



On Topological Indices of *mth* Chain Hex-Derived Network of Third Type

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In theoretical chemistry, the numerical parameters that are used to characterize the molecular topology of graphs are called topological indices. Several physical and chemical properties like boiling point, entropy, heat formation, and vaporization enthalpy of chemical compounds can be determined through these topological indices. Graph theory has a considerable use in evaluating the relation of various topological indices of some derived graphs. In this article, we will compute the topological indices like Randić, first Zagreb, harmonic, augmented Zagreb, atom-bond connectivity, and geometric-arithmetic indices for chain hex-derived network of type 3 *CHDN3*(m,n) for different cases of m and n. We will also compute the numerical computation and graphical view to justify our results.

OPEN ACCESS

Edited by:

Jinjin Li, Shanghai Jiao Tong University, China

Reviewed by:

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Specialty section:

This article was submitted to Computational Physics, a section of the journal Frontiers in Physics

Received: 24 August 2020 Accepted: 23 September 2020 Published: 20 November 2020

Citation:

Huo Y, Ali H, Binyamin MA, Asghar SS, Babar U and Liu J-B (2020) On Topological Indices of mth Chain Hex-Derived Network of Third Type. Front. Phys. 8:593275. doi: 10.3389/fphy.2020.593275 Keywords: *Randić*, index, first and second Zagreb index, augmented Zagreb index, harmonic index, atom-bond connectivity and geometric-arithmetic index

INTRODUCTION AND PRELIMINARY RESULTS

Mathematics Subject Classification: 05C12, 05C90

A branch of numerical science called graph theory is the one in which we use tools of graph parameters to reveal the compound phenomenon precisely. Graph theory, for instance, when used in the study of molecular structures, characterizes a field among various disciplines of science known as molecular topology or chemical graph theory.

Chemical graph theory has provided a considerable part of study to chemist through which they can execute graph theory to mathematical demonstrating of chemical marvel. We are usually interested in estimating the structural characters to elaborate quantitative structure-activity relationships using techniques taken from graph theory.

Topological description of chemical structures with required properties can be used to categorize the molecules and to model unknown structures. Molecules and molecular compounds are frequently demonstrated by molecular graph. In graph theory, a molecular graph is the illustration of structural formula of chemical compounds. The vertices are expressed by the atoms of molecule while the edges suggest the covalent bonds between the atoms.

Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to analyze the organic activities and properties of biological compounds can be studied by the help of a new subject known as cheminformatics, which is the composition of mathematics, information science, and chemistry.

At present, the numerical programming of biological structure with topological descriptors is increasing in consequence in invigorating science, bioinformatics, and pharmaceutics.

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In QSAR/QSPR study, physicochemical properties of the topological descriptors like Wiener index, Randić index, sieged index, first and second Zagreb index, augmented Zagreb index, harmonic index, and geometric–arithmetic index are useful to classify the bioactivity of the chemical compounds.

A graph can be characterized by a polynomial, a numeric number, and a sequence of numbers or a matrix. A numeric quantity interrelated with a graph that remains invariant under the graph automorphism and differentiate the topology of graph is called molecular descriptor. A graph theoretical characteristic that is sustained by an isomorphism is called topological descriptor.

At present, in the field of computational chemistry, topological indices have a rising interest, which is actually associated to their use in nonempirical quantitative structure–property relationship and quantitative structure–activity relationship.

Topological descriptor, Top (*G*), may also be defined with the property of isomorphism, that is, for every graph *H* isomorphic to *G*, Top (*G*) = Top (*H*). The idea of topological indices was first introduced by Weiner [35] during the laboratory work on boiling point of paraffin and named this result as path number, which was later named as Weiner index.

This article takes into account the topological indices of hexagonal networks derived from a hexagonal graph, which contain molecular graphs of unbranched benzene hydrocarbons. Hexagonal structure graphs consist of hexagons that are fused together. Theoretical chemists pay great attention to this class of chemical compounds. Topological index theory has been intensively developed over the past four decades for the individual molecular graphs. Benzene hydrocarbons are not only the major chemical industry raw materials but also harmful pollutants [15, 16, 28].

Chen et al. [9] derived a hexagonal mesh. Hexagonal mesh made by a set of triangles is shown in **Figure 1**. There exists no hexagonal mesh with one dimension. A two dimensional hexagonal mesh HX(2) can be generated from six triangles. A three dimensional hexagonal mesh HX(3) can be obtained by adding a layer of triangles around the each wall of HX(2).

In the similar way, HX(n) can be produced by adding *n* layers around all the sides of every proceeding hexagonal mesh. Drawing algorithm of *HDN3* networks.

Step-1: First, we draw a hexagonal network of dimension *n*. **Step-2:** All the K_3 subgraphs are converted into planar octahedron network *POH* and the graph obtained is known as *HDN3* [29] [see **Figures 1, 2**)] network.

Step-3: An mth *CHDN*3 (m, n) can be easily formed from the *HDN*3 network (see **Figures 2, 3**).

In CHDN3(m, n), *m* represents the number of rows and *n* are the number of triangles in each row.

In this article, \mathcal{G} is considered a network with a $V(\mathcal{G})$ vertex set and an edge set of $E(\mathcal{G})$, and d_r is the degree of vertex $r \in V(\mathcal{G})$.

The Randić index [27] is denoted by $R_{\frac{-1}{2}}(\mathcal{G})$ and makes us aware of Milan Randić and is represented as follows:

$$R_{\frac{-1}{2}}(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \frac{1}{\sqrt{d_r d_s}}.$$
 (1)

The general Randić index is the sum of $(d_r d_s)^{\alpha}$ over all edges $e = rs \in E(\mathcal{G})$, represented as

$$R_{\alpha}(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} (d_r d_s)^{\alpha} \quad \text{for } \alpha = 1, \frac{1}{2}, -1, \frac{-1}{2}.$$
 (2)

Trinajstić [31] makes us aware of TI's, which are the first and second Zagreb indices, denoted by $M_1(\mathcal{G})$ and formalized as follows:

$$M_1(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} (d_r + d_s).$$
(3)

Furtula et al. [13] introduced the augmented Zagreb index and described it as





$$AZI(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \left(\frac{d_r d_s}{d_r + d_s - 2} \right)^3.$$
(4)

Zhong [37] introduced the harmonic index and described it as

$$H(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \left(\frac{2}{d_r + d_s}\right).$$
 (5)

The index atom-bond connectivity (ABC) is one of the wellknown degree-based topological indices, given by Estrada et al. [12] and defined as

$$ABC(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}.$$
 (6)

Vukićević and Furtula [33] invented the famous geometric-arithmetic index and represented it as

$$GA(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \frac{2\sqrt{d_r d_s}}{(d_r + d_s)}.$$
(7)

Cases for mth chain hex-derived network of third type. CHDN3(m, n)

There are three cases for CHDN3(m, n).

Case-1: For m = n, $(m, n) \ge 1$.

Case-2: For m < n, m is odd and $n \in \mathbb{N}$. For m > n, m is odd and $n \in \mathbb{N}$. For m < n, m and n both are even. For m > n, m and n both are even.

Case-3: For m < n, m is even and n is odd. For m > n, m is even and n is odd.

MAIN RESULTS

Simonraj et al. [29] discovered hex-derived networks and found the metric dimension of *HDN3*. We discuss the newly derived third type of hex-derived networks in this article and calculate the exact results for topological indexes based on degrees. These topological indices and their variants are currently subjected to extensive research activity, see [1–8, 14, 18–25, 30, 32, 34, 36]. For Basic notations and definitions, see [10, 17, 26, 31].

Results for the First Case mth Chain Hex-Derived Network of Third Type *CHDN3* (*m*, *n*)

In this section, for the very first time, we discuss CHDN3(m, n), which is derived from hex-derived network and compute the exact results for Randic, Zagreb, harmonic, augmented Zagreb, atom-bond connectivity, and geometric-arithmetic indices for case 1.

Theorem 2.1.1. Consider the *mth* chain hex-derived network of type 3 *CHDN3* (m, n), the general Randić index is equal to



$$R_{\alpha}(\mathcal{G}) = \begin{cases} 16(2-9m+27mn-9n), & \alpha = 1; \\ 4(6-4\sqrt{2}-3m+(9+6\sqrt{2})mn-3n), & \alpha = \frac{1}{2}; \\ \frac{1}{8}(6-4\sqrt{2}+3m+(9+6\sqrt{2})mn+3n), & \alpha = \frac{-1}{2}; \\ \frac{1}{64}(2+9m+27mn+9n), & \alpha = -1. \end{cases}$$

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. Table 1 shows such an edge partition of \mathcal{G} for m = n. Using Equation (2), we have

$$R_{\alpha}(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} (d_r d_s)^{\alpha}.$$

Using edge partitions in Table 1, we get the following. For $\alpha = 1$, **Eq. 2** becomes

$$R_{1}(\mathcal{G}) = (16)^{1} (3mn + 3m + 3n + 2) + (32)^{1} (6mn - 4) + (64)^{1} (3mn - 3m - 3n + 2).$$

By making some calculations, we get

.

$$\Rightarrow R_1(\mathcal{G}) = 16(2 - 9m + 27mn - 9n).$$

For $\alpha = \frac{1}{2}$, Eq. 2 becomes

$$R_{\frac{1}{2}}(\mathcal{G}) = (16)^{\frac{1}{2}}(3mn+3m+3n+2) + (32)^{\frac{1}{2}}(6mn-4) + (64)^{\frac{1}{2}}(3mn-3m-3n+2).$$

By making some calculations, we get

$$\Rightarrow R_{\frac{1}{2}}(\mathcal{G}) = 4\left(6 - 4\sqrt{2} - 3m + \left(9 + 6\sqrt{2}\right)mn - 3n\right).$$

For $\alpha = -\frac{1}{2}$, Eq. 2 becomes

$$R_{-\frac{1}{2}}(\mathcal{G}) = (16)^{-\frac{1}{2}}(3mn + 3m + 3n + 2) + (32)^{-\frac{1}{2}}(6mn - 4) + (64)^{-\frac{1}{2}}(3mn - 3m - 3n + 2).$$

By making some calculations, we get

$$\Rightarrow R_{-\frac{1}{2}}(\mathcal{G}) = \frac{1}{8} \left(6 - 4\sqrt{2} + 3m + (9 + 6\sqrt{2})mn + 3n \right).$$

For $\alpha = -1$, Eq. 2 becomes $R_{-1}(\mathcal{G}) = (16)^{-1}(3mn + 3m + 3n + 2) + (32)^{-1}(6mn - 4)$ $+ (64)^{-1} (3mn - 3m - 3n + 2).$

TABLE 1 Degree-Based Edge partition for $m = n$		
(d_r, d_s) where $rs \in \boldsymbol{E}(\mathcal{G})$	Number of Edges	
(4, 4)	(3mn + 3m + 3n + 2)	
(4, 8)	(6 <i>mn</i> – 4)	
(8, 8)	(3mn - 3m - 3n + 2)	

By making some calculations, we get

$$\Rightarrow R_{-1}(\mathcal{G}) = \frac{1}{64} \left(2 + 9m + 27mn + 9n\right).$$

Theorem 2.1.2. Consider the *mth* chain hex-derived network of type 3 CHDN3(m, n), the first Zagreb index is equal to

$$M_1(\mathcal{G}) = -24(m - 6mn + n).$$

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. In **Table 1**, there is an edge partition of \mathcal{G} for m = n. Using **Eq. 3**, we have

$$M_1(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} (d_r + d_s).$$

Using edge partitions in Table 1, we get

$$M_1(\mathcal{G}) = (4+4)(3mn+3m+3n+2) + (4+8)(6mn-4) + (8+8)(3mn-3m-3n+2), = (8)(3mn+3m+3n+2) + (12)(6mn-4) + (16)(3mn-3m-3n+2),$$

By making some calculations, we get

$$\Rightarrow M_1(\mathcal{G}) = -24(m - 6mn + n).$$

Theorem 2.1.3. Consider the *mth* chain hex-derived network of type 3 *CHDN3*(m, n), the augmented Zagreb index and harmonic index are equal to

$$AZI(\mathcal{G}) = \frac{512}{1157625} (221398 - 519375m + 1221153mn - 519375n).$$
$$H(\mathcal{G}) = \frac{1}{24} (2 + 9m + 51mn + 9n).$$

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. Using Eq. 4, we have

$$AZI(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \left(\frac{d_r d_s}{d_r + d_s - 2}\right)^3.$$

From **Table 1**, using the edge partition, the outcome can be obtained as

$$AZI(\mathcal{G}) = \left(\frac{4 \times 4}{4 + 4 - 2}\right)^3 (3mn + 3m + 3n + 2) + \left(\frac{4 \times 8}{4 + 8 - 2}\right)^3 (6mn - 4) + \left(\frac{8 \times 8}{8 + 8 - 2}\right)^3 (3mn - 3m - 3n + 2),$$

$$= \left(\frac{8}{3}\right)^{3} (3mn + 3m + 3n + 2) + \left(\frac{16}{5}\right)^{3} (6mn - 4) + \left(\frac{32}{7}\right)^{3} (3mn - 3m - 3n + 2).$$

By making some calculations, we get

$$\Rightarrow AZI(\mathcal{G}) = \frac{512}{1157625} (221398 - 519375m + 1221153mn - 519375n).$$

Using Eq. 5, we have

$$H(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \left(\frac{2}{d_r + d_s}\right).$$

From **Table 1**, using the edge partition, the outcome can be obtained as

$$H(\mathcal{G}) = \left(\frac{2}{4+4}\right)(3mn+3m+3n+2) + \left(\frac{2}{4+8}\right)(6mn-4) \\ + \left(\frac{2}{8+8}\right)(3mn-3m-3n+2), \\ = \left(\frac{1}{8}\right)(3mn+3m+3n+2) + \left(\frac{1}{6}\right)(6mn-4) \\ + \left(\frac{1}{8}\right)(3mn-3m-3n+2).$$

By making some calculations, we get

$$\Rightarrow H(\mathcal{G}) = \frac{1}{24} \left(2 + 9m + 51mn + 9n\right).$$

Theorem 2.1.4. Let \mathcal{G} be the *mth* chain hex-derived network of third type *CHDN3*(*m*, *n*), then atom–bond connectivity index and geometric–arithematic index are equal to

$$ABC(\mathcal{G}) = \frac{1}{8} \left(4\sqrt{5} \left(3mn - 2 \right) + \sqrt{14} \left(2 - 3m + 3mn - 3n \right) \right.$$
$$\left. + 2\sqrt{6} \left(2 + 3m + 3mn + 3n \right) \right].$$
$$GA(\mathcal{G}) = 4 + 6mn + \frac{4\sqrt{2}}{3} \left(3mn - 2 \right).$$

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. Using Eq. 6, we have

$$ABC(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}.$$

From Table 1, using the edge partition, the outcome can be obtained as

$$ABC(\mathcal{G}) = \sqrt{\frac{4+4-2}{4\times4}}(3mn+3m+3n+2) + \sqrt{\frac{4+8-2}{4\times8}}(6mn-4) + \sqrt{\frac{8+8-2}{8\times8}}(3mn-3m-3n+2)$$

$$= \sqrt{\frac{3}{8}}(3mn + 3m + 3n + 2) + \sqrt{\frac{14}{64}}(6mn - 4) + \sqrt{\frac{7}{32}}(3mn - 3m - 3n + 2),$$

By making some calculations, we get

$$\Rightarrow ABC(\mathcal{G}) = \frac{1}{8} \left(4\sqrt{5} \left(3mn - 2 \right) + \sqrt{14} \left(2 - 3m + 3mn - 3n \right) \right.$$
$$+ 2\sqrt{6} \left(2 + 3m + 3mn + 3n \right) \right).$$

Using Eq. 7,

$$GA(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \frac{2\sqrt{d_r d_s}}{d_r + d_s}$$

From Table 1, using the edge partition, we get the outcome as,

$$GA(\mathcal{G}) = \frac{2\sqrt{4 \times 4}}{(4+4)} (3mn+3m+3n+2) + \frac{2\sqrt{4 \times 8}}{(4+8)} (6mn-4) + \frac{2\sqrt{8 \times 8}}{(8+8)},$$

(3mn-3m-3n+2)
= (1)(3mn+3m+3n+2) + $\frac{2\sqrt{2}}{3} (6mn-4) + (1)(3mn-3m-3n+2).$

By making some calculations, we get

$$\Rightarrow GA(\mathcal{G}) = 4 + 6mn + \frac{4\sqrt{2}}{3}(3mn - 2).$$

Results for the Second Case of Chain Hex-Derived Networks of Third Type *CHDN3* (*m*, *n*)

In this section, for the very first time, we discuss CHDN3(m, n) derived from of hex-derived network and compute the exact results forRandic, Zagreb, harmonic, augmented Zagreb, atom-bond connectivity, and geometric-arithmetic indices for case 2.

Theorem 2.2.1. Consider the *mth* chain hex-derived network of type 3 *CHDN3* (*m*, *n*), the general Randic index for second case is equal to

$$R_{\alpha}(\mathcal{G}) = \begin{cases} 16(2-12m+27mn-6n), & \alpha = 1; \\ 4(6-4\sqrt{2}-4m+(9+6\sqrt{2})mn-2n), & \alpha = \frac{1}{2}; \\ \frac{1}{8}(6-4\sqrt{2}+4m+(9+6\sqrt{2})mn+2n,) & \alpha = \frac{-1}{2}; \\ \frac{1}{64}(2+12m+27mn+6n), & \alpha = -1. \end{cases}$$

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. Table 2 shows such an edge partition of \mathcal{G} for second case.

Using Eq. 2, we get

$$R_{\alpha}(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} (d_r d_s)^{\alpha}$$

Using edge partitions in **Table 2**, we get, for $\alpha = 1$,

$$R_1(\mathcal{G}) = (16)^1 (3mn + 4m + 2n + 2) + (32)^1 (6mn - 4) + (64)^1 (3mn - 4m - 2n + 2),$$

By making some calculations, we get

$$\Rightarrow R_1(\mathcal{G}) = 16(2 - 12m + 27mn - 6n).$$

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

$$\begin{aligned} R_{\frac{1}{2}}(\mathcal{G}) &= (16)^{\frac{1}{2}}(3mn+4m+2n+2) + (32)^{\frac{1}{2}}(6mn-4) \\ &+ (64)^{\frac{1}{2}}(3mn-4m-2n+2), \end{aligned}$$

By making some calculations, we get

$$\Rightarrow R_{\frac{1}{2}}(\mathcal{G}) = 4(6 - 4\sqrt{2} - 4m + (9 + 6\sqrt{2})mn - 2n).$$

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

$$R_{\frac{1}{2}}(\mathcal{G}) = (16)^{-\frac{1}{2}}(3mn + 4m + 2n + 2) + (32)^{-\frac{1}{2}}(6mn - 4)$$

+ $(64)^{-\frac{1}{2}}(3mn - 4m - 2n + 2).$

By making some calculations, we get

$$\Rightarrow R_{\frac{-1}{2}}(\mathcal{G}) = \frac{1}{8} \left(6 - 4\sqrt{2} + 4m + (9 + 6\sqrt{2})mn + 2n \right).$$

For $\alpha = -1$,

$$R_{-1}(\mathcal{G}) = (16)^{-1} (3mn + 4m + 2n + 2) + (32)^{-1} (6mn - 4) + (64)^{-1} (3mn - 4m - 2n + 2).$$

By making some calculations, we get

$$\Rightarrow R_{-1}(\mathcal{G}) = \frac{1}{64} (2 + 12m + 27mn + 6n).$$

Theorem 2.2.2. Consider the *mth* chain hex-derived network of type 3 CHDN3(m, n), the first Zagreb index is equal to

$$M_1(\mathcal{G}) = -16(2m - 9mn + n).$$

TABLE 2	Degree-Based	Edge	partition	for	Case 2.

(d_r, d_s) where $rs \in \boldsymbol{E}(\mathcal{G})$	Number of Edges
(4, 4)	(3mn + 4m + 2n + 2)
(4, 8)	(6 <i>mn</i> – 4)
(8, 8)	(3mn - 4m - 2n + 2)

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. Table 2 shows such an edge partition of \mathcal{G} for second case.

Using Eq. 3,

$$M_1(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} (d_r + d_s).$$

Using edge partitions in Table 2, we get

$$M_{1}(\mathcal{G}) = (4+4)(3mn+4m+2n+2) + (4+8)(6mn-4) + (8+8)(3mn-4m-2n+2), = (8)(3mn+4m+2n+2) + (12)(6mn-4) + (16)(3mn-4m-2n+2).$$

By making some calculations, we get

$$\Rightarrow M_1(\mathcal{G}) = -16(2m - 9mn + n).$$

Theorem 2.2.3. Let \mathcal{G} be the *CHDN3*(*m*, *n*) *mth* chain hexderived network of third type, the augmented Zagreb index and harmonic index are equal to

$$AZI(\mathcal{G}) = \frac{512}{1157625} (221398 - 692500m + 1221153mn - 346250n).$$
$$H(\mathcal{G}) = \frac{1}{24} (2 + 12m + 51mn + 6n).$$

Proof. Consider G be the CHDN3(m, n) mth chain hexderived network of third type. Using Eq. 4, we get

$$AZI(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \left(\frac{d_r d_s}{d_r + d_s - 2}\right)^3.$$

From **Table 1**, using the edge partition, the outcome can be obtained as

$$\begin{split} AZI\left(\mathcal{G}\right) &= \left(\frac{4\times4}{4+4-2}\right)^{3} (3mn+4m+2n+2) \\ &+ \left(\frac{4\times8}{4+8-2}\right)^{3} (6mn-4) \\ &+ \left(\frac{8\times8}{8+8-2}\right)^{3} (3mn-4m-2n+2), \\ &= \left(\left(\frac{8}{3}\right)^{3}\right) (3mn+4m+2n+2) \\ &+ \left(\frac{16}{5}\right)^{3} (6mn-4) + \left(\frac{32}{7}\right)^{3} (3mn-4m-2n+2). \end{split}$$

By making some calculations, we get

$$\Rightarrow AZI(\mathcal{G}) = \frac{512}{1157625} (221398 - 692500m + 1221153mn - 346250n).$$

By using Eq. 5, we have

$$H(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \left(\frac{2}{d_r + d_s}\right).$$

From Table 1, using the edge partition, the outcome can be obtained as

$$H(\mathcal{G}) = \left(\frac{2}{4+4}\right)(3mn+4m+2n+2) + \left(\frac{2}{4+8}\right)(6mn-4) \\ + \left(\frac{2}{8+8}\right)(3mn-4m-2n+2), \\ = \left(\frac{1}{8}\right)(3mn+4m+2n+2) + \left(\frac{1}{6}\right)(6mn-4) \\ + \left(\frac{1}{8}\right)(3mn-4m-2n+2).$$

By making some calculations, we get

$$\Rightarrow H(\mathcal{G}) = \frac{1}{24} \left(2 + 12m + 51mn + 6n \right).$$

Theorem 2.2.4. Let \mathcal{G} be the *CHDN3*(*m*, *n*) *mth* chain hexderived network of third type, then atom–bond connectivity and geometric–arithematic index are equal to

$$ABC(\mathcal{G}) = \frac{1}{8} \left(4\sqrt{5} (3mn-2) + \sqrt{14} (2-4m+3mn-2n) + 2\sqrt{6} (2+4m+3mn+2n) \right).$$
$$GA(\mathcal{G}) = 4 + 6mn + \frac{4\sqrt{2}}{3} (3mn-2).$$

Proof. Consider $\mathcal{G} \cong CHDN3(m, n)$. By using **Eq. 6**, we have

$$ABC(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}.$$

From **Table 2**, by using the edge partition, we get the outcome as,

$$ABC(\mathcal{G}) = \sqrt{\frac{4+4-2}{4\times 4}}(3mn+4m+2n+2) + \sqrt{\frac{4+8-2}{4\times 8}}(6mn-4) + \sqrt{\frac{8+8-2}{8\times 8}}(3mn-4m-2n+2),$$
$$= \sqrt{\frac{3}{8}}(3mn+4m+2n+2) + \sqrt{\frac{14}{64}}(6mn-4) + \sqrt{\frac{7}{32}}(3mn-4m-2n+2).$$

By making some calculations, we get

$$\Rightarrow ABC(\mathcal{G}) = \frac{1}{8} \left(4\sqrt{5} \left(3mn - 2 \right) + \sqrt{14} \left(2 - 4m + 3mn - 2n \right) \right.$$
$$+ 2\sqrt{6} \left(2 + 4m + 3mn + 2n \right) \right).$$

Using Eq. 7, we have

$$GA(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \frac{2\sqrt{d_r d_s}}{(d_r + d_s)}.$$

From Table 2, using the edge partition, we get the outcome as,

$$GA(\mathcal{G}) = \frac{2\sqrt{4\times4}}{(4+4)} (3mn+4m+2n+2) + \frac{2\sqrt{4\times8}}{(4+8)} (6mn-4) + \frac{2\sqrt{8\times8}}{(8+8)} (3mn-4m-2n+2), = (1)(3mn+4m+2n+2) + \frac{2\sqrt{2}}{3} (6mn-4) + (1)(3mn-4m-2n+2).$$

By making some calculations, we get

$$\Rightarrow GA(\mathcal{G}) = 4 + 6mn + \frac{4\sqrt{2}}{3}(3mn - 2).$$

Results for the Third Case of CHDN3(m, n)Chain Hex Derived Networks of Third Type

In this section, for the very first time, we discuss CHDN3(m, n)-derived hex-derived network and compute the exact results forRandic, Zagreb, harmonic, augmented Zagreb, atom-bond connectivity, and geometric-arithmetic indices for case 3.

Theorem 2.3.1. Consider the *mth* chain hex-derived network of type 3 *CHDN3* (m, n), the general *Randic* index for third case is equal to

$$R_{\alpha}(\mathcal{G}) = \begin{cases} -16(2+12m-27mn+6n), & \alpha = 1; \\ 4(-4m+(9+6\sqrt{2})mn-2(-5+4\sqrt{2}+n)), & \alpha = \frac{1}{2}; \\ \frac{1}{8}(4m+(9+6\sqrt{2})mn+2(7-4\sqrt{2}+n)), & \alpha = \frac{-1}{2}; \\ \frac{1}{64}(10+12m+27mn+6n), & \alpha = -1. \end{cases}$$

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. Using Eq. 2, we get

$$R_{\alpha}(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} (d_r d_s)^{\alpha}.$$

Using edge partitions in **Table 3**, we get, for $\alpha = 1$

$$R_{1}(\mathcal{G}) = (16)^{1} (3mn + 4m + 2n + 6) + (32)^{1} (6mn - 8) + (64)^{1} (3mn - 4m - 2n + 2).$$

By making some calculations, we get

$$\Rightarrow R_1(\mathcal{G}) = -16(2 + 12m + 27mn + 6n).$$

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

$$R_{\frac{1}{2}}(\mathcal{G}) = (16)^{\frac{1}{2}}(3mn+4m+2n+6) + (32)^{\frac{1}{2}}(6mn-8) + (64)^{\frac{1}{2}}(3mn-4m-2n+2).$$

By making some calculations, we get

$$\Rightarrow R_{\frac{1}{2}}(\mathcal{G}) = 4(-4m + (9 + 6\sqrt{2})mn - 2(-5 + 4\sqrt{2} + n)).$$

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

$$R_{\frac{1}{2}}(\mathcal{G}) = (16)^{-\frac{1}{2}}(3mn + 4m + 2n + 6) + (32)^{-\frac{1}{2}}(6mn - 8) + (64)^{-\frac{1}{2}}(3mn - 4m - 2n + 2).$$

By making some calculations, we get

$$\Rightarrow R_{-\frac{1}{2}}(\mathcal{G}) = \frac{1}{8} \left(4m + \left(9 + 6\sqrt{2}\right)mn + 2\left(7 - 4\sqrt{2} + n\right) \right).$$

For $\alpha = -1$,

$$R_{-1}(\mathcal{G}) = (16)^{-1} (3mn + 4m + 2n + 6) + (32)^{-1} (6mn - 8) + (64)^{-1} (3mn - 4m - 2n + 2).$$

By making some calculations, we get

$$\Rightarrow R_{-1}(\mathcal{G}) = \frac{1}{64} (10 + 12m + 27mn + 6n).$$

Theorem 2.3.2. Consider the *mth* chain hex-derived network of type 3 CHDN3(m, n), the first Zagreb index is equal to

$$M_1(\mathcal{G}) = -16(1 + 2m - 9mn + n).$$

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. Table 3 shows such an edge partition of \mathcal{G} for third case. Using Eq. 3, we get

$$M_1(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} (d_r + d_s).$$

Using edge partitions in Table 3, we get

$$M_{1}(\mathcal{G}) = (4+4)(3mn+4m+2n+6) + (4+8)(6mn-8) + (8+8)(3mn-4m-2n+2), = (8)(3mn+4m+2n+6) + (12)(6mn-8) + (16)(3mn-4m-2n+2).$$

By making some calculations, we get

$$\Rightarrow M_1(\mathcal{G}) = -16(1 + 2m - 9mn + n).$$

TABLE 3 Degree-Based Edge partition for Case 3.		
(d_r, d_s) where $rs \in \boldsymbol{E}(\mathcal{G})$	Number of Edges	
(4, 4)	(3 <i>mn</i> + 4 <i>m</i> + 2 <i>n</i> + 6)	
(4, 8)	(6 <i>mn</i> – 8)	
(8, 8)	(3mn - 4m - 2n + 2)	

Theorem 2.3.3. Consider the *mth* chain hex-derived network of type 3 CHDN3(m, n), the augmented Zagreb index and Harmonic Zagreb index are equal to

$$AZI(\mathcal{G}) = \frac{512}{1157625} (96546 - 692500m + 1221153mn - 346250n).$$
$$H(\mathcal{G}) = \frac{1}{24} (10 + 12m + 51mn + 6n).$$

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. Using Eq. 4,

$$AZI(\mathcal{G}) = \sum_{r \in E(\mathcal{G})} \left(\frac{d_r d_s}{d_r + d_s - 2} \right)^3.$$

From **Table 3**, using the edge partition, the outcome can be obtained as

$$\begin{aligned} AZI(\mathcal{G}) &= \left(\frac{4 \times 4}{4 + 4 - 2}\right)^3 (3mn + 4m + 2n + 6) \\ &+ \left(\frac{4 \times 8}{4 + 8 - 2}\right)^3 (6mn - 8) \\ &+ \left(\frac{8 \times 8}{8 + 8 - 2}\right)^3 (3mn - 4m - 2n + 2), \\ &= \left(\left(\frac{8}{3}\right)^3\right) (3mn + 4m + 2n + 6) + \left(\frac{16}{5}\right)^3 (6mn - 8) \\ &+ \left(\frac{32}{7}\right)^3 (3mn - 4m - 2n + 2). \end{aligned}$$

By making some calculations, we get

$$\Rightarrow AZI(\mathcal{G}) = \frac{512}{1157625} (96546 - 692500m + 1221153mn - 346250n).$$

Using Eq. 5,

$$H(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \left(\frac{2}{d_r + d_s}\right).$$

From **Table 3**, using the edge partition, the outcome can be obtained as

$$H(\mathcal{G}) = = \left(\frac{2}{4+4}\right)(3mn+4m+2n+2) + \left(\frac{2}{4+8}\right)(6mn-8) + \left(\frac{2}{8+8}\right)(3mn-4m-2n+2),$$
$$= \left(\frac{1}{8}\right)(3mn+4m+2n+6) + \left(\frac{1}{6}\right)(6mn-8) + \left(\frac{1}{8}\right)(3mn-4m-2n+2).$$

By making some calculations, we get

$$\Rightarrow H(\mathcal{G}) = \frac{1}{24} \left(10 + 12m + 51mn + 6n \right).$$

Theorem 2.3.4. Let \mathcal{G} be the *CHDN3* (*m*, *n*) *mth* chain hexderived network of third type, then atom-bond connectivity index is equal to

$$ABC(\mathcal{G}) = \frac{1}{8} \left(4\sqrt{5} \left(3mn - 4 \right) + \sqrt{14} \left(2 - 4m + 3mn - 2n \right) \right.$$
$$+ 2\sqrt{6} \left(6 + 4m + 3mn + 2n \right) \right).$$
$$GA(\mathcal{G}) = 8 + 6mn + \frac{4\sqrt{2}}{3} \left(3mn - 4 \right).$$

Proof. Let $\mathcal{G} \cong CHDN3(m, n)$. Using Eq. 6, we get

$$ABC(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}.$$

From **Table 3**, by using the edge partition, the outcome can be obtained as

$$ABC(\mathcal{G}) = \sqrt{\frac{4+4-2}{4\times 4}}(3mn+4m+2n+6) + \sqrt{\frac{4+8-2}{4\times 8}}(6mn-8) + \sqrt{\frac{8+8-2}{8\times 8}}(3mn-4m-2n+2),$$
$$= \sqrt{\frac{3}{8}}(3mn+4m+2n+6) + \sqrt{\frac{14}{64}}(6mn-8) + \sqrt{\frac{7}{32}}(3mn-4m-2n+2).$$

By making some calculations, we get

$$\Rightarrow ABC(\mathcal{G}) = \frac{1}{8} \left(4\sqrt{5} \left(3mn - 4 \right) + \sqrt{14} \left(2 - 4m + 3mn - 2n \right) \right.$$
$$+ 2\sqrt{6} \left(6 + 4m + 3mn + 2n \right) \right).$$

Using Eq. 7, we have

$$GA(\mathcal{G}) = \sum_{rs \in E(\mathcal{G})} \frac{2\sqrt{d_r d_s}}{d_r + d_s}.$$

From **Table 3**, using the edge partition, the outcome can be obtained as

$$GA(\mathcal{G}) = \frac{2\sqrt{4\times4}}{(4+4)} (3mn+4m+2n+6) + \frac{2\sqrt{4\times8}}{(4+8)} (6mn-8) + \frac{2\sqrt{8\times8}}{(8+8)} (3mn-4m-2n+2),$$

TABLE 4 | Numerical computation of *CHDN*3(m,n) for m = n.

	M₁	н	ABC	GA
(2.2)	480	10.08	28.04	46.86
(3.3)	1,152	21.46	61.88	105.14
(4.4)	2,112	37.08	108.91	186.74
(5.5)	3,360	56.96	169.12	291.65
(6.6)	4,896	81.08	242.53	419.88
(7.7)	6,720	109.46	329.12	571.41
(8.8)	8,832	142.08	428.91	746.27
(9.9)	11,232	178.96	541.88	944.43
(10.10)	13,920	220.08	668.04	1,165.93

$$= (1)(3mn + 4m + 2n + 6) + \frac{2\sqrt{2}}{3}(6mn - 8) + (1)(3mn - 4m - 2n + 2).$$

By making some calculations, we get

$$\Rightarrow GA(\mathcal{G}) = 8 + 6mn + \frac{4\sqrt{2}}{3}(3mn - 4).$$

- For the comparison of First Zagreb, harmonic, atom-bond connectivity, and geometric-arithmetic indices of CHDN3(m, n) for m = n, we computed the indices for different values of m and n. By increasing the values of m and n, we can clearly check from the following **Table 4**, the order of indices is also increasing, and their graphical structure is shown in **Figure 4**.
- For the comparison of first Zagreb, harmonic, atom-bond connectivity, and geometric-arithmetic indices of



TABLE 5 Numerical computation of *CHDN*3 (m, n) network for m < n, where *m* is odd and *n* is natural number.

	M 1	н	ABC	GA
(3.4)	1,568	28.08	84.75	140.11
(3.5)	1984	34.70	105.76	175.08
(3.6)	2,400	41.33	126.77	210.05
(3.7)	2,816	47.95	147.77	245.02
(3.8)	3,232	54.58	168.78	279.99
(3.9)	3,648	61.20	189.79	314.96
(3.10)	4,064	67.83	210.80	349.93
(3.11)	4,480	74.45	231.81	384.90
(3.12)	4,896	81.08	252.81	419.87
(3.13)	5,312	87.70	273.82	454.84

CHDN3(m, n) for m < n, where m is odd and n is natural number. By increasing the values of m and n, we can clearly check from the following **Table 5**, the order of indices is also increasing, and their graphical structure is shown in **Figure 5**.

- For the comparison of first Zagreb, harmonic, atom-bond connectivity, and geometric-arithmetic indices of CHDN3(m, n) for m < n, where m and n both are even. By increasing the values of m and n, we can clearly check from the following **Table 6**, the order of indices is also increasing, and their graphical structure is shown in **Figure 6**.
- For the comparison of first Zagreb, harmonic, atom-bond connectivity, and geometric-arithmetic indices of CHDN3(m, n) for m < n, where *m* is even and *n* is odd. By increasing the values of *m* and *n*, we can clearly check from the following **Table** 7, the order of indices is also increasing, and their graphical structure is shown in **Figure** 7.



TABLE 6 | Numerical computation of *CHDN3* (m, n) network for m < n, where m and n both are even.

TABLE 7 Numerical computation of *CHDN3* (m, n) network for m < n, where *m* is even and *n* is odd.

	M ₁	н	ABC	GA
(2.4)	1,024	19.08	57.79	93.48
(2.6)	1,568	28.08	86.62	140.11
(2.8)	2,112	37.08	115.45	186.73
(2.10)	2,656	46.08	144.28	233.36
(2.12)	3,200	55.08	173.10	279.99
(2.14)	3,744	64.08	201.93	226.62
(2.16)	4,288	73.08	230.76	373.24
(2.18)	4,832	82.08	259.58	419.87
(2.20)	5,376	91.08	288.41	466.50
(2.22)	5,920	100.08	317.24	513.13





CONCLUSION

In this article, we have calculated the exact solutions for degree-based indices for mth-hex-derived networks of third type. Hex-derived network has a variety of useful applications in pharmacy, electronics, and networking. We obtained the degree-based indices such as Randić, first Zagreb, augmented Zagreb, harmonic, atom-bond connectivity index, and geometric-arithmetic index for hex derived networks. For this network, we have also given the tabular and graphical comparison between indices. We came to know that by increasing the values of m and n, there is also increase in the indices, which shows the correctness of our results. These results may be helpful for people working in computer science and chemistry who encounter hex-derived networks.



DATA AVAILABILITY STATEMENT

All datasets presented in this study are included in the article/ Supplementary Material.

AUTHOR CONTRIBUTIONS

All the authors participated in the preparation and presenting of the manuscript.

SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fphy.2020.593275/full#supplementary-material

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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