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Comparative Study of rth Chain Benzenoid Hex-Derived Network

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Abstract. This study integrates advanced algorithms with chemical graph theory to analyze the topological indices of benzenoid-derived nanostructures, focusing on their applications in computational chemistry and drug design. By developing novel mathematical formulations for degree-based indices (R_α, M_1, H, AZI, ABC, and GA), we establish quantitative relationships between structural parameters (r, s) and physicochemical properties of hexagonal networks. Our results reveal that increasing network dimensions enhances molecular stability and electron delocalization in these nanostructures, offering critical insights for optimizing antiviral agents and energy storage materials. The proposed computational framework, validated through rigorous graphical and tabular comparisons, provides a robust tool for predicting structure-activity relationships in drug discovery and designing next-generation nanomaterials. This work bridges theoretical graph theory with practical applications in nanotechnology and pharmaceutical sciences, demonstrating significant potential for sustainable innovation in medical and energy technologies.

AMS (MOS) Subject Classification Codes: 05C12; 05C90
Key Words: general Randić index, harmonic index, augmented Zagreb index, atom-bond connectivity (ABC) index, geometric-arithmetic (GA) index, algorithms, rth Chain Benzenoid Hex-Derived Network, $CBHDN(r, s)$, drug design, nanostructures, edge computing, network structures.

1. INTRODUCTION

Graph theory provides powerful mathematical tools for modeling complex molecular structures, with chemical graph theory emerging as a vital interdisciplinary field that bridges mathematics and chemistry [4]. This approach represents molecules as graphs where vertices correspond to atoms and edges represent chemical bonds, enabling quantitative analysis of structural properties through topological indices. While topological indices like the Wiener index, R_α, M_1, AZI, H, ABC, and GA have been widely used in quantitative structure-activity relationship (QSAR) and structure-property relationship (QSPR) studies [5], significant gaps remain in their application to hexagonal mesh networks.

The present work makes several novel contributions to this field. First, we develop new analytical formulations for six topological indices (R_α, M_1, H, AZI, ABC, and GA) applied to Chain Benzenoid Hex-Derived Networks ($CBHDN$), extending beyond previous work on simple hexagonal meshes [4]. Our approach systematically addresses all three structural configurations: when $r = s$, when $r < s$ with parity constraints, and when $r > s$ with mixed parity conditions. These formulations provide a more complete mathematical framework for analyzing complex benzenoid structures.

Second, we establish previously unknown mathematical relationships between network dimensionality (r, s) and topological index behavior through rigorous derivations. This theoretical advancement provides fundamental insights into how structural variations affect molecular properties in benzenoid systems, particularly in understanding the connection between network geometry and chemical reactivity. The derived relationships offer predictive capabilities for molecular behavior that were not available in previous studies [3].

Third, we demonstrate practical applications through comprehensive graphical analysis, revealing how index variations correlate with stability and reactivity in polycyclic aromatic hydrocarbons. These materials are crucial for pharmaceutical and materials science applications, and our results provide valuable tools for molecular design. The graphical representations allow for intuitive understanding of complex relationships between structure and properties [2].

Building upon the foundational work of on hexagonal mesh construction, we significantly advance the theoretical framework by considering more complex chain benzenoid structures. Our results provide both theoretical advancements in chemical graph theory and practical tools for molecular design, addressing current limitations in predicting properties of extended benzenoid networks. The combination of rigorous mathematical analysis with practical applications distinguishes this work from previous studies in the field [8].

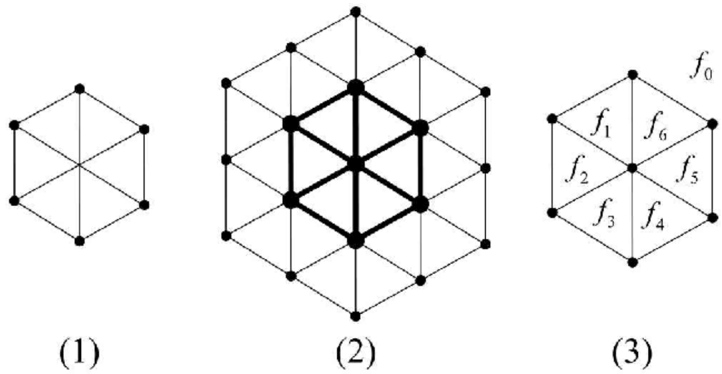

FIGURE 1. Hexagonal meshes: (1)HX(2), (2)HX(3), and(3), all facing HX(2).

The topological indices of polygonal mesh produced by a polygonal graph, which comprise molecular graphs of unbranched benzene hydrocarbons, are considered in this article. Hexagonal structure graphs are made up of hexagons that have been joined together. This class of chemical compounds is very important to theoretical chemists. For individual molecule graphs, topological index theory has been extensively explored during the last four decades. Benzene hydrocarbons are not only important raw materials in the chemical industry, but they are also dangerous pollutants. Chen et al. [4] introduced a novel hexagonal mesh structure. This mesh consists of interconnected triangles, forming a hexagonal pattern. Notably, a single layer of triangles cannot constitute a hexagonal mesh. A fundamental 2-dimensional hexagonal mesh, denoted as $HX(2)$, is formed by arranging six triangles (Figure 1(1)). To create a 3-dimensional hexagonal mesh, $HX(3)$, an additional layer of triangles is added around the perimeter of $HX(2)$ (Figure 1(2)). This iterative process is extended to construct higher-dimensional hexagonal meshes, $HX(r)$, by recursively adding r layers of triangles around the boundary of each preceding mesh.

The Wiener index was the earliest topological index to be applied in chemistry. Harold Wiener [21] developed the term in 1947. A computer network can be represented to use the Wiener index.

$$W(G) = \frac{1}{2} \sum_{x,y \subseteq V(G)} d(x,y). \tag{1. 1}$$

Milan Randić [17] created the Randić index in 1975. The Randić index is the earliest and most primitive degree-based topological index.

$$R_\alpha(G) = \sum_{xy \in E(G)} (d_x d_y)^\alpha, \tag{1. 2}$$

Estrada et al. [6] recognized's degree-based topological indices is the atom-bond connectivity (ABC) index.

$$ABC(G) = \sum_{xy \in E(G)} \sqrt{\frac{d_x + d_y - 2}{d_x d_y}}. \quad (1.\ 3)$$

Another recognized connectivity topological caption established by Vukicevic et al. [19] is the Geometric-arithmetic (GA) index.

$$GA(G) = \sum_{xy \in E(G)} \frac{2\sqrt{d_x d_y}}{d_x + d_y}. \quad (1.\ 4)$$

Gutman [9] established a significant topological index. The Zagreb index is represented by $M_1(G)$ and has the following

$$M_1(G) = \sum_{xy \in E(G)} (d_x + d_y). \quad (1.\ 5)$$

Zhong [22] introduced the harmonic index, which is defined as

$$H(G) = \sum_{xy \in E(G)} \frac{2}{d_x + d_y}. \quad (1.\ 6)$$

Furtula et al. [7] proposed the augmented Zagreb index, which is defined as

$$AZI(G) = \sum_{xy \in E(G)} (\frac{d_x d_y}{d_x + d_y - 2}). \quad (1.\ 7)$$

2. Cases for rth Chain Benzenoid Hex-Derived Network. $CBHDN(r, s)$

There are three cases for $CBHDN(r, s)$.
Case-1: For $r = s$, $(r, s) \geq 1$.
Case-2: For $r < s$, r is odd and $s \in N$. For $r > s$, r is odd and $s \in N$. For $r < s$, r and s both are even. For $r > s$, r and s both are even.
Case-3: For $r < s$, r is even and s is odd. For $r > s$, r is even and s is odd.

3. Results

Simonraj et al. [18] found hex-derived networks and calculated the metric dimension of $(BHDN)$. In this article, we analyze the newly found $(CBHDN(r, s))$'s and calculate the precise results for topological indexes that are degree-based. These derived topological indices are currently use in the subject of rigorous examination [1, 10, 11, 12, 13, 14, 15, 16, 20].

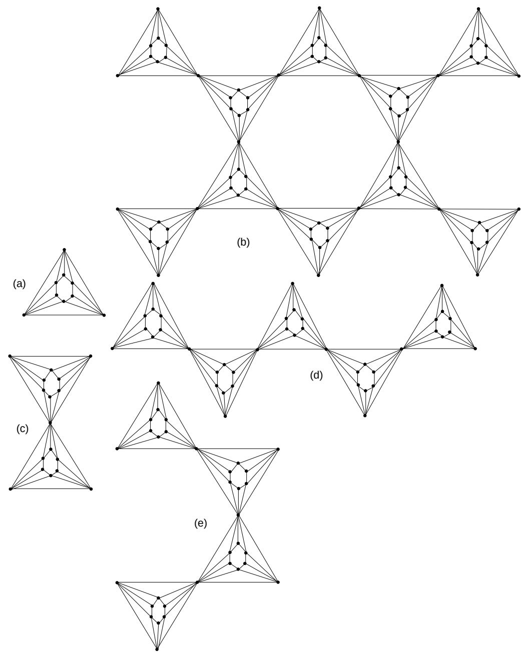

FIGURE 2. Chain Benzenoid Hex-Derived Networks $(CBHDN)$

(d_x, d_y)	Number of Edges	(d_x, d_y)	Number of Edges
(3,4)	6rs	(4,10)	6rs-6s
(3,5)	3s	(5,5)	2
(3,10)	3rs-6s	(5,10)	6s-4
(4,5)	6s	(10,10)	3rs-3r-3s+2

TABLE 1. Edge Partition for $r = s$

3.1. **Results for the First Case rth Chain Benzenoid Hex-Derived Network,** $CBHDN(r, s)$**.** In this part, we examine $CBHDN(r, s)$, which is formed from a HDN, for the first time, and estimate the exact findings for R_α, M_1, H, AZI, ABC, and GA indices for case 1.

Theorem 3.2. *Consider Chain Benzenoid Hex-Derived Network $CBHDN(r,s)$, the Randić index is*

$$R_\alpha(CBHDN(r,s)) = \begin{cases} 702rs - 300r - 165s + 50, & \alpha = 1; \\ \frac{78rs-3r+24s+2}{100}, & \alpha = -1; \\ 3(10+4\sqrt{3}+4\sqrt{10}+\sqrt{30})rs \\ +10(3-3r-3s) - 3(4\sqrt{10} \\ +\sqrt{30}+4\sqrt{5}+\sqrt{15}+10\sqrt{2})s \\ -20\sqrt{2}, & \alpha = \frac{1}{2}; \\ \frac{1}{10}(6-4\sqrt{2}-3r-3s+(3 \\ +10\sqrt{3}+3\sqrt{10}+\sqrt{30})rs \\ +(6\sqrt{2}-3\sqrt{10}+2\sqrt{15}-\sqrt{30})s), & \alpha = \frac{-1}{2}. \end{cases}$$

Proof. Let $G \cong CBHDN(r,s)$ be the chain hex derived network. Using edge partition from Table 1 and equation 1. 2 , we obtained.
For $\alpha = 1$,

$$\begin{aligned} R_1(G) &= 12(6rs) + 15(3s) + 30(3rs-3s) + 20(6s) + 40(6rs-6s) \\ &\quad +25(2) + 50(6s-4) + 100(3rs-3r-3s+2), \\ R_1(G) &= 702rs - 300r - 165s + 50. \end{aligned}$$

For $\alpha = -1$,

$$\begin{aligned} R_{-1}(G) &= \frac{6rs}{12} + \frac{3s}{15} + \frac{3rs-6s}{30} + \frac{6s}{20} + \frac{6rs-6s}{40} + \frac{2}{25} + \frac{6s-4}{50} + \\ &\quad \frac{3rs-3r-3s+2}{100}, \\ R_{-1}(G) &= \frac{78rs-3r+24s+2}{100}. \end{aligned}$$

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

$$\begin{aligned} R_{\frac{1}{2}}(G) &= 6rs\sqrt{12} + 3s\sqrt{15} + (3rs-3s)\sqrt{30} + 6s\sqrt{20} \\ &\quad +(6rs-6s)\sqrt{40} + 2\sqrt{25} + (6s-4)\sqrt{50} \\ &\quad +(3rs-3r-3s+2)\sqrt{100} \\ R_{\frac{1}{2}}(G) &= 3(10+4\sqrt{3}+4\sqrt{10}+\sqrt{30})rs + 10(3-3r-3s) \\ &\quad -3(4\sqrt{10}+\sqrt{30}+4\sqrt{5}+\sqrt{15}+10\sqrt{2})s - 20\sqrt{2}. \end{aligned}$$

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

$$\begin{aligned} R_{-\frac{1}{2}}(G) &= \frac{6rs}{\sqrt{12}} + \frac{3s}{\sqrt{15}} + \frac{3rs-3s}{\sqrt{30}} + \frac{6s}{\sqrt{20}} + \frac{6rs-6s}{\sqrt{40}} + \frac{2}{\sqrt{25}} \\ &\quad + \frac{6s-4}{\sqrt{50}} + \frac{3rs-3r-3s+2}{\sqrt{100}} \\ R_{-\frac{1}{2}}(G) &= \frac{1}{10}(6-4\sqrt{2}-3r-3s+(3+10\sqrt{3}+3\sqrt{10}+\sqrt{30})rs \\ &\quad +(6\sqrt{2}-3\sqrt{10}+2\sqrt{15}-\sqrt{30})s). \end{aligned}$$

□

Theorem 3.3. *Consider Chain Benzenoid Hex-Derived Network $CBHDN(r,s)$, the atom-bond connectivity index is*

$$\begin{aligned} ABC(G) &= \frac{1}{10}(8\sqrt{2}+10\sqrt{15}rs+3\sqrt{2}(3rs-3r-3s+2) \\ &+(6\sqrt{30}+\sqrt{330})(rs-s)+(6\sqrt{10}+6\sqrt{35})s \\ &+2\sqrt{26}(3s-2)). \end{aligned}$$

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 1 and the equation 1. 3 , we easily prove it.

$$\begin{aligned} ABC(G) &= 6rs\sqrt{\frac{5}{12}}+3s\sqrt{\frac{6}{15}}+(3rs-6s)\sqrt{\frac{11}{30}}+6s\sqrt{\frac{7}{20}} \\ &+(6rs-6s)\sqrt{\frac{12}{40}}+2\sqrt{\frac{8}{25}}+(6s-4)\sqrt{\frac{13}{50}} \\ &+(3rs-3r-3s+2)\frac{3\sqrt{2}}{10}, \\ ABC(G) &= \frac{1}{10}(8\sqrt{2}+10\sqrt{15}rs+3\sqrt{2}(3rs-3r-3s+2) \\ &+(6\sqrt{30}+\sqrt{330})(rs-s)+(6\sqrt{10}+6\sqrt{35})s \\ &+2\sqrt{26}(3s-2)). \end{aligned}$$

□

Theorem 3.4. *Consider $CBHDN(r,s)$, the geometric arithmetic is*

$$\begin{aligned} GA(G) &= 3rs-3r-3s+4+\frac{24\sqrt{3}}{7}rs+(\frac{12\sqrt{10}}{7} \\ &+\frac{\sqrt{30}}{5})(rs-s)+(\frac{8\sqrt{5}}{3}+\frac{3\sqrt{15}}{4})s \\ &+\frac{4\sqrt{2}}{3}(3s-2). \end{aligned}$$

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 1 and the equation 1. 4 , we easily prove it.

$$\begin{aligned}
GA(G) &= 6rs(\frac{2\sqrt{12}}{7}) + 3s(\frac{2\sqrt{15}}{8}) + (3rs-6s)(\frac{2\sqrt{30}}{13}) \\
&+6s(\frac{2\sqrt{20}}{9}) + (6rs-6s)(\frac{2\sqrt{40}}{14}) + 2(\frac{2\sqrt{25}}{10}) \\
&+(6s-4)(\frac{2\sqrt{50}}{15}) + (3rs-3r-3s+2)(\frac{2\sqrt{100}}{20}) \\
GA(G) &= 3rs-3r-3s+4+\frac{24\sqrt{3}}{7}rs + (\frac{12\sqrt{10}}{7} \\
&+\frac{\sqrt{30}}{5})(rs-s) + (\frac{8\sqrt{5}}{3} + \frac{3\sqrt{15}}{4})s \\
&+\frac{4\sqrt{2}}{3}(3s-2).
\end{aligned}$$

□

Theorem 3.5. *Consider $CBHDN(r,s)$, Zagreb index is*

$$M_1(G) = 15(15rs-4r-s).$$

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 1 and the equation 1. 5 , we easily prove it.

$$\begin{aligned}
M_1(G) &= 7(6rs) + 8(3s) + 13(3rs-6s) + 9(6s) \\
&+14(6rs-6s) + 10(2) + 15(6s-4) \\
&+20(3rs-3r-3s+2) \\
M_1(G) &= 15(15rs-4r-s).
\end{aligned}$$

□

Theorem 3.6. *Consider $CBHDN(r,s)$, the Zagreb index is*

$$M_2(G) = 702rs - 300r - 165s + 50.$$

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 1 and the equation 1. 3 for $\alpha = 1$, we easily prove it.

$$\begin{aligned}
M_2(G) &= 12(6rs) + 15(3s) + 30(3rs-6s) + 20(6s) + 40(6rs-6s) \\
&+25(2) + 50(6s-4) + 100(3rs-3r-3s+2) \\
M_2(G) &= 702rs - 300r - 165s + 50.
\end{aligned}$$

□

Theorem 3.7. *Consider $CBHDN(r,s)$, the harmonic index is*

$$H(G) = \frac{18198rs - 1638r + 6905s + 364}{5460}.$$

(d_x, d_y)	Number of Edges	(d_x, d_y)	Number of Edges
(3,4)	6rs	(4,10)	6rs-4r-2s
(3,5)	2r+s	(5,5)	2
(3,10)	3rs-2r-s	(5,10)	4r+2s-4
(4,5)	4r+2s	(10,10)	3rs-4r-2s+2

TABLE 2. Edge Partition for Case 2

Proof. Let G be the $CBHDN(r, s)$. The proof is just calculation based. Using the edge partition given in Table 1 and the equation 1. 7 , we easily prove it.

$$\begin{aligned} H(G) &= 6rs(\frac{2}{7}) + 3s(\frac{2}{8}) + (3rs - 6s)(\frac{2}{13}) + 6s(\frac{2}{9}) \\ &\quad +(6rs - 6s)(\frac{2}{14}) + 2(\frac{2}{10}) + (6s - 4)(\frac{2}{15}) \\ &\quad +(3rs - 3r - 3s + 2)(\frac{2}{20}) \\ H(G) &= \frac{18198rs - 1638r + 6905s + 364}{5460}. \end{aligned}$$

□

Theorem 3.8. *Consider $CBHDN(r, s)$, the augmented Zagreb index is*

$$\begin{aligned} AZI(G) &= \frac{35594853344}{40429125}rs - \frac{125000}{243}r - \frac{525073235325875}{1949837833944}s \\ &\quad +\frac{72321203125}{410012928}. \end{aligned}$$

Proof. Let G be the $CBHDN(r, s)$. The proof is just calculation based. Using the edge partition given in Table 1 and the equation 1. 7 , we easily prove it.

$$\begin{aligned} AZI(G) &= 6rs(\frac{12}{5})^3 + 3s(\frac{15}{6})^3 + (3rs - 6s)(\frac{30}{11})^3 + 6s(\frac{20}{7})^3 \\ &\quad +(6rs - 6s)(\frac{40}{12})^3 + 2(\frac{25}{8})^3 + (6s - 4)(\frac{50}{13})^3 \\ &\quad +(3rs - 3r - 3s + 2)(\frac{100}{18})^3 \\ AZI(G) &= \frac{35594853344}{40429125}rs - \frac{125000}{243}r - \frac{525073235325875}{1949837833944}s \\ &\quad +\frac{72321203125}{410012928}. \end{aligned}$$

□

3.9. **Results for the Second Case rth Chain Benzenoid Hex-Derived Network, $CBHDN(r, s)$.** In this part, we examine $CBHDN(r, s)$, which is formed from a HDN, for the first time, and estimate the exact findings for R_α, M_1, H, AZI, ABC, and GA indices for case 2.

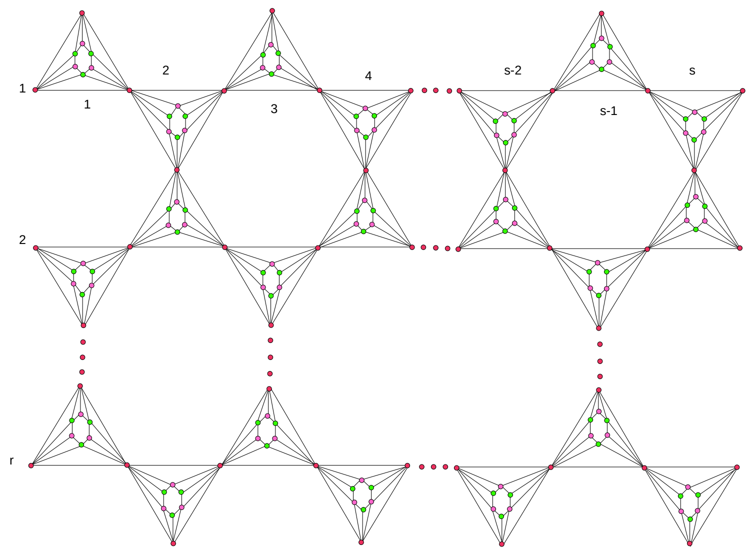

FIGURE 3. Chain Benzenoid Hex-Derived Networks $(CBHDN)$

Theorem 3.10. *Consider Chain Hex Derived Network $CBHDN(r,s)$, the Randić index is*

$$R_\alpha(CBHDN(r,s)) = \begin{cases} 702rs - 310r - 155s + 50, & \alpha = 1; \\ \frac{234rs+62r+31sn+6}{300}, & \alpha = -1; \\ 10 + 12\sqrt{3}rs + 10(3rs \\ -4r - 2s + 2) + 10\sqrt{2}(2r \\ +s - 2) + (4\sqrt{5} + \sqrt{15})(2r \\ +s) + (4\sqrt{10} + \sqrt{30})(3rs \\ -2r - sn), & \alpha = \frac{1}{2}; \\ \frac{1}{30}(9rs - 12r - 6s + 18 \\ +30\sqrt{3}rs + 6\sqrt{2}(2r + s \\ -2) + (6\sqrt{5} + 2\sqrt{15})(2r + s) \\ +(3\sqrt{10} + \sqrt{30})(3rs \\ -2r - s)), & \alpha = \frac{-1}{2}; \end{cases}$$

Proof. Let $G \cong CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 2 and the equation 1. 2 , we easily prove it.
For $\alpha = 1$,

$$\begin{aligned} R_1(G) &= 12(6rs) + 15(2r+s) + 30(3rs - 2r - s) \\ &\quad +20(4r+2s) + 40(6rs - 4r - 2s) + 25(2) \\ &\quad +50(4r + 2s - 4) + 100(3rs - 4r - 2s + 2), \\ R_1(G) &= 702rs - 310r - 155s + 50. \end{aligned}$$

For $\alpha = -1$,

$$\begin{aligned}
R_{-1}(G) &= \frac{6rs}{12} + \frac{2r+s}{15} + \frac{3rs-2r-s}{30} + \frac{4r+2s}{20} + \frac{6rs-4r-2s}{40} \\
&\quad + \frac{2}{25} + \frac{4r+2s-4}{50} + \frac{3rs-4r-2s+2}{100}, \\
R_{-1}(G) &= \frac{234rs+62r+31s+6}{300}.
\end{aligned}$$

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

$$\begin{aligned}
R_{\frac{1}{2}}(G) &= 6rs\sqrt{12} + (2r+s)\sqrt{15} + (3rs-2r-s)\sqrt{30} + (4r+2s)\sqrt{20} \\
&\quad +(6rs-4r-2s)\sqrt{40} + 2\sqrt{25} + (4r+2s-4)\sqrt{50} \\
&\quad +(3rs-4r-2s+2)\sqrt{100}, \\
R_{\frac{1}{2}}(G) &= 10 + 12\sqrt{3}rs + 10(3rs-4r-2s+2) + 10\sqrt{2}(2r+s-2) \\
&\quad +(4\sqrt{5}+\sqrt{15})(2r+s) + (4\sqrt{10}+\sqrt{30})(3rs-2r-s).
\end{aligned}$$

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

$$\begin{aligned}
R_{-\frac{1}{2}}(G) &= \frac{6rs}{\sqrt{12}} + \frac{2r+s}{\sqrt{15}} + \frac{3rs-2r-s}{\sqrt{30}} + \frac{4r+2s}{\sqrt{20}} \\
&\quad + \frac{6rs-4r-2s}{\sqrt{40}} + \frac{2}{\sqrt{25}} + \frac{4r+2s-4}{\sqrt{50}} \\
&\quad + \frac{3rs-4r-2s+2}{\sqrt{100}}, \\
R_{-\frac{1}{2}}(G) &= \frac{1}{30}(9rs-12r-6s+18+30\sqrt{3}rs+6\sqrt{2}(2r+s-2) \\
&\quad +(6\sqrt{5}+2\sqrt{15})(2r+s) + (3\sqrt{10}+\sqrt{30})(3rs-2r-s)).
\end{aligned}$$

□

Theorem 3.11. *For Chain Hex Derived Network, the atom-bond connectivity index is*

$$\begin{aligned}
ABC(G) &= \frac{1}{30}(24\sqrt{2} + 30\sqrt{15}rs + 9\sqrt{2}(3rs-4r-2s+2) \\
&\quad +6\sqrt{26}(2r+s-2) + (6\sqrt{10}+6\sqrt{35})(2r+s) \\
&\quad +(6\sqrt{30}+\sqrt{330})(3rs-2r-s)).
\end{aligned}$$

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 2 and the equation 1. 3 , we easily prove it.

$$\begin{aligned} ABC(G) &= 6rs\sqrt{\frac{5}{12}}+(2r+s)\sqrt{\frac{6}{15}}+(3rs-2r-s)\sqrt{\frac{11}{30}} \\ &\quad +(4r+2s)\sqrt{\frac{7}{20}}+(6rs-4r-2s)\sqrt{\frac{12}{40}}+2\sqrt{\frac{8}{25}} \\ &\quad +(4r+2s-4)\sqrt{\frac{13}{50}}+(3rs-4r-2s+2)\sqrt{\frac{18}{100}}, \\ ABC(G) &= \frac{1}{30}(24\sqrt{2}+30\sqrt{15}rs+9\sqrt{2}(3rs-4r-2s+2) \\ &\quad +6\sqrt{26}(2r+s-2)+(6\sqrt{10}+6\sqrt{35})(2r+s) \\ &\quad +(6\sqrt{30}+\sqrt{330})(3rs-2r-s)). \end{aligned}$$

□

Theorem 3.12. *Consider $CBHDN(r,s)$, the geometric arithmetic index is*

$$\begin{aligned} GA(G) &= 3rs-4r-2s+4+\frac{24\sqrt{3}}{7}rs+\frac{4\sqrt{2}}{3}(2r+s-2) \\ &\quad +(\frac{8\sqrt{5}}{9}+\frac{\sqrt{15}}{4}(2r+s)+(\frac{4\sqrt{10}}{7}+\frac{2\sqrt{30}}{13})(3rs-2r-s)). \end{aligned}$$

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 2 and the equation 1. 4 , we easily prove it.

$$\begin{aligned} GA(G) &= 6rs(\frac{2\sqrt{12}}{7})+(2r+s)(\frac{2\sqrt{15}}{8})+(3rs-2r-s)(\frac{2\sqrt{30}}{13}) \\ &\quad +(4r+2s)(\frac{2\sqrt{20}}{9})+(6rs-4r-2s)(\frac{2\sqrt{40}}{14})+2(\frac{2\sqrt{25}}{10}) \\ &\quad +(4r+2s-4)(\frac{2\sqrt{50}}{15})+(3rs-4r-2s+2)(\frac{2\sqrt{100}}{20}) \\ GA(G) &= 3rs-4r-2s+4+\frac{24\sqrt{3}}{7}rs+\frac{4\sqrt{2}}{3}(2r+s-2) \\ &\quad +(\frac{8\sqrt{5}}{9}+\frac{\sqrt{15}}{4}(2r+s)+(\frac{4\sqrt{10}}{7}+\frac{2\sqrt{30}}{13})(3rs-2r-s)). \end{aligned}$$

□

Theorem 3.13. *For $CBHDN(r,s)$, the Zagreb index is*

$$M_1(G) = 25(9rs-2r-s).$$

Proof. Let G be the $CBHDN(r, s)$. The proof is just calculation based. Using the edge partition given in Table 2 and the equation 1. 5 , we easily prove it.

$$\begin{aligned} M_1(G) &= 7(6rs) + 8(2r + s) + 13(3rs - 2r - s) + 9(4r + 2s) \\ &\quad +14(6rs - 4r - 2s) + 10(2) + 15(4r + 2s - 4) \\ &\quad +20(3rs - 4r - 2s + 2) \\ M_1(G) &= 25(9rs - 2r - s). \end{aligned}$$

□

Theorem 3.14. *For $CBHDN(r, s)$, the Zagreb index is*

$$M_2(G) = 702rs - 310r - 155s + 50.$$

Proof. Let G be the $CBHDN(r, s)$. The proof is just calculation based. Using the edge partition given in Table 2 and the equation 1. 2 for $\alpha = 1$, we easily prove it.

$$\begin{aligned} M_2(G) &= 12(6rs) + 15(2r + s) + 30(3rs - 2r - s) \\ &\quad +20(4r + 2s) + 40(6rs - 4r - 2s) + 25(2) \\ &\quad +50(4r + 2sn - 4) + 100(3rs - 4r - 2s + 2) \\ M_2(G) &= 702rs - 310r - 155s + 50. \end{aligned}$$

□

Theorem 3.15. *For $CBHDN(r, s)$, the harmonic index is*

$$H(G) = \frac{54594rs + 10534r + 5267s + 1092}{16380}.$$

Proof. Let G be the $CBHDN(r, s)$. The proof is just calculation based. Using the edge partition given in Table 2 and the equation 1. 6 , we easily prove it.

$$\begin{aligned} H(G) &= 6rs(\frac{2}{7}) + (2r + s)(\frac{2}{8}) + (3rs - 2r - s)(\frac{2}{13}) \\ &\quad +(4r + 2s)(\frac{2}{9}) + (6rs - 4r - 2s)(\frac{2}{14}) + 2(\frac{2}{10}) \\ &\quad +(4r + 2s - 4)(\frac{2}{15}) + (3rs - 4r - 2s + 2)(\frac{2}{20}) \\ H(G) &= \frac{54594rs + 10534r + 5267s + 1092}{16380}. \end{aligned}$$

□

Theorem 3.16. *Consider $CBHDN(r, s)$, augmented Zagreb index is*

$$AZI(G) = \frac{(1.2224r + 2.0600rs) \times 10^{19} - 15625(3.9118s - 2.6413) \times 10^{14}}{2.3398 \times 10^{16}}.$$

(d_x, d_y)	Number of Edges	(d_x, d_y)	Number of Edges
(3,4)	6rs	(4,10)	6rs-4r-2s
(3,5)	2r+s+1	(5,5)	4
(3,10)	3rs-2r-s	(5,10)	4r+2s-6
(4,5)	4r+2s+2	(10,10)	3rs-4r-2s+2

TABLE 3. Edge Partition for Case 3

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 2 and the equation 1. 7 , we easily prove it.

$$\begin{aligned}
AZI(G) &= 6rs(\frac{12}{5})^3 + (2r+s)(\frac{15}{6})^3 + (3rs-2r-s)(\frac{30}{11})^3 \\
&\quad +(4r+2s)(\frac{20}{7})^3 + (6rs-4r-2s)(\frac{40}{12})^3 + 2(\frac{25}{8})^3 \\
&\quad +(4r+2s-4)(\frac{50}{13})^3 + (3rs-4r-2s+2)(\frac{100}{18})^3 \\
AZI(G) &= \frac{(1.2224r + 2.0600rs)\times 10^{19} - 15625(3.9118s - 2.6413)\times 10^{14}}{2.3398\times 10^{16}}.
\end{aligned}$$

□

3.17. **Results for the Third Case rth Chain Benzenoid Hex-Derived Network, $CBHDN(r,s)$.** In this part, we examine $CBHDN(r,s)$, which is formed from a HDN, for the first time, and estimate the exact findings for R_α, M_1, H, AZI, ABC, and GA indices for case 3.

Theorem 3.18. *For Chain Hex Derived Network $CBHDN(r,s)$, the Randić index is*

$$R_\alpha(CBHDN(r,s)) = \begin{cases} 702rs - 310r - 155s + 55, & \alpha = 1; \\ \frac{234rs+62r+31s+68}{300}, & \alpha = -1; \\ 20 + 12\sqrt{3}rs + 10(3rs \\ -4r - 2s + 2) + 10\sqrt{2}(2r \\ +s-3) + (4\sqrt{5}+\sqrt{15})(2r \\ +s+1) + (4\sqrt{10}+ \\ \sqrt{30})(3rs-2r-s), & \alpha = \frac{1}{2}; \\ \frac{1}{30}(30 - 12r + 9rs \\ +30\sqrt{3}rs - 6s + 6\sqrt{2}(2r \\ +s-3) + (6\sqrt{5}+2\sqrt{15})(2r \\ +s+1) + (3\sqrt{10}+ \\ \sqrt{30})(3rs-2r-s)), & \alpha = \frac{-1}{2}. \end{cases}$$

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 3 and the equation 1. 2 , we easily prove it.
For $\alpha = 1$,

$$\begin{aligned}
R_1(G) &= 12(6rs) + 15(2r+s+1) + 30(3rs-2r-s) \\
&\quad +20(4r+2s+2) + 40(6rs-4r-2s) + 25(4) \\
&\quad +50(4r+2s-6) + 100(3rs-4r-2s+2), \\
R_1(G) &= 702rs - 310r - 155s + 55.
\end{aligned}$$

For $\alpha = -1$,

$$\begin{aligned}
R_{-1}(G) &= \frac{6rs}{12} + \frac{2r+s+1}{15} + \frac{3rs-2r-s}{30} \\
&\quad + \frac{4r+2s+2}{20} + \frac{6rs-4r-2s}{40} + \frac{4}{25} \\
&\quad + \frac{4r+2s-6}{50} + \frac{3rs-4r-2s+2}{100}, \\
R_{-1}(G) &= \frac{234rs+62r+31s+68}{300}.
\end{aligned}$$

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

$$\begin{aligned}
R_{\frac{1}{2}}(G) &= 6rs\sqrt{12} + (2r+s+1)\sqrt{15} + (3rs-2r-s)\sqrt{30} \\
&\quad +(4r+2s+2)\sqrt{20} + (6rs-4r-2s)\sqrt{40} + 4\sqrt{25} \\
&\quad +(4r+2s-6)\sqrt{50} + (3rs-4r-2s+2)\sqrt{100}, \\
R_{\frac{1}{2}}(G) &= 20 + 12\sqrt{3}rs + 10(3rs-4r-2s+2) + 10\sqrt{2}(2r+s-3), \\
&\quad +(4\sqrt{5}+\sqrt{15})(2r+s+1) + (4\sqrt{10}+\sqrt{30})(3rs-2r-s).
\end{aligned}$$

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

$$\begin{aligned}
R_{-\frac{1}{2}}(G) &= \frac{6rs}{\sqrt{12}} + \frac{2r+s+1}{\sqrt{15}} + \frac{3rs-2r-s}{\sqrt{30}} + \frac{4r+2s+2}{\sqrt{20}} \\
&\quad + \frac{6rs-4r-2s}{\sqrt{40}} + \frac{4}{\sqrt{25}} + \frac{4r+2s-6}{\sqrt{50}} \\
&\quad + \frac{3rs-4r-2s+2}{\sqrt{100}}, \\
R_{-\frac{1}{2}}(G) &= \frac{1}{30}(30 - 12r + 9rs + 30\sqrt{3}rs - 6s + 6\sqrt{2}(2r+s-3) \\
&\quad +(6\sqrt{5}+2\sqrt{15})(2r+s+1) + (3\sqrt{10}+\sqrt{30})(3rs-2r-s)).
\end{aligned}$$

□

Theorem 3.19. *Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 3 and the equation 1. 3 , we easily prove it.*

$$\begin{aligned}
ABC(G) &= \frac{1}{30}(48\sqrt{2} + 30\sqrt{15}rs + 9\sqrt{2}(3rs-4r-2s+2) \\
&\quad +6\sqrt{26}(2r+s-3) + (6\sqrt{10}+6\sqrt{35})(2r+s+1) \\
&\quad +(6\sqrt{30}+\sqrt{330})(3rs-2r-s)).
\end{aligned}$$

Proof. Let $CBHDN$ using edge partition, we obtained

$$\begin{aligned}
ABC(G) &= 6rs\sqrt{\frac{5}{12}}+(2r+s+1)\sqrt{\frac{6}{15}}+(3rs-2r-s)\sqrt{\frac{11}{30}} \\
&+(4r+2s+2)\sqrt{\frac{7}{20}}+(6rs-4r-2s)\sqrt{\frac{12}{40}}+4\sqrt{\frac{8}{25}} \\
&+(4r+2s-6)\sqrt{\frac{13}{50}}+(3rs-4r-2s+2)\sqrt{\frac{18}{100}} \\
ABC(G) &= \frac{1}{30}(48\sqrt{2}+30\sqrt{15}rs+9\sqrt{2}(3rs-4r-2s+2) \\
&+6\sqrt{26}(2r+s-3)+(6\sqrt{10}+6\sqrt{35})(2r+s+1) \\
&+(6\sqrt{30}+\sqrt{330})(3rs-2r-s)).
\end{aligned}$$

□

Theorem 3.20. *Consider $CBHDN(r,s)$, geometric arithmetic index is*

$$\begin{aligned}
GA(G) &= 3rs-4r-2s+6+\frac{24\sqrt{3}}{7}rs+\frac{4(2r+s-3)\sqrt{2}}{3} \\
&+(\frac{8\sqrt{5}}{9}+\frac{\sqrt{15}}{4})(2r+s+1)+(\frac{4\sqrt{10}}{7} \\
&+\frac{2\sqrt{30}}{13})(3rs-2r-s).
\end{aligned}$$

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 3 and the equation 1. 4 , we easily prove it.

$$\begin{aligned}
GA(G) &= 6rs\frac{2\sqrt{12}}{7}+(2r+s+1)\frac{2\sqrt{15}}{8}+(3rs-2r-s)\frac{2\sqrt{30}}{13} \\
&+(4r+2s+2)\frac{2\sqrt{20}}{9}+(6rs-4r-2s)\frac{2\sqrt{40}}{14}+4\frac{2\sqrt{25}}{10} \\
&+(4r+2s-6)\frac{2\sqrt{50}}{15}+(3rs-4r-2s+2)\frac{2\sqrt{100}}{20} \\
GA(G) &= 3rs-4r-2s+6+\frac{24\sqrt{3}}{7}rs+\frac{4(2r+s-3)\sqrt{2}}{3} \\
&+(\frac{8\sqrt{5}}{9}+\frac{\sqrt{15}}{4})(2r+s+1)+(\frac{4\sqrt{10}}{7} \\
&+\frac{2\sqrt{30}}{13})(3rs-2r-s).
\end{aligned}$$

□

Theorem 3.21. *Consider $CBHDN(r,s)$, Zagreb index is*

$$M_1(G) = 225rs-50r-25s+16.$$

Proof. Let G be the $CBHDN(r, s)$. The proof is just calculation based. Using the edge partition given in Table 3 and the equation 1. 5 , we easily prove it.

$$\begin{aligned}
M_1(G) &= 7(6rs) + 8(2r + s + 1) + 13(3rs - 2r - s) + 9(4r + 2s + 2) \\
&\quad +14(6rs - 4r - 2s) + 10(4) + 15(4r + 2s - 6) \\
&\quad +20(3rs - 4r - 2s + 2) \\
M_1(G) &= 225rs - 50r - 25s + 16.
\end{aligned}$$

□

Theorem 3.22. *Consider $CBHDN(r, s)$, the Zagreb index is*

$$M_2(G) = 702rs - 310r - 155s + 55.$$

Proof. Let G be the $CBHDN(r, s)$. The proof is just calculation based. Using the edge partition given in Table 3 and the equation 1. 2 for $\alpha = 1$, we easily prove it.

$$\begin{aligned}
M_2(G) &= 12(6rs) + 15(2r + s + 1) + 30(3rs - 2r - s) \\
&\quad +20(4r + 2s + 2) + 40(6rs - 4r - 2s) + 25(4) \\
&\quad +50(4r + 2s - 6) + 100(3rs - 4r - 2s + 2) \\
M_2(G) &= 702rs - 310r - 155s + 55.
\end{aligned}$$

□

Theorem 3.23. *Consider $CBHDN(r, s)$, the harmonic index is*

$$H(G) = \frac{54594rs + 10534r + 5267s + 14651}{16380}.$$

Proof. Let G be the $CBHDN(r, s)$. The proof is just calculation based. Using the edge partition given in Table 3 and the equation 1. 6 , we easily prove it.

$$\begin{aligned}
H(G) &= 6rs(\frac{2}{7}) + (2r + s + 1)(\frac{2}{8}) + (3rs - 2r - s)(\frac{2}{13}) \\
&\quad +(4r + 2s + 2)(\frac{2}{9}) + (6rs - 4r - 2s)(\frac{2}{14}) + 4(\frac{2}{10}) \\
&\quad +(4r + 2s - 6)(\frac{2}{15}) + (3rs - 4r - 2s + 2)(\frac{2}{20}) \\
H(G) &= \frac{54594rs + 10534r + 5267s + 14651}{16380}.
\end{aligned}$$

□

Theorem 3.24. *Consider $CBHDN(r, s)$, the augmented Zagreb index is*

$$AZI(G) = \frac{1.03001 \times 10^{19}rs - 6.1123 \times 10^{18}r - 15625 \times 10^{14}(1.9559s - 1.3919)}{1.1699 \times 10^{16}}.$$

Proof. Let G be the $CBHDN(r,s)$. The proof is just calculation based. Using the edge partition given in Table 3 and the equation 1. 7 , we easily prove it.

$$\begin{aligned} AZI(G) &= 6rs(\frac{12}{5})^3 + (2r+s+1)(\frac{15}{6})^3 + (3rs-2r-s)(\frac{30}{11})^3 \\ &+(4r+2s+2)(\frac{20}{7})^3 + (6rs-4r-2s)(\frac{40}{12})^3 + 4(\frac{25}{8})^3 \\ &+(4r+2s-6)(\frac{50}{13})^3 + (3rs-4r-2s+2)(\frac{100}{18})^3 \\ AZI(G) &= \frac{1.03001\times 10^{19}rs - 6.1123\times 10^{18}r - 15625\times 10^{14}(1.9559s-1.3919)}{1.1699\times 10^{16}}. \end{aligned}$$

□

• We estimated the indices for distinct characteristics of r and s to compare the M_1, H, ABC, and GA indices of $CBHDN(r,s)$ for $r = s$. We can plainly see from the accompanying Table 4 that when we increase the values of r and s, the order of the indices increases, and their graphical structure is illustrated in Figure 4.
• For comparing the M_1, H, ABC, and GA indices of $CBHDN(r,s)$ for rs, where r is an odd number and n is a natural number. The order of the indices increases as the values of r and s increase, as shown in Table 5, and their graphical structure is given in Figure 5.
• For comparing the M_1, H, ABC, and GA indices of $CBHDN(r,s)$ for rs, where r and s are both even. We can see from Table 6 that when we increase the values of r and s, the order of the indices increases, and their graphical structure is displayed in Figure 6.
• For the evaluation of the indices M_1, H, ABC, and GA of $CBHDN(r,s)$ for rs, where r is even and s is odd. We can see from Table 7 that when we increase the values of r and s, the order of the indices increases, and their graphical structure is displayed in Figure 7.

(m,n)	M_1	H	ABC	GA
(2,2)	750	15.327	42.651	66.064
(3,3)	1800	32.957	94.752	145.347
(4,4)	3300	57.252	167.351	255.54
(5,5)	5250	88.214	260.447	396.642
(6,6)	7650	125.841	375.041	568.655
(7,7)	10500	170.134	508.132	771.577
(8,8)	13800	221.093	662.72	1005.41
(9,9)	17550	278.718	837.006	1270.15
(10,10)	21750	343.009	1033.39	1565.8

TABLE 4. Numerical computation of $CBHDN(r,s)$ for $r = s$

(m,n)	M_1	H	ABC	GA
(3,4)	2450	43.278	125.784	186.908
(3,5)	3100	53.598	156.817	235.774
(3,6)	3750	63.918	187.849	284.641
(3,7)	4400	74.239	218.881	333.508
(3,8)	5050	84.559	249.913	382.374
(3,9)	5700	94.880	280.945	431.241
(3,10)	6350	105.201	311.977	480.107
(3,11)	7000	115.521	343.009	528.974
(3,12)	7650	125.841	374.041	577.84

TABLE 5. Numerical computation of $CBHDN(r,s)$ for $r < s$, where r is odd and s is natural number.

(m,n)	M_1	H	ABC	GA
(2,4)	1600	29.302	84.218	122.95
(2,6)	2450	43.277	125.784	186.908
(2,8)	3300	57.252	167.351	250.866
(2,10)	4150	71.227	208.918	314.824
(2,12)	5000	85.202	250.485	378.783
(2,14)	5850	99.177	292.051	442.741
(2,16)	6700	113.152	333.618	506.699
(2,18)	7550	127.127	375.185	570.657
(2,20)	8400	141.102	416.752	634.615

TABLE 6. Numerical computation of $CBHDN(r,s)$ for $r < s$, where r and s both are even.

(m,n)	M_1	H	ABC	GA
(2,3)	1191	23.1431	65.362	105.966
(4,5)	4191	71.7339	210.559	343.542
(6,7)	8991	146.9885	437.746	716.217
(8,9)	15591	248.9068	746.923	1223.99
(10,11)	23991	377.4889	1138.09	1866.87
(12,13)	34191	532.7347	1611.25	2644.84
(14,15)	46191	714.6442	2166.39	3557.91
(16,17)	59991	923.2175	2803.53	4606.09
(18,19)	75591	1158.4545	3522.65	5789.36

TABLE 7. Numerical computation of $CBHDN(r,s)$ for $r < s$, where r is even and s is odd.

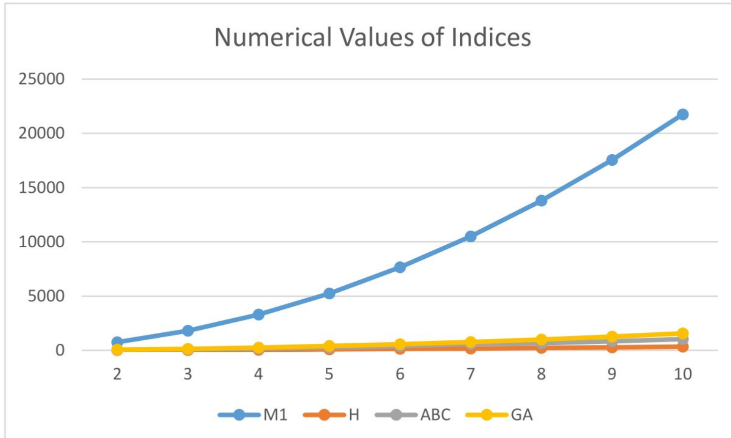

FIGURE 4. Graphical representation of $CBHDN(r, s)$ for different values of $r = s$.

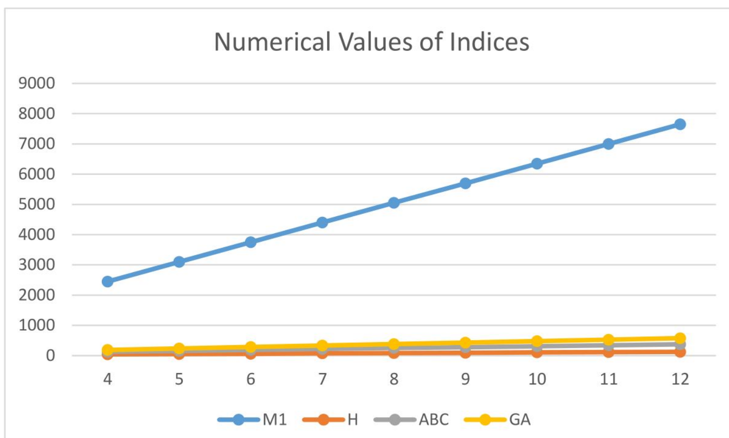

FIGURE 5. Graphical representation of $CBHDN(r, s)$ for $r < s$, where r is odd and s is natural number.

4. DISCUSSION

The computed topological indices reveal fundamental structure-property relationships in Chain Benzenoid Hex-Derived Networks that have significant theoretical and practical implications. Our results demonstrate that increasing the network dimensions (r, s) leads to predictable growth patterns in all six indices (R_α, M_1, H, AZI, ABC, and GA), with the ABC and GA indices showing particularly strong correlations with molecular stability. The consistent mathematical relationships we established between network parameters

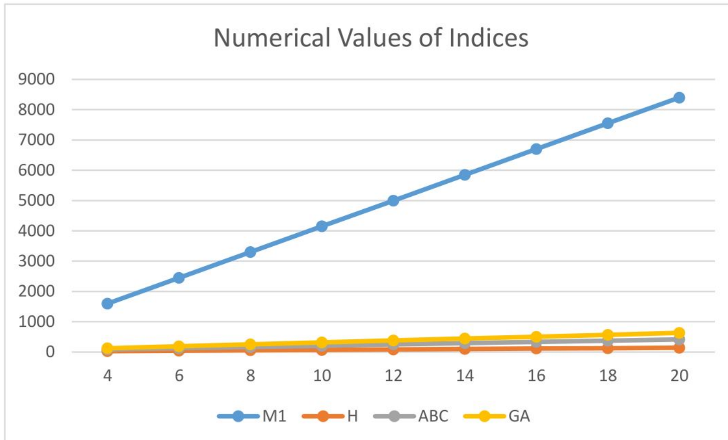

FIGURE 6. Graphical representation of $CBHDN(r, s)$ for $r < s$, where r and s both are even.

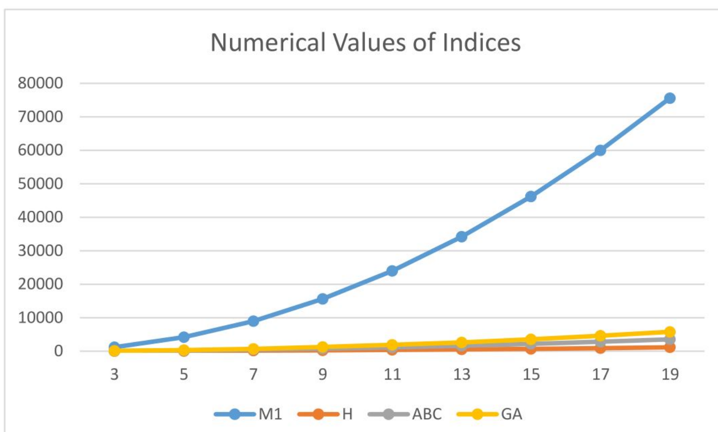

FIGURE 7. Graphical representation of $CBHDN(r, s)$ for $r < s$, where r is even and s is odd.

and index values suggest that these topological descriptors can serve as reliable predictors for physicochemical properties in benzenoid systems, including aromaticity, electron delocalization, and thermal stability. The distinct behaviors observed in the three structural cases ($r = s$, $r < s$, and $r > s$) provide new insights into how symmetry breaking affects molecular properties, which could guide the design of benzenoid-based materials with tailored characteristics. Particularly noteworthy is the nonlinear response of the AZI index to dimensional changes, indicating its potential as a sensitive marker for structural defects in hexagonal networks. These findings advance computational chemistry methodologies by providing a quantitative framework for structure-activity predictions in complex benzenoid systems, with immediate applications in drug design (through QSAR modeling of polycyclic aromatic compounds) and materials science (for optimizing graphene-like nanostructures). The graphical representations further enhance the utility of these results by enabling visual identification of property trends across different network configurations, offering researchers an intuitive tool for molecular design.

5. Conflict of interest

The authors declare no conflict of interest.

6. Conclusion

It became evident that a psychological perspective alone could not account for the complexity of the events occurring in the classroom. Establishing social norms that provided the setting in which children engaged in meaningful activity was an aspect of social interaction not considered prior to the classroom teaching experiment. As these norms became accepted, the students participated in a type of discourse in which they were expected to explain and justify their solutions and listen to others. The teacher acted to initiate and guide students' learning by posing questions and highlighting children's expectations. As students engaged in this discourse, their personal meanings were negotiated until an agreement was reached. The establishment of taken-as-shared meanings between the participants enabled mathematical ideas to be established by members of the class.

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