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Research Article

Computation of Benzenoid Planar Octahedron Networks by Using Topological Indices

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Chemical descriptors are numeric numbers that contain a basic chemical structure and describe the structure of a graph. A graph's topological indices are linked to its chemical characteristics. Biological activity of chemical compounds can be predicted using topological indices. Numerous chemical indices have been developed in theoretical chemistry, including the Zagreb index, the Randić index, the Wiener index, and many others. In this paper, we compute the exact results for the Randić, Zagreb, Harmonic, augmented Zagreb, atom-bond connectivity, and geometric-arithmetic indices for the Benzenoid networks theoretically.

1. Introduction and Preliminary Results

Topological indices, which are particularly useful tools for chemists, are provided by graph theory. In terms of graph theory, vertices represent atoms and edges indicate chemical bonding in a molecular graph [1]. Topological indices such as the ABC index, Wiener index, Randić index, Szeged index, and Zagreb index are highly useful for predicting the bioactivity of chemical compounds.

A graph can be represented by polynomials, numeric numbers, a sequence of integers, or a matrix. All graphs are simple, finite, and connected. All graphs discussed in this article are simple, finite, and connected.

A topological index is a numerical quantity for the chemical graph and it is expressed through chemical graph theory. Interest in topological descriptors has already increased in the computer chemistry sector, and is mostly related with the use of unexpected quantities, the relationship between structure properties, and the relationship between structure quantities.

Topological indices based on distance, degree, and polynomials are some of the most popular forms [2]. Chemical graphs play an important part in theory and theoretical chemistry, and degree-based indices are often utilized in a number of these segments. In this article, we explore at some important topological indices and how they areused to assess benzenoid graphs' chemical activity. Chemists can benefit from these topological indices.the

2. Construction for Benzenoid Planar Octahedron Networks

Step 1: consider a sheet oxide network [3] of dimension n

Step 2: then, place C_6 in each C_3 of oxide network

Step 3: connecting alternating adjacent vertices of C_6 to each opposite vertex, the resultant graph is called benzenoid planar octahedron network BPOH

Step 4: by using the previous algorithm, we can construct the benzenoid dominating planar octahedron network $\mathrm{BDPOH}(r)$ and the benzenoid hex planar octahedron network $\mathrm{BHPOH}(r)$

We defined B to be a network with $V(B)$ as a set of vertices and $E(B)$ as a set of edges in this article, where $\delta(m)$ is the degree of vertex $m \in V(B)$.

The Estrada index is a graph-spectrum-based structural descriptor that was introduced in 2000 by Estrada and is defined as follows [4]:

$$\mathrm{EE}(B) = \sum_{j=1}^{n} e^{\lambda i}. \tag{1}$$

In full resemblance with the Estrada index, Fath-Tabar et al. in [5] introduced the Laplacian Estrada index, which is formalised as follows:

$$\mathrm{LEE}(B) = \sum_{j=1}^{n} e^{\mu i}. \tag{2}$$

Randić index [6] is an oldest degree-based topological index, denoted by $R_{-1/2}(B)$, and was proposed by Milan Randić and is defined as follows:

$$R_{-1/2}(B) = \sum_{mn\in E(B)} \frac{1}{\sqrt{\delta(m)\delta(n)}}. \tag{3}$$

The sum of $(\delta(m)\delta(n))^{\alpha}$ over all the edges $e = mn \in E(B)$ is general Randić index $R_{\alpha}(B)$ [6] and is defined as follows:

$$R_{\alpha}(B) = \sum_{mn\in E(B)} (\delta(m)\delta(n))^{\alpha} \text{ for } \alpha = 1, \frac{1}{2}, -1, -\frac{1}{2}. \tag{4}$$

The Zagreb index, represented by $M_1(B)$ and defined by Gutman and Das [7], is an important topological index:

$$M_1(B) = \sum_{mn\in E(B)} (\delta(m) + \delta(n)). \tag{5}$$

Zhong [8] established the most important harmonic index, which is defined as follows:

$$H(B) = \sum_{mn\in E(B)} \frac{2}{\delta(m) + \delta(n)}. \tag{6}$$

The prominent topological index is augmented Zagreb index which was proposed by Furtula et al. in [9], and it is defined as follows:

$$\mathrm{AZI}(B) = \sum_{mn\in E(B)} \left(\frac{\delta(m)\delta(n)}{\delta(m) + \delta(n) - 2}\right)^{3}. \tag{7}$$

The atom-bond connectivity (ABC) index, proposed by Estrada et al. in [10], is a prominent degree-based topological indicator that is defined as follows:

$$\mathrm{ABC}(B) = \sum_{mn\in E(B)} \sqrt{\frac{\delta(m) + \delta(n) - 2}{\delta(m)\delta(n)}}. \tag{8}$$

Another prominent topological index is the Geometric-arithmetic (GA) index, which was proposed by Furtula in reference [11] and described as follows:

$$\mathrm{GA}(B) = \sum_{mn\in E(B)} \frac{2\sqrt{\delta(m)\delta(n)}}{\delta(m) + \delta(n)}. \tag{9}$$

3. Primary Results of Benzenoid Networks

In this article, the general Randić, first Zagreb, H, AZI, ABC, and GA indices are studied and closed equations for these indices for the benzenoid planar octahedron networks are given. The ABC and GA indices, also their derivatives, are now the subject of substantial research, see [12, 13] topological indices and their invariants in different graph families for more information.

3.1. Results for the Benzenoid Planar Octahedron Network. We construct some degree-based topological indices of the benzenoid planar octahedron network, denoted by $B_1(r)$, in this section. We calculate the general Randić $R_{\alpha}(B)$ for $\alpha = \{1, -1, 1/2, -1/2\}$, first Zagreb, H, AZI, ABC, and GA indices for benzenoid planar octahedron network in this section.

In the following theorem, we calculate the general Randić index for the benzenoid planar octahedron network.

Theorem 1. *Let $B_1(r)$ be the benzenoid planar octahedron network, then its general Randić index is equal to the following equation:*

$$R_\alpha(B_1(r)) = \begin{cases} 2340r^2 - 528r, & \alpha = 1, \\ 12(21+6\sqrt{6})r^2 + 12(2\sqrt{3}-8)r, & \alpha = \frac{1}{2}, \\ \frac{185}{32}r^2 + \frac{11}{16}r, & \alpha = -1, \\ \frac{3}{4}(19+4\sqrt{6})r^2 + \frac{1}{4}(-6+6\sqrt{2}+8\sqrt{3}-4\sqrt{6})r, & \alpha = -\frac{1}{2}. \end{cases} \tag{10}$$

Proof. Let $B_1(r)$ be the benzenoid planar octahedron network BPOH(r) as shown in Figure 1, with $r \geq 2$ and $B_1(r)$ edge set divided into five divisions based on the degree of end vertices. The first edge partition $E_1(B_1(r))$ has $36r^2$ edges, having $\delta(m) = \delta(n) = 3$. The second edge division $E_2(B_1(r))$ has $12r$ edges, having $\delta(m) = 3$ and $\delta(n) = 4$. The third edge division $E_3(B_1(r))$ has $36r^2 - 12r$ edges, having $\delta(m) = 3$ and $\delta(n) = 8$. The fourth edge division $E_4(B_1(r))$ has $12r$ edges, having $\delta(m) = 4$ and $\delta(n) = 8$. The fifth edge division has $18r^2 - 12r$ edges, having $\delta(m) = \delta(n) = 8$.

$$R_\alpha(B) = \sum_{mn \in E(B)} (\delta(m)\delta(n))^\alpha. \tag{11}$$

For $\alpha = 1$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_1(B) = \sum_{j=1}^{5} \sum_{mn \in E_j(B)} \delta(m) \cdot \delta(n). \tag{12}$$

We can achieve the following result by using Table 1 edge division:

$$\begin{aligned} R_1(B) &= 9|E_1(B_1(r))| + 12|E_2(B_1(r))| + 24|E_3(B_1(r))| + 32|E_4(B_1(r))| + 64|E_5(B_1(r))|, \\ \Rightarrow R_1(B) &= 2340r^2 - 528r. \end{aligned} \tag{13}$$

For $\alpha = 1/2$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_{1/2}(B) = \sum_{j=1}^{5} \sum_{mn \in E_j(B)} \sqrt{\delta(m) \cdot \delta(n)}. \tag{14}$$

We can achieve the following result by using the Table 1 edge division:

$$\begin{aligned} R_{1/2}(B) &= 3|E_1(B_1(r))| + 2\sqrt{3}|E_2(B_1(r))| + 2\sqrt{6}|E_3(B_1(r))| + 4\sqrt{2}|E_4(B_1(r))| + 8|E_5(B_1(r))|, \\ \Rightarrow R_{1/2}(B) &= 36(7+2\sqrt{6})r^2 + 12(-8+4\sqrt{2}+2\sqrt{3}-2\sqrt{6})r. \end{aligned} \tag{15}$$

For $\alpha = -1$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_{-1}(B) = \sum_{j=1}^{5} \sum_{mn\in E_j(B)} \frac{1}{\delta(m)\cdot\delta(n)},$$

$$R_{-1}(B) = \frac{1}{9}\left|E_1(B_1(r))\right| + \frac{1}{12}\left|E_2(B_1(r))\right| + \frac{1}{24}\left|E_3(B_1(r))\right| + \frac{1}{32}\left|E_4(B_1(r))\right| + \frac{1}{64}\left|E_5(B_1(r))\right|, \tag{16}$$

$$\Rightarrow R_{-1}(B) = \frac{185}{32}r^2 + \frac{11}{16}r.$$

For $\alpha = -1/2$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_{-1/2}(B) = \sum_{mn\in E_j(B)} \frac{1}{\sqrt{\delta(m)\cdot\delta(n)}},$$

$$R_{-1/2}(B) = \frac{1}{3}\left|E_1(B_1(r))\right| + \frac{1}{2\sqrt{3}}\left|E_2(B_1(r))\right| + \frac{1}{2\sqrt{6}}\left|E_3(B_1(r))\right| + \frac{1}{4\sqrt{2}}\left|E_4(B_1(r))\right| + |\frac{1}{8}\left|E_5(B_1(r))\right|, \tag{17}$$

$$\Rightarrow R_{-1/2}(B) = \frac{3}{4}(19 + 4\sqrt{6})r^2 + \frac{1}{4}(-6 + 6\sqrt{2} + 8\sqrt{3} - 4\sqrt{6})r.$$

The first Zagreb index of the benzenoid planar octahedron network is computed in the following theorem. □

Theorem 2. *For the benzenoid planar octahedron network $B_1(r)$, the first Zagreb index is equal to the following equation:*

$$M_1(B_1(r)) = 900r^2 - 96r. \tag{18}$$

Proof. Let $B_1(r)$ denote the bezenoid planar octahedron network. The following is the result of using the edge division from Table 1. As a result of equation (5), we have

$$M_1(B) = \sum_{mn\in E(B)} (\delta(m) + \delta(n)) = \sum_{j=1}^{5} \sum_{mn\in E_j(B)} (\delta(m) + \delta(n)),$$
$$M_1(B_1(r)) = 6\left|E_1(B_1(r))\right| + 7\left|E_2(B_1(r))\right| + 11\left|E_3(B_2(r))\right| + 12\left|E_4(B_1(r))\right| + 16\left|E_5(B_1(r))\right|. \tag{19}$$

We get following result by doing calculation:

$$\Rightarrow M_1(B_1(r)) = 900r^2 - 96r. \tag{20}$$

□

Theorem 3. *Let $B_1(r)$ be the benzenoid planar octahedron network $r \geq 2$; then, we have*

$$H(B_1(r)) = \frac{915}{44}r^2 + \frac{269}{154}r,$$
$$\mathrm{AZI}(B_1(r)) = \frac{46302245}{16464}r^2 - \frac{314431744}{38587}r,$$
$$\mathrm{ABC}(B_1(r)) = \frac{1}{4}(36\sqrt{6} + 9\sqrt{14} + 96)r^2 + \frac{1}{2}(6\sqrt{5} + 4\sqrt{15} - 3\sqrt{14} - 6\sqrt{6})r,$$
$$\mathrm{GA}(B_1(r)) = \frac{18}{11}(33 + 4\sqrt{6})r^2 + \frac{3}{154}(429\sqrt{3} - 112\sqrt{6} - 616)r. \tag{21}$$

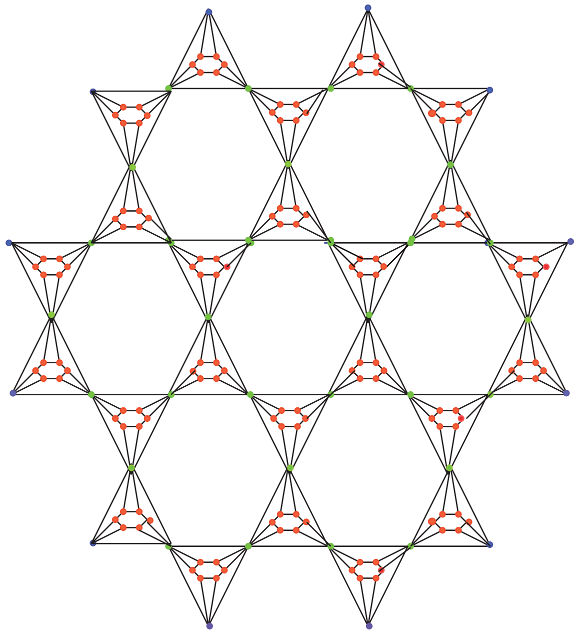

Figure 1: Benzenoid planar octahedron network BPOH(2).

Table 1: Edge division of benzenoid planar octahedron network $(B_1(r))$ based on the sum of the degrees of each edge's end vertices.

$(\delta(m), \delta(n))$, where $mn \in E(B_1)$	Number of edges	$(\delta(m), \delta(n))$, where $mn \in E(B_1)$	Number of edges
$E_1 = (3,3)$	$36r^2$	$E_4 = (4,8)$	$12r$
$E_2 = (3,4)$	$12r$	$E_5 = (8,8)$	$18r^2 - 12r$
$E_3 = (3,8)$	$36r^2 - 12r$		

Proof. We get the required result by finding the edge division in Table 1, and then, applying the definition. It follows from equation (6) that

$$H(B) = \sum_{mn \in E(B)} \frac{2}{\delta(m) + \delta(n)} = \sum_{j=1}^{5} \sum_{mn \in E(B)} \frac{2}{\delta(m) + \delta(n)},$$
$$H(B_1(r)) = \frac{1}{3}|E_1(B_1(r))| + \frac{2}{7}|E_2(B_1(r))| + \frac{2}{11}|E_3(B_1(r))| + \frac{1}{6}|E_4(B_1(r))| + \frac{1}{8}|E_5(B_1(r))|. \tag{22}$$

By doing the calculation, we obtained the following result:

$$H(B_1(r)) = \frac{915}{44} r^2 + \frac{269}{154} r. \tag{23}$$

Equation (7) can be used to compute the augmented Zagreb index as follows:

$$\mathrm{AZI}(B) = \sum_{mn \in E(B)} \left(\frac{\delta(m)\delta(n)}{\delta(m) + \delta(n) - 2}\right)^3 = \sum_{j=1}^{5} \sum_{mn \in E(B)} \left(\frac{\delta(m)\delta(n)}{\delta(m) + \delta(n) - 2}\right)^3,$$
$$\mathrm{AZI}(B_1(r)) = \frac{1}{3}|E_1(B_1(r))| + \frac{1}{2\sqrt{3}}|E_2(B_1(r))| + \frac{1}{2\sqrt{6}}|E_3(B_1(r))| + \frac{1}{4\sqrt{2}}|E_4(B_1(r))| + \frac{1}{8}|E_5(B_1(r))|. \tag{24}$$

By doing the calculation, we obtained the following result:

$$\mathrm{AZI} = \frac{46302245}{16464} r^2 - \frac{314431744}{38587} r. \tag{25}$$

Equation (8) can be used to compute the atom-bond connectivity index as follows:

$$\begin{aligned} \mathrm{ABC}(B) &= \sum_{mn \in E(B)} \sqrt{\frac{\delta(m) + \delta(n) - 2}{\delta(m) \cdot \delta(n)}} = \sum_{j=1}^{5} \sum_{mn \in E_j(B)} \sqrt{\frac{\delta(m) + \delta(n) - 2}{\delta(m) \cdot \delta(n)}}, \\ \mathrm{ABC}(B_1(r)) &= \frac{2}{3}\left|E_1(B_1(r))\right| + \frac{\sqrt{15}}{6}\left|E_2(B_1(r))\right| + \frac{\sqrt{6}}{4}\left|E_3(B_1(r))\right| + \frac{\sqrt{15}}{4}\left|E_4(B_1(r))\right| + \frac{\sqrt{14}}{8}\left|E_5(B_1(r))\right|. \end{aligned} \tag{26}$$

By doing the calculation, we obtained the following result:

$$\Rightarrow \mathrm{ABC}(B_1(r)) = \frac{1}{4}(36\sqrt{6} + 9\sqrt{14} + 96)r^2 + \frac{1}{2}(6\sqrt{5} + 4\sqrt{15} - 3\sqrt{14} - 6\sqrt{6})r. \tag{27}$$

Equation (9) can be used to compute the geometric-arithmetic index as follows:

$$\mathrm{GA}(B) = \sum_{mn \in E(B)} \frac{2\sqrt{\delta(m)\delta(n)}}{(\delta(m) + \delta(n))} = \sum_{j=1}^{6} \sum_{mn \in E_j(B)} \frac{2\sqrt{\delta(m)\delta(n)}}{(\delta(m) + \delta(n))}. \tag{28}$$

By doing the calculation, we obtained the following result:

$$\begin{aligned} \mathrm{GA}(B_1(r)) &= \left|E_1(B_1(r))\right| + \frac{4\sqrt{3}}{7}\left|E_2(B_1(r))\right| + \frac{4\sqrt{6}}{11}\left|E_3(B_1(r))\right| + \frac{2\sqrt{2}}{11}\left|E_4(B_1(r))\right| + \left|E_5(B_1(r))\right|, \\ \Rightarrow \mathrm{GA}(B_1(r)) &= \frac{18}{11}(33 + 4\sqrt{6})r^2 + \frac{3}{154}(429\sqrt{3} - 112\sqrt{6} - 616)r. \end{aligned} \tag{29}$$

□

3.2. Results for the Benzenoid Dominating Planar Octahedron Network. We construct some degree-based topological indices of the benzenoid planar octahedron network, denoted by $B_2(r)$. We compute the general Randić $R_\alpha(B)$ for $\alpha = \{1, -1, 1/2, -1/2\}$, first Zagreb, H, AZI, ABC, and GA indices for benzenoid dominating planar octahedron network in this section.

We compute the general Randić index for benzenoid dominating planar octahedron network in the following theorem.

Theorem 4. *Let $B_2(r)$ be the benzenoid dominating planar octahedron network, and then, its general Randić index is equal to the following equation:*

$$R_\alpha(B_2(r)) = \begin{cases} 7020r^2 - 8076r + 2868, & \alpha = 1, \\ 108(7+2\sqrt{6})r^2 + 12(-79+8\sqrt{2}+4\sqrt{3}-22\sqrt{6})r + 12(29-4\sqrt{2}-2\sqrt{3}+8\sqrt{6}), & \alpha = \frac{1}{2}, \\ \frac{555}{32}r^2 - \frac{511}{32} + \frac{163}{32}, & \alpha = -1, \\ \frac{9}{4}(19+4\sqrt{6})n^2 + \left(3\sqrt{2}+4\sqrt{3}-11\sqrt{6}-\frac{183}{4}\right)n + \left(\frac{63}{4}-3\sqrt{2}-2\sqrt{3}+4\sqrt{6}\right), & \alpha = -\frac{1}{2}. \end{cases} \tag{30}$$

Proof. Let $B_2(r)$ be the benzenoid planar octahedron network BPOH(r) as shown in Figure 2, with $r \geq 2$ and B_2 edge set divided into five divisions based on the degree of end vertices. The first edge division $E_1(B_2(n))$ has $108r^2 - 108r + 36$ edges, having $\delta(m) = \delta(n) = 3$. The second edge division $E_2(B_2(n))$ has $24r - 12$ edges, having $\delta(m) = 3$ and $\delta(n) = 4$. The third edge division $E_3(B_2(r))$ has $108r^2 - 132r + 48$ edges, having $\delta(m) = 3$ and $\delta(n) = 8$. The fourth edge division $E_4(B_2(r))$ has $24r - 12$ edges, having $\delta(m) = 4$ and $\delta(n) = 8$. The fifth edge division $E_5(B_2(r))$ has $54r^2 - 78r + 30$ edges, having $\delta(m) = \delta(n) = 8$.

$$R_\alpha(B) = \sum_{mn \in E(B)} (\delta(m)\delta(n))^\alpha. \tag{31}$$

For $\alpha = 1$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_1(B) = \sum_{j=1}^{5} \sum_{mn \in E_j(B)} \delta(m) \cdot \delta(n). \tag{32}$$

We can achieve the following results by using the edge division in Table 2.

$$\begin{aligned} &R_1(B) = 9|E_1(B_2(r))| + 12|E_2(B_2(r))| + 24|E_3(B_2(r))| + 32|E_4(B_2(r))| + 64|E_5(B_2(r))|, \\ &\Rightarrow R_1(B) = 7020r^2 - 8076r + 2868. \end{aligned} \tag{33}$$

For $\alpha = 1/2$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_{1/2}(B) = \sum_{j=1}^{5} \sum_{mn \in E_j(B)} \sqrt{\delta(m) \cdot \delta(n)}. \tag{34}$$

We can achieve the following results by using the edge division in Table 2.

$$\begin{aligned} &R_{1/2}(B) = 3|E_1(B_2(r))| + 2\sqrt{3}|E_2(B_2(r))| + 2\sqrt{6}|E_3(B_2(r))| + 4\sqrt{2}|E_4(B_2(r))| + 8|E_5(B_2(r))|, \\ &\Rightarrow R_{1/2}(B) = 108(7+2\sqrt{6})n^2 + 12(-79+8\sqrt{2}+4\sqrt{3}-22\sqrt{6})n + 12(29-4\sqrt{2}-2\sqrt{3}+8\sqrt{6}). \end{aligned} \tag{35}$$

For $\alpha = -1$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_{-1}(B) = \sum_{j=1}^{5} \sum_{mn\in E_j(B)} \frac{1}{\delta(m)\cdot\delta(n)},$$
$$R_{-1}(B) = \frac{1}{9}\left|E_1(B_2(r))\right| + \frac{1}{12}\left|E_2(B_2(r))\right| + \frac{1}{24}\left|E_3(B_2(r))\right| + \frac{1}{32}\left|E_4(B_2(r))\right| + \frac{1}{64}\left|E_5(B_2(r))\right|, \tag{36}$$
$$\Rightarrow R_{-1}(B) = \frac{555}{32}n^2 - \frac{511}{32} + \frac{163}{32}.$$

For $\alpha = -1/2$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_{-1/2}(B) = \sum_{mn\in E_j(B)} \frac{1}{\sqrt{\delta(m)\cdot\delta(n)}},$$
$$R_{-1/2}(B) = \frac{1}{3}\left|E_1(B_2(r))\right| + \frac{1}{2\sqrt{3}}\left|E_2(B_2(r))\right| + \frac{1}{2\sqrt{6}}\left|E_3(B_2(r))\right| + \frac{1}{4\sqrt{2}}\left|E_4(B_2(r))\right| + \frac{1}{8}\left|E_5(B_2(r))\right|, \tag{37}$$
$$R_{-1/2}(B) = \frac{9}{4}(19+4\sqrt{6})n^2 + \left(3\sqrt{2} + 4\sqrt{3} - 11\sqrt{6} - \frac{183}{4}\right)n + \left(\frac{63}{4} - 3\sqrt{2} - 2\sqrt{3} + 4\sqrt{6}\right).$$

The first Zagreb index of the benzenoid dominating planar octahedron network is computed in the following theorem. □

Theorem 5. *For the benzenoid dominating planar octahedron network $B_2(n)$, the first Zagreb index is equal to the following equation:*

$$M_1(B_2(r)) = 2700r^2 - 2892r + 996. \tag{38}$$

Proof. Let $B_2(n)$ be the bezenoid dominating planar octahedron network. The following is the result of using the edge division from Table 2. As a result of equation (5), we have

$$M_1(B) = \sum_{mn\in E(B)} (\delta(m)+\delta(n)) = \sum_{j=1}^{5} \sum_{mn\in E_j(B)} (\delta(m)+\delta(n)),$$
$$M_1(B_2(r)) = 6\left|E_1(B_2(r))\right| + 7\left|E_2(B_2(r))\right| + 11\left|E_3(B_2(r))\right| + 12\left|E_4(B_2(r))\right| + 16\left|E_5(B_2(r))\right|. \tag{39}$$

By doing the calculation, we obtained the following result:

$$\Rightarrow M_1(B_2(r)) = 2700r^2 - 2892r + 996. \tag{40}$$

□

Theorem 6. *Let $B_2(r)$ be the benzenoid dominating planar octahedron network $r \geq 2$; then, we have*

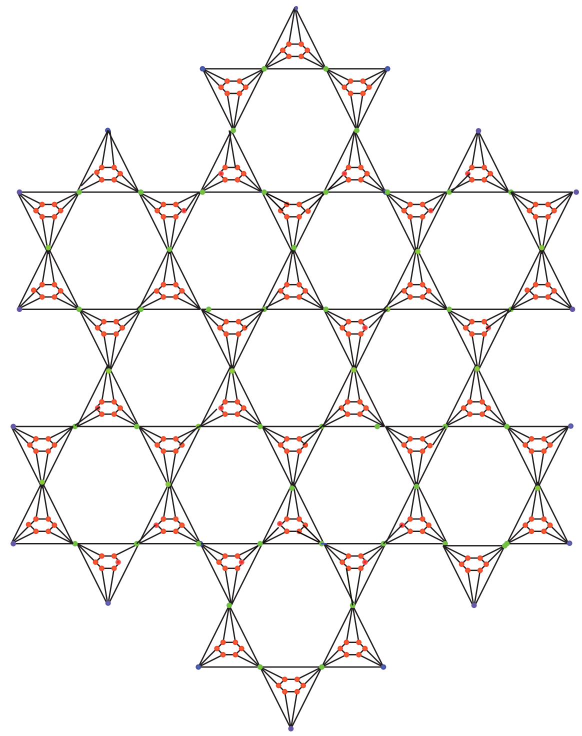

Figure 2: Benzenoid dominating planar octahedron network BDPOH(2).

Table 2: Edge division of benzenoid dominating planar octahedron network $(B_2(r))$ based on the sum of the degrees of each edge's end vertices.

$(\delta(m), \delta(n))$, where $mn \in E(B_2)$	Number of edges	$(\delta(m), \delta(n))$, where $mn \in E(B_2)$	Number of edges
$E_1 = (3,3)$	$108r^2 - 108r + 36$	$E_4 = (4,8)$	$24r - 12$
$E_2 = (3,4)$	$24r - 12$	$E_5 = (8,8)$	$54r^2 - 78r + 30$
$E_3 = (3,8)$	$108r^2 - 132r + 48$		

$$
\begin{aligned}
H(B_2(r)) &= \frac{2745}{44}r^2 - \frac{1649}{28}r + \frac{5867}{308},\\
\mathrm{AZI}(B_2(r)) &= \frac{46302245}{5488}r^2 - \frac{62151841433}{6174000}r + \frac{22394249779}{6174000},\\
\mathrm{ABC}(B_2(r)) &= \frac{1}{4}(288 + 108\sqrt{6} + 27\sqrt{14})r^2 + \frac{1}{4}(-288 + 24\sqrt{5} - 132\sqrt{6} - 39\sqrt{14} + 16\sqrt{15})r\\
&\quad + \frac{1}{4}(96 - 12\sqrt{5} + 48\sqrt{6} + 15\sqrt{14} - 8\sqrt{15}),\\
\mathrm{GA}(B_2(r)) &= \left(162 + \frac{432\sqrt{6}}{11}\right)r^2 + \left(-186 + 16\sqrt{2} + \frac{96\sqrt{3}}{7} - 48\sqrt{6}\right)r + 66 - 8\sqrt{2} - \frac{48\sqrt{3}}{7} + \frac{192\sqrt{6}}{11}.
\end{aligned}
\tag{41}
$$

Proof. We get the required result by finding the edge division in Table 1, and then, applying the definition. It follows from equation (6) that

$$H(B)=\sum_{mn\in E(B)}\frac{2}{\delta(m)+\delta(n)}=\sum_{j=1}^{5}\sum_{mn\in E(B)}\frac{2}{\delta(m)+\delta(n)},$$
$$H(B_2(r))=\frac{1}{3}|E_1(B_2(r))|+\frac{2}{7}|E_2(B_2(r))|+\frac{2}{11}|E_3(B_2(r))|+\frac{1}{6}|E_4(B_2(r))|+\frac{1}{8}|E_5(B_2(r))|, \tag{42}$$

By doing the calculation, we obtained the following result:

$$H(B_2(r))=\frac{2745}{44}r^2-\frac{1649}{28}r+\frac{5867}{308}. \tag{43}$$

Equation (7) can be used to compute the augmented Zagreb index as follows:

$$\mathrm{AZI}(B_2(r))=\sum_{mn\in E(B)}\left(\frac{\delta(m)\delta(n)}{\delta(m)+\delta(n)-2}\right)^3=\sum_{j=1}^{5}\sum_{mn\in E(B)}\left(\frac{\delta(m)\delta(n)}{\delta(m)+\delta(n)-2}\right)^3,$$
$$\mathrm{AZI}(B_2(r))=\frac{1}{3}|E_1(B_2(r))|+\frac{1}{2\sqrt{3}}|E_2(B_2(r))|+\frac{1}{2\sqrt{6}}|E_3(B_2(r))|+\frac{1}{4\sqrt{2}}|E_4(B_2(r))|+\frac{1}{8}|E_5(B_2(r))|. \tag{44}$$

By doing the calculation, we obtained the following result:

$$\mathrm{AZI}=\frac{46302245}{5488}r^2-\frac{62151841433}{6174000}r+\frac{22394249779}{6174000}. \tag{45}$$

Equation (8) can be used to compute the atom-bond connectivity index as follows:

$$\mathrm{ABC}(B)=\sum_{mn\in E(B)}\sqrt{\frac{\delta(m)+\delta(n)-2}{\delta(m)\cdot\delta(n)}}$$
$$=\sum_{j=1}^{5}\sum_{mn\in E_j(B)}\sqrt{\frac{\delta(m)+\delta(n)-2}{\delta(m)\cdot\delta(n)}},$$
$$\mathrm{ABC}(B_2(r))=\frac{2}{3}|E_1(B_2(r))|+\frac{\sqrt{15}}{6}|E_2(B_2(r))|+\frac{\sqrt{6}}{4}|E_3(B_2(r))|+\frac{\sqrt{15}}{4}|E_4(B_2(r))|+\frac{\sqrt{14}}{8}|E_5(B_2(r))|. \tag{46}$$

By doing the calculation, we obtained the following result:

$$\Rightarrow\mathrm{ABC}(B_2(r))=\frac{1}{4}(288+108\sqrt{6}+27\sqrt{14})r^2+\frac{1}{4}(-288+24\sqrt{5}-132\sqrt{6}-39\sqrt{14}+16\sqrt{15})r$$
$$+\frac{1}{4}(96-12\sqrt{5}+48\sqrt{6}+15\sqrt{14}-8\sqrt{15}). \tag{47}$$

Equation (9) can be used to compute the geometric-arithmetic index as follows:

$$\begin{aligned}\mathrm{GA}(B) &= \sum_{mn\in E(B)} \frac{2\sqrt{\delta(m)\delta(n)}}{(\delta(m)+\delta(n))}\\ &= \sum_{j=1}^{5}\sum_{mn\in E_j(B)} \frac{2\sqrt{\delta(m)\delta(n)}}{(\delta(m)+\delta(n))}.\end{aligned} \tag{48}$$

By doing the calculation, we obtained the following result:

$$\begin{aligned}\mathrm{GA}(B_2(r)) &= |E_1(B_2(r))| + \frac{4\sqrt{3}}{7}|E_2(B_2(r))| + \frac{4\sqrt{6}}{11}|E_3(B_2(r))| + \frac{2\sqrt{2}}{11}|E_4(B_2(r))| + |E_5(B_2(r))|,\\ \Rightarrow \mathrm{GA}(B_2(r)) &= \left(162 + \frac{432\sqrt{6}}{11}\right)r^2 + \left(-186 + 16\sqrt{2} + \frac{96\sqrt{3}}{7} - 48\sqrt{6}\right)r + \left(66 - 8\sqrt{2} - \frac{48\sqrt{3}}{7} + \frac{192\sqrt{6}}{11}.\right.\end{aligned} \tag{49}$$

□

3.3. Results for Benzenoid Hex Planar Octahedron Network. We construct some degree-based topological indices of the benzenoid planar octahedron network, denoted by $B_3(r)$, in this section. We compute the general Randić $R_\alpha(B)$ for $\alpha = \{1, -1, 1/2, -1/2\}$, H, AZI, ABC, and GA indices for benzenoid hex planar octahedron network in this section.

We compute the general Randić index for benzenoid hex planar octahedron network in the following theorem.

Theorem 7. *Let $B_3(r)$ be the benzenoid hex planar octahedron network, then its general Randić index is equal to the following:*

$$R_\alpha(B_3(r)) = \begin{cases} 2340r^2 + 1752r - 30, & \alpha = 1,\\ 36(7+2\sqrt{6})r^2 + 24(7+\sqrt{6}+\sqrt{10}+\sqrt{15})r + 6(2\sqrt{10}-5), & \alpha = \dfrac{1}{2},\\ \dfrac{185}{32}r^2 + \dfrac{175}{25}r + \dfrac{24}{25}, & \alpha = -1,\\ \left(\dfrac{57}{4} + 3\sqrt{6}\right)r^2 + \left(\dfrac{72}{5} + 3\sqrt{\dfrac{2}{5}} + 8\sqrt{\dfrac{3}{5}} + \sqrt{6}\right)r + \dfrac{6}{5}(-1+\sqrt{10}), & \alpha = -\dfrac{1}{2}.\end{cases} \tag{50}$$

Proof. Let $B_3(r)$ be the benzenoid hex planar octahedron network BHPOH(r) as shown in Figure 3, with $r \geq 2$ and $B_3(r)$ edge set divided into seven divisions based on the degree of end vertices. The first edge division $E_1(B_3(r))$ has 12 edges, having $\delta(m) = 2$ and $\delta(r) = 5$. The second edge division $E_2(B_3(r))$ has $36r^2 - 36r$ edges, having $\delta(m) = \delta(n) = 3$. The third edge division $E_3(B_3(r))$ has $24r$ edges, having $\delta(m) = 3$ and $\delta(n) = 5$. The fourth edge division $E_4(B_1(r))$ has $36r^2 + 12r$ edges, having $\delta(m) = 3$ and $\delta(n) = 8$. The fifth edge division $E_5(B_3(r))$ has $12r - 6$ edges, having $\delta(m) = 5 = \delta(n)$. The sixth edge division $E_6(B_3(r))$ has $12r$ edges, having $\delta(m) = 5$ and $\delta(n) = 8$. The seventh edge division $E_7(B_3(r))$ has $18r^2$ edges, having $\delta(m) = \delta(n) = 8$.

$$R_\alpha(B) = \sum_{mn\in E(B)} (\delta(m)\delta(n))^\alpha. \tag{51}$$

For $\alpha = 1$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_1(B) = \sum_{j=1}^{7}\sum_{mn\in E_j(B)} \delta(m)\cdot\delta(n). \tag{52}$$

We can obtain the following results by using the edge division in Table 3.

$$\begin{aligned}R_1(B) &= 10|E_1(B_3(r))| + 9|E_2(B_3(r))| + 15|E_3(B_3(r))| + 24|E_4(B_3(r))| + 25|E_5(B_3(r))| + 40|E_6(B_3(r))| + 64|E_7(B_3(r))|,\\ \Rightarrow R_1(B) &= 2340r^2 + 1752r - 30.\end{aligned} \tag{53}$$

For $\alpha = 1/2$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$R_{1/2}(B) = \sum_{j=1}^{7} \sum_{mn \in E_j(B)} \sqrt{\delta(m) \cdot \delta(n)}. \tag{54}$$

We can achieve the following result by using the edge division in Table 3.

$$\begin{aligned} R_{1/2}(B) &= \sqrt{10}\left|E_1(B_3(r))\right| + 3\left|E_2(B_3(r))\right| + \sqrt{15}\left|E_3(B_3(r))\right| + 2\sqrt{6}\left|E_4(B_3(r))\right| + 5\left|E_5(B_3(r))\right| + 2\sqrt{10}\left|E_6(B_3(r))\right| + 8\left|E_7(B_3(r)\right|, \\ \Rightarrow R_{1/2}(B) &= 36(7 + 2\sqrt{6})r^2 + 24(7 + \sqrt{6} + \sqrt{10} + \sqrt{15})r + 6(2\sqrt{10} - 5). \end{aligned} \tag{55}$$

For $\alpha = -1$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$\begin{aligned} R_{-1}(B) &= \sum_{j=1}^{7} \sum_{mn \in E_j(B)} \frac{1}{\delta(m) \cdot \delta(n)}, \\ R_{-1}(B) &= \frac{1}{10}\left|E_1(B_3(r))\right| + \frac{1}{9}\left|E_2(B_3(r))\right| + \frac{1}{15}\left|E_3(B_3(r))\right| + \frac{1}{24}\left|E_4(B_3(r))\right| + \frac{1}{25}\left|E_5(B_3(r))\right| + \frac{1}{40}\left|E_6(B_3(r))\right| + \frac{1}{64}\left|E_7(B_3(r))\right|, \\ \Rightarrow R_{-1}(B) &= \frac{185}{32}r^2 + \frac{175}{25}r + \frac{24}{25}. \end{aligned} \tag{56}$$

For $\alpha = -1/2$

The general Randić index $R_\alpha(B)$ formula from equation (4) is used as follows:

$$\begin{aligned} R_{-1/2}(B) &= \sum_{mn \in E_j(B)} \frac{1}{\sqrt{\delta(m) \cdot \delta(n)}}. \\ R_{-1/2}(B) &= \frac{1}{\sqrt{10}}\left|E_1(B_3(r))\right| + \frac{1}{3}\left|E_2(B_3(r))\right| + \frac{1}{\sqrt{15}}\left|E_3(B_3(r))\right| + \frac{1}{2\sqrt{6}}\left|E_4(B_3(r))\right| + \frac{1}{5}\left|E_5(B_3(r))\right| \\ &\quad + \frac{1}{2\sqrt{10}}\left|E_6(B_3(r))\right| + \frac{1}{8}\left|E_7(B_3(r))\right|, \\ \Rightarrow R_{-1/2}(B) &= \left(\frac{57}{4} + 3\sqrt{6}\right)r^2 + \left(\frac{72}{5} + 3\sqrt{\frac{2}{5}} + 8\sqrt{\frac{3}{5}} + \sqrt{6}\right)r + \frac{6}{5}(-1 + \sqrt{10}). \end{aligned} \tag{57}$$

The first Zagreb index of the benzenoid hex planar octahedron network is computed in the following theorem. □

Theorem 8. *For the benzenoid planar octahedron network $B_3(r)$, the first Zagreb index is equal to the following equation:*

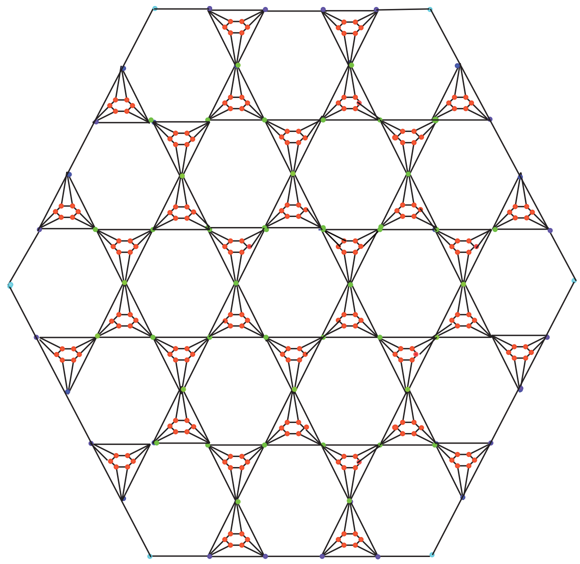

Figure 3: Benzenoid hex planar octahedron network BHPOH(2).

Table 3: Edge division of benzenoid hex planar octahedron network $(B_3(r))$ based on the sum of the degrees of each edge's end vertices.

$(\delta(m), \delta n)$, where $mn \in E(B_3)$	Number of edges	$(\delta(m), \delta(n))$, where $mn \in E(B_3)$	Number of edges
$E_1 = (2,5)$	12	$E_5 = (5,5)$	$12r - 6$
$E_2 = (3,3)$	$36r^2 - 36r$	$E_6 = (5,8)$	$12r$
$E_3 = (3,5)$	$24r$	$E_7 = (8,8)$	$18r^2$
$E_4 = (3,8)$	$36r^2 + 12r$		

$$M_1(B_3(r)) = 900r^2 + 816r + 24. \tag{58}$$

Proof. Let $B_3(r)$ be the bezenoid hex planar octahedron network. The following is the result of using the edge division from Table 3. As a result of equation (5), we have

$$\begin{aligned} M_1(B) &= \sum_{mn\in E(B)} (\delta(m) + \delta(n)) \\ &= \sum_{j=1}^{7} \sum_{mn\in E_j(B)} (\delta(m) + \delta(n)), \end{aligned}$$

$$M_1(B_3(r)) = 7|E_1(B_3(r))| + 6|E_2(B_3(r))| + 8|E_3(B_3(r))| + 11|E_4(B_3(r))| + 10|E_5(B_3(r))| + 13|E_6(B_3(r))| + 16|E_7(B_3(r))|. \tag{59}$$

By doing the calculation, we obtained the following result:

$$\Rightarrow M_1(B_3(r)) = 900r^2 + 816r + 24. \tag{60}$$

□

Theorem 9. *Let $B_3(r)$ be the benzenoid hex planar octahedron network $r \geq 2$; then, we have*

$$\begin{aligned}
H\left(B_3(r)\right) &= \frac{915}{44}r^2 + \frac{17466}{715} + \frac{78}{35},\\
\mathrm{AZI}\left(B_3(r)\right) &= \frac{46302245}{16464}r^2 + \frac{38645819}{23958} + \frac{2697}{32},\\
\mathrm{ABC}\left(B_3(r)\right) &= \left(24 + \frac{9\sqrt{14}}{4} + 9\sqrt{6}\right)r^2 + \frac{3}{5}\left(40 + 8\sqrt{5} + 5\sqrt{6} + 8\sqrt{10} + \sqrt{110}\right)r + \left(6\sqrt{2} - \frac{12}{\sqrt{5}}\right),\\
\mathrm{GA}\left(B_3(r)\right) &= \left(54 + \frac{144\sqrt{6}}{11}\right)r^2 + \left(48 + \frac{48\sqrt{6}}{11} + \frac{48\sqrt{10}}{13} + 6\sqrt{15}\right)r + \left(\frac{24\sqrt{10}}{7} - 6\right).
\end{aligned} \tag{61}$$

Proof. We obtained the required result by finding the edge division in Table 3, and then, applying the definition. It follows from equation (6) that

$$\begin{aligned}
H(B) &= \sum_{mn\in E(B)} \frac{2}{\delta(m)+\delta(n)} = \sum_{j=1}^{7} \sum_{mn\in E(B)} \frac{2}{\delta(m)+\delta(n)},\\
H\left(B_3(r)\right) &= \frac{2}{7}\left|E_1\left(B_3(r)\right)\right| + \frac{1}{3}\left|E_2\left(B_3(r)\right)\right| + \frac{1}{4}\left|E_3\left(B_3(r)\right)\right| + \frac{2}{11}\left|E_4\left(B_3(r)\right)\right| + \frac{1}{5}\left|E_5\left(B_3(r)\right)\right| + \frac{2}{13}\left|E_6\left(B_3(r)\right)\right| + \frac{1}{8}\left|E_7\left(B_3(r)\right)\right|.
\end{aligned} \tag{62}$$

By doing the calculation, we obtained the following result:

$$H\left(B_3(r)\right) = \frac{915}{44}r^2 + \frac{17466}{715} + \frac{78}{35}. \tag{63}$$

Equation (7) can be used to compute the augmented Zagreb index as follows:

$$\begin{aligned}
\mathrm{AZI}\left(B_3(r)\right) &= \sum_{mn\in E(B)} \left(\frac{\delta(m)\delta(n)}{\delta(m)+\delta(n)-2}\right)^3\\
&= \sum_{j=1}^{7} \sum_{mn\in E(B)} \left(\frac{\delta(m)\delta(n)}{\delta(m)+\delta(n)-2}\right)^3.\\
\mathrm{AZI}\left(B_3(r)\right) &= 8\left|E_1\left(B_3(r)\right)\right| + \frac{729}{64}\left|E_2\left(B_3(r)\right)\right| + \frac{125}{8}\left|E_3\left(B_3(r)\right)\right| + \frac{512}{27}\left|E_4\left(B_3(r)\right)\right| + \frac{15625}{512}\left|E_5\left(B_3(r)\right)\right| + \frac{6400}{1331}\left|E_6\left(B_3(r)\right)\right|\\
&\quad + \frac{32768}{343}\left|E_7\left(B_3(r)\right)\right|.
\end{aligned} \tag{64}$$

By doing the calculation, we obtained the following result:

$$\mathrm{AZI} = \frac{46302245}{16464}r^2 + \frac{38645819}{23958}r + \frac{2697}{32}. \tag{65}$$

Table 4: Numerical computation for BPOH(r).

$[r]$	R_1	$R_{1/2}$	R_{-1}	$R_{-1/2}$	M_1	H	AZI	GA	
4	35328	6672.47	95.25	352.119	14016	339.714	12402.7	877.399	1109.05
5	110964	10482.4	147.969	548.141	22020	528.62	29565.1	10482.4	1736.48
6	55860	15149.1	212.25	787.36	31824	759.117	52352.1	15149.1	2503.97
7	81072	20672.4	288.094	10969.78	43428	1031.2	80763.8	20672.4	3411.53

Equation (8) can be used to compute the atom-bond connectivity index as follows:

$$\begin{aligned}\mathrm{ABC}(B) &= \sum_{mn\in E(B)} \sqrt{\frac{\delta(m)+\delta(n)-2}{\delta(m)\cdot\delta(n)}}\\ &= \sum_{j=1}^{7}\sum_{mn\in E_j(B)} \sqrt{\frac{\delta(m)+\delta(n)-2}{\delta(m)\cdot\delta(n)}},\\ \mathrm{ABC}(B_3(r)) &= \frac{\sqrt{2}}{2}\left|E_1(B_3(r))\right| + \frac{2}{3}\left|E_2(B_3(r))\right| + \frac{\sqrt{10}}{5}\left|E_3(B_3(r))\right| + \frac{\sqrt{6}}{4}\left|E_4(B_3(r))\right| + \frac{2\sqrt{2}}{5}\left|E_5(B_3(r))\right|\\ &\quad + \frac{\sqrt{110}}{20}\left|E_6(B_3(r))\right| + \frac{\sqrt{14}}{8}\left|E_7(B_3(r))\right|.\end{aligned} \tag{66}$$

By doing the calculation, we obtained the following result:

$$\Rightarrow \mathrm{ABC}(B_3(r)) = \left(24 + \frac{9\sqrt{14}}{4} + 9\sqrt{6}\right)r^2 + \frac{3}{5}\left(40 + 8\sqrt{5} + 5\sqrt{6} + 8\sqrt{10} + \sqrt{110}\right)r + \left(6\sqrt{2} - \frac{12}{\sqrt{5}}\right). \tag{67}$$

Equation (9) can be used to compute the geometric-arithmetic index as follows:

$$\mathrm{GA}(B) = \sum_{mn\in E(B)} \frac{2\sqrt{\delta(m)\delta(n)}}{(\delta(m)+\delta(n))} = \sum_{j=1}^{7}\sum_{mn\in E_j(B)} \frac{2\sqrt{\delta(m)\delta(n)}}{(\delta(m)+\delta(n))}. \tag{68}$$

By doing the calculation, we obtained the following result:

$$\begin{aligned}\mathrm{GA}(B_3(r)) &= \frac{2\sqrt{10}}{5}\left|E_1(B_3(r))\right| + \left|E_2(B_3(r))\right| + \frac{\sqrt{2}}{2}\left|E_3(B_3(r))\right| + \frac{2}{\sqrt{11}}\left|E_4(B_3(r))\right| + \frac{\sqrt{10}}{5}\left|E_5(B_3(r))\right|\\ &\quad + \frac{2}{\sqrt{13}}\left|E_6(B_3(r))\right| + \frac{1}{2}\left|E_7(B_3(r))\right|\\ \Rightarrow \mathrm{GA}(B_3(r)) &= \left(54 + \frac{144\sqrt{6}}{11}\right)r^2 + \left(48 + \frac{48\sqrt{6}}{11} + \frac{48\sqrt{10}}{13} + 6\sqrt{15}\right)r + \left(\frac{24\sqrt{10}}{7} - 6\right).\end{aligned} \tag{69}$$

Table 5: Numerical computation for BDPOH (r).

$[r]$	R_1	$R_{1/2}$	R_{-1}	$R_{-1/2}$	M_1	H	AZI	ABC	GA
4	12884	15532.1	218.719	810595	32628	781.659	98352.3	2025.63	1633.58
5	137988	25327.4	358.844	1332.23	54036	1284.24	164219	3335.75	2678.18
6	207132	38087.6	533.656	1983.46	80844	1911.6	246959	4972.66	3980.99
7	290316	53481.0	743.156	2764.27	113052	2663.73	346573	6936.36	5542

Table 6: Numerical computation BHPOH (r).

$[r]$	R_1	$R_{1/2}$	R_{-1}	$R_{-1/2}$	M_1	H	AZI	ABC	GA
4	44418	844.3	120.98	447.945	176888	432.668	51533.9	1128.76	1756.31
5	67230	12695.2	179.891	667.275	26604	644.2	78457.9	1682.49	2624.51
6	94722	17802.8	250.365	929.801	37320	897.433	111007	2345.15	3664.84
7	126894	23767.2	332.401	1235.53	49836	1192.2	149180	3116.74	4877.3

To compare topological indices numerically for BPOH, BDPOH, and BHPOH, we calculated all of the indices for different values of r. Tables 4–6 clearly show that when the value of r increases, all indices increase in ascending order. □

4. Conclusion

In this paper, we computed the required results of Randić, Zagreb, Harmonic, augmented Zagreb, atom-bond connectivity, and geometric-arithmetic indices for BPOH, BDPOH, and BHPOH. We also discovered all of the networks, numerical computations. These key insights lay the groundwork for understanding the underlying topologies of the following networks, which are useful from a variety of chemical and pharmaceutical perspectives. In the future, we want to create some networks and then analyse their topological indices to learn more about their underlying topologies.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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