ and $\mathcal{C}_\eta$ for $1 \le \eta \le \rho - 1$ are symmetric and satisfy $|\mathcal{B}_\eta| = |\mathcal{C}_\eta| = \eta + 1$. Their parameters are

$$ccn_{B_\eta}(r) = n_{C_\eta}(r) = \eta(\eta+2), n_{B_\eta}(s) = n_{C_\eta}(s) = 2\rho(\rho+2) - \eta(\eta+2), \quad (10)$$

$$m_{B_\eta}(r) = m_{C_\eta}(r) = \frac{3}{2}\eta(\eta+1) - 1, m_{B_\eta}(s) = m_{C_\eta}(s) = 3\rho^2 + 4\rho - 1 - \frac{3}{2}\eta^2 - \frac{5}{2}\eta. \quad (11)$$

The matching pairs of degrees are

$$\left(d_{\mathcal{B}_\eta}(r), d_{\mathcal{B}_\eta}(s)\right) = \left(d_{\mathcal{C}_\eta}(r), d_{\mathcal{C}_\eta}(s)\right) = \begin{cases} (2,3), & if\ 1 \le \eta \le \rho - 1\ and\ size\ is\ 2; \\ (3,3), & if\ 1 \le \eta \le \rho\ and\ size\ is\ \eta - 1; \\ (2,2), & if\ \eta = \rho\ and\ size\ is\ 2. \end{cases} \quad (12)$$

We now determine the Mostar index of the hexagonal boron nitride network using the expressions (4), (5),

and (??), as well as the previously calculated cut parameters.

Theorem 2.1 *For $\rho \geq 2$, the Mostar indices for the network of hexagonal boron nitride are*

- $Mo_v(\mathbb{BN}) = \rho^4 + 4\rho^3 + \rho^2 - 6\rho + 8\left\lceil\frac{\rho}{2}\right\rceil(\rho+1)^2\left(\rho - \left\lceil\frac{\rho}{2}\right\rceil\right)$.
- $Mo_e(\mathbb{BN}) = \frac{3\rho^4}{2} + \frac{16\rho^3}{3} - \frac{\rho^2}{2} - \frac{19\rho}{3} + 4\left\lceil\frac{\rho}{2}\right\rceil(\rho+1)(3\rho+2)\left(\rho - \left\lceil\frac{\rho}{2}\right\rceil\right)$.
- $Mo_t(\mathbb{BN}) = \frac{5\rho^4}{2} + \frac{28\rho^3}{3} - \frac{\rho^2}{2} - \frac{37\rho}{3} + 4\left\lceil\frac{\rho}{2}\right\rceil(\rho+1)(5\rho+4)\left(\rho - \left\lceil\frac{\rho}{2}\right\rceil\right)$.

Proof. • By using the equations (4), we acquire

$$\begin{aligned}
Mo_v(\mathbb{BN}) = \; & 2\sum_{\eta=1}^{\rho}(\rho+1)|2(\rho+1)\eta - 1 - (2\rho(\rho+2) - 2(\rho+1)\eta + 1)| \\
& +2\sum_{\eta=1}^{\rho-1}(\eta+1)|(2\rho(\rho+2) - \eta(\eta+2)) - \eta(\eta+2)| \\
& = 2(\rho+1)\sum_{\eta=1}^{\lceil\frac{\rho}{2}\rceil}(2\rho^2 + 4\rho + 2 - 4(\rho+1)\eta) + 2(\rho+1)\sum_{i=\lceil\frac{\rho}{2}\rceil+1}^{\rho}(4(\rho+1)\eta - 2\rho^2 \\
& -4\rho - 2) + 2\sum_{\eta=1}^{\rho-1}(\eta+1)(2\rho(\rho+2) - 2\eta(\eta+2)) \\
& = 4(\rho+1)^3\left\lceil\frac{\rho}{2}\right\rceil - 4(\rho+1)^3\left(\rho - \left\lceil\frac{\rho}{2}\right\rceil\right) - 4(\rho+1)^2\left(\left\lceil\frac{\rho}{2}\right\rceil\left(\left\lceil\frac{\rho}{2}\right\rceil + 1\right)\right) \\
& +4(\rho+1)^2\left(\rho - \left\lceil\frac{\rho}{2}\right\rceil\right)\left(\rho + 1 + \left\lceil\frac{\rho}{2}\right\rceil\right) + 4\rho(\rho+2)\left(\frac{\rho^2+\rho-2}{2}\right) \\
& -(4\times\frac{\rho}{4})(\rho-1)(\rho+1)(\rho+2) \\
& = \rho^4 + 4\rho^3 + \rho^2 - 6\rho + 8\left\lceil\frac{\rho}{2}\right\rceil(\rho+1)^2\left(\rho - \left\lceil\frac{\rho}{2}\right\rceil\right).
\end{aligned}$$

• By using the equations (5), we acquire

$$
\begin{aligned}
Mo_e(\mathbb{BN}) &= 2\sum_{\eta=1}^{\rho}(\rho+1)|(3\rho+2)\eta-(\rho+2)-(3\rho^2+4\rho-(3\rho+2)\eta)| \\
&+2\sum_{\eta=1}^{\rho-1}(\eta+1)\left|\frac{3}{2}\eta^2+\frac{3}{2}\eta-1-(3\rho^2+4\rho-1-\frac{3}{2}\eta^2-\frac{5}{2}\eta)\right| \\
&= 2(\rho+1)\sum_{\eta=1}^{\lceil\frac{\rho}{2}\rceil}(3\rho^2+5\rho+2)-4\sum_{\eta=1}^{\lceil\frac{\rho}{2}\rceil}(\rho+1)(3\rho+2)\eta-2(\rho+1)\sum_{\eta=\lceil\frac{\rho}{2}\rceil+1}^{\rho}(3\rho^2 \\
&+5\rho+2)+4\sum_{\eta=\lceil\frac{\rho}{2}\rceil+1}^{\rho}(\rho+1)(3\rho+2)\eta+2\sum_{\eta=1}^{\rho-1}(\eta+1)(3\rho^2+4\rho-3\eta^2-4\eta) \\
&= 2\left\lceil\frac{\rho}{2}\right\rceil(\rho+1)(3\rho^2+5\rho+2)-2(\rho+1)(3\rho+2)\left\lceil\frac{\rho}{2}\right\rceil\left(\left\lceil\frac{\rho}{2}\right\rceil+1\right) \\
&-2\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right)(\rho+1)(3\rho^2+5\rho+2)+2(\rho+1)(3\rho+2)\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right) \\
&\left(\left\lceil\frac{\rho}{2}\right\rceil+\rho+1\right)+(3\rho^2+4\rho)(\rho^2+\rho-2)-\frac{\rho}{6}(\rho^2-1)(9\rho+10). \\
&= \frac{3\rho^4}{2}+\frac{16\rho^3}{3}-\frac{\rho^2}{2}-\frac{19\rho}{3}+4\left\lceil\frac{\rho}{2}\right\rceil(\rho+1)(3\rho+2)\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right).
\end{aligned}
$$

- By adding the values of $Mo_v(\mathbb{BN})$ and $Mo_e(\mathbb{BN})$, we get

$$Mo_t(\mathbb{BN}) = \frac{5\rho^4}{2}+\frac{28\rho^3}{3}-\frac{\rho^2}{2}-\frac{37\rho}{3}+4\left\lceil\frac{\rho}{2}\right\rceil(\rho+1)(5\rho+4)\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right).$$

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Theorem 2.2 *For $\rho \geq 2$, the Szeged indices for the network of hexagonal boron nitride are*

- $Sz_v(\mathbb{BN}) = \rho(\rho+1)\left[2\rho^4+10\rho^3+\frac{77}{6}\rho^2+\frac{5}{2}\rho-\frac{1}{3}\right]$.
- $Sz_e(\mathbb{BN}) = \frac{9}{2}\rho^6+\frac{157}{10}\rho^5+\frac{34}{3}\rho^4-10\rho^3-\frac{29}{6}\rho^2+\frac{83}{10}\rho-1$.
- $Sz_t(\mathbb{BN}) = \frac{13}{2}\rho^6+\frac{277}{10}\rho^5+\frac{205}{6}\rho^4+\frac{16}{3}\rho^3-\frac{8}{3}\rho^2+\frac{239}{30}\rho-1$.

Proof. • From the help of equation (2), we acquire

$$Sz_v(\mathbb{BN}) = 2\sum_{\eta=1}^{\rho}(\rho+1)[2(\rho+1)\eta-1][(2\rho(\rho+2)-2(\rho+1)\eta+1]$$
$$+2\sum_{\eta=1}^{\rho-1}(\eta+1)[\eta(\eta+2)][(2\rho(\rho+2)-\eta(\eta+2)]+(\rho+1)[\rho(\rho+2)\times\rho(\rho+2)]$$
$$=2(\rho+1)\sum_{\eta=1}^{\rho}[2(\rho+1)(2\rho^2+4\rho+1)\eta-(2\rho^2+4\rho+1)-4(\rho+1)^2\eta^2$$
$$+2(\rho+1)\eta]+2\sum_{\eta=1}^{\rho-1}[2\rho(\rho+2)\eta(\eta+1)(\eta+2)-\eta^2(\eta+1)(\eta+2)^2]$$
$$+\rho^2(\rho+1)(\rho+2)^2$$
$$=4(\rho+1)^2(2\rho^2+4\rho+2)\sum_{\eta=1}^{\rho}\eta-2\rho(\rho+1)(2\rho^2+4\rho+1)-8(\rho+1)^3\sum_{\eta=1}^{\rho}\eta^2$$
$$+4\rho(\rho+2)\sum_{\eta=1}^{\rho-1}\eta(\eta+1)(\eta+2)-2\sum_{\eta=1}^{\rho-1}\eta^2(\eta+1)(\eta+2)^2$$
$$+\rho^2(\rho+1)(\rho^2+4\rho+4)$$
$$=4(\rho+1)^2(2\rho^2+4\rho+2)\times\frac{1}{2}\rho(\rho+1)-2\rho(\rho+1)(2\rho^2+4\rho+1)$$
$$-8(\rho+1)^3\times\frac{\rho}{6}(\rho+1)(2\rho+1)+4\rho(\rho+2)\times\frac{\rho}{4}(\rho-1)(\rho+1)(\rho+2)$$
$$-2\times\frac{\rho}{12}(\rho-1)(\rho+1)(\rho+2)(2\rho^2+2\rho-3)+\rho^2(\rho+1)(\rho^2+4\rho+4)$$
$$=\rho(\rho+1)\left[2\rho^4+10\rho^3+\frac{77}{6}\rho^2+\frac{5}{2}\rho-\frac{1}{3}\right].$$

- From the help of equation (2), we acquire

$$Sz_e(\mathbb{BN}) = 2\sum_{\eta=1}^{\rho}(\rho+1)[(3\rho+2)\eta-(\rho+2)][3\rho^2+4\rho-(3\rho+2)\eta]$$
$$+2\sum_{\eta=1}^{\rho-1}(\eta+1)\left(\frac{3}{2}\eta^2+\frac{3}{2}\eta-1\right)\left[3\rho^2+4\rho-1-\frac{3}{2}\eta^2-\frac{5}{2}\eta\right]$$
$$+(\rho+1)\left(\frac{3}{2}\rho(\rho+1)-1\right)\left(\frac{3}{2}\rho(\rho+1)-1\right)$$
$$=2(\rho+1)\sum_{\eta=1}^{\rho}[(3\rho^2+4\rho)(3\rho+2)\eta-(3\rho^2+4\rho)(\rho+2)-(3\rho+2)^2\eta^2$$
$$+\eta(3\rho+2)(\rho+2)]+2\sum_{\eta=1}^{\rho-1}(\eta+1)[\frac{3}{2}(3\rho^2+4\rho-1)\big(\eta(\eta+1)\big)$$

$$
\begin{aligned}
& -(3\rho^2+4\rho-1)-\frac{9}{4}\eta^4-\frac{9}{4}\eta^3-\frac{15}{4}\eta^3-\frac{15}{4}\eta^2+\frac{3}{2}\eta^2+\frac{5}{2}\eta] \\
& +(\rho+1)\left(\frac{9}{4}\rho^4+\frac{9}{4}\rho^2+\frac{9}{2}\rho^3-3\rho^2-3\rho\right) \\
= \quad & \rho(\rho+1)^2(3\rho+2)(3\rho^2+5\rho+2)-2\rho^2(\rho+1)(\rho+2)(3\rho+4)-\frac{\rho}{3}(\rho+1)^2 \\
& (2\rho+1)(3\rho+2)^2-2(3\rho^2+4\rho-1)\frac{1}{2}(\rho^2+\rho-2)+\sum_{\eta=1}^{\rho-1}(\eta+1)(-\frac{9}{2}\eta^4-12\eta^3 \\
& +(9\rho^2+12\rho-\frac{15}{2})\eta^2+(9\rho^2+12\rho+2)\eta)+(\rho+1)(\frac{9}{4}\rho^4+\frac{9}{2}\rho^3-\frac{3}{4}\rho^2-3\rho+1) \\
= \quad & \rho(\rho+1)^2(3\rho+2)(3\rho^2+5\rho+2)-2\rho^2(\rho+1)(\rho+2)(3\rho+4) \\
& -\frac{\rho}{3}(\rho+1)^2(2\rho+1)(3\rho+2)^2-(3\rho^2+4\rho-1)(\rho^2+\rho-2)+\frac{\rho}{60}(\rho-1)(\rho+1) \\
& (90\rho^3+207\rho^2+165\rho+82)+(\rho+1)(\frac{9}{4}\rho^4+\frac{9}{2}\rho^3-\frac{3}{4}\rho^2-3\rho+1) \\
= \quad & \frac{9}{2}\rho^6+\frac{157}{10}\rho^5+\frac{34}{3}\rho^4-10\rho^3-\frac{29}{6}\rho^2+\frac{83}{10}\rho-1.
\end{aligned}
$$

- By adding the values of $Sz_v(\mathbb{BN})$ and $Sz_e(\mathbb{BN})$, we get

$$Sz_t(\mathbb{BN})=\frac{13}{2}\rho^6+\frac{277}{10}\rho^5+\frac{205}{6}\rho^4+\frac{16}{3}\rho^3-\frac{8}{3}\rho^2+\frac{239}{30}\rho-1.$$

Theorem 2.3 *For $\rho \geq 2$, the weighted PI indices for hexagonal boron nitride are*

- $w^+PI_v(\mathbb{BN})=36\rho^4+104\rho^3+44\rho^2-40\rho.$
- $w^+PI_e(\mathbb{BN})=54\rho^4+92\rho^3-16\rho^2-46\rho+12.$
- $w^+PI_t(\mathbb{BN})=90\rho^4+196\rho^3+28\rho^2-86\rho+12.$

Proof. • By using the equation (1), we acquire

$$
\begin{aligned}
w^{+}PI_{v}(\mathbb{BN}) = \; & 2\sum_{\eta=2}^{\rho-1}(2(2+3)+(3+3)(\rho-1))[2(\rho+1)\eta-1+2\rho(\rho+2)-2(\rho+1)\eta+1] \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))[2(\rho+1)-1+2\rho(\rho+2)-2(\rho+1)+1] \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))[2(\rho+1)\rho-1+2\rho(\rho+2)-2(\rho+1)\rho+1] \\
& +2\sum_{\eta=1}^{\rho-1}(2(2+3)+(3+3)(\eta-1))[\eta(\eta+2)+(2\rho(\rho+2)-\eta(\eta+2))] \\
& +(2(2+2)+(3+3)(\rho-1))[2\rho(\rho+2)-\rho(\rho+2)+\rho(\rho+2)] \\
& =4(3\rho+2)[2\rho(\rho+2)]\sum_{\eta=2}^{\rho-1}(1)+12(2\rho+1)[2\rho(\rho+2)]+4[2\rho(\rho+2)]\sum_{\eta=1}^{\rho-1}(3\eta+2) \\
& +4\rho(3\rho+1)(\rho+2) \\
& =8\rho(3\rho+2)(\rho+2)(\rho-2)+24\rho(2\rho+1)(\rho+2)+8\rho(\rho+2)\times\frac{1}{2}(3\rho^{2}+\rho-4) \\
& +4\rho(3\rho+1)(\rho+2) \\
& =36\rho^{4}+104\rho^{3}+44\rho^{2}-40\rho.
\end{aligned}
$$

- By using the equation (1), we acquire

$$
\begin{aligned}
w^{+}PI_{e}(\mathbb{BN}) = \; & 2\sum_{\eta=2}^{\rho-1}(2(2+3)+(3+3)(\rho-1))[(3\rho+2)\eta-(\rho+2)+3\rho^{2}+4\rho-(3\rho+2)\eta] \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))[(3\rho+2)-(\rho+2)+3\rho^{2}+4\rho-(3\rho+2)] \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))[(3\rho+2)\rho-(\rho+2)+3\rho^{2}+4\rho-(3\rho+2)\rho] \\
& +2\sum_{\eta=1}^{\rho-1}(2(2+3)+(3+3)(\eta-1))\left[\frac{3}{2}\eta^{2}+\frac{3}{2}\eta-1+3\rho^{2}+4\rho-1-\frac{3}{2}\eta^{2}-\frac{5}{2}\eta\right] \\
& +(2(2+2)+(3+3)(\rho-1))\left[\frac{3}{2}\rho^{2}+\frac{3}{2}\rho-1+3\rho^{2}+4\rho-1-\frac{3}{2}\rho^{2}-\frac{5}{2}\rho\right] \\
& =4(3\rho+2)(3\rho^{2}+3\rho-2)\sum_{\eta=2}^{\rho-1}(1)+12(2\rho+1)(3\rho^{2}+3\rho-2)+4\sum_{\eta=1}^{\rho-1}(3\eta+1) \\
& +(3\rho^{2}+4\rho-2-\eta)+2(3\rho+1)(3\rho^{2}+3\rho-2) \\
& =4(3\rho+2)(3\rho^{2}+3\rho-2)(\rho-2)+12(2\rho+1)(3\rho^{2}+3\rho-2)+4(\frac{9}{2}\rho^{4}+\frac{7}{2}\rho^{3} \\
& -7\rho^{2}-3\rho+2)+2(3\rho+1)(3\rho^{2}+3\rho-2) \\
& =54\rho^{4}+92\rho^{3}-16\rho^{2}-46\rho+12.
\end{aligned}
$$

- By adding the values of $w^{+}PI_{v}(\mathbb{BN})$ and $w^{+}PI_{e}(\mathbb{BN})$, we get

$$w^{+}PI_{t}(\mathbb{BN}) = 90\rho^{4}+196\rho^{3}+28\rho^{2}-86\rho+12.$$

Theorem 2.4 *For $\rho \geq 2$, the weighted PI indices for hexagonal boron nitride are*

- $w^{*}PI_{v}(\mathbb{BN}) = 54\rho^{4}+144\rho^{3}+30\rho^{2}-84\rho.$

- $w^*PI_e(\mathbb{BN}) = 81\rho^4 + 120\rho^3 - 60\rho^2 - 75\rho + 30.$
- $w^*PI_t(\mathbb{BN}) = 135\rho^4 + 264\rho^3 - 30\rho^2 - 159\rho + 30.$

Proof. • By using the equation (1), we acquire

$$\begin{aligned}
w^*PI_v(\mathbb{BN}) = \; & 2\sum_{\eta=2}^{\rho-1}(2(2\times 3)+(3\times 3)(\rho-1))[2(\rho+1)\eta-1+2\rho(\rho+2)-2(\rho+1)\eta+1] \\
& +2((2\times 3)+(2\times 2)+(3\times 3)(\rho-1))[2(\rho+1)-1+2\rho(\rho+2)-2(\rho+1)+1] \\
& +2((2\times 3)+(2\times 2)+(3\times 3)(\rho-1))[2(\rho+1)\rho-1+2\rho(\rho+2)-2(\rho+1)\rho+1] \\
& +2\sum_{\eta=1}^{\rho-1}(2(2\times 3)+(3\times 3)(\eta-1))[\eta(\eta+2)+(2\rho(\rho+2)-\eta(\eta+2))] \\
& +(2(2\times 2)+(3\times 3)(\rho-1))[2\rho(\rho+2)-\rho(\rho+2)+\rho(\rho+2)] \\
& = 6(3\rho+1)[2\rho(\rho+2)]\sum_{\eta=2}^{\rho-1}(1)+4(9\rho+1)[2\rho(\rho+2)]+6[2\rho(\rho+2)]\sum_{\eta=1}^{\rho-1}(3\eta+1) \\
& +2\rho(9\rho-1)(\rho+2) \\
& = 12\rho(3\rho+1)(\rho+2)(\rho-2)+8\rho(9\rho+1)(\rho+2)+12\rho(\rho+2)\times\frac{1}{2}(3\rho^2+\rho-4) \\
& +2\rho(9\rho-1)(\rho+2) \\
& = 54\rho^4+144\rho^3+30\rho^2-84\rho.
\end{aligned}$$

• By using the equation (1), we acquire

$$\begin{aligned}
w^*PI_e(\mathbb{BN}) = \; & 2\sum_{\eta=2}^{\rho-1}(2(2\times 3)+(3\times 3)(\rho-1))[(3\rho+2)\eta-(\rho+2)+3\rho^2+4\rho-(3\rho+2)\eta] \\
& +2((2\times 3)+(2\times 2)+(3\times 3)(\rho-1))[(3\rho+2)-(\rho+2)+3\rho^2+4\rho-(3\rho+2)] \\
& +2((2\times 3)+(2\times 2)+(3\times 3)(\rho-1))[(3\rho+2)\rho-(\rho+2)+3\rho^2+4\rho-(3\rho+2)\rho] \\
& +2\sum_{\eta=1}^{\rho-1}(2(2\times 3)+(3\times 3)(\eta-1))\left[\frac{3}{2}\eta^2+\frac{3}{2}\eta-1+3\rho^2+4\rho-1-\frac{3}{2}\eta^2-\frac{5}{2}\eta\right] \\
& +(2(2\times 2)+(3\times 3)(\rho-1))\left[\frac{3}{2}\rho^2+\frac{3}{2}\rho-1+3\rho^2+4\rho-1-\frac{3}{2}\rho^2-\frac{5}{2}\rho\right] \\
& = 6(3\rho+1)(3\rho^2+3\rho-2)\sum_{\eta=2}^{\rho-1}(1)+4(9\rho+1)(3\rho^2+3\rho-2)+6\sum_{\eta=1}^{\rho-1}(3\eta+1)
\end{aligned}$$

$$\begin{aligned}
& (3\rho^2+4\rho-2-\eta)+(9\rho-1)(3\rho^2+3\rho-2) \\
= \; & 6(3\rho+1)(3\rho^2+3\rho-2)(\rho-2)+4(9\rho+1)(3\rho^2+3\rho-2)+6(\frac{9}{2}\rho^4+\frac{7}{2}\rho^3 \\
& -7\rho^2-3\rho+2)+(9\rho-1)(3\rho^2+3\rho-2) \\
= \; & 81\rho^4+120\rho^3-60\rho^2-75\rho+30.
\end{aligned}$$

• By adding the values of $w^*PI_v(\mathbb{BN})$ and $w^*PI_e(\mathbb{BN})$, we get

$$w^*PI_t(\mathbb{BN}) = 135\rho^4 + 264\rho^3 - 30\rho^2 - 159\rho + 30.$$

Theorem 2.5 *For $\rho \geq 2$, the weighted Szeged indices for hexagonal boron nitride are*

- $w^+Sz_v(\mathbb{BN}) = 12\rho^6 + \frac{328}{5}\rho^5 + 105\rho^4 + \frac{116}{3}\rho^3 - 11\rho^2 + \frac{26}{15}\rho + 4.$
- $w^+Sz_e(\mathbb{BN}) = 27\rho^6 + \frac{399}{5}\rho^5 + 32\rho^4 - \frac{218}{3}\rho^3 - 9\rho^2 + \frac{613}{15}\rho - 2.$
- $w^+Sz_t(\mathbb{BN}) = 39\rho^6 + \frac{727}{5}\rho^5 + 137\rho^4 - 34\rho^3 - 20\rho^2 + \frac{213}{5}\rho + 2.$

Proof. • By using the equation (3), we acquire

$$\begin{aligned}
w^+Sz_v(\mathbb{BN}) = \; & 2\sum_{\eta=2}^{\rho-1}(2(2+3)+(3+3)(\rho-1))[2(\rho+1)\eta-1][2\rho(\rho+2)-2(\rho+1)\eta+1] \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))[2(\rho+1)-1][2\rho(\rho+2)-2(\rho+1)+1] \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))[2(\rho+1)\rho-1][2\rho(\rho+2)-2(\rho+1)\rho+1] \\
& +2\sum_{\eta=1}^{\rho-1}(2(2+3)+(3+3)(\eta-1))[\eta(\eta+2)][(2\rho(\rho+2)-\eta(\eta+2))] \\
& +(2(2+2)+(3+3)(\rho-1))[2\rho(\rho+2)-\rho(\rho+2)][\rho(\rho+2)] \\
& = 4(3\rho+2)\sum_{\eta=2}^{\rho-1}[4(\rho+1)(\rho^2+2\rho+1)\eta-(2\rho^2+4\rho+1)-4(\rho+1)^2\eta^2] \\
& +12(2\rho+1)^2(2\rho^2+2\rho-1)+4\sum_{\eta=1}^{\rho-1}[2\rho(\rho+2)\eta(3\eta+1)(\eta+2)-\eta^2(3\eta+1) \\
& (\eta+2)^2]+2\rho^2(3\rho+1)(\rho+2)^2 \\
& = \frac{4}{3}(3\rho+2)(2\rho^5+10\rho^4-12\rho^3-34\rho^2+\rho+6)+12(2\rho+1)^2(2\rho^2+2\rho-1) \\
& +\frac{1}{15}\rho(60\rho^5+214\rho^4+65\rho^3-260\rho^2-65\rho-14)+2\rho^2(3\rho+1)(\rho+2)^2 \\
& = 12\rho^6+\frac{328}{5}\rho^5+105\rho^4+\frac{116}{3}\rho^3-11\rho^2+\frac{26}{15}\rho+4.
\end{aligned}$$

• By using the equation (3), we acquire

$$
\begin{aligned}
w^{+}Sz_e(\mathbb{BN}) = \; & 2\sum_{\eta=2}^{\rho-1}(2(2+3)+(3+3)(\rho-1))[(3\rho+2)\eta-(\rho+2)][3\rho^2+4\rho-(3\rho+2)\eta] \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))[(3\rho+2)-(\rho+2)][3\rho^2+4\rho-(3\rho+2)] \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))[(3\rho+2)\rho-(\rho+2)][3\rho^2+4\rho-(3\rho+2)\rho] \\
& +2\sum_{\eta=1}^{\rho-1}(2(2+3)+(3+3)(\eta-1))\left[\frac{3}{2}\eta^2+\frac{3}{2}\eta-1\right]\left[3\rho^2+4\rho-1-\frac{3}{2}\eta^2-\frac{5}{2}\eta\right] \\
& +(2(2+2)+(3+3)(\rho-1))\left[\frac{3}{2}\rho^2+\frac{3}{2}\rho-1\right]\left[3\rho^2+4\rho-1-\frac{3}{2}\rho^2-\frac{5}{2}\rho\right] \\
& = 4(3\rho+2)\sum_{\eta=2}^{\rho-1}[(3\rho^2+4\rho)(3\rho+2)\eta-(3\rho^2+4\rho)(\rho+2)-(3\rho+2)^2\eta^2+\eta(3\rho+2) \\
& (\rho+2)]+24\rho(2\rho+1)(3\rho^2+\rho-2)+4\sum_{\eta=1}^{\rho-1}(3\eta+1)[\frac{3}{2}\eta(\eta+1)(3\rho^2+4\rho-1) \\
& -(3\rho^2+4\rho-1)-\frac{9}{4}\eta^4-\frac{9}{4}\eta^3-\frac{15}{4}\eta^3-\frac{15}{4}\eta^2+\frac{3}{2}\eta^2+\frac{5}{2}\eta] \\
& +2(3\rho+1)\left(\frac{3}{2}\rho^2+\frac{3}{2}\rho-1\right)^2 \\
& = \frac{2}{3}\rho(3\rho+2)(9\rho^4+21\rho^3-74\rho^2-36\rho+56)+24\rho(2\rho+1)(3\rho^2+\rho-2)+\frac{1}{10}(90\rho^6 \\
& +123\rho^5-235\rho^4-265\rho^3+185\rho^2+142\rho-40)+2(3\rho+1)\left(\frac{3}{2}\rho^2+\frac{3}{2}\rho-1\right)^2 \\
& = 27\rho^6+\frac{399}{5}\rho^5+32\rho^4-\frac{218}{3}\rho^3-9\rho^2+\frac{613}{15}\rho-2.
\end{aligned}
$$

- By adding the values of $w^{+}Sz_v(\mathbb{BN})$ and $w^{+}Sz_e(\mathbb{BN})$, we get

$$w^{+}Sz_t(\mathbb{BN}) = 39\rho^6+\frac{727}{5}\rho^5+137\rho^4-34\rho^3-20\rho^2+\frac{213}{5}\rho+2.$$

Theorem 2.6 *For $\rho \geq 2$, the weighted Szeged indices for hexagonal boron nitride are*

- $w^{*}Sz_v(\mathbb{BN}) = 18\rho^6+\frac{472}{5}\rho^5+\frac{267}{2}\rho^4+10\rho^3-\frac{97}{2}\rho^2+\frac{3}{5}\rho+8.$
- $w^{*}Sz_e(\mathbb{BN}) = \frac{81}{2}\rho^6+\frac{1107}{10}\rho^5+18\rho^4-137\rho^3-\frac{5}{2}\rho^2+\frac{733}{10}\rho-7.$
- $w^{*}Sz_t(\mathbb{BN}) = \frac{117}{2}\rho^6+\frac{2051}{10}\rho^5+\frac{303}{2}\rho^4-127\rho^3-51\rho^2+\frac{739}{10}\rho+1.$

Proof. • By using the equation (3), we acquire

$$w^*Sz_v(\mathbb{BN}) = 2\sum_{\eta=2}^{\rho-1}(2(2\times3)+(3\times3)(\rho-1))[2(\rho+1)\eta-1][2\rho(\rho+2)-2(\rho+1)\eta+1]$$
$$+2((2\times3)+(2\times2)+(3\times3)(\rho-1))[2(\rho+1)-1][2\rho(\rho+2)-2(\rho+1)+1]$$
$$+2((2\times3)+(2\times2)+(3\times3)(\rho-1))[2(\rho+1)\rho-1][2\rho(\rho+2)-2(\rho+1)\rho+1]$$
$$+2\sum_{\eta=1}^{\rho-1}(2(2\times3)+(3\times3)(\eta-1))[\eta(\eta+2)][(2\rho(\rho+2)-\eta(\eta+2))]$$
$$+(2(2\times2)+(3\times3)(\rho-1))[2\rho(\rho+2)-\rho(\rho+2)][\rho(\rho+2)]$$
$$=6(3\rho+1)\sum_{\eta=2}^{\rho-1}[4(\rho+1)(\rho^2+2\rho+1)\eta-(2\rho^2+4\rho+1)-4(\rho+1)^2\eta^2]$$
$$+4(9\rho+1)(2\rho+1)(2\rho^2+2\rho-1)+6\sum_{\eta=1}^{\rho-1}[2\rho(\rho+2)\eta(3\eta+1)(\eta+2)-\eta^2(3\eta+1)$$
$$(\eta+2)^2]+\rho^2(9\rho-1)(\rho+2)^2$$
$$=2(3\rho+1)(2\rho^5+10\rho^4-12\rho^3-34\rho^2+\rho+6)+4(9\rho+1)(2\rho+1)(2\rho^2+2\rho-1)$$
$$+\frac{1}{10}\rho(60\rho^5+214\rho^4+65\rho^3-260\rho^2-65\rho-14)+\rho^2(9\rho-1)(\rho+2)^2$$
$$=18\rho^6+\frac{472}{5}\rho^5+\frac{267}{2}\rho^4+10\rho^3-\frac{97}{2}\rho^2+\frac{3}{5}\rho+8.$$

- By using the equation (3), we acquire

$$w^*Sz_e(\mathbb{BN}) = 2\sum_{\eta=2}^{\rho-1}(2(2\times3)+(3\times3)(\rho-1))[(3\rho+2)\eta-(\rho+2)][3\rho^2+4\rho-(3\rho+2)\eta]$$
$$+2((2\times3)+(2\times2)+(3\times3)(\rho-1))[(3\rho+2)-(\rho+2)][3\rho^2+4\rho-(3\rho+2)]$$
$$+2((2\times3)+(2\times2)+(3\times3)(\rho-1))[(3\rho+2)\rho-(\rho+2)][3\rho^2+4\rho-(3\rho+2)\rho]$$
$$+2\sum_{\eta=1}^{\rho-1}(2(2\times3)+(3\times3)(\eta-1))\left[\frac{3}{2}\eta^2+\frac{3}{2}\eta-1\right]\left[3\rho^2+4\rho-1-\frac{3}{2}\eta^2-\frac{5}{2}\eta\right]$$
$$+(2(2\times2)+(3\times3)(\rho-1))\left[\frac{3}{2}\rho^2+\frac{3}{2}\rho-1\right]\left[3\rho^2+4\rho-1-\frac{3}{2}\rho^2-\frac{5}{2}\rho\right]$$
$$=6(3\rho+1)\sum_{\eta=2}^{\rho-1}[(3\rho^2+4\rho)(3\rho+2)\eta-(3\rho^2+4\rho)(\rho+2)-(3\rho+2)^2\eta^2+\eta(3\rho+2)$$
$$(\rho+2)]+8\rho(9\rho+1)(3\rho^2+\rho-2)+6\sum_{\eta=1}^{\rho-1}(3\eta+1)[\frac{3}{2}\eta(\eta+1)(3\rho^2+4\rho-1)$$
$$-(3\rho^2+4\rho-1)-\frac{9}{4}\eta^4-\frac{9}{4}\eta^3-\frac{15}{4}\eta^3-\frac{15}{4}\eta^2+\frac{3}{2}\eta^2+\frac{5}{2}\eta]$$

$$+(9\rho-1)\left(\frac{3}{2}\rho^2+\frac{3}{2}\rho-1\right)^2$$

$$= \rho(3\rho+1)(9\rho^4+21\rho^3-74\rho^2-36\rho+56)+8\rho(9\rho+1)(3\rho^2+\rho-2)+\frac{3}{20}(90\rho^6$$

$$+123\rho^5-235\rho^4-265\rho^3+185\rho^2+142\rho-40)+(9\rho-1)\left(\frac{3}{2}\rho^2+\frac{3}{2}\rho-1\right)^2$$

$$= \frac{81}{2}\rho^6+\frac{1107}{10}\rho^5+18\rho^4-137\rho^3-\frac{5}{2}\rho^2+\frac{733}{10}\rho-7.$$

- By adding the values of $w^*Sz_v(\mathbb{BN})$ and $w^*Sz_e(\mathbb{BN})$, we get

$$w^*Sz_t(\mathbb{BN})=\frac{117}{2}\rho^6+\frac{2051}{10}\rho^5+\frac{303}{2}\rho^4-127\rho^3-51\rho^2+\frac{739}{10}\rho+1.$$

Theorem 2.7 *For $\rho \geq 2$, the weighted Mostar indices of hexagonal boron nitride are*

- $w^+Mo_v(\mathbb{BN})=6\rho^4+\frac{56}{3}\rho^3-6\rho^2-\frac{80}{3}\rho+8+16(3\rho+2)(\rho+1)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right)$.
- $w^+Mo_e(\mathbb{BN})=9\rho^4+16\rho^3-19\rho^2-14\rho+8+8(3\rho+2)^2\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right)$.
- $w^+Mo_t(\mathbb{BN})=15\rho^4+\frac{104}{3}\rho^3-25\rho^2-\frac{122}{3}\rho+16+8(3\rho+2)(5\rho+4)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right)$.

Proof. • By using the equations (6), we acquire

$$\begin{aligned}
w^+Mo_v(\mathbb{BN}) = {} & 2\sum_{\eta=2}^{\rho-1}(2(2+3)+(3+3)(\rho-1))|2(\rho+1)\eta-1-(2\rho(\rho+2)-2(\rho+1)\eta+1)| \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))|2\rho(\rho+2)-2(\rho+1)+1-2(\rho+1)+1| \\
& +2((2+3)+(2+2)+(3+3)(\rho-1))|2(\rho+1)\rho-1-(2\rho(\rho+2)-2(\rho+1)\rho \\
& +1)|+2\sum_{\eta=1}^{\rho-1}(2(2+3)+(3+3)(\eta-1))|(2\rho(\rho+2)-\eta(\eta+2))-\eta(\eta+2)| \\
& +(2(2+2)+(3+3)(\rho-1))|(2\rho(\rho+2)-\rho(\rho+2))-\rho(\rho+2)| \\
& = 4(3\rho+2)\sum_{\eta=2}^{\lceil\frac{\rho}{2}\rceil}(2\rho^2+4\rho+2-4(\rho+1)\eta)+4(3\rho+2)\sum_{i=\lceil\frac{\rho}{2}\rceil+1}^{\rho-1}(4(\rho+1)\eta \\
& -2\rho^2-4\rho-2)+24(2\rho+1)(\rho^2-1)+8\sum_{\eta=1}^{\rho-1}(3\eta+2)(\rho(\rho+2)-\eta(\eta+2)) \\
& = 8(3\rho+2)(\rho+1)\left(\left\lceil\frac{\rho}{2}\right\rceil-1\right)\left(-\left\lceil\frac{\rho}{2}\right\rceil+\rho-1\right)+8(3\rho+2)(\rho+1)\left(\left\lceil\frac{\rho}{2}\right\rceil-1\right) \\
& \left(-\left\lceil\frac{\rho}{2}\right\rceil+\rho-1\right)+24(2\rho+1)(\rho^2-1)+\frac{2}{3}\rho(9\rho^3+28\rho^2+3\rho-40) \\
& = 6\rho^4+\frac{56}{3}\rho^3-6\rho^2-\frac{80}{3}\rho+8+16(3\rho+2)(\rho+1)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right).
\end{aligned}$$

- By using the equations (6), we acquire

$$
\begin{aligned}
w^{+}Mo_{e}(\mathbb{BN}) &= 2\sum_{\eta=2}^{\rho-1}(2(2+3)+(3+3)(\rho-1))|(3\rho+2)\eta-(\rho+2)-(3\rho^{2}+4\rho-(3\rho+2)\eta)|\\
&+2((2+3)+(2+2)+(3+3)(\rho-1))|(3\rho^{2}+4\rho-(3\rho+2))-(3\rho+2)+(\rho+2)|\\
&+2((2+3)+(2+2)+(3+3)(\rho-1))|(3\rho+2)\rho-(\rho+2)-(3\rho^{2}+4\rho-(3\rho+2)\rho)|\\
&+2\sum_{\eta=1}^{\rho-1}(2(2+3)+(3+3)(\eta-1))\left|\frac{3}{2}\eta^{2}+\frac{3}{2}\eta-1-(3\rho^{2}+4\rho-1-\frac{3}{2}\eta^{2}-\frac{5}{2}\eta)\right|\\
&+(2(2+2)+(3+3)(\rho-1))\left|\frac{3}{2}\rho^{2}+\frac{3}{2}\rho-1-(3\rho^{2}+4\rho-1-\frac{3}{2}\rho^{2}-\frac{5}{2}\rho)\right|\\
&=4(3\rho+2)\sum_{\eta=2}^{\lceil\frac{\rho}{2}\rceil}(3\rho^{2}+5\rho+2-2(3\rho+2)\eta)+4(3\rho+2)\sum_{\eta=\lceil\frac{\rho}{2}\rceil+1}^{\rho-1}(2(3\rho+2)\eta-3\rho^{2}-5\rho-2)\\
&+12(2\rho+1)(3\rho^{2}-\rho-2)+4\sum_{\eta=1}^{\rho-1}(3\eta+1)(3\rho^{2}+4\rho-3\eta^{2}-4\eta)\\
&=4(3\rho+2)^{2}\left(\left\lceil\frac{\rho}{2}\right\rceil-1\right)\left(-\left\lceil\frac{\rho}{2}\right\rceil+\rho-1\right)+4(3\rho+2)^{2}\left(\left\lceil\frac{\rho}{2}\right\rceil-1\right)\left(-\left\lceil\frac{\rho}{2}\right\rceil+\rho-1\right)\\
&+12(2\rho+1)(3\rho^{2}-\rho-2)+9\rho^{4}+16\rho^{3}-7\rho^{2}-18\rho\\
&=9\rho^{4}+16\rho^{3}-19\rho^{2}-14\rho+8+8(3\rho+2)^{2}\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right).
\end{aligned}
$$

- By adding the values of $w^{+}Mo_{v}(\mathbb{BN})$ and $w^{+}Mo_{e}(\mathbb{BN})$, we get

$$w^{+}Mo_{t}(\mathbb{BN})=15\rho^{4}+\frac{104}{3}\rho^{3}-25\rho^{2}-\frac{122}{3}\rho+16+8(3\rho+2)(5\rho+4)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right).$$

Theorem 2.8 *For $\rho\geq 2$, the weighted Mostar indices of hexagonal boron nitride are*

- $w^{*}Mo_{v}(\mathbb{BN})=9\rho^{4}+20\rho^{3}-19\rho^{2}-26\rho+16+24(3\rho+1)(\rho+1)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right)$.
- $w^{*}Mo_{e}(\mathbb{BN})=\frac{27}{2}\rho^{4}+24\rho^{3}-\frac{69}{2}\rho^{2}-19\rho+16+12(3\rho+1)(3\rho+2)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right)$.
- $w^{*}Mo_{t}(\mathbb{BN})=\frac{45}{2}\rho^{4}+44\rho^{3}-\frac{107}{2}\rho^{2}-45\rho+32+12(3\rho+1)(5\rho+4)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right)$.

Proof. • By using the equations (6), we acquire

$$
\begin{aligned}
w^{*}Mo_{v}(\mathbb{BN})= \; & 2\sum_{\eta=2}^{\rho-1}(2(2\times 3)+(3\times 3)(\rho-1))|2(\rho+1)\eta-1-(2\rho(\rho+2)-2(\rho+1)\eta+1)|\\
&+2((2\times 3)+(2\times 2)+(3\times 3)(\rho-1))|2\rho(\rho+2)-2(\rho+1)+1-2(\rho+1)+1|\\
&+2((2\times 3)+(2\times 2)+(3\times 3)(\rho-1))|2(\rho+1)\rho-1-(2\rho(\rho+2)-2(\rho+1)\rho\\
&+1)|+2\sum_{\eta=1}^{\rho-1}(2(2\times 3)+(3\times 3)(\eta-1))|(2\rho(\rho+2)-\eta(\eta+2))-\eta(\eta+2)|
\end{aligned}
$$

$$+(2(2\times 2)+(3\times 3)(\rho-1))|(2\rho(\rho+2)-\rho(\rho+2))-\rho(\rho+2)|$$

$$= 12(3\rho+1)\sum_{\eta=2}^{\lceil\frac{\rho}{2}\rceil}(\rho^2+2\rho+1-2(\rho+1)\eta)+12(3\rho+1)\sum_{i=\lceil\frac{\rho}{2}\rceil+1}^{\rho-1}(2(\rho+1)\eta$$

$$-\rho^2-2\rho-1)+8(9\rho+1)(\rho^2-1)+12\sum_{\eta=1}^{\rho-1}(3\eta+1)(\rho(\rho+2)-\eta(\eta+2))$$

$$= 12(3\rho+1)(\rho+1)\left(\left\lceil\frac{\rho}{2}\right\rceil-1\right)\left(-\left\lceil\frac{\rho}{2}\right\rceil+\rho-1\right)+12(3\rho+1)(\rho+1)\left(\left\lceil\frac{\rho}{2}\right\rceil-1\right)$$

$$\left(-\left\lceil\frac{\rho}{2}\right\rceil+\rho-1\right)+8(9\rho+1)(\rho^2-1)+9\rho^4+20\rho^3-3\rho^2-26\rho$$

$$= 9\rho^4+20\rho^3-19\rho^2-26\rho+16+24(3\rho+1)(\rho+1)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right).$$

- By using the equations (6), we acquire

$$w^*Mo_e(\mathbb{BN}) = 2\sum_{\eta=2}^{\rho-1}(2(2\times 3)+(3\times 3)(\rho-1))|(3\rho+2)\eta-(\rho+2)-(3\rho^2+4\rho-(3\rho+2)\eta)|$$

$$+2((2\times 3)+(2\times 2)+(3\times 3)(\rho-1))|(3\rho^2+4\rho-(3\rho+2))-(3\rho+2)+(\rho+2)|$$

$$+2((2\times 3)+(2\times 2)+(3\times 3)(\rho-1))|(3\rho+2)\rho-(\rho+2)-(3\rho^2+4\rho-(3\rho+2)\rho)|$$

$$+2\sum_{\eta=1}^{\rho-1}(2(2\times 3)+(3\times 3)(\eta-1))\left|\frac{3}{2}\eta^2+\frac{3}{2}\eta-1-(3\rho^2+4\rho-1-\frac{3}{2}\eta^2-\frac{5}{2}\eta)\right|$$

$$+(2(2\times 2)+(3\times 3)(\rho-1))\left|\frac{3}{2}\rho^2+\frac{3}{2}\rho-1-(3\rho^2+4\rho-1-\frac{3}{2}\rho^2-\frac{5}{2}\rho)\right|$$

$$= 6(3\rho+1)\sum_{\eta=2}^{\lceil\frac{\rho}{2}\rceil}(3\rho^2+5\rho+2-2(3\rho+2)\eta)+6(3\rho+1)\sum_{\eta=\lceil\frac{\rho}{2}\rceil+1}^{\rho-1}(2(3\rho+2)\eta-3\rho^2-5\rho-2)$$

$$+4(9\rho+1)(3\rho^2-\rho-2)+6\sum_{\eta=1}^{\rho-1}(3\eta+1)(3\rho^2+4\rho-3\eta^2-4\eta)$$

$$= 6(3\rho+1)(3\rho+2)\left(\left\lceil\frac{\rho}{2}\right\rceil-1\right)\left(-\left\lceil\frac{\rho}{2}\right\rceil+\rho-1\right)+6(3\rho+1)(3\rho+2)\left(\left\lceil\frac{\rho}{2}\right\rceil-1\right)$$

$$\left(-\left\lceil\frac{\rho}{2}\right\rceil+\rho-1\right)+4(9\rho+1)(3\rho^2-\rho-2)+\frac{27}{2}\rho^4+24\rho^3-\frac{21}{2}\rho^2-27\rho$$

$$= \frac{27}{2}\rho^4+24\rho^3-\frac{69}{2}\rho^2-19\rho+16+12(3\rho+1)(3\rho+2)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right).$$

- By adding the values of $w^*Mo_v(\mathbb{BN})$ and $w^*Mo_e(\mathbb{BN})$, we get

$$w^*Mo_t(\mathbb{BN}) = \frac{45}{2}\rho^4+44\rho^3-\frac{107}{2}\rho^2-45\rho+32+12(3\rho+1)(5\rho+4)\left\lceil\frac{\rho}{2}\right\rceil\left(\rho-\left\lceil\frac{\rho}{2}\right\rceil\right).$$

3 Numerical and Graphical Comparison of Results for Hexagonal Boron Nitride and Carbon Nanotube

The Mostar, PI, and Szeged-type indices for the hexagonal boron nitride network and carbon nanotube structures are evaluated numerically in this section. For values of ρ between 2 and 10, we calculate these indices using the closed formulas developed in Sections 2 and ??. The growth behavior of the indices varies by type, as we can see from the analytical expressions: the Szeged-type indices show a hexic (degree six) growth pattern, while the Mostar and PI indices both increase in a quadric manner with respect to ρ. Both the numerical values and the graphical plots shown below clearly reflect these tendencies. The calculated numerical values of the vertex-based, edge-based, and total-based indices are presented in Tables 1, 2, and 3. The tables provide a comprehensive comparative overview by listing the corresponding Mostar, PI, and Szeged values along with their weighted forms for each ρ. These tables are supplemented by graphical comparisons of the three index families in Figures 2. Figure 2 shows how the vertex-based indices, the edge-based indices and the total indices behave as ρ increases. The numerical observations and plots validate the previously derived theoretical growth rates by showing a consistent and predictable trend across all three index families.

Table 1: Vertex based Mostar, PI and Szeged indices of Hexagonal Boron nitride

$[\rho]$	Mo_v	Sz_v	w^+PI_v	w^+Sz_v	w^+Mo_v	w^*PI_v	w^*Sz_v	w^*Mo_v
2	112	1008	1504	4820	560	1968	6204	696
3	436	6656	6000	34148	2272	8280	46718	2956
4	1304	27340	16416	145516	7016	23184	204444	9432
5	2848	84990	36400	462696	15600	52080	659736	21360
6	5688	219604	70464	1214028	31600	101664	1747304	43888
7	9924	497168	123984	2779172	55664	179928	4025862	78060
8	16528	1019016	203200	5744500	93448	296160	8360736	132096
9	25504	1932630	315216	10967128	145056	460944	16019432	206272
10	38240	3443880	468000	19647588	218608	686160	28780164	312456

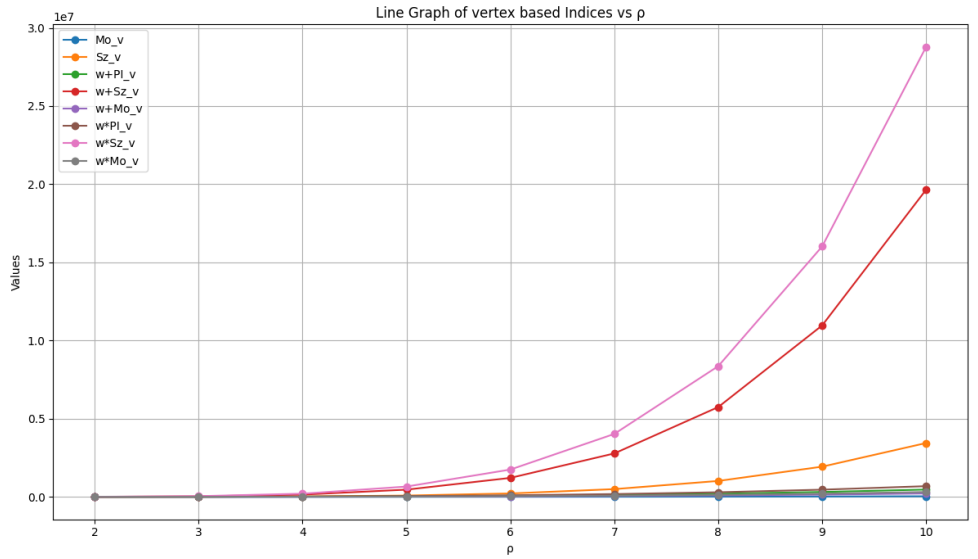
Table 2: Edge based Mostar, PI and Szeged indices of Hexagonal Boron nitride

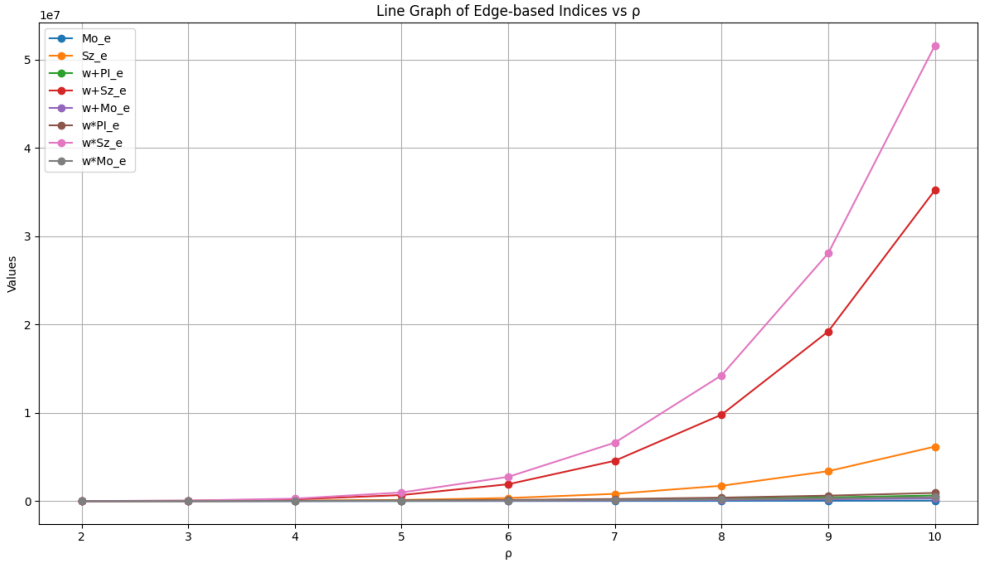
$[\rho]$	Mo_e	Sz_e	w^+PI_e	w^+Sz_e	w^+Mo_e	w^*PI_e	w^*Sz_e	w^*Mo_e
2	148	888	1456	4256	688	1896	5456	920
3	594	7724	6588	39744	2892	9066	54374	4030
4	1812	36725	19284	195866	9248	27186	275331	13116
5	4008	125128	44632	682144	20960	63780	973172	30080
6	8080	344438	89016	1905932	43160	128316	2744450	62380
7	14194	816892	160116	4569472	76860	232206	6621930	111702
8	23768	1735163	266908	9786390	130264	388806	14248253	190040
9	36832	3385304	419664	19217632	203616	613416	28078760	298000
10	55420	6172932	629952	35226840	308768	923280	51613476	452976

Table 3: Total based Mostar, PI and Szeged indices of Hexagonal Boron nitride

$[\rho]$	Mo_t	Sz_t	w^+PI_t	w^+Sz_t	w^+Mo_t	w^*PI_t	w^*Sz_t	w^*Mo_t
2	256	1896	2960	9076	1248	1896	11660	1616
3	1021	14380	12588	73892	5164	9066	101092	6986
4	3100	64065	35700	341382	16264	27186	479775	22548
5	6831	210118	81032	1144840	36560	63780	1632908	51440
6	13732	564042	159480	3119960	74760	128316	4491754	106268

7	24069	1314060	284100	7348644	132524	232206	10647792	189762
8	40232	2754179	470108	15530890	223712	388806	22608989	322136
9	62255	5317934	734880	30184760	348672	613416	44098192	504272
10	93560	9616812	1097952	54874428	527376	923280	80393640	765432





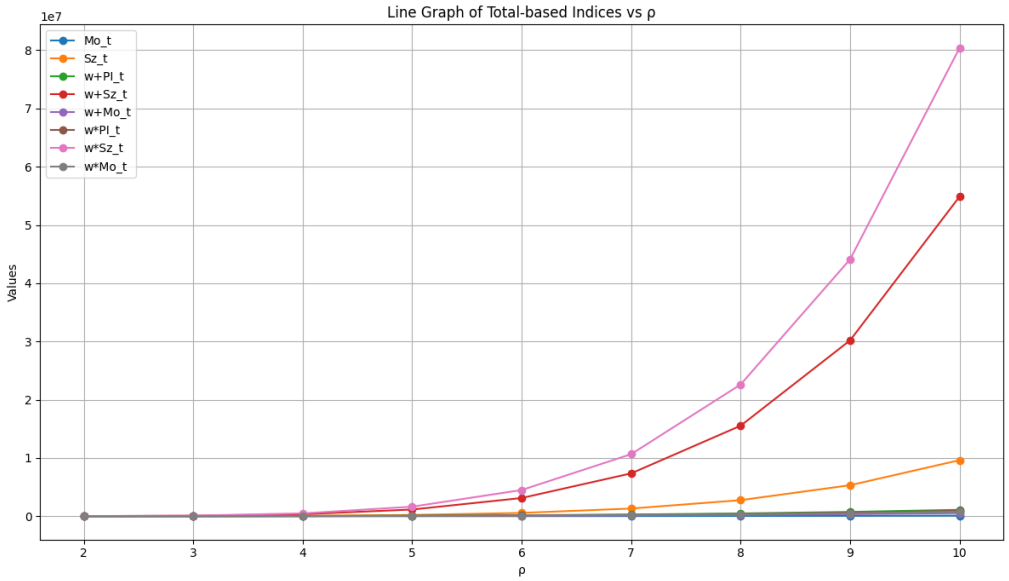


Figure 2: Comparison of Vertex-distance based, edge-distance based and total-distance based Mostar, PI and Szeged indices of CHexagonal Boron nitride

Conclusion

In this work, we have used the cut method to examine the Mostar, PI, and Szeged-type indices of the hexagonal boron nitride network. In terms of the parameter ρ, closed-form expressions for the vertex-based, edge-based, and total variants of these indices were successfully obtained. The obtained results show different growth patterns for the indices under consideration. Specifically, the Szeged index shows a higher-order (hexic) growth behavior, whereas the Mostar and PI indices show quadric growth. These results demonstrate the hexagonal boron nitride network's structural richness and complexity. Additionally, the variation of these indices for various values of ρ was shown through numerical calculations and graphical representations. Although both networks have similar hexagonal frameworks, the comparison with carbon nanotube structures reveals that their topological indices differ noticeably, indicating differences in their structural characteristics. The findings of this study add to the expanding corpus of research on topological descriptors of nano structures and could be helpful in forecasting the physicochemical characteristics of materials based on boron nitride. Other topological indices, such as Zagreb-type or entropy-based measures, as well as extensions to three-dimensional nanostructures and doped systems, might be the subject of future research.

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