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Computing Degree Based Topological Properties of Third Type of Hex-Derived Networks

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Abstract: In chemical graph theory, a topological index is a numerical representation of a chemical network, while a topological descriptor correlates certain physicochemical characteristics of underlying chemical compounds besides its chemical representation. The graph plays a vital role in modeling and designing any chemical network. Simonraj et al. derived a new type of graphs, which is named a third type of hex-derived networks. In our work, we discuss the third type of hex-derived networks $HDN3(r)$, $THDN3(r)$, $RHDN3(r)$, $CHDN3(r)$, and compute exact results for topological indices which are based on degrees of end vertices.

Keywords: general randić index; Harmonic index; augmented Zagreb index; atom–bond connectivity (ABC) index; geometric–arithmetic (GA) index; third type of hex-derived networks; $HDN3(r)$; $THDN3(r)$; $RHDN3(r)$; $CHDN3(r)$

1. Introduction and Preliminary Results

Graph theory has provided chemists with a variety of useful tools, such as topological indices. Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. *Cheminformatics* is new subject which is a combination of chemistry, mathematics, and information science. It studies quantitative structure–activity (QSAR) and structure–property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds. Biological indicators such as the Randić Index, Zagreb Index, Wiener Index, and Balaban index are used to predict and study the physical and chemical properties of chemical structures. The topological index is a numeric quantity associated with chemical constitutions purporting the correlation of chemical structures with many physicochemical properties, chemical reactivity or biological activity. Topological indices are made on the grounds of the transformation of a chemical network into a number that characterizes the topology of the chemical network. Some of the major types of topological indices of graphs are distance-based topological indices, degree-based topological indices, and counting-related topological indices.

Recently, many researchers have found topological indices vital for the study of structural properties of molecular graph or network or chemical tree. An acyclic connected graph is called a tree graph. The degree 3 or greater of every vertex of a tree is called the branching point of the tree. A chemical tree is a connected acyclic graph having maximum degree 4. The first and second Zagreb index of star-like trees and sun-like graphs and also caterpillar trees containing the hydrocarbons, especially ethane, propane, and butane, was studied and computed in Reference [1]. Imran et al. [2] also computed the topological indices of fractal and cayley tree type dendrimers.

For any graph, $G = (V, E)$ where V is be the vertex set and E to be the edge set of G. The degree $\kappa(x)$ of vertex x is the amount of edges of G episode with x. A graph can be spoken by a polynomial, a numerical esteem or by network shape.

In the present paper, we consider the topological indices of hex-derived networks which are derived from a hexagonal graph that include molecular graphs of unbranched benzenoid hydrocarbons [3]. Graphs of hexagonal systems consist of mutually fused hexagons. Since this class of chemical compounds is attracting the great attention of theoretical chemists, the theory of the topological index of the respective molecular graphs have been intensively developed in the last 4 decades. Benzenoid hydrocarbons are important raw materials of the chemical industry (used, for instance, for the production of dyes and plastics) but are also dangerous pollutants [3–5]. A hexagonal mesh was derived by Chen et al. [6]. A set of triangles made a *hexagonal mesh*, as shown in Figure 1. No hexagonal mesh with dimension 1 exists. A composition of six triangles made a 2-dimensional hexagonal mesh $HX(2)$ (see Figure 1 (1)). By adding a new layer of triangles around the boundary of $HX(2)$, we have a 3-dimensional hexagonal mesh $HX(3)$ (see Figure 1 (2)). Similarly, we formed $HX(n)$ by adding n layers around the boundary of each proceeding hexagonal mesh.

Drawing algorithm of $HDN3$ networks

Step-1: First, we draw a hexagonal network of dimension r.
Step-2: Replace all K_3 subgraphs into a planar octahedron POH once. The resulting graph is called an $HDN3$ (see Figure 2) network.
Step-3: From the $HDN3$ network, we can easily form $THDN3$ (see Figure 3), $RHDN3$ (see Figure 4), and $CHDN3$ (see Figure 5).

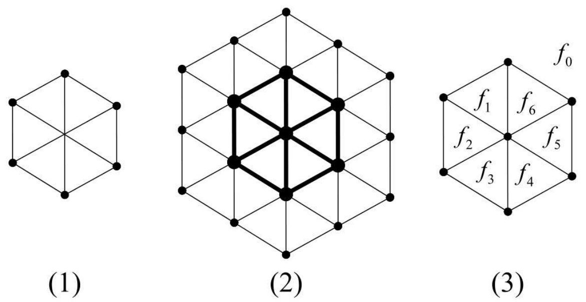

Figure 1. Hexagonal meshes: (1) HX(2) , (2) HX(3), and (3), all facing HX(2).

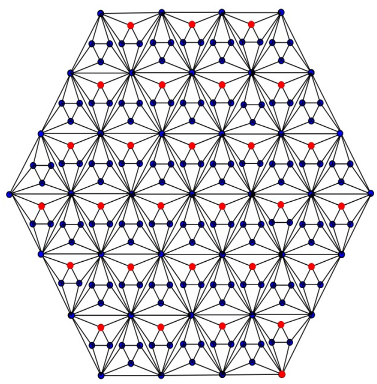

Figure 2. Hex-derived network of type 3 ($HDN3(4)$).

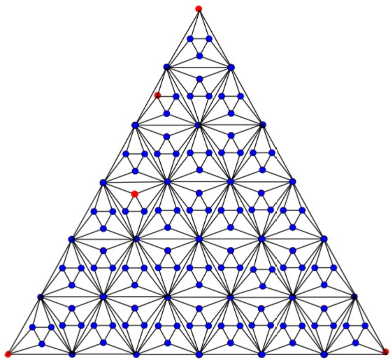

Figure 3. Triangular hex-derived network of type 3 ($THDN3(7)$).

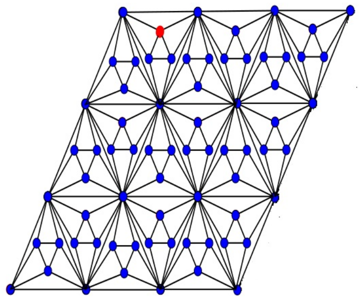

Figure 4. Rectangular hex-derived network of type 3 ($RHDN3(4,4)$).

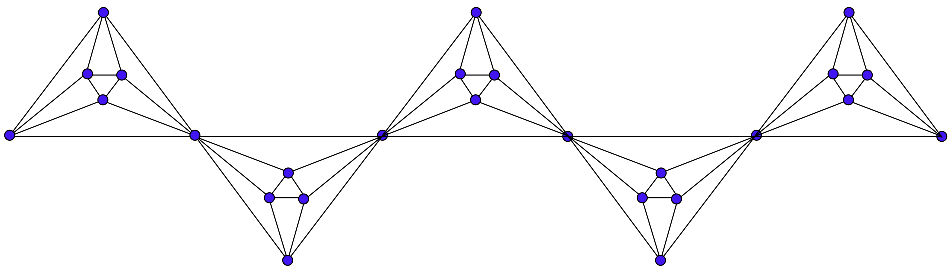

Figure 5. Chain hex-derived network of type 3 ($CHDN3(5)$).

In this article, we consider G as a network, with $V(\mathrm{G})$ as the set of vertices and edge set $E(\mathrm{G})$; the degree of any vertex $\acute{p} \in V(\mathrm{G})$ is denoted by $\kappa(\acute{p})$.

The Estrada index is a graph–spectrum-based topological index, which is defined as [7]:

$$EE(\mathrm{G}) = \sum_{i=1}^{n} e^{\lambda_i}. \tag{1}$$

In full analogy with the Estrada index, Fath-Tabar et al. [8] proposed the Laplacian Estrada index, which is defined as:

$$LEE(\mathrm{G}) = \sum_{i=1}^{n} e^{\mu_i}. \tag{2}$$

The *Randić* index [9] was denoted by $R_{-\frac{1}{2}}(\mathrm{G})$ and acquainted by Milan Randić and written as:

$$R_{-\frac{1}{2}}(\mathrm{G}) = \sum_{\acute{p}\acute{q} \in \mathrm{E}(\mathrm{G})} \frac{1}{\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}. \tag{3}$$

The general Randić index $R_\alpha(\mathrm{G})$ is the sum of $(\kappa(\acute{p})\kappa(\acute{q}))^\alpha$ over all edges $e = \acute{p}\acute{q} \in \mathrm{E}(\mathrm{G})$, defined as:

$$R_{\alpha}(G) = \sum_{\acute{p}\acute{q} \in E(G)} (\kappa(\acute{p})\kappa(\acute{q}))^{\alpha} \;\; \text{for} \;\; \alpha = 1, \frac{1}{2}, -1, -\frac{1}{2}. \tag{4}$$

Gutman and Trinajstić were acquainted with a substantial topological index, which is the *Zagreb* index denoted by $M_1(G)$ and formalised as:

$$M_1(G) = \sum_{\acute{p}\acute{q} \in E(G)} (\kappa(\acute{p}) + \kappa(\acute{q})). \tag{5}$$

The augmented Zagreb index was presented by Furtula et al. [10], and it is defined as:

$$AZI(G) = \sum_{\acute{p}\acute{q} \in E(G)} \left(\frac{\kappa(\acute{p})\kappa(\acute{q})}{\kappa(\acute{p}) + \kappa(\acute{q}) - 2} \right)^3. \tag{6}$$

The harmonic index was presented by Zhong [11], and it is defined as:

$$H(G) = \sum_{\acute{p}\acute{q} \in E(G)} \left(\frac{2}{\kappa(\acute{p}) + \kappa(\acute{q})} \right) \tag{7}$$

The *Atom-bond connectivity* (ABC) index is one of the famous degree-based topological indices denoted by Estrada et al. in Reference [12] and formalised as:

$$ABC(G) = \sum_{\acute{p}\acute{q} \in E(G)} \sqrt{\frac{\kappa(\acute{p}) + \kappa(\acute{q}) - 2}{\kappa(\acute{p})\kappa(\acute{q})}}. \tag{8}$$

The *Geometric-arithmetic* (GA) index is another famous connectivity topological descriptor, which was introduced by Vukičević et al. in Reference [13] and written as:

$$GA(G) = \sum_{\acute{p}\acute{q} \in E(G)} \frac{2\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}{(\kappa(\acute{p}) + \kappa(\acute{q}))}. \tag{9}$$

By taking $\alpha = 1$, the general Randić index is the second Zagreb index for any graph G.

2. Main Results for Third Type of Hex-Derived Networks

Simonraj et al. [14] derived a new third type of hex-derived networks and found the metric dimension of $HDN3$ and $PHDN3$. In this work, we discuss the newly derived third type of hex-derived networks and compute the exact results for degree-based topological indices. At present, there is an extensive research activity on these topological indices and their variants, see [15–26]. For basic definitions and notations, see [27–31].

2.1. Results for Third Type of Hex-Derived Network $HDN3(r)$

In this section, we discuss the newly derived third type of hex-derived network and compute the exact results for Randić, Zagreb, Harmonic, augmented Zagreb, atom–bond connectivity and geometric–arithmetic indices for the very first time.

Theorem 1. *Consider the hex-derived network of type 3 $HDN3(n)$, the general Randić index is equal to:*

$$R_\alpha(HDN3(n)) = \begin{cases} 12(777 + r(-1237 + 483r)), & \alpha = 1; \\ 6(72 + 84\sqrt{2} - 24\sqrt{5} + 8\sqrt{7} - 24\sqrt{10} & \\ +3\sqrt{14} + 2\sqrt{70} + r(-113 - 108\sqrt{2} & \\ +12\sqrt{5}(1+\sqrt{2}) + (39 + 36\sqrt{2})r)), & \alpha = \frac{1}{2}; \\ \frac{(50921+7r(-15256+8925r))}{37800}, & \alpha = -1; \\ \frac{131}{30} + 6\sqrt{\frac{2}{35}} + \sqrt{\frac{2}{7}} - 18\sqrt{\frac{2}{5}} + 7\sqrt{2} - \frac{4}{\sqrt{5}} + \frac{12}{\sqrt{7}} & \\ +(\frac{-307}{30} + 9\sqrt{\frac{2}{5}} - 9\sqrt{2} + \frac{2}{\sqrt{5}})r + (5 + 3\sqrt{2})r^2, & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let G_1 be the hex-derived network of type 3, $HDN3(r)$ shown in Figure 2, where $r \geq 4$. The hex-derived network G_1 has $21r^2 - 39r + 19$ vertices, and the edge set of G_1 is divided into nine partitions based on the degree of end vertices. The first edge partition $E_1(G_1)$ contains $18r^2 - 36r + 18$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 4$. The second edge partition $E_2(G_1)$ contains 24 edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 4$ and $\kappa(\acute{q}) = 7$. The third edge partition $E_3(G_1)$ contains $36r - 72$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 4$ and $\kappa(\acute{q}) = 10$. The fourth edge partition $E_4(G_1)$ contains $36r^2 - 108r + 84$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 4$ and $\kappa(\acute{q}) = 18$. The fifth edge partition $E_5(G_1)$ contains 12 edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 7$ and $\kappa(\acute{q}) = 10$. The sixth edge partition $E_6(G_1)$ contains 6 edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 7$ and $\kappa(\acute{q}) = 18$. The seventh edge partition $E_7(G_1)$ contains $6r - 18$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 10$, the eighth edge partition $E_8(G_1)$ contains $12r - 24$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 10$ and $\kappa(\acute{q}) = 18$, and the ninth edge partition $E_9(G_1)$ contains $9r^2 - 33r + 30$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 18$. Table 1 shows such an edge partition of G_1. Thus, from Equation (3), it follows that:

Table 1. Edge partition of hex-derived network of type 3 $HDN3(r)$ based on degrees of end vertices of each edge.

(κ_x, κ_y) where $\acute{p}\acute{q} \in E(G_1)$	Number of Edges	(κ_u, κ_v) where $\acute{p}\acute{q} \in E(G_1)$	Number of Edges
$(4,4)$	$18r^2 - 36r + 18$	$(7,18)$	6
$(4,7)$	24	$(10,10)$	$6r - 18$
$(4,10)$	$36r - 72$	$(10,18)$	$12r - 24$
$(4,18)$	$36r^2 - 108r + 84$	$(18,18)$	$9r^2 - 33r + 30$
$(7,10)$	12		

$$R_\alpha(G_1) = \sum_{\acute{p}\acute{q} \in E(G_1)} (\kappa(\acute{p})\kappa(\acute{q}))^\alpha.$$

For $\alpha = 1$
The general Randić index $R_\alpha(G_1)$ can be computed as follows:

$$R_1(G_1) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(G_1)} (\kappa(\acute{p}) \cdot \kappa(\acute{q})).$$

Using the edge partition given in Table 1, we get:

$$\begin{aligned} R_1(G_1) \quad = \quad & 16|E_1(G_1)| + 28|E_2(G_1)| + 40|E_3(G_1)| + 72|E_4(G_1)| + 70|E_5(G_1)| + 126|E_6(G_1)| + \\ & 100|E_7(G_1)| + 180|E_8(G_1)| + 324|E_9(G_1)| \end{aligned}$$

$$\Longrightarrow R_1(G_1) = 12(777 + r(-1237 + 483r)).$$

For $\alpha = \frac{1}{2}$
We apply the formula of $R_\alpha(G_1)$:

$$R_{\frac{1}{2}}(G_1) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(G_1)} \sqrt{\kappa(\acute{p}) \cdot \kappa(\acute{q})}.$$

Using the edge partition given in Table 1, we get:

$$\begin{aligned} R_{\frac{1}{2}}(G_1) &= 4|E_1(G_1)| + 2\sqrt{7}|E_2(G_1)| + 2\sqrt{10}|E_3(G_1)| + 6\sqrt{2}|E_4(G_1)| + \sqrt{70}|E_5(G_1)| + \\ &\quad 2\sqrt{14}|E_6(G_1)| + 10|E_7(G_1)| + 6\sqrt{5}|E_8(G_1)| + 18|E_9(G_1)| \end{aligned}$$

$$\begin{aligned} \Longrightarrow R_{\frac{1}{2}}(G_1) &= 6(72 + 84\sqrt{2} - 24\sqrt{5} + 8\sqrt{7} - 24\sqrt{10} + 3\sqrt{14} + 2\sqrt{70} + \\ &\quad r(-113 - 108\sqrt{2} + 12\sqrt{5}(1 + \sqrt{2}) + (39 + 36\sqrt{2})r)). \end{aligned}$$

For $\alpha = -1$

We apply the formula of $R_\alpha(G_1)$:

$$R_{-1}(G_1) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(G_1)} \frac{1}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}$$

$$\begin{aligned} R_{-1}(G_1) &= \frac{1}{16}|E_1(G_1)| + \frac{1}{28}|E_2(G_1)| + \frac{1}{40}|E_3(G_1)| + \frac{1}{72}|E_4(G_1)| + \frac{1}{70}|E_5(G_1)| + \\ &\quad \frac{1}{126}|E_6(G_1)| + \frac{1}{100}|E_7(G_1)| + \frac{1}{180}|E_8(G_1)| + \frac{1}{324}|E_9(G_1)| \end{aligned}$$

$$\Longrightarrow R_{-1}(G_1) = \frac{(50921 + 7r(-15256 + 8925r))}{37800}.$$

For $\alpha = -\frac{1}{2}$

We apply the formula of $R_\alpha(G_1)$:

$$R_{-\frac{1}{2}}(G_1) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(G_1)} \frac{1}{\sqrt{\kappa(\acute{p}) \cdot \kappa(\acute{q})}}$$

$$\begin{aligned} R_{-\frac{1}{2}}(G_1) &= \frac{1}{\sqrt{4}}|E_1(G_1)| + \frac{1}{2\sqrt{7}}|E_2(G_1)| + \frac{1}{2\sqrt{10}}|E_3(G_1)| + \frac{1}{6\sqrt{2}}|E_4(G_1)| + \frac{1}{\sqrt{70}}|E_5(G_1)| + \\ &\quad \frac{1}{3\sqrt{14}}|E_6(G_1)| + \frac{1}{10}|E_7(G_1)| + \frac{1}{6\sqrt{5}}|E_8(G_1)| + \frac{1}{18}|E_9(G_1)| \end{aligned}$$

$$\begin{aligned} \Longrightarrow R_{-\frac{1}{2}}(G_1) &= \frac{131}{30} + 6\sqrt{\frac{2}{35}} + \sqrt{\frac{2}{7}} - 18\sqrt{\frac{2}{5}} + 7\sqrt{2} - \frac{4}{\sqrt{5}} + \frac{12}{\sqrt{7}} + (\frac{-307}{30} + 9\sqrt{\frac{2}{5}} - \\ &\quad 9\sqrt{2} + \frac{2}{\sqrt{5}})r + (5 + 3\sqrt{2})r^2. \end{aligned}$$

□

In the following theorem, we compute the first Zagreb index of hex-derived network G_1.

Theorem 2. *For hex-derived network* G_1*, the first Zagreb index is equal to:*

$$M_1(G_1) = 6(275 - 482r + 210r^2).$$

Proof. Let G_1 be the hex-derived network $HDN3(r)$. Using the edge partition from Table 1, the result follows. The Zagreb index can be calculated using Equation (5) as follows:

$$M_1(G_1) = \sum_{\acute{p}\acute{q}\in E(G_1)} (\kappa(\acute{p}) + \kappa(\acute{q})) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q}\in E_j(G_1)} (\kappa(\acute{p}) + \kappa(\acute{q}))$$

$$\begin{aligned} M_1(G_1) &= 8|E_1(G_1)| + 11|E_2(G_1)| + 14|E_3(G_1)| + 22|E_4(G_1)| + 17|E_5(G_1)| + 25|E_6(G_1)| + \\ &\quad 20|E_7(G_1)| + 28|E_8(G_1)| + 36|E_9(G_1)|. \end{aligned}$$

By doing some calculations, we get:

$$\Longrightarrow M_1(G_1) = 6(275 - 482r + 210r^2).$$

□

Now, we compute H, AZI, ABC, and GA indices of the third type of hex-derived network G_1.

Theorem 3. *Let G_1 be the third type of hex-derived network, then:*

- $H(G_1) = \frac{15959}{2550} + \frac{1}{330}r(-4637 + 2730r)$;
- $AZI(G_1) = \frac{8(9690243075343773626+85169r(-163548617818123+57430071805041r))}{3989115543655125}$;
- $ABC(G_1) = 6\sqrt{\frac{6}{7}} + \sqrt{\frac{46}{7}} + \frac{36}{\sqrt{7}} + \frac{9}{5}\sqrt{2}(-3 + r) + 18\sqrt{\frac{6}{5}}(-2 + r) + 2\sqrt{\frac{26}{5}}(-2 + r) + 9\sqrt{\frac{3}{2}}(-1 + r)^2 + \frac{1}{3}\sqrt{\frac{17}{2}}(-2 + r)(-5 + 3r) + 2\sqrt{10}(7 + 3(-3 + r)r)$;
- $GA(G_1) = 30 + 96\frac{\sqrt{7}}{11} + 36\frac{\sqrt{14}}{25} + 24\frac{\sqrt{70}}{11} + \frac{36}{7}\sqrt{5}(-2 + r) + \frac{72}{7}\sqrt{10}(-2 + r) + 2\sqrt{\frac{26}{5}}(-2 + r) + 9\sqrt{\frac{3}{2}}(-1 + r)^2 + \frac{1}{3}\sqrt{\frac{17}{2}}(-2 + r)(-5 + 3r) + 2\sqrt{10}(7 + 3(-3 + r)r)$.

Proof. Using the edge partition given in Table 1, The Harmonic index can be calculated using Equation (7) as follows:

$$H(G_1) = \sum_{\acute{p}\acute{q}\in E(G_1)} \left(\frac{2}{\kappa(\acute{p}) + \kappa(\acute{q})}\right) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q}\in E_j(G_1)} \left(\frac{2}{\kappa(\acute{p}) + \kappa(\acute{q})}\right)$$

$$\begin{aligned} H(G_1) &= \frac{1}{4}|E_1(G_1)| + \frac{2}{11}|E_2(G_1)| + \frac{1}{7}|E_3(G_1)| + \frac{1}{11}|E_4(G_1)| + \frac{2}{17}|E_5(G_1)| + \frac{2}{25}|E_6(G_1)| + \\ &\quad \frac{1}{10}|E_7(G_1)| + \frac{1}{14}|E_8(G_1)| + \frac{1}{18}|E_9(G_1)|. \end{aligned}$$

By doing some calculations, we get:

$$\Longrightarrow H(G_1) = \frac{15959}{2550} + \frac{1}{330}r(-4637 + 2730r).$$

The augmented Zagreb index can be calculated from Equation (6) as follows:

$$AZI(G_1) = \sum_{\acute{p}\acute{q}\in E(G_1)} \left(\frac{\kappa(\acute{p}) \cdot \kappa(\acute{q})}{\kappa(\acute{p}) + \kappa(\acute{q}) - 2}\right)^3 = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q}\in E_j(G_1)} \left(\frac{\kappa(\acute{p}) \cdot \kappa(\acute{q})}{\kappa(\acute{p}) + \kappa(\acute{q}) - 2}\right)^3$$

$$
\begin{aligned}
AZI(\mathrm{G}_1) \quad = \quad & \frac{512}{27}|E_1(\mathrm{G}_1)| + \frac{21952}{729}|E_2(\mathrm{G}_1)| + \frac{1000}{27}|E_3(\mathrm{G}_1)| + \frac{5832}{125}|E_4(\mathrm{G}_1)| + \frac{2744}{27}|E_5(\mathrm{G}_1)| + \\
& \frac{2000376}{12167}|E_6(\mathrm{G}_1)| + \frac{125000}{729}|E_7(\mathrm{G}_1)| + \frac{729000}{2197}|E_8(\mathrm{G}_1)| + \frac{4251528}{4913}|E_9(\mathrm{G}_1)|.
\end{aligned}
$$

By doing some calculations, we get:

$$
\Longrightarrow AZI(\mathrm{G}_1) = \frac{8(9690243075343773626 + 85169r(-163548617818123 + 57430071805041r))}{3989115543655125}.
$$

The atom–bond conectivity index can be calculated from Equation (8) as follows:

$$
ABC(\mathrm{G}_1) = \sum_{\acute{p}\acute{q}\in E(\mathrm{G}_1)} \sqrt{\frac{\kappa(\acute{p}) + \kappa(\acute{q}) - 2}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}} = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q}\in E_j(\mathrm{G}_1)} \sqrt{\frac{\kappa(\acute{p}) + \kappa(\acute{q}) - 2}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}}
$$

$$
\begin{aligned}
ABC(\mathrm{G}_1) \quad = \quad & \frac{1}{2}\sqrt{\frac{3}{2}}|E_1(\mathrm{G}_1)| + \frac{3}{2\sqrt{7}}|E_2(\mathrm{G}_1)| + \sqrt{\frac{3}{10}}|E_3(\mathrm{G}_1)| + \frac{1}{3}\sqrt{\frac{5}{2}}|E_4(\mathrm{G}_1)| + \sqrt{\frac{3}{14}}|E_5(\mathrm{G}_1)| + \\
& \frac{1}{3}\sqrt{\frac{23}{14}}|E_6(\mathrm{G}_1)| + \frac{3}{5\sqrt{2}}|E_7(\mathrm{G}_1)| + \frac{1}{3}\sqrt{\frac{13}{10}}|E_8(\mathrm{G}_1)| + \frac{1}{9}\sqrt{\frac{17}{2}}|E_9(\mathrm{G}_1)|.
\end{aligned}
$$

By doing some calculations, we get:

$$
\begin{aligned}
\Longrightarrow ABC(\mathrm{G}_1) \quad = \quad & 6\sqrt{\frac{6}{7}} + \sqrt{\frac{46}{7}} + \frac{36}{\sqrt{7}} + \frac{9}{5}\sqrt{2}(-3+r) + 18\sqrt{\frac{6}{5}}(-2+r) + 2\sqrt{\frac{26}{5}} \\
& (-2+r) + 9\sqrt{\frac{3}{2}}(-1+r)^2 + \frac{1}{3}\sqrt{\frac{17}{2}}(-2+r)(-5+3r) + 2\sqrt{10} \\
& (7+3(-3+r)r).
\end{aligned}
$$

The geometric–arithmetic index can be calculated from Equation (9) as follows:

$$
GA(\mathrm{G}_1) = \sum_{\acute{p}\acute{q}\in E(\mathrm{G}_1)} \frac{2\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}{(\kappa(\acute{p}) + \kappa(\acute{q}))} = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q}\in E_j(\mathrm{G}_1)} \frac{2\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}{(\kappa(\acute{p}) + \kappa(\acute{q}))}.
$$

By doing some calculations, we get:

$$
\begin{aligned}
GA(\mathrm{G}_1) \quad = \quad & |E_1(\mathrm{G}_1)| + \frac{4\sqrt{7}}{11}|E_2(\mathrm{G}_1)| + \frac{2\sqrt{10}}{7}|E_3(\mathrm{G}_1)| + \frac{6\sqrt{2}}{11}|E_4(\mathrm{G}_1)| + \frac{2\sqrt{70}}{17}|E_5(\mathrm{G}_1)| + \\
& \frac{6\sqrt{14}}{25}|E_6(\mathrm{G}_1)| + |E_7(\mathrm{G}_1)| + \frac{3\sqrt{5}}{7}|E_8(\mathrm{G}_1)| + |E_9(\mathrm{G}_1)|
\end{aligned}
$$

$$
\begin{aligned}
\Longrightarrow GA(\mathrm{G}_1) \quad = \quad & 30 + 96\frac{\sqrt{7}}{11} + 36\frac{\sqrt{14}}{25} + 24\frac{\sqrt{70}}{11} + \frac{36}{7}\sqrt{5}(-2+r) + \frac{72}{7}\sqrt{10}(-2+r) + \\
& 2\sqrt{\frac{26}{5}}(-2+r) + 9\sqrt{\frac{3}{2}}(-1+r)^2 + \frac{1}{3}\sqrt{\frac{17}{2}}(-2+r)(-5+3r) + \\
& 2\sqrt{10}(7+3(-3+r)r).
\end{aligned}
$$

□

2.2. Results for Third Type of Triangular Hex-Derived Network $THDN3(r)$

In this section, we calculate certain degree-based topological indices of a triangular hex-derived network of type 3, $THDN3(r)$ of dimension r. We compute general Randić index $R_\alpha(THDN3(r))$ with $\alpha = \{1, -1, \frac{1}{2}, -\frac{1}{2}\}$, M_1, H, AZI ABC, and GA indices in the coming theorems of $THDN3(r)$.

Theorem 4. *Consider the triangular hex-derived network of type 3, $THDN3(r)$, the general Randić index is equal to:*

$$R_\alpha(THDN3(r)) = \begin{cases} 6(588 + r(-593 + 161r)), & \alpha = 1; \\ 3(4(25 + 18\sqrt{2} - 9\sqrt{5} - 5\sqrt{10}) + \\ r(-61 - 60\sqrt{2} + 12\sqrt{5}(1 + \sqrt{2}) + (13 + 12\sqrt{2})r)), & \alpha = \frac{1}{2}; \\ \frac{(2247 + r(-3356 + 2975r))}{10800}, & \alpha = -1; \\ \frac{53}{20} + 3\sqrt{2} - 3\sqrt{\frac{5}{2}} - \frac{3}{\sqrt{5}} + (-\frac{107}{60} - \frac{5}{\sqrt{2}} + \frac{1}{\sqrt{5}} + \frac{9}{\sqrt{10}})r + \\ (\frac{5}{6} + \frac{1}{\sqrt{2}})r^2, & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let G_2 be the third type of a triangular hex-derived network of type 3, $THDN3(r)$ shown in Figure 3, where $r \geq 4$. The triangular hex-derived network G_2 has $\frac{(7r^2-11r+6)}{2}$ vertices and the edge set of G_2 is divided into six partitions based on the degree of end vertices. The first edge partition $E_1(G_2)$ contains $3r^2 - 6r + 9$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 4$. The second edge partition $E_2(G_2)$ contains $18r - 30$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 4$ and $\kappa(\acute{q}) = 10$. The third edge partition $E_3(G_2)$ contains $6r^2 - 30r + 36$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 4$ and $\kappa(\acute{q}) = 18$. The fourth edge partition $E_4(G_2)$ contains $3r - 6$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 10$. The fifth edge partition $E_5(G_2)$ contains $6r - 18$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 10$ and $\kappa(\acute{q}) = 18$, and the sixth edge partition $E_6(G_2)$ contains $\frac{3r^2-21r+36}{2}$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 18$. Table 2 shows such an edge partition of G_2. Thus, from Equation (3), it follows that:

Table 2. Edge partition of a hex-derived network of type 3 $HDN3(r)$ based on degrees of end vertices of each edge.

(κ_x, κ_y) where $\acute{p}\acute{q} \in E(G_1)$	Number of Edges	(κ_u, κ_v) where $\acute{p}\acute{q} \in E(G_1)$	Number of Edges
$(4,4)$	$3r^2 - 6r + 9$	$(10,10)$	$3r - 6$
$(4,10)$	$18r - 30$	$(10,18)$	$6r - 18$
$(4,18)$	$6r^2 - 30r + 36$	$(18,18)$	$\frac{3r^2-21r+36}{2}$

$$R_\alpha(G_2) = \sum_{\acute{p}\acute{q} \in E(G_2)} (\kappa(\acute{p})\kappa(\acute{q}))^\alpha.$$

For $\alpha = 1$
The general Randić index $R_\alpha(G_2)$ can be computed as follows:

$$R_1(G_1) = \sum_{j=1}^{6} \sum_{\acute{p}\acute{q} \in E_j(G_2)} (\kappa(\acute{p}) \cdot \kappa(\acute{q})).$$

Using the edge partition given in Table 2, we get:

$$\begin{aligned} R_1(G_2) &= 16|E_1(G_2)| + 40|E_2(G_2)| + 72|E_3(G_2)| + 100|E_4(G_2)| + 180|E_5(G_2)| + \\ & \quad 324|E_6(G_2)| \end{aligned}$$

$$\Longrightarrow R_1(G_2) = 6(588 + r(-593 + 161r)).$$

For $\alpha = \frac{1}{2}$

We apply the formula of $R_\alpha(G_2)$:

$$R_{\frac{1}{2}}(G_2) = \sum_{j=1}^{6} \sum_{\acute{p}\acute{q} \in E_j(G_2)} \sqrt{\kappa(\acute{p}) \cdot \kappa(\acute{q})}.$$

Using the edge partition given in Table 2, we get:

$$\begin{aligned} R_{\frac{1}{2}}(G_2) &= 4|E_1(G_2)| + 2\sqrt{10}|E_2(G_2)| + 6\sqrt{2}|E_3(G_2)| + 10|E_4(G_2)| + 6\sqrt{5}|E_5(G_2)| + \\ &\quad 18|E_6(G_2)| \end{aligned}$$

$$\begin{aligned} \Longrightarrow R_{\frac{1}{2}}(G_2) &= 3(4(25 + 18\sqrt{2} - 9\sqrt{5} - 5\sqrt{10}) + r(-61 - 60\sqrt{2} + 12\sqrt{5}(1 + \sqrt{2}) + \\ &\quad (13 + 12\sqrt{2})r)). \end{aligned}$$

For $\alpha = -1$

We apply the formula of $R_\alpha(G_2)$:

$$R_{-1}(G_2) = \sum_{j=1}^{6} \sum_{\acute{p}\acute{q} \in E_j(G_2)} \frac{1}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}$$

$$\begin{aligned} R_{-1}(G_2) &= \frac{1}{16}|E_1(G_2)| + \frac{1}{40}|E_2(G_2)| + \frac{1}{72}|E_3(G_2)| + \frac{1}{100}|E_4(G_2)| + \\ &\quad \frac{1}{180}|E_5(G_2)| + \frac{1}{324}|E_6(G_2)| \end{aligned}$$

$$\Longrightarrow R_{-1}(G_2) = \frac{(2247 + r(-3356 + 2975r))}{10800}.$$

For $\alpha = -\frac{1}{2}$

We apply the formula of $R_\alpha(G_2)$:

$$R_{-\frac{1}{2}}(G_2) = \sum_{j=1}^{6} \sum_{\acute{p}\acute{q} \in E_j(G_2)} \frac{1}{\sqrt{\kappa(\acute{p}) \cdot \kappa(\acute{q})}}$$

$$\begin{aligned} R_{-\frac{1}{2}}(G_2) &= \frac{1}{\sqrt{4}}|E_1(G_2)| + \frac{1}{2\sqrt{10}}|E_2(G_2)| + \frac{1}{6\sqrt{2}}|E_3(G_2)| + \frac{1}{10}|E_4(G_2)| + \\ &\quad \frac{1}{6\sqrt{5}}|E_5(G_2)| + \frac{1}{18}|E_6(G_2)| \end{aligned}$$

$$\begin{aligned} \Longrightarrow R_{-\frac{1}{2}}(G_2) &= \frac{53}{20} + 3\sqrt{2} - 3\sqrt{\frac{5}{2}} - \frac{3}{\sqrt{5}} + (-\frac{107}{60} - \frac{5}{\sqrt{2}} + \frac{1}{\sqrt{5}} + \frac{9}{\sqrt{10}})r + (\frac{5}{6} + \\ &\quad \frac{1}{\sqrt{2}})r^2. \end{aligned}$$

□

In the following theorem, we compute the first Zagreb index of the third type of triangular hex-derived network G_2.

Theorem 5. *For the third type of triangular hex-derived network* G_2*, the first Zagreb index is equal to:*

$$M_1(G_2) = 6(78 + r(-101 + 35r)).$$

Proof. Let G_2 be the triangular hex-derived network $THDN3(r)$. Using the edge partition from Table 2, the result follows. The first Zagreb index can be calculated using Equation (5) as follows:

$$M_1(G_2) = \sum_{\acute{p}\acute{q}\in E(G_2)} (\kappa(\acute{p}) + \kappa(\acute{q})) = \sum_{j=1}^{6} \sum_{\acute{p}\acute{q}\in E_j(G_2)} (\kappa(\acute{p}) + \kappa(\acute{q}))$$

$$\begin{aligned} M_1(G_2) &= 8|E_1(G_2)| + 14|E_2(G_2)| + 17|E_3(G_2)| + 20|E_4(G_2)| + 28|E_5(G_2)| + \\ &\quad 36|E_6(G_2)|. \end{aligned}$$

By doing some calculations, we get:

$$\Longrightarrow M_1(G_2) = 6(78 + r(-101 + 35r)).$$

□

Now, we compute the H, AZI, ABC, and GA indices of the third type of triangular hex-derived network G_2.

Theorem 6. *Let* G_2 *be the third type of a triangular hex-derived network, then:*

- $H(G_2) = \frac{(1623+7r(-997+910r))}{4620}$;
- $AZI(G_2) = \frac{(4(763447224726824+7r(-86975188744735+19143357268347r)))}{327863527875}$;
- $ABC(G_2) = \frac{12\sqrt{65}(-3+r)+5\sqrt{17}(-4+r)(-3+r)+54(-2+r)+60\sqrt{5}(-3+r)(-2+r)}{30\sqrt{2}} + \frac{36\sqrt{15}(-5+3r)+45\sqrt{45}(3+(-2+r)r)}{30\sqrt{2}}$;
- $GA(G_2) = 3 + \frac{18}{7}\sqrt{5}(-3+r) + \frac{3}{2}(-4+r)(-3+r) + \frac{36}{11}\sqrt{2}(-3+r)(-2+r) - 3r + 3r^2 + \frac{12}{7}\sqrt{10}(-5+3r))$.

Proof. Using the edge partition given in Table 2, The Harmonic index can be calculated using Equation (7) as follows:

$$H(G_2) = \sum_{\acute{p}\acute{q}\in E(G_2)} \left(\frac{2}{\kappa(\acute{p}) + \kappa(\acute{q})}\right) = \sum_{j=1}^{6} \sum_{\acute{p}\acute{q}\in E_j(G_2)} \left(\frac{2}{\kappa(\acute{p}) + \kappa(\acute{q})}\right)$$

$$\begin{aligned} H(G_2) &= \frac{1}{4}|E_1(G_2)| + \frac{1}{7}|E_2(G_2)| + \frac{1}{11}|E_3(G_2)| + \frac{1}{10}|E_4(G_2)| + \frac{1}{14}|E_5(G_2)| + \\ &\quad \frac{1}{18}|E_6(G_2)|. \end{aligned}$$

By doing some calculations, we get:

$$\Longrightarrow H(G_2) = \frac{(1623 + 7r(-997 + 910r))}{4620}.$$

The augmented Zagreb index can be calculated from Equation (6) as follows:

$$AZI(G_2) = \sum_{\acute{p}\acute{q}\in E(G_2)} \left(\frac{\kappa(\acute{p})\cdot\kappa(\acute{q})}{\kappa(\acute{p})+\kappa(\acute{q})-2}\right)^3 = \sum_{j=1}^{6}\sum_{\acute{p}\acute{q}\in E_j(G_2)} \left(\frac{\kappa(\acute{p})\cdot\kappa(\acute{q})}{\kappa(\acute{p})+\kappa(\acute{q})-2}\right)^3$$

$$\begin{aligned} AZI(G_2) \quad = \quad & \frac{512}{27}|E_1(G_2)| + \frac{1000}{27}|E_2(G_2)| + \frac{5832}{125}|E_3(G_2)| + \frac{125000}{729}|E_4(G_2)| + \\ & \frac{729000}{2197}|E_5(G_2)| + \frac{4251528}{4913}|E_6(G_2)|. \end{aligned}$$

By doing some calculations, we get:

$$\Longrightarrow AZI(G_2) = \frac{(4(763447224726824 + 7r(-86975188744735 + 19143357268347r)))}{327863527875}.$$

The atom–bond connectivity index can be calculated from Equation (8) as follows:

$$ABC(G_2) = \sum_{\acute{p}\acute{q}\in E(G_2)} \sqrt{\frac{\kappa(\acute{p})+\kappa(\acute{q})-2}{\kappa(\acute{p})\cdot\kappa(\acute{q})}} = \sum_{j=1}^{6}\sum_{\acute{p}\acute{q}\in E_j(G_2)} \sqrt{\frac{\kappa(\acute{p})+\kappa(\acute{q})-2}{\kappa(\acute{p})\cdot\kappa(\acute{q})}}$$

$$\begin{aligned} ABC(G_2) \quad = \quad & \frac{1}{2}\sqrt{\frac{3}{2}}|E_1(G_2)| + \sqrt{\frac{3}{10}}|E_2(G_2)| + \frac{1}{3}\sqrt{\frac{5}{2}}|E_3(G_2)| + \frac{3}{5\sqrt{2}}|E_4(G_2)| \\ & +\frac{1}{3}\sqrt{\frac{13}{10}}|E_5(G_2)| + \frac{1}{9}\sqrt{\frac{17}{2}}|E_6(G_2)|. \end{aligned}$$

By doing some calculations, we get:

$$\begin{aligned} \Longrightarrow ABC(G_2) \quad = \quad & \frac{12\sqrt{65}(-3+r) + 5\sqrt{17}(-4+r)(-3+r) + 54(-2+r)}{30\sqrt{2}} + \\ & \frac{60\sqrt{5}(-3+r)(-2+r) + 36\sqrt{15}(-5+3r) + 45\sqrt{45}(3+(-2+r)r)}{30\sqrt{2}}. \end{aligned}$$

The geometric–arithmetic index can be calculated from Equation (9) as follows:

$$GA(G_2) = \sum_{\acute{p}\acute{q}\in E(G_2)} \frac{2\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}{(\kappa(\acute{p})+\kappa(\acute{q}))} = \sum_{j=1}^{6}\sum_{\acute{p}\acute{q}\in E_j(G_2)} \frac{2\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}{(\kappa(\acute{p})+\kappa(\acute{q}))}.$$

By doing some calculations, we get:

$$\begin{aligned} GA(G_2) \quad = \quad & |E_1(G_2)| + \frac{2\sqrt{10}}{7}|E_2(G_2)| + \frac{6\sqrt{2}}{11}|E_3(G_2)| + |E_4(G_2)| + \frac{3\sqrt{5}}{7}|E_5(G_2)| + \\ & |E_6(G_2)| \end{aligned}$$

$$\begin{aligned} \Longrightarrow GA(G_2) \quad = \quad & 3 + \frac{18}{7}\sqrt{5}(-3+r) + \frac{3}{2}(-4+r)(-3+r) + \frac{36}{11}\sqrt{2}(-3+r)(-2+r) - \\ & 3r + 3r^2 + \frac{12}{7}\sqrt{10}(-5+3r)). \end{aligned}$$

□

2.3. Results of the Third Type of Rectangular Hex-Derived Network $RHDN3(r,s)$

In this section, we compute certain degree-based topological indices of the third type of rectangular hex-derived network $RHDN3(r,s)$ of dimension $r = s$. We compute general Randić index $R_\alpha(RHDN3(r))$ with the $\alpha = \{1, -1, \frac{1}{2}, -\frac{1}{2}\}$, M_1, H, AZI ABC, and GA indices in the coming theorems of $RHDN3(r,s)$.

Theorem 7. *Consider the rectangular hex-derived network of type 3, $RHDN3(r)$, the general Randić index is equal to:*

$$R_\alpha(RHDN3(r)) = \begin{cases} 4816 + 4r(-1508 + 483r), & \alpha = 1; \\ 2(159 + 144\sqrt{2} - 60\sqrt{5} + 8\sqrt{7} - 44\sqrt{10} + 3\sqrt{14} + \\ 2\sqrt{70} + 4(-37 - 36\sqrt{2} + 6\sqrt{5}(1 + \sqrt{2}))r + \\ (39 + 36\sqrt{2})r^2), & \alpha = \frac{1}{2}; \\ \frac{(45825 + 7r(-12662 + 8925r))}{113400}, & \alpha = -1; \\ \frac{8}{3} + 2\sqrt{\frac{2}{35}} + \frac{1}{3}\sqrt{\frac{2}{7}} - 11\sqrt{\frac{2}{5}} + 4\sqrt{2} - \frac{1}{3}2\sqrt{5} + \frac{4}{\sqrt{7}} + \\ (\frac{-157}{45} + 6\sqrt{\frac{2}{5}} - 4\sqrt{2} + ^{4}\sqrt{5})r + (\frac{5}{3} + \sqrt{2})r^2, & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let G_3 be the rectangular hex-derived network of type 3, $RHDN3(r)$ shown in Figure 4, where $r = s \geq 4$. The rectangular hex-derived network G_3 has $7r^2 - 12r + 6$ vertices and the edge set of G_3 is divided into nine partitions based on the degree of end vertices. The first edge partition $E_1(G_3)$ contains $6r^2 - 12r + 10$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 4$. The second edge partition $E_2(G_3)$ contains 8 edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 4$ and $\kappa(\acute{q}) = 7$. The third edge partition $E_3(G_3)$ contains $24r - 44$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 4$ and $\kappa(\acute{q}) = 10$. The fourth edge partition $E_4(G_3)$ contains $12r^2 - 48r + 48$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 4$ and $\kappa(\acute{q}) = 18$. The fifth edge partition $E_5(G_3)$ contains 4 edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 7$ and $\kappa(\acute{q}) = 10$. The sixth edge partition $E_6(G_3)$ contains 2 edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 7$ and $\kappa(\acute{q}) = 18$. The seventh edge partition $E_7(G_3)$ contains $4r - 10$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 10$, the eighth edge partition $E_8(G_3)$ contains $8r - 20$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 10$ and $\kappa(\acute{q}) = 18$, and the ninth edge partition $E_9(G_3)$ contains $3r^2 - 16r + 21$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 18$, Table 3 shows such an edge partition of G_3. Thus, from Equation (3), it follows that:

Table 3. Edge partition of rectangular hex-derived network of type 3, $RHDN3(r)$ based on degrees of end vertices of each edge.

(κ_x, κ_y) where $\acute{p}\acute{q} \in E(G_1)$	Number of Edges	(κ_u, κ_v) where $\acute{p}\acute{q} \in E(G_1)$	Number of Edges
$(4,4)$	$6r^2 - 12r + 10$	$(7,18)$	2
$(4,7)$	8	$(10,10)$	$4r - 10$
$(4,10)$	$24r - 44$	$(10,18)$	$8r - 20$
$(4,18)$	$12r^2 - 48r + 48$	$(18,18)$	$3r^2 - 16r + 21$
$(7,10)$	4		

$$R_\alpha(G_3) = \sum_{\acute{p}\acute{q} \in E(G_3)} (\kappa(\acute{p})\kappa(\acute{q}))^\alpha.$$

For $\alpha = 1$

The general Randić index $R_\alpha(G_3)$ can be computed as follows:

$$R_1(G_3) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(G_3)} (\kappa(\acute{p}) \cdot \kappa(\acute{q})).$$

Using the edge partition given in Table 3, we get:

$$\begin{aligned} R_1(\mathrm{G}_3) &= 16|E_1(\mathrm{G}_3)| + 28|E_2(\mathrm{G}_3)| + 40|E_3(\mathrm{G}_3)| + 72|E_4(\mathrm{G}_3)| + 70|E_5(\mathrm{G}_3)| + \\ &\quad 126|E_6(\mathrm{G}_3)| + 100|E_7(\mathrm{G}_3)| + 180|E_8(\mathrm{G}_3)| + 324|E_9(\mathrm{G}_3)| \end{aligned}$$

$$\Longrightarrow R_1(\mathrm{G}_3) = 4816 + 4r(-1508 + 483r).$$

For $\alpha = \frac{1}{2}$
We apply the formula of $R_\alpha(\mathrm{G}_3)$:

$$R_{\frac{1}{2}}(\mathrm{G}_3) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(G)} \sqrt{\kappa(\acute{p}) \cdot \kappa(\acute{q})}.$$

Using the edge partition given in Table 3, we get:

$$\begin{aligned} R_{\frac{1}{2}}(\mathrm{G}_3) &= 4|E_1(\mathrm{G}_3)| + 2\sqrt{7}|E_2(\mathrm{G}_3)| + 2\sqrt{10}|E_3(\mathrm{G}_3)| + 6\sqrt{2}|E_4(\mathrm{G}_3)| + \\ &\quad \sqrt{70}|E_5(\mathrm{G}_3)| + 2\sqrt{14}|E_6(\mathrm{G}_3)| + 10|E_7(\mathrm{G}_3)| + 6\sqrt{5}|E_8(\mathrm{G}_3)| + \\ &\quad 18|E_9(\mathrm{G}_3)| \end{aligned}$$

$$\begin{aligned} \Longrightarrow R_{\frac{1}{2}}(\mathrm{G}_3) &= 2(159 + 144\sqrt{2} - 60\sqrt{5} + 8\sqrt{7} - 44\sqrt{10} + 3\sqrt{14} + 2\sqrt{70} + \\ &\quad 4(-37 - 36\sqrt{2} + 6\sqrt{5}(1 + \sqrt{2}))r + (39 + 36\sqrt{2})r^2). \end{aligned}$$

For $\alpha = -1$
We apply the formula of $R_\alpha(\mathrm{G}_3)$:

$$R_{-1}(\mathrm{G}_3) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(\mathrm{G}_3)} \frac{1}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}$$

$$\begin{aligned} R_{-1}(\mathrm{G}_3) &= \frac{1}{16}|E_1(\mathrm{G}_3)| + \frac{1}{28}|E_2(\mathrm{G}_3)| + \frac{1}{40}|E_3(\mathrm{G}_3)| + \frac{1}{72}|E_4(\mathrm{G}_3)| + \frac{1}{70}|E_5(\mathrm{G}_3)| + \\ &\quad \frac{1}{126}|E_6(\mathrm{G}_3)| + \frac{1}{100}|E_7(\mathrm{G}_3)| + \frac{1}{180}|E_8(\mathrm{G}_3)| + \frac{1}{324}|E_9(\mathrm{G}_3)| \end{aligned}$$

$$\Longrightarrow R_{-1}(\mathrm{G}_3) = \frac{(45825 + 7r(-12662 + 8925r))}{113400}.$$

For $\alpha = -\frac{1}{2}$
We apply the formula of $R_\alpha(\mathrm{G}_3)$:

$$R_{-\frac{1}{2}}(\mathrm{G}_3) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(\mathrm{G}_3)} \frac{1}{\sqrt{\kappa(\acute{p}) \cdot \kappa(\acute{q})}}$$

$$\begin{aligned} R_{-\frac{1}{2}}(\mathrm{G}_3) &= \frac{1}{\sqrt{4}}|E_1(\mathrm{G}_3)| + \frac{1}{2\sqrt{7}}|E_2(\mathrm{G}_3)| + \frac{1}{2\sqrt{10}}|E_3(\mathrm{G}_3)| + \frac{1}{6\sqrt{2}}|E_4(\mathrm{G}_3)| + \\ &\quad \frac{1}{\sqrt{70}}|E_5(\mathrm{G}_3)| + \frac{1}{3\sqrt{14}}|E_6(\mathrm{G}_3)| + \frac{1}{10}|E_7(\mathrm{G}_3)| + \frac{1}{6\sqrt{5}}|E_8(\mathrm{G}_3)| + \\ &\quad \frac{1}{18}|E_9(\mathrm{G}_3)| \end{aligned}$$

$$\Longrightarrow R_{-\frac{1}{2}}(G_3) = \frac{8}{3}+2\sqrt{\frac{2}{35}}+\frac{1}{3}\sqrt{\frac{2}{7}}-11\sqrt{\frac{2}{5}}+4\sqrt{2}-\frac{1}{3}2\sqrt{5}+ \frac{4}{\sqrt{7}}+(\frac{-157}{45}+6\sqrt{\frac{2}{5}}-4\sqrt{2}+\frac{4}{-}\sqrt{5})r+(\frac{5}{3}+\sqrt{2})r^2.$$

□

In the following theorem, we compute the first Zagreb index of rectangular hex-derived network G_3.

Theorem 8. *For the third type of rectangular hex-derived network* G_3*, the first Zagreb index is equal to:*

$$M_1(G_3) = 722 + 4r(-272 + 105r).$$

Proof. Let G_3 be the hex-derived network $RHDN3(r)$. Using the edge partition from Table 3, the result follows. The Zagreb index can be calculated using Equation (5) as follows:

$$M_1(G_3) = \sum_{\acute{p}\acute{q}\in E(G_3)} (\kappa(\acute{p}) + \kappa(\acute{q})) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q}\in E_j(G_3)} (\kappa(\acute{p}) + \kappa(\acute{q}))$$

$$M_1(G_3) = 8|E_1(G_3)| + 11|E_2(G_3)| + 14|E_3(G_3)| + 22|E_4(G_3)| + 17|E_5(G_3)| + 25|E_6(G_3)| + 20|E_7(G_3)| + 28|E_8(G_3)| + 36|E_9(G_3)|.$$

By doing some calculations, we get:

$$\Longrightarrow M_1(G_3) = 722 + 4n(-272 + 105n).$$

□

Now, we compute the H, AZI, ABC, and GA indices of the third type of rectangular hex-derived network G_3.

Theorem 9. *Let* G_3 *be the third type of rectangular hex-derived network, then:*

- $H(G_3) = \frac{137558}{98175} + \frac{1}{495}r(-1907 + 1365r)$;
- $AZI(G_3) = \frac{(8(17348684863407195591+85169n(-212237092026164+57430071805041n)))}{11967346630965375}$;
- $ABC(G_3) = \frac{1}{1260}(2160\sqrt{7} + 360\sqrt{42} + 60\sqrt{322} + 2520\sqrt{10}(-2 + n)^2 + 756\sqrt{2}(-5 + 2r) + 168\sqrt{130}(-5 + 2r) + 504\sqrt{30}(-11 + 6r) + 70\sqrt{34}(21 - 16r + 3r^2) + 630\sqrt{6}(5 - 6r + 3r^2))$;
- $GA(G_3) = 21 + \frac{(32\sqrt{7})}{11} + \frac{(12v14)}{25} + \frac{(8v70)}{17} + \frac{72}{11}\sqrt{2}(-2 + n)^2 - 24r + 9r^2 + \frac{12}{7}\sqrt{5}(-5 + 2r) + \frac{8}{7}\sqrt{10}(-11 + 6r)$.

Proof. Using the edge partition given in Table 3, The Harmonic index can be calculated using Equation (7) as follows:

$$H(G_3) = \sum_{\acute{p}\acute{q}\in E(G_3)} \left(\frac{2}{\kappa(\acute{p}) + \kappa(\acute{q})}\right) = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q}\in E_j(G_3)} \left(\frac{2}{\kappa(\acute{p}) + \kappa(\acute{q})}\right)$$

$$
\begin{aligned}
H(\mathrm{G}_3) \quad = \quad & \frac{1}{4}|E_1(\mathrm{G}_3)| + \frac{2}{11}|E_2(\mathrm{G}_3)| + \frac{1}{7}|E_3(\mathrm{G}_3)| + \frac{1}{11}|E_4(\mathrm{G}_3)| + \frac{2}{17}|E_5(\mathrm{G}_3)| + \\
& \frac{2}{25}|E_6(\mathrm{G}_3)| + \frac{1}{10}|E_7(\mathrm{G}_3)| + \frac{1}{14}|E_8(\mathrm{G}_3)| + \frac{1}{18}|E_9(\mathrm{G}_3)|.
\end{aligned}
$$

By doing some calculations, we get:

$$\Longrightarrow H(\mathrm{G}_3) = \frac{137558}{98175} + \frac{1}{495}r(-1907 + 1365r).$$

The augmented Zagreb index can be calculated from Equation (6) as follows:

$$AZI(\mathrm{G}_3) = \sum_{\acute{p}\acute{q} \in E(\mathrm{G}_3)} \left(\frac{\kappa(\acute{p}) \cdot \kappa(\acute{q})}{\kappa(\acute{p}) + \kappa(\acute{q}) - 2} \right)^3 = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(\mathrm{G}_3)} \left(\frac{\kappa(\acute{p}) \cdot \kappa(\acute{q})}{\kappa(\acute{p}) + \kappa(\acute{q}) - 2} \right)^3$$

$$
\begin{aligned}
AZI(\mathrm{G}_3) \quad = \quad & \frac{512}{27}|E_1(\mathrm{G}_3)| + \frac{21952}{729}|E_2(\mathrm{G}_3)| + \frac{1000}{27}|E_3(\mathrm{G}_3)| + \frac{5832}{125}|E_4(\mathrm{G}_3)| + \\
& \frac{2744}{27}|E_5(\mathrm{G}_3)| + \frac{2000376}{12167}|E_6(\mathrm{G}_3)| + \frac{125000}{729}|E_7(\mathrm{G}_3)| + \\
& \frac{729000}{2197}|E_8(\mathrm{G}_3)| + \frac{4251528}{4913}|E_9(\mathrm{G}_3)|.
\end{aligned}
$$

By doing some calculations, we get:

$$\Longrightarrow AZI(\mathrm{G}_3) = \frac{(8(17348684863407195591 + 85169n(-212237092026164 + 57430071805041n)))}{11967346630965375}.$$

The atom–bond connectivity index can be calculated from Equation (8) as follows:

$$ABC(\mathrm{G}_3) = \sum_{\acute{p}\acute{q} \in E(\mathrm{G}_3)} \sqrt{\frac{\kappa(\acute{p}) + \kappa(\acute{q}) - 2}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}} = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(\mathrm{G}_3)} \sqrt{\frac{\kappa(\acute{p}) + \kappa(\acute{q}) - 2}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}}$$

$$
\begin{aligned}
ABC(\mathrm{G}_3) \quad = \quad & \frac{1}{2}\sqrt{\frac{3}{2}}|E_1(\mathrm{G}_3)| + \frac{3}{2\sqrt{7}}|E_2(\mathrm{G}_3)| + \sqrt{\frac{3}{10}}|E_3(\mathrm{G}_3)| + \frac{1}{3}\sqrt{\frac{5}{2}}|E_4(\mathrm{G}_3)| + \\
& \sqrt{\frac{3}{14}}|E_5(\mathrm{G}_3)| + \frac{1}{3}\sqrt{\frac{23}{14}}|E_6(\mathrm{G}_3)| + \frac{3}{5\sqrt{2}}|E_7(\mathrm{G}_3)| + \frac{1}{3}\sqrt{\frac{13}{10}}|E_8(\mathrm{G}_3)| + \\
& \frac{1}{9}\sqrt{\frac{17}{2}}|E_9(\mathrm{G}_3)|.
\end{aligned}
$$

By doing some calculations, we get:

$$
\begin{aligned}
\Longrightarrow ABC(\mathrm{G}_3) \quad = \quad & \frac{1}{1260}(2160\sqrt{7} + 360\sqrt{42} + 60\sqrt{322} + 2520\sqrt{10}(-2+n)^2 + \\
& 756\sqrt{2}(-5+2r) + 168\sqrt{130}(-5+2r) + 504\sqrt{30}(-11+6r) + \\
& 70\sqrt{34}(21 - 16r + 3r^2) + 630\sqrt{6}(5 - 6r + 3r^2)).
\end{aligned}
$$

The geometric–arithmetic index can be calculated from Equation (9) as follows:

$$GA(\mathrm{G}_3) = \sum_{\acute{p}\acute{q} \in E(\mathrm{G}_3)} \frac{2\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}{(\kappa(\acute{p}) + \kappa(\acute{q}))} = \sum_{j=1}^{9} \sum_{\acute{p}\acute{q} \in E_j(\mathrm{G}_3)} \frac{2\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}{(\kappa(\acute{p}) + \kappa(\acute{q}))}.$$

By doing some calculations, we get:

$$\begin{aligned} GA(G_3) &= |E_1(G_3)| + \frac{4\sqrt{7}}{11}|E_2(G_3)| + \frac{2\sqrt{10}}{7}|E_3(G_3)| + \frac{6\sqrt{2}}{11}|E_4(G_3)| + \\ & \frac{2\sqrt{70}}{17}|E_5(G_3)| + \frac{6\sqrt{14}}{25}|E_6(G_3)| + |E_7(G_3)| + \frac{3\sqrt{5}}{7}|E_8(G_3)| + |E_9(G_3)| \end{aligned}$$

$$\begin{aligned} \Longrightarrow GA(G_3) &= 21 + \frac{(32\sqrt{7})}{11} + \frac{(12v14)}{25} + \frac{(8v70)}{17} + \frac{72}{11}\sqrt{2}(-2+n)^2 - 24r + 9r^2 + \\ & \frac{12}{7}\sqrt{5}(-5+2r) + \frac{8}{7}\sqrt{10}(-11+6r). \end{aligned}$$

□

2.4. Results of the Third Type of Chain Hex-Derived Network, $CHDN3(r)$

In this section, we compute certain degree-based topological indices of the third type of chain hex-derived network, $CHDN3(r)$ of dimension r. We compute general Randić index $R_\alpha(CHDN3(r))$ with the $\alpha = \{1, -1, \frac{1}{2}, -\frac{1}{2}\}$, M_1, H, AZI ABC, and GA indices in the coming theorems of $CHDN3(r)$.

Theorem 10. *Consider the chain hex-derived network of type 3, $CHDN3(r)$, the general Randić index is equal to:*

$$R_\alpha(CHDN3(r)) = \begin{cases} 336r - 160, & \alpha = 1; \\ 4(2 - 4\sqrt{2} + (7 + 6\sqrt{2})r), & \alpha = \frac{1}{2}; \\ \frac{1}{64}(14 + 33r), & \alpha = -1; \\ \frac{1}{8}(10 - 4\sqrt{2} + (11 + 6\sqrt{2})r), & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let G_4 be the chain hex-derived network of type 3, $CHDN3(r)$ shown in Figure 5, where $r \geq 2$. The chain hex-derived network G_4 has $5r + 1$ vertices, and the edge set of G_4 is divided into three partitions based on the degree of end vertices. The first edge partition $E_1(G_4)$ contains $5r + 6$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 4$. The second edge partition $E_2(G_4)$ contains $6r - 4$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = 4$ and $\kappa(\acute{q}) = 8$, and the third edge partition $E_3(G_4)$ contains $r - 2$ edges $\acute{p}\acute{q}$, where $\kappa(\acute{p}) = \kappa(\acute{q}) = 8$. Table 4 shows such an edge partition of G_4. Thus, from Equation (3), it follows that:

Table 4. Edge partition of chain hex-derived network of type 3, $CHDN3(r)$ based on degrees of end vertices of each edge.

(κ_x, κ_y) where $\acute{p}\acute{q} \in E(G_1)$	Number of Edges
$(4,4)$	$6r^2 - 12r + 10$
$(4,8)$	8
$(8,8)$	$24r - 44$

$$R_\alpha(G_4) = \sum_{\acute{p}\acute{q} \in E(G_4)} (\kappa(\acute{p})\kappa(\acute{q}))^\alpha.$$

For $\alpha = 1$

The general Randić index $R_\alpha(G_4)$ can be computed as follows:

$$R_1(G_4) = \sum_{j=1}^{3} \sum_{\acute{p}\acute{q} \in E_j(G_4)} (\kappa(\acute{p}) \cdot \kappa(\acute{q})).$$

Using the edge partition given in Table 4, we get:

$$R_1(G_4) \quad = \quad 16|E_1(G_4)| + 32|E_2(G_4)| + 64|E_3(G_4)|$$
$$\Longrightarrow R_1(G_4) = 336r - 160.$$

For $\alpha = \frac{1}{2}$

We apply the formula of $R_\alpha(G_4)$:

$$R_{\frac{1}{2}}(G_4) = \sum_{j=1}^{3} \sum_{\acute{p}\acute{q} \in E_j(G)} \sqrt{\kappa(\acute{p}) \cdot \kappa(\acute{q})}.$$

Using the edge partition given in Table 4, we get:

$$R_{\frac{1}{2}}(G_4) \quad = \quad 4|E_1(G_4)| + 4\sqrt{2}|E_2(G_4)| + 8|E_3(G_4)|$$

$$\Longrightarrow R_{\frac{1}{2}}(G_4) \quad = \quad 4(2 - 4\sqrt{2} + (7 + 6\sqrt{2})r).$$

For $\alpha = -1$

We apply the formula of $R_\alpha(G_4)$:

$$R_{-1}(G_4) = \sum_{j=1}^{3} \sum_{\acute{p}\acute{q} \in E_j(G_4)} \frac{1}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}$$

$$R_{-1}(G_4) \quad = \quad \frac{1}{16}|E_1(G_4)| + \frac{1}{32}|E_2(G_4)| + \frac{1}{64}|E_3(G_4)|$$
$$\Longrightarrow R_{-1}(G_4) = \frac{1}{64}(14 + 33r).$$

For $\alpha = -\frac{1}{2}$

We apply the formula of $R_\alpha(G_4)$:

$$R_{-\frac{1}{2}}(G_4) = \sum_{j=1}^{3} \sum_{\acute{p}\acute{q} \in E_j(G_4)} \frac{1}{\sqrt{\kappa(\acute{p}) \cdot \kappa(\acute{q})}}$$

$$R_{-\frac{1}{2}}(G_4) \quad = \quad \frac{1}{\sqrt{4}}|E_1(G_4)| + \frac{1}{4\sqrt{2}}|E_2(G_4)| + \frac{1}{8}|E_3(G_4)|$$

$$\Longrightarrow R_{-\frac{1}{2}}(G_4) \quad = \quad \frac{1}{8}(10 - 4\sqrt{2} + (11 + 6\sqrt{2})r).$$

□

In the following theorem, we compute the first Zagreb index of chain hex-derived network G_4.

Theorem 11. *For the third type of chain hex-derived network* G_4*, the first Zagreb index is equal to:*

$$M_1(G_4) = 32(-1+4n).$$

Proof. Let G_4 be the hex-derived network $CHDN3(r)$. Using the edge partition from Table 4, the result follows. The Zagreb index can be calculated using Equation (5) as follows:

$$M_1(G_4) = \sum_{\acute{p}\acute{q}\in E(G_4)} (\kappa(\acute{p})+\kappa(\acute{q})) = \sum_{j=1}^{3}\sum_{\acute{p}\acute{q}\in E_j(G_4)} (\kappa(\acute{p})+\kappa(\acute{q}))$$

$$M_1(G_4) = 8|E_1(G_4)| + 12|E_2(G_4)| + 16|E_3(G_4)|.$$

By doing some calculations, we get:

$$\Longrightarrow M_1(G_4) = 32(-1+4n).$$

□

Now, we compute the H, AZI, ABC and GA indices of the third type of chain hex-derived network G_4.

Theorem 12. *Let* G_4 *be the third type of rectangular hex-derived network, then:*

- $H(G_4) = \frac{7}{12} + \frac{19}{8}r$;
- $AZI(G_4) = \frac{512(-471102+874903r)}{1157625}$;
- $ABC(G_4) = \frac{1}{8}(\sqrt{14}(-2+r) + 4\sqrt{5}(-2+3r) + 2\sqrt{6}(6+5r))$;
- $GA(G_4) = 4 + 6r + \frac{4}{3}\sqrt{2}(-2+3r)$.

Proof. Using the edge partition given in Table 4, the Harmonic index can be calculated using Equation (7) as follows:

$$H(G_4) = \sum_{\acute{p}\acute{q}\in E(G_4)} \left(\frac{2}{\kappa(\acute{p})+\kappa(\acute{q})}\right) = \sum_{j=1}^{3}\sum_{\acute{p}\acute{q}\in E_j(G_4)} \left(\frac{2}{\kappa(\acute{p})+\kappa(\acute{q})}\right)$$

$$H(G_4) = \frac{1}{4}|E_1(G_4)| + \frac{1}{6}|E_2(G_4)| + \frac{1}{8}|E_3(G_4)|.$$

By doing some calculations, we get:

$$\Longrightarrow H(G_4) = \frac{7}{12} + \frac{19}{8}r.$$

The augmented Zagreb index can be calculated from Equation (6) as follows:

$$AZI(G_4) = \sum_{\acute{p}\acute{q}\in E(G_4)} \left(\frac{\kappa(\acute{p})\cdot\kappa(\acute{q})}{\kappa(\acute{p})+\kappa(\acute{q})-2}\right)^3 = \sum_{j=1}^{3}\sum_{\acute{p}\acute{q}\in E_j(G_4)} \left(\frac{\kappa(\acute{p})\cdot\kappa(\acute{q})}{\kappa(\acute{p})+\kappa(\acute{q})-2}\right)^3$$

$$AZI(G_4) = \frac{512}{27}|E_1(G_4)| + \frac{4096}{125}|E_2(G_4)| + \frac{32768}{343}|E_3(G_4)|.$$

By doing some calculations, we get:

$$\Longrightarrow AZI(G_4) = \frac{512(-471102 + 874903r)}{1157625}.$$

The atom–bond connectivity index can be calculated from Equation (8) as follows:

$$ABC(G_4) = \sum_{\acute{p}\acute{q}\in E(G_4)} \sqrt{\frac{\kappa(\acute{p}) + \kappa(\acute{q}) - 2}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}} = \sum_{j=1}^{3} \sum_{\acute{p}\acute{q}\in E_j(G_4)} \sqrt{\frac{\kappa(\acute{p}) + \kappa(\acute{q}) - 2}{\kappa(\acute{p}) \cdot \kappa(\acute{q})}}$$

$$ABC(G_4) = \frac{1}{2}\sqrt{\frac{3}{2}}|E_1(G_4)| + \frac{1}{4}\sqrt{5}|E_2(G_4)| + \frac{1}{4}\sqrt{\frac{7}{2}}|E_3(G_4)|.$$

By doing some calculations, we get:

$$\Longrightarrow ABC(G_4) = \frac{1}{8}(\sqrt{14}(-2 + r) + 4\sqrt{5}(-2 + 3r) + 2\sqrt{6}(6 + 5r)).$$

The geometric–arithmetic index can be calculated from Equation (9) as follows:

$$GA(G_4) = \sum_{\acute{p}\acute{q}\in E(G_4)} \frac{2\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}{(\kappa(\acute{p}) + \kappa(\acute{q}))} = \sum_{j=1}^{3} \sum_{\acute{p}\acute{q}\in E_j(G_4)} \frac{2\sqrt{\kappa(\acute{p})\kappa(\acute{q})}}{(\kappa(\acute{p}) + \kappa(\acute{q}))}.$$

By doing some calculations, we get:

$$GA(G_4) = |E_1(G_4)| + \frac{2\sqrt{2}}{3}|E_2(G_4)| + |E_3(G_4)|$$

$$\Longrightarrow GA(G_4) = 4 + 6r + \frac{4}{3}\sqrt{2}(-2 + 3r).$$

□

For the comparison of topological indices numerically for $HDN3$, $THDN3$, $RHDN3$, and $CHDN3$, we computed all indices for different values of r. From Tables 5–8, we can easily see that all indices are in increasing order as the values of r increases.

The Zagreb and augmented Zagreb indices were found to occur for the computation of the total π-electron energy of molecules [30]. Thus, the total π-electron energy is in increasing order in the case of all networks.

Table 5. Numerical computation of all indices for $HDN3(r)$.

$[r]$	R_1	$R_{\frac{1}{2}}$	R_{-1}	$R_{-\frac{1}{2}}$	M_1	H	AZI	ABC	GA
4	42,684	4470.75	16.49	89.98	10,242	82.41	64,642.58	305.8	514.21
5	80,004	8120.25	28.54	156.78	18,690	142.81	124,991	539.17	904.86
6	128,916	12,848.69	43.89	242.08	29,658	219.76	204,958	838.37	1405.05
7	189,420	18,656.07	62.55	345.86	43,146	313.26	304,543	1203.39	2014.77

Table 6. Numerical computation of all indices for $THDN3(r)$.

$[r]$	R_1	$R_{\frac{1}{2}}$	R_{-1}	$R_{-\frac{1}{2}}$	M_1	H	AZI	ABC	GA
4	4752	639.95	3.37	17.35	1404	16.36	5760.91	54.36	91.95
5	9888	1205.94	5.54	29.19	2688	27.26	13,046.93	94.25	159.48
6	16,956	1951.75	8.26	44.10	4392	40.92	23,602.69	145.12	245.26
7	25,956	2877.38	11.53	62.10	6516	49.92	37,428.2	206.95	349.30

Table 7. Numerical computation of all indices for $RHDN3(r)$.

$[r]$	R_1	$R_{\frac{1}{2}}$	R_{-1}	$R_{-\frac{1}{2}}$	M_1	H	AZI	ABC	GA
4	11,600	1377.42	6.09	32.32	3090	30.11	15,578.92	105.26	177.94
5	22,956	2551.65	10.27	55.29	5782	51.08	32,923	184.05	310.57
6	38,176	4085.54	15.55	84.43	9314	77.56	56,206.57	284.78	479.72
7	57,260	5979.54	21.93	119.72	13,686	109.56	87,229.60	407.45	685.38

Table 8. Numerical computation of all indices for $CHDN3(r)$.

$[r]$	R_1	$R_{\frac{1}{2}}$	R_{-1}	$R_{-\frac{1}{2}}$	M_1	H	AZI	ABC	GA
4	1184	233.14	2.28	10.28	480	10.08	1339.46	28.04	46.86
5	1520	295.08	2.79	12.72	608	12.46	1726.42	34.92	58.51
6	1856	357.02	3.31	15.16	736	14.83	2113.38	41.80	70.17
7	2192	418.96	3.83	17.59	864	17.21	2500.33	48.69	81.83

3. Conclusions

In this paper, we studied a newly formed third type of hex-derived networks, $HDN3$, $THDN3$, $RHDN3$, and $CHDN3$. The exact results were computed for Randić, Zagreb, Harmonic, augmented Zagreb, atom–bond connectivity, and geometric–arithmetic indices for the very first time of the third type of hex-derived networks, and we also found the numerical computation for all the networks. As these important results are helpful from many chemical points of view as well as for pharmaceutical sciences, these results also provide the basis to understand the deep underlying topologies of the above networks. In future, we are interested in computing the distance-based and counting-related topological indices and polynomials for these networks. We are looking to find Estrada and L-Estrada indices of edge-independent random graphs [32]. We also put forward computing topological indices for random graphs in future.

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