

EDGE SZEGED INDICES OF BENZENE RING

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ABSTRACT. Consider a connected molecular graph $G = (V, E)$ where V is the set of vertices and E is the set of edges. In G , vertices represent the atoms and edges represent the covalent bonds between atoms. In graph G , every edge (say) $e = uv$ will be connected by two atoms u and v . The edge Szeged index is a topological index which has been introduced by Ivan Gutman. In this paper, we have computed edge Szeged indices of a hydrocarbon family called Benzene ring and is denoted by $(BR)_{n \times n}$.

1. Introduction

In chemical graph theory, the vertices of a molecular graph G represent the atoms and edges represent the bonds. The shape derived from a chemical compound is often called its molecular graph and can be a path, a tree or in general a graph. A topological index is a single number which is derived by following certain rules and it can be used to characterize the molecule. In this article we have computed the topological indices called edge Szeged [7], Padmakar-Iven [3] and Geometric Arithmetic index of an $n \times n$ molecular graph of benzene ring (BR) shown in the Figure 1 and Figure 2.

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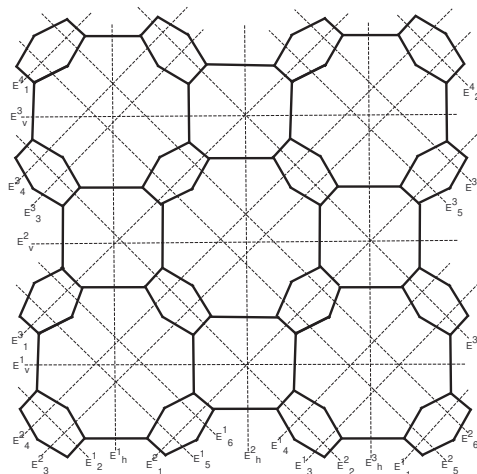


FIGURE 1. Benzene ring

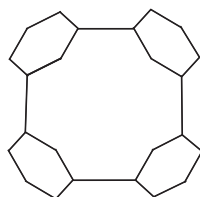


FIGURE 2. Unit of Benzene ring

The Wiener index $W(G)$ [14] is one of the oldest topological index introduced by chemist Harold Wiener in 1947, with many chemical applications and mathematical properties and is probably the most studied index from both theoretical and practical points of view; (see [4] for further details). It demonstrates correlations between physio-chemical properties of organic compounds. This index is defined as the sum of all distances between pairs of vertices in a graph,

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u, v)$$

where $d(u, v)$ is the distance between vertices u and v of G and is defined as the number of edges in the shortest path connecting them. Let G be a chemical graph. Two vertices u and v are called incident if there is an

edge between u and v . The Zagreb indices were introduced more than thirty years ago by Gutman and Trinajestic [7]. They are defined as:

$$M_1(G) = \sum_{uv \in E(G)} (deg(u) + deg(v)),$$

$$M_2(G) = \sum_{uv \in E(G)} deg(u)deg(v),$$

where $deg(u)$ is the number of vertices of G that are incident to u same goes for $deg(v)$. Another topological index of a chemical graph was introduced by Gutman in 1994 that is called the Szeged index [6, 10, 11] denoted as $Sz(G)$. The vertex Szeged index is a modification of Wiener index and it is define as:

$$Sz_v(G) = \sum_{e=uv \in E(G)} (n_u|e \times n_v|e)$$

where $n_u|e$ is the number of vertices of G closer to u as compared to v and $n_v|e$ is the number of vertices of G closer to v as compared to u . To understand $n_u|e$ and $n_v|e$ for an edge $e = \{u, v\}$ we consider the graph H in Figure 3. With respect to edge e of graph H the vertices v, b, c, d are closer to v than u and the vertices u, a are closer to u than v thus $n_u|e = 2$ and $n_v|e = 4$.

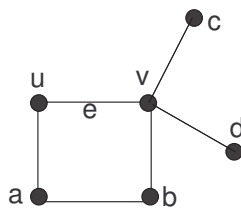


FIGURE 3. Graph H

The edge version of Szeged index has been introduced very recently by Gutman and Ashrafi [7]. It is defined as:

$$Sz_e(G) = \sum_{e=uv \in E(G)} (m_u|e \times m_v|e)$$

where $m_u|e$ is the number edges of G closer to u as compared to v and $m_v|e$ is the number of edges of G closer to v as compared to u . The Zagreb version of Szeged indices was introduced by H. Deng and J. Hou [3] it is known as Padmaker-Iven index and defined as:

$$PI_e(G) = \sum_{e=uv \in E(G)} (m_u|e + m_v|e)$$

A somewhat new member of the class of Geometric-Arithmetic indices, which is also tentatively-referred to as the second geometric-arithmetical index is discussed in [1] and characterized as;

$$(1) \quad GA_{vs}(G) = \sum_{e \in E(G)} \left[\frac{2\sqrt{n_u|e \times n_v|e}}{n_u|e + n_v|e} \right]$$

The edge version of this index will be $GA_e(G) = \sum_{e \in E(G)} \left[\frac{2\sqrt{m_u|e \times m_v|e}}{m_u|e + m_v|e} \right]$

Recently, in [5] 2018, a new edge Szeged type topological index was introduced by Doslic et al known as Mostar index which is defined as,

$$MI(G) = \sum_{e=uv \in (G)} \left| m_u|e - m_v|e \right|,$$

where $m_u|e$ and $m_v|e$ are defined as before.

The applications or the so called chemical applications of the Szeged indices are in great correlation with the Wiener index. So firstly, one has to recall that the Wiener index has many such applications, which can be found in number of reviews like [8,9]. The Wiener index is correlated with a large number of physico-chemical properties of organic molecules through their chemical graphs, especially for the case for alkanes, whose molecular graphs are trees. Since in the case of trees the Wiener and the Szeged index coincide, with $Sz(G)$ and $W(G)$ depend on molecular structure in a remarkably similar manner for unicyclic molecules. It also has been shown in Systematic numerical testing [2,12,13] that the correlations between $Sz(G)$ Szeged Indices and various physico-chemical properties of monocycloalkanes are of comparable. The $Sz(G)$ and $W(G)$ values of benzenoid molecules were also found to be well correlated yet for very large benzenoids this correlation is curvilinear. This means that

also for this class of polycyclic molecules the structural information contained in Sz is quite similar to that contained in W . So very application of literature which is related to $W(G)$ can associate with $Sz(G)$. This gives us motivation to compute and compare the different Szeged indices of Benzene ring $(BR)_{n \times n}$.

After computation of $m_u|e$ and $m_v|e$ for each edge, we have partitioned the edges of $G \cong BR$ as follows. Let e be an edge in Figure 1. we denote: $E_h^i = e \in E(G)$ = The set of horizontal edges. Horizontal levels increase from left to right but the values of $m_u|e$ and $m_v|e$ remain unchanged from bottom to top.

$E_v^i = e \in E(G)$ = The set of vertical edges. Vertical levels increase from bottom to top but the values of $m_u|e$ and $m_v|e$ remain unchanged from left to right.

$E_1^i = e \in E(G)$ = The set of edges making angle of 140° with positive x-axis in anticlockwise direction. E_1^i levels increase from right bottom to left top but the values of $m_u|e$ and $m_v|e$ remain unchanged from left to right.

$E_2^i = e \in E(G)$ = The set of edges making angle of 45° with positive x-axis in anticlockwise direction. E_2^i levels increase from left bottom to right top but the values of $m_u|e$ and $m_v|e$ remain unchanged from left to right.

$E_3^i = e \in E(G)$ = The set of edges making angle of 155° with positive x-axis in anticlockwise direction. E_3^i levels increase from right bottom to left top but the values of $m_u|e$ and $m_v|e$ remain unchanged from left to right.

$E_4^i = e \in E(G)$ = The set of edges making angle of 120° and 150° with positive x-axis in anticlockwise direction. E_4^i levels increase from right bottom to left top but the values of $m_u|e$ and $m_v|e$ remain unchanged from left to right.

$E_5^i = e \in E(G)$ = The set of edges making angle of 30° and 60° with positive x-axis in anticlockwise direction. E_5^i levels increase from left bottom to right top but the values of $m_u|e$ and $m_v|e$ remain unchanged from left to right.

$E_6^i = e \in E(G)$ = The set of edges making angle of 35° and 65° with positive x-axis in anticlockwise direction. E_6^i levels increase from left bottom to right top but the values of $m_u|e$ and $m_v|e$ remain unchanged from left to right.

2. General Formulas

We compute $m_u|e$ and $m_v|e$ for every edge of above sets, where $m_u|e$ is the edges close to u as compared to v and $m_v|e$ is the edges close to v as compared to u . General formulas for each edge is computed in the table given below. All the calculations are made by using symmetric property of benzene ring network which is a connected $n \times n$ dimensional graph.

TABLE 1. Partition of edges based on $(m_u|e, m_v|e)$ for each edge $e = \{u, v\} \in E(BR)$

| Edges | $(m_u e, m_v e)$ | Frequency | Range |
|---------|---|-------------|-----------------------|
| E_h^i | $(16ni - 2n - i, 32n^2 - 4n - 16ni + i)$ | $4n$ | $1 \leq i \leq n - 1$ |
| E_h^i | $(16n^2 - 3n, 16n^2 - 3n)$ | $2n$ | $n=n$ |
| E_v^i | $(16ni - 2n - i, 32n^2 - 4n - 16ni + i)$ | $4n$ | $1 \leq i \leq n - 1$ |
| E_v^i | $(16n^2 - 3n, 16n^2 - 3n)$ | $2n$ | $n = n$ |
| E_1^i | $(16n^2 - 20n + 6, 32n^2 - 4n - 32i + 28)$ | $4(2i - 1)$ | $1 \leq i \leq n$ |
| E_2^i | $(16n^2 - 20n + 32ni - 32i + 28,$ $16n^2 + 12n - 32ni + 36i - 30)$ | $4(2i - 1)$ | $1 \leq i \leq n$ |
| E_3^i | $(16n^2 - 38n + 32ni - 14i + 15,$ $16n^2 + 30n - 32ni + 18i - 19)$ | $8i$ | $1 \leq i \leq n - 1$ |
| E_3^i | $(16n^2 - 6n + 1, 16n^2 - 2n - 1)$ | $4n$ | $n = n$ |
| E_4^i | $(16n^2 - 34n + 32ni - 18i + 17,$ $16n^2 - 38n + 32ni - 22i + 23)$ | $8i$ | $1 \leq i \leq n - 1$ |
| E_4^i | $(16n^2 - 2n - 1, 16n^2 - 6n + 1)$ | $4n$ | $n = n$ |
| E_5^i | $(46i - 33, 32n^2 - 4n - 50i + 3)$ | $8i$ | $1 \leq i \leq n - 1$ |
| E_5^i | $(16n^2 - 6n + 1, 16n^2 - 2n - 1)$ | $4n$ | $n = n$ |
| E_6^i | $(42i - 31, 31n^2 + n + n^2i - 5ni - 40i + 25)$ | $8i$ | $1 \leq i \leq n - 1$ |
| E_6^i | $(16n^2 - 6n + 1, 16n^2 - 2n - 1)$ | $4n$ | $n = n$ |

THEOREM 2.1. Let $G \cong BR$ be the benzene ring graph then edge Szeged index of graph is

$$S_{ze}(BR) = 7252n^6 - 3684n^5 - \frac{38812n^4}{3} + \frac{86012n^3}{3} - \frac{71084n^2}{3} + \frac{23224n}{3}$$

Proof. As we know, the formula to calculate edge Szeged index of a connected graph is

$$S_{ze}(G) = \sum_{e=uv \in E(G)} (m_u|e \times m_v|e)$$

Then by using above formula and Table 1 we compute the edge Szeged index of $G \cong BR$ as follows:

$$\begin{aligned}
S_{ze}(BR) &= 4 \sum_{i=1}^{n-1} n(16ni - 2n - i)(32n^2 + i - 4n - 16ni) + 2n(16n^2 - 3n)^2 \\
&+ 4 \sum_{i=1}^{n-1} n(16ni - 2n - i)(32n^2 + i - 4n - 16ni) + 2n(16n^2 - 3n)^2 \\
&+ 4 \sum_{i=1}^n (2i - 1)(16n^2 - 20n + 6) \times (32n^2 - 32i - 4n + 28) \\
&+ 4 \sum_{i=1}^n (2i - 1)(16n^2 - 32i - 20n + 32ni + 28) \\
&\times (16n^2 - 32ni + 36i + 12n - 30) \\
&+ 8 \sum_{i=1}^{n-1} i(16n^2 - 14i - 38n + 32ni + 15) \times (16n^2 + 18i + 30n - 32ni - 19) \\
&+ 4n(16n^2 - 6n + 1)(16n^2 - 2n - 1) \\
&+ 8 \sum_{i=1}^{n-1} i(16n^2 - 18i - 34n + 32ni + 17)(16n^2 - 22i - 38n + 32ni + 23) \\
&+ 4n(16n^2 - 2n - 1)(16n^2 - 6n + 1) \\
&+ 8 \sum_{i=1}^{n-1} i(46i - 33)(32n^2 - 50i - 4n + 3) + 4n(16n^2 - 6n + 1)(16n^2 - 2n - 1) \\
&+ 8 \sum_{i=1}^{n-1} i(42i - 31)(31n^2 + in^2 - 40i + n - 5ni + 25) \\
&+ 4n(16n^2 - 6n + 1)(16n^2 - 2n - 1)
\end{aligned}$$

After some simplifications, we get the result

$$S_{ze}(BR) = 7252n^6 - 3684n^5 - \frac{38812n^4}{3} + \frac{86012n^3}{3} - \frac{71084n^2}{3} + \frac{23224n}{3}$$

□

THEOREM 2.2. Let $G \cong BR$ be the benzene ring graph then edge Padmakar – Ivan (PI_e) index of graph is

$$PI_e(BR) = \frac{8n}{3}(n^4 + 464n^3 - 391n^2 + 199n - 12)$$

Proof. As we know, the edge Padmakar–Ivan (PI_e) index of a connected graph is

$$PI_e(G) = \sum_{e=uv \in E(G)} (m_u|e + m_v|e)$$

Therefore by using above formula and Table 1 we compute the Padmakar–Ivan (PI_e) of $G \cong BR$ as follows:

$$\begin{aligned} & PI_e(BR) \\ = & \sum_{i=1}^{n-1} 4n(16ni - 2n - i + 32n^2 + i - 4n - 16ni) + 2n(16n^2 - 3n + 16n^2 - 3n) \\ + & \sum_{i=1}^{n-1} 4n(16ni - 2n - i + 32n^2 + i - 4n - 16ni) + 2n(16n^2 - 3n + 16n^2 - 3n) \\ + & \sum_{i=1}^n 4(2i - 1)(16n^2 - 20n + 6 + 32n^2 - 32i - 4n + 28) \\ + & \sum_{i=1}^n 4(2i - 1)(16n^2 - 32i - 20n + 32ni + 28 - 32ni + 16n^2 + 36i + 12n - 30) \\ + & \sum_{i=1}^{n-1} 8i(16n^2 - 14i - 38n + 32ni + 15 + 16n^2 + 18i + 30n - 32ni - 19) \\ + & 4n(16n^2 - 6n + 1 + 16n^2 - 2n - 1) \\ + & \sum_{i=1}^{n-1} 8i(16n^2 - 18i - 34n + 32ni + 17 + 16n^2 - 22i - 38n + 32ni + 23) \\ + & 4n(16n^2 - 2n - 1 + 16n^2 - 6n + 1) \\ + & \sum_{i=1}^{n-1} 8i(46i - 33 + 32n^2 - 50i - 4n + 3) + 4n(16n^2 - 6n + 1 + 16n^2 - 2n - 1) \\ + & \sum_{i=1}^{n-1} 8i(42i - 31 + n^2i + 31n^2 - 40i + n - 5ni + 25) \\ + & 4n(16n^2 - 6n + 1 + 16n^2 - 2n - 1) \end{aligned}$$

After some necessary simplifications, we get the result

$$PI_e(BR) = \frac{8n}{3}(n^4 + 464n^3 - 391n^2 + 199n - 12)$$

□

□

THEOREM 2.3. *Let $G \cong BR$ then edge szeged Geometric Arithmetic index of Benzene ring is*

$$\begin{aligned}
& GA_e(BR) \\
= & \frac{512n^2 - 224n + 24}{64n^2 - 8n + 3} \sqrt{2} \\
& \times \left(\sum_{i=1}^n \frac{(2i-1) \sqrt{-(8ni + 4n^2 - 8i - 5n + 7)(16ni - 8n^2 - 18i - 6n + 15)}}{16n^2 + 2i - 4n - 1} \right) \\
+ & (256n^2 - 112n + 12) \\
& \times \left(\sum_{i=1}^{n-1} \frac{i \sqrt{-(32ni + 16n^2 - 14i - 38n + 15)(32ni - 16n^2 - 18i - 30n + 19)}}{8n^2 + i + 2n - 1} \right) \\
+ & (-512n^2 + 224n - 24) \sqrt{2} \left(\sum_{i=1}^n \frac{(2i-1) \sqrt{-(8n^2 - 10n + 3)(-8n^2 + 8i + n - 7)}}{-24n^2 + 16i + 12n - 17} \right) \\
+ & (-512n^2 + 224n - 24) \sum_{i=1}^{n-1} \frac{i \sqrt{-(46i - 33)(-32n^2 + 50i + 4n - 3)}}{-16n^2 + 2i + 2n + 15} \\
+ & (32n - 8) \left(\sum_{i=1}^{n-1} \sqrt{-(16ni - i - 2n)(16ni - 32n^2 - i + 4n)} \right) \\
+ & (64n - 12) \sqrt{256n^4 - 128n^3 + 12n^2 + 4n - 1} \\
+ & 128 \left(n - \frac{1}{4} \right) \left(\frac{\sqrt{n^2(16n-3)^2}}{8} \right) \\
+ & \frac{16n-3}{16} \sum_{i=1}^{n-1} \frac{i \sqrt{(32ni + 16n^2 - 18i - 34n + 17)(32ni + 16n^2 - 22i - 38n + 23)}}{(8n-5)i + 4n^2 - 9n + 5} \\
+ & 8 \left(\sum_{i=1}^{n-1} \frac{i \sqrt{42} \sqrt{\left(i - \frac{31}{42}\right) \left((n^2 - 5n - 40)i + 31n^2 + n + 25\right) \left(i - \frac{31}{42}\right)}}{(n^2 - 5n + 2)i + 31n^2 + n - 6} \right)
\end{aligned}$$

Proof. We know that the Geometric Arithmetic index of a connected graph is given by;

$$GA_e(BR) = \sum_{e=uv \in E(G)} \left(\frac{2 \times \sqrt{m_u \times m_v}}{m_u + m_v} \right)$$

Therefore by using above formula and Table 1 we compute the edge Szeged version of Geometric Arithmetic index of $G \cong BR$ as follows:

$$\begin{aligned}
& GA_e(BR) \\
= & \sum_{i=1}^{n-1} 8n \frac{\sqrt{(16ni - 2n - i)(32n^2 + i - 4n - 16ni)}}{(16ni - 2n - i + 32n^2 + i - 4n - 16ni)} \\
& + 4n \frac{\sqrt{(16n^2 - 3n)(16n^2 - 3n)}}{(16n^2 - 3n + 16n^2 - 3n)} \\
& + \sum_{i=1}^{n-1} 8n \frac{\sqrt{(16ni - 2n - i)(32n^2 + i - 4n - 16ni)}}{(16ni - 2n - i + 32n^2 + i - 4n - 16ni)} \\
& + 4n \frac{\sqrt{(16n^2 - 3n)(16n^2 - 3n)}}{(16n^2 - 3n + 16n^2 - 3n)} \\
& + \sum_{i=1}^n 8(2i - 1) \frac{\sqrt{(16n^2 - 20n + 6)(32n^2 - 4n - 32i + 28)}}{(16n^2 - 20n + 6 + 32n^2 - 4n - 32i + 28)} \\
& + \sum_{i=1}^n 8(2i - 1) \frac{\sqrt{(16n^2 - 20n + 32ni - 32i + 28)(16n^2 + 12n - 32ni + 36i - 30)}}{(16n^2 - 20n + 32ni - 32i + 28 + 16n^2 + 12n - 32ni + 36i - 30)} \\
& + \sum_{i=1}^{n-1} 16i \frac{\sqrt{(16n^2 - 38n + 32ni - 14i + 15)(16n^2 + 30n - 32ni + 18i - 19)}}{(16n^2 - 38n + 32ni - 14i + 15 + 16n^2 + 30n - 32ni + 18i - 19)} \\
& + 8n \frac{\sqrt{(16n^2 - 6n + 1)(16n^2 - 2n - 1)}}{(16n^2 - 6n + 1 + 16n^2 - 2n - 1)} \\
& + \sum_{i=1}^{n-1} 16i \frac{\sqrt{(16n^2 - 34n + 32ni - 18i + 17)(16n^2 - 38n + 32ni - 22i + 23)}}{(16n^2 - 34n + 32ni - 18i + 17 + 16n^2 - 38n + 32ni - 22i + 23)} \\
& + 8n \frac{\sqrt{(16n^2 - 2n - 1)(16n^2 - 6n + 1)}}{(16n^2 - 2n - 1 + 16n^2 - 6n + 1)} \\
& + \sum_{i=1}^{n-1} 16i \frac{\sqrt{(46i - 33)(32n^2 - 4n - 50i + 3)}}{(46i - 33 + 32n^2 - 4n - 50i + 3)} \\
& + 8n \frac{\sqrt{(16n^2 - 6n + 1)(16n^2 - 2n - 1)}}{(16n^2 - 6n + 1 + 16n^2 - 2n - 1)} \\
& + \sum_{i=1}^{n-1} 16i \frac{\sqrt{(42i - 31)(31n^2 + n + n^2i - 5ni - 40i + 25)}}{(42i - 31 + 31n^2 + n + n^2i - 5ni - 40i + 25)} \\
& + 8n \frac{\sqrt{(16n^2 - 6n + 1)(16n^2 - 2n - 1)}}{(16n^2 - 6n + 1 + 16n^2 - 2n - 1)}
\end{aligned}$$

After some necessary simplifications, we get the result

$$\begin{aligned}
& GA_e(BR) \\
= & \frac{\sqrt{2}(512n^2 - 224n + 24)}{64n^2 - 8n + 3} \\
& \times \left(\sum_{i=1}^n \frac{(2i-1)\sqrt{-(8ni+4n^2-8i-5n+7)(16ni-8n^2-18i-6n+15)}}{16n^2+2i-4n-1} \right) \\
+ & (256n^2 - 112n + 12) \\
& \times \left(\sum_{i=1}^{n-1} \frac{i\sqrt{-(32ni+16n^2-14i-38n+15)(32ni-16n^2-18i-30n+19)}}{8n^2+i+2n-1} \right) \\
+ & \sqrt{2}(-512n^2 + 224n - 24) \sum_{i=1}^n \frac{(2i-1)\sqrt{-(8n^2-10n+3)(-8n^2+8i+n-7)}}{-24n^2+16i+12n-17} \\
+ & (-512n^2 + 224n - 24) \sum_{i=1}^{n-1} \frac{i\sqrt{-(46i-33)(-32n^2+50i+4n-3)}}{-16n^2+2i+2n+15} \\
+ & (32n-8) \sum_{i=1}^{n-1} \sqrt{-(16ni-i-2n)(16ni-32n^2-i+4n)} \\
+ & 48n-9\sqrt{256n^4-128n^3+12n^2+4n-1} \\
+ & (16n-4)\sqrt{16n(16n^2-3n)^2-3n(16n^2-3n)} \\
+ & 128(n-\frac{1}{4})\frac{\sqrt{256n^4-96n^3+6n-1}}{3} \\
+ & \frac{1}{16}(16n-1) \sum_{i=1}^{n-1} \frac{\sqrt{(32ni+16n^2-18i-34n+17)(32ni+16n^2-22i-38n+23)}}{(8n-5)i+4n^2-3n+5} \\
+ & 8 \sum_{i=1}^{n-1} \frac{i\sqrt{42}\sqrt{(i-\frac{31}{42})((n^2-5n-40)i+31n^2+n+25)}}{(n^2-5n+2)i+31n^2+n-6}
\end{aligned}$$

□

THEOREM 2.4. Let $G \cong (BR)_{n \times n}$ then its Mostar index is,

$$\begin{aligned}
MI(BR_{n \times n}) &= 8|16n^4 - 17n^3 + n^2| + 8|-\frac{8}{3}n^3 + 3n^2 + \frac{8}{3}n + 8n^4| \\
&+ \frac{8}{3}|64n^4 - 68n^3 + 20n^2 + 17n| \\
&+ \frac{8}{3}|64n^4 - 230n^3 + 233n^2 + 67n| + 32|2n^2 - n| \\
&+ 8|\frac{10}{3}n^3 - 7n^2 + \frac{11}{3}n| + |\frac{272}{3}n^3 - 255n^2 + \frac{484}{3}n + 3| \\
&+ |\frac{1}{2}n^4 - 84n^3 + \frac{489}{2}n^2 - 136n - 25| + |48n^2 - 22n + 5|.
\end{aligned}$$

Proof. As we know that the Mostar index is defined as

$$MI(G) = \sum_{e=uv \in (G)} \left| m_u|e - m_v|e \right|$$

Thus by using above formula and Table 1 we compute the Mostar index of $G \cong BR$ as follows:

$$\begin{aligned} & MI \\ &= \sum_{i=1}^{n-1} |4n((16ni - 2n - i) - (32n^2 + i - 4n - 16ni))| + |2n((16n^2 - 3n) - (16n^2 - 3n))| \\ &+ \sum_{i=1}^{n-1} |4n((16ni - 2n - i) - (32n^2 + i - 4n - 16ni))| + |2n((16n^2 - 3n) - (16n^2 - 3n))| \\ &+ \sum_{i=1}^n |4(2i - 1)((16n^2 - 20n + 6) - (32n^2 - 4n - 32i + 28))| \\ &+ \sum_{i=1}^n |4(2i - 1)((16n^2 - 20n + 32ni - 32i + 28) - (16n^2 + 12n - 32ni + 36i - 30))| \\ &+ \sum_{i=1}^{n-1} |8i((16n^2 - 38n + 32ni - 14i + 15) - (16n^2 + 30n - 32ni + 18i - 19))| \\ &+ |4n((16n^2 - 6n + 1) - (16n^2 - 2n - 1))| \\ &+ \sum_{i=1}^{n-1} |8i((16n^2 - 34n + 32ni - 18i + 17) - (16n^2 - 38n + 32ni - 22i + 23))| \\ &+ |4n((16n^2 - 2n - 1) - (16n^2 - 6n + 1))| + \sum_{i=1}^{n-1} |8i((46i - 33) - (32n^2 - 4n - 50i + 3))| \\ &+ |4n((16n^2 - 6n + 1) - (16n^2 - 2n - 1))| \\ &+ \sum_{i=1}^{n-1} |8i((42i - 31) - (31n^2 + n + n^2i - 5ni - 40i + 25))| \\ &+ |4n((16n^2 - 6n + 1) - (16n^2 - 2n - 1))| \end{aligned}$$

After some simplifications, we get the result

$$\begin{aligned}
 &= 8|16n^4 - 17n^3 + n^2| + 8|-\frac{8}{3}n^3 + 3n^2 + \frac{8}{3}n + 8n^4| \\
 &+ \frac{8}{3}|64n^4 - 68n^3 + 20n^2 + 17n| \\
 &+ \frac{8}{3}|64n^4 - 230n^3 + 233n^2 + 67n| + 32|2n^2 - n| \\
 &+ 8|\frac{10}{3}n^3 - 7n^2 + \frac{11}{3}n| + |\frac{272}{3}n^3 - 255n^2 + \frac{484}{3}n + 3| \\
 &+ |\frac{1}{2}n^4 - 84n^3 + \frac{489}{2}n^2 - 136n - 25| + |48n^2 - 22n + 5|
 \end{aligned}$$

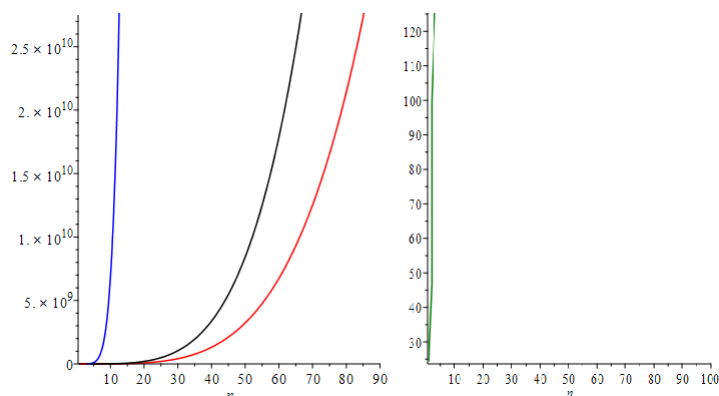
□

□Now we compare the values of Sz , PI , GA and MI indices for some initial values of n and then construct a comparison table for these values. Graphs of the above mentioned indices are given

TABLE 2. Comparison table of indices.

| n | Sz | PI | $GA(\text{approx.})$ | MI |
|-----|------------|----------|----------------------|---------|
| 1 | 3348 | 696 | 24 | 239 |
| 2 | 289312 | 13600 | 100 | 4057 |
| 3 | 3927652 | 77400 | 222 | 25775 |
| 4 | 24106592 | 261120 | 377 | 93249 |
| 5 | 96744340 | 664440 | 570 | 246603 |
| 6 | 298322048 | 1418016 | 798 | 538879 |
| 7 | 768938212 | 2683800 | 1064 | 1035907 |
| 8 | 1740584512 | 4655360 | 1362 | 1816305 |
| 9 | 3570643092 | 7558200 | 1698 | 2971479 |
| 10 | 6780605280 | 11650080 | 2065 | 4605623 |

below. Blue curve represents the Sz index, black curve represents the PI index, green curve represents the GA index and red curve represents the MI index.

FIGURE 4. Graphs of S_z , PI , GA and MI indices

3. Conclusion

In this article, we discussed the edge Szeged index, edge Padmakar–Ivan (PI_e) index and geometric arithmetic index. We consider the molecular graph of Benzene Ring and we have computed the edge Szeged index, edge Padmakar–Ivan (PI_e) index, geometric arithmetic index and Mostar index of this chemical graph for n -levels.

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