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Some Degree-Based Topological Indices of Hexagonal Cacti

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Abstract Applications of graph theory in the theoretical investigation of molecular physiochemical properties are the focus of mathematical chemistry. Atoms without hydrogen are the nodes of a chemical network, and covalent bonds between them serve as the edges. Cactus graphs are specially connected graphs in which no edge is part of more than one cycle. A topological index is a number calculated from the graph. In this work, we develop precise formulas for the randic index, geometric arithmetic index, and the atom bond connectivity index and second zagreb index, ABC_4 index and GA_5 index of hexagonal cacti, many of which are not a hexagonal chain.

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1. Introduction

Chemical graph theory is a sub-field of mathematical chemistry with applications in science, engineering, and chemistry. Edge set $E(G)$ and vertex set $V(G)$ form an ordered pair of two sets that together make up a graph $G = (V(G), E(G))$. The *degree* of a vertex is the total number of vertices in the graph G excluding v and that are adjacent to v denoted by $d_G(v)$.

A connected graph having no edge that is part of more than one cycle is known as *cactus graph*. This graph was studied in statistical mechanics in 1956 [1], communication networks in 2005 [2] and chemistry by Zmazek et al. in 2003 [3]. Graphs of benzenoid hydrocarbon can be represented by hexagonal systems, and they have a significant role in theoretical chemistry, See Qu et al. [4] for example. A cactus graph having cycles of 6 vertices, i.e. hexagons, as blocks is known as a *hexagonal cactus*. A graph in which

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every hexagon has at most two cut-vertices is known as *hexagonal cactus chain* where each cut-vertex is allocated by two hexagons exactly.

For a hexagonal cactus C, a *leaf hexagon* is a block that shares a cut vertex with exactly one other block. A *branching hexagon* is a block that shares a cut vertex with at least three other blocks. Hence, an *internal hexagon* is a hexagon, which is neither branching nor leaf that shares a cut vertex to exactly two other blocks. An internal hexagon in the cactus H_n whose cut-vertices are adjacent is called an *ortho-hexagon*. If the cut-vertices of an internal hexagon are at distance 2, it is called a *meta-hexagon* and it is called a *para-hexagon*, if the distance between the two cut-vertices is 3. A hexagonal cactus chain of n hexagons is called *ortho*, denoted by O_n, if all internal hexagons are ortho, is called *meta*, denoted by M_n, if all internal hexagons are meta and is called *para*, denoted by L_n, if the internal hexagons are para. Not long ago, Sadeghieh et al. [5] calculated degree-based topological indices of some cactus chain and their Hosoya polynomial as well. Further, Sadeghieh et al. [6] also computed Gutman index of some cactus chains.

A numeric quantity that is mathematically derived from the graph is the *topological index* of a graph, which is always the same for isomorphic graphs. Different researchers have recently defined many topological indices; these have many uses in chemistry, medicine, biochemistry, and other fields to theoretically understand the physicochemical properties of the chemical compounds. Degree-related topological invariants having ability to predict the biological activity of particular classes of chemical compounds make them highly desirable for utilization in QSAR/QSPR studies known as the degree-based topological indices[7]. For some references on topological indices, the readers can see in [8]. Xu et.al. [9] published a survey on graphs extremel based on distance-based topological indices. Recently, there has been a spike in interest in topological indices research. A huge number of topological descriptors have been found and used in theoretical chemistry, particularly in QSPR or QSAR [[10],[11]]. In this paper, G is considered to be a connected and simple graph with edge set $E(G)$ and $V(G)$ vertex set; $d(v)$ is considered as *degree* of vertex $v \in V(G)$ and the *open neighbourhood* of v is $S_v = \sum_{u\in N_G(v)} d(v)$, where $N_G(v) = \{u \in V(G)|uv \in E(G)\}$.

The *Wiener index* was the first and most thoroughly studied in QSPR [12–14]. Many new topological indices have been introduced to predict different physical properties of the compounds ever since. The first topological index based on degree is the *Randic connectivity index*, denoted by $R_{-\frac{1}{2}}(G)$ defined in [15] introduced by Milan Randić is

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

K.C.Das and S. Sorgun calculated Randic energy of graphs in [16]. The *Atom-Bond Connectivity* (ABC) index is the regularly used connectivity index that was initiated by Estrada et al. [17] and can be described as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

The *Geometric-Arithmetic* (GA) index was introduces in [18] by Vukičević *et al.* and is calculated as

$$GA\left(G\right)=\sum_{uv\in E(G)}\frac{2\sqrt{d_u d_v}}{(d_u+d_v)}.$$

A survey on geometric-arithmetic indices of graphs was published by K.C. Das, I. Gutman [19] in 2011. The *second Zagreb index* ($ZG_2(G)$) is calculated as

$$ZG_2\left(G\right)=\sum_{uv\in E(G)}(d_u d_v).$$

where d_u and d_v represent degrees of u and v. M. Azari and A. Iranmanesh calculated Zagreb indices of some Chemical graphs [20]. In 2010, Ghorbani et al. [21] introduced the ABC_4 index which is the fourth version of ABC index and is defined as

$$ABC_4\left(G\right)=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_u S_v}}.$$

In 2011, Graovac et al. [22] proposed fifth version GA_5 of GA index and defined as

$$GA_5\left(G\right)=\sum_{uv\in E(G)}\frac{2\sqrt{S_u S_v}}{(S_u+S_v)}.$$

From the above discussion, it is clear that one can find the randic index, atom-bond connectivity index, geometric arithmetic index, Zagreb index, fourth atom bond connectivity index and fifth geometric arithmetic index if we know what types of edges are there and what is the sum of degrees of end vertices of these edges are in the graphs.

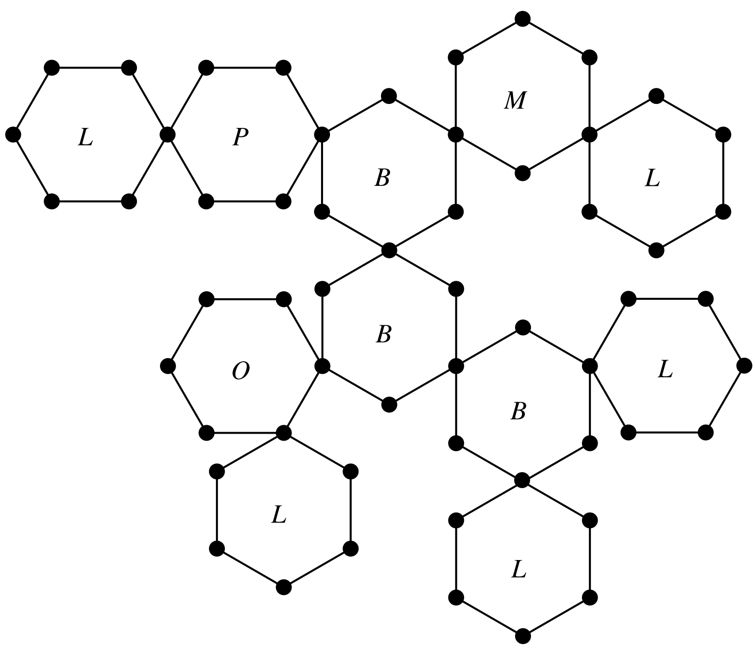

FIGURE 1. A cactus C_{11}.

Definition 1.1. Let C_n be a hexagonal cactus with n hexagons whose each branching hexagon is adjacent to exactly 3 other hexagons via the 3 vertices that are distance 2 apart.

Figure 1 shows an example of a graph C_{11}. Thus, the problem that arises is:

Problem 1.2. What are the structures of C_n such that their degree based topological indices are maximum or minimum?

In this paper, we partially answer Problem 1.2 (in Theorems 2.5 and 2.6) by establishing upper and lower bounds of Randic connectivity index, Atom-bond connectivity index, Geometric-arithmetic index, second zagreb index, the fourth version of ABC index and the fifth version GA index of C_n as well as characterizing all C_n satisfying the upper or lower bounds. This paper is organized in the following manner: we state our main results of this paper in the next section, while proofs are given in Section 3.

2. Main Results

In this section, we state all our main results. The first observation is obvious but necessary in the proofs of main theorem.

Observation 2.1. For a hexagonal cactus C_n, we let h be the number of internal hexagons, b be number of branching hexagons and l be number of leave hexagons. Then,

$$n = b + h + l.$$

The following lemma is an upper bound of the number of leaves of a tree in terms of the maximum degree and order. We provide the proof in Section 3.

Lemma 2.2. *Let G be a tree of order n having maximum degree Δ. If G has b branching vertices and l leaves, then*

$$(\Delta - 2)b \geq l - 2$$

and the equality holds when every branching vertex has degree Δ. In particular, if $\Delta = 3$, then $b = l - 2$.

In the following, for a Cactus C_n of n hexagons, we let

- l be the number of leaf hexagons,
- m be the number of meta-hexagons,
- p be the number of para-hexagons,
- o be the number of otho-hexagons
- h be the number of internal hexagons and
- b be the number of branching hexagons.

Hence, $h = m + p + o$.

Our first main theorem establishes the exact values of $\chi(C_n)$, $ABC(C_n)$, $GA(C_n)$ and $ZG_2(C_n)$ in terms of the numbers of hexagons with different types.

Theorem 2.3. *Let C_n be a cactus of n hexagons. Then*

$$\chi(C_n) = (\frac{1+2\sqrt{2}}{\sqrt{2}})l + (\frac{4+7\sqrt{2}}{4\sqrt{2}})o + (1+\sqrt{2})(m+p) + \frac{3b}{\sqrt{2}} \tag{2.1}$$

$$ABC(C_n) = 3\sqrt{2}(l+m+p+b) + \frac{10+\sqrt{3}}{2\sqrt{2}}o \tag{2.2}$$

$$GA(C_n) = (\frac{4\sqrt{2}}{3}+4)(l+o) + (\frac{8\sqrt{2}}{3}+2)(m+p) + 4\sqrt{2}b \tag{2.3}$$

$$ZG_2(C_n) = 32l + 40(m+p) + 44o + 48b. \tag{2.4}$$

Further, we let

- $\tilde{b}$ be the number of branching hexagons that are not attached to any ortho-hexagon,
- $\bar{b}$ be the number of branching hexagons that are attached to at least one ortho-hexagon,
- $\tilde{l}$ be the number of leave hexagons that are not attached to any ortho-hexagons,
- $\bar{l}$ be the number of leave hexagons that are attached to at least one ortho-hexagon.

Hence, $l = \bar{l} + \tilde{l}$ and $b = \bar{b} + \tilde{b}$. Our second main theorem establishes the exact values of $ABC_4(C_n)$ and $GA_5(C_n)$.

Theorem 2.4. *Let C_n be a cactus of n hexagons. Then*

$$\begin{aligned} ABC_4(C_n) = {} & (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)\tilde{l} + (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}})\bar{l} \\ & + (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})o \\ & + (\frac{\sqrt{10}}{3} + 2)p + (\frac{2}{\sqrt{3}} + 1 + \frac{\sqrt{14}}{4})m \\ & + (\frac{3\sqrt{14}}{4})\tilde{b} + (\frac{\sqrt{14}}{2} + \frac{2}{\sqrt{5}})\bar{b} \end{aligned} \tag{2.5}$$

$$\begin{aligned} GA_5(C_n) = {} & (3 + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{10}}{7} + \frac{\sqrt{15}}{4})o + (2 + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7})(\tilde{l}+m) \\ & + (2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{15}}{2})\bar{l} + (2 + \frac{16\sqrt{3}}{7})p + (4 + \frac{8\sqrt{5}}{9})\bar{b} + 6\tilde{b}. \end{aligned} \tag{2.6}$$

By applying the results in Theorems 2.3 and 2.4, we establish upper and lower bounds of the topological indices and characterize the graphs C_n satisfying the bounds as detailed in Theorems 2.5 and 2.6.

Theorem 2.5. *Let n be any positive number and C_n be a cactus of n hexagons. Then*

$$\begin{aligned} 2.414n + 0.586 \leq \chi(C_n) &\leq 2.457n + 0.5 \\ 4.148n + 0.189 \leq ABC(C_n) &\leq 4.243n \\ 5.771n + 0.229 \leq GA(C_n) &\leq 5.886n \\ 40n - 16 \leq ZG_2\,(C_n) &\leq 44n - 24. \end{aligned}$$

For atom bond connectivity index, the lower bound holds if there is no branching hexagon and all the internal hexagons are ortho hexagon while the upper bound holds if there is no branching hexagon and all the internal hexagons are either para or meta hexagons. For randic index, geometric arithmetic index and second zagreb index the lower bound holds if all the internal hexagons are either para or meta and there is no branching hexagon while the upper bounds holds if all the hexagons are ortho and there is no branching hexagons.

Theorem 2.6. *Let n be any positive number and C_n be a cactus of n hexagons. Then*

$$3.054n - 5.457 \leq ABC_4(C_n) \leq 3.257n + 0.177.$$

The upper bound holds if there are no branching hexagons and all internal hexagons are ortho while the lower bound holds if all internal hexagons are para with no branching hexagon. Further,

$$5.852n + 4.089 \leq GA_5\,(C_n) \leq 5.97n - 0.061.$$

The upper bound holds if C_n is a cactus of n hexagons having only branching hexagons and leaf hexagons while the lower bound holds if all inner hexagons are ortho with no branching hexagons.

From Theorems 2.3 and 2.4, we also obtain the following corollaries when all the internal hexagons of C_n are the same type. We skip the proofs as they are obvious.

Corollary 2.7. *If the cactus C_n has no para or ortho hexagons, i.e. $p = o = 0$, then $l = \tilde{l}, b = \tilde{b}$ and*

$$\begin{aligned} \chi(C_n) &= (\frac{1+2\sqrt{2}}{\sqrt{2}})l + (1+\sqrt{2})m + \frac{3b}{\sqrt{2}} \\ ABC(C_n) &= 3\sqrt{2}(l+m+b) \\ GA(C_n) &= (\frac{4\sqrt{2}}{3}+4)l + (\frac{8\sqrt{2}}{3}+2)m + 4\sqrt{2}b \\ ZG_2\,(C_n) &= 32l + 40m + 48b \\ ABC_4(C_n) &= (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)l + (\frac{2}{\sqrt{3}} + 1 + \frac{\sqrt{14}}{4})m + (\frac{3\sqrt{14}}{4})b \\ GA_5\,(C_n) &= (2 + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7})(l+m) + 6b. \end{aligned}$$

Corollary 2.8. *If the cactus C_n has no para and meta hexagons, i.e. $m = p = 0$, then*

$$\chi(C_n) = (\frac{1+2\sqrt{2}}{\sqrt{2}})l + (\frac{4+7\sqrt{2}}{4\sqrt{2}})o + \frac{3b}{\sqrt{2}}$$
$$ABC(C_n) = 3\sqrt{2}(l+b) + \frac{10+\sqrt{6}}{2\sqrt{2}}o$$
$$GA(C_n) = (\frac{4\sqrt{2}}{3}+4)(l+o) + 4\sqrt{2}b$$
$$ZG_2(C_n) = 32l + 44o + 48b$$
$$ABC_4(C_n) = (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)\tilde{l} + (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}})\bar{l} + (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})o + (\frac{3\sqrt{14}}{4})\tilde{b} + (\frac{\sqrt{14}}{2} + \frac{2}{\sqrt{5}})\bar{b}$$
$$GA_5(C_n) = (3 + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{10}}{7} + \frac{\sqrt{15}}{4})o + (2 + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7})\tilde{l} + (2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{15}}{2})\bar{l} + (4 + \frac{8\sqrt{5}}{9})\bar{b} + 6\tilde{b}.$$

Corollary 2.9. *If the cactus C_n has no meta and ortho hexagons, i.e. $m = o = 0$, then $l = \tilde{l}, b = \tilde{b}$ and*

$$\chi(C_n) = (\frac{1+2\sqrt{2}}{\sqrt{2}})l + (1+\sqrt{2})p + \frac{3b}{\sqrt{2}}$$
$$ABC(C_n) = 3\sqrt{2}(l+p+b)$$
$$GA(C_n) = (\frac{4\sqrt{2}}{3}+4)l + (\frac{8\sqrt{2}}{3}+2)p + 4\sqrt{2}b$$
$$ZG_2(C_n) = 32l + 40p + 48b$$
$$ABC_4(C_n) = (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)l + (\frac{\sqrt{10}}{3} + 2)p + (\frac{3\sqrt{14}}{4})b$$
$$GA_5(C_n) = (2 + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7})l + (2 + \frac{16\sqrt{3}}{7})p + 6b.$$

Finally, from Theorems 2.3 and 2.4, we also obtain the following corollaries when C_n is a hexagonal cactus chain, i.e. $b = 0$. Thus,

$$l = 2 \text{ and } n = h + b + l = h + 2.$$

We have that:

Corollary 2.10. *If C_n is a meta-hexagonal cactus chain, i.e. $b = 0$ and $p = o = 0$, then $l = \tilde{l} = 2, m = h$ and $n = h + b + l = m + 2$. Further, we have that*

$$\begin{aligned}
\chi(C_n) &= 2.414n + 0.586 \\
ABC(C_n) &= 4.243n \\
GA(C_n) &= 5.771n + 0.229 \\
ZG_2\,(C_n) &= 40n - 16 \\
ABC_4(C_n) &= 3.09n + 0.579 \\
GA_5\,(C_n) &= 5.939n.
\end{aligned}$$

Corollary 2.11. *If C_n is an otho-hexagonal cactus chain, i.e. $b = 0$ and $p = m = 0$, then $l = \bar{l} = 2, o = h$ and $n = h + b + l = o + 2$. Further, we have that*

$$\begin{aligned}
\chi(C_n) &= 2.457n + 0.5 \\
ABC(C_n) &= 4.148n + 0.189 \\
GA(C_n) &= 5.886n \\
ZG_2\,(C_n) &= 44n - 24 \\
ABC_4(C_n) &= 3.257n + 0.177 \\
GA_5\,(C_n) &= 5.852n + 4.089.
\end{aligned}$$

Corollary 2.12. *If C_n is an para-hexagonal cactus chain, i.e. $b = 0$ and $o = m = 0$, then $l = \bar{l} = 2, p = h$ and $n = h + b + l = p + 2$. Further, we have that*

$$\begin{aligned}
\chi(C_n) &= 2.414n + 0.586 \\
ABC(C_n) &= 4.243n \\
GA(C_n) &= 5.77n + 0.229 \\
ZG_2\,(C_n) &= 40n - 16 \\
ABC_4(C_n) &= 3.054n - 5.457 \\
GA_5\,(C_n) &= 5.959n - 0.04.
\end{aligned}$$

3. Proofs

3.1. Proof of Lemma 2.2

Let B and L be the sets of branching vertices and leaves of G, respectively. Hence, $V(G) \setminus (B \cup L)$ is the set of vertices of degree two of G. If $B = \emptyset$, then $b = 0$ and the graph G is a path. Thus, $(\Delta - 2)b = 0 \geq 2 - 2 = l - 2$ because every path has $l = 2$. This proves the lemma.

Thus, we may assume that $B \neq \emptyset$. We call a path P of length at least 2 in G a "bad path" if both end vertices of P are in $B \cup L$ and all the internal vertices of P are in $V(G) \setminus (B \cup L)$ (P always has internal vertices as it has length at least two).

We construct a tree T from G by replacing each bad path $v_1 v_2 ... v_\ell$ by the edge $v_1 v_\ell$ and remove all vertices $v_2, ..., v_{\ell-1}$. Figure (2) shows example to obtain T from G.

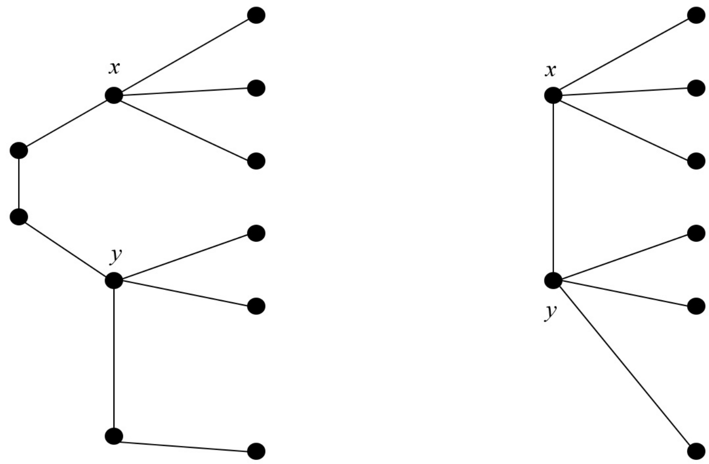

FIGURE 2. A tree G (left) and the corresponding tree T (right).

Let B' and L' be the sets of all branching vertices and leaves of T, respectively. By the construction of T, we see that:

(a) $B = B'$ and $L = L'$,

(b) $V(T) = B' \cup L'$ and

(c) $d_{u,T} = d_{u,G}$ for all $u \in V(T)$.

By (a), $|B'| = b$. It can be checked that $T[B']$ is a tree. Thus, $T[B']$ has $b-1$ edges We further let

$d_{u,B'} = |N_T(u) \cap B'|$ and $d_{u,L'} = |N_T(u) \cap L'|$.

Thus, by (b), we have that

$$\sum_{u \in B'} d_{u,L'} = |L'| = l \tag{3.1}$$

and

$$\Delta \geq d_{u,T} = d_{u,B'} + d_{u,L'} \tag{3.2}$$

for all $u \in V(T)$. We sum (3.2) overall $u \in B'$ and have that

$$\sum_{u \in B'} \Delta \geq \sum_{u \in B'} d_{u,B'} + \sum_{u \in B'} d_{u,L'}. \tag{3.3}$$

Because $T[B']$ has $b-1$ edges, it follows that $\sum_{u \in B'} d_{u,B'} = 2(b-1)$. By (3.1), we have that

$$b\Delta \geq 2(b-1) + l \tag{3.4}$$

and this proves the first inequality of Lemma 2.2.

It can be observed that the equality (3.4) holds if the equality (3.2) holds implying that every vertex in B' has degree Δ. Hence, by (a), the equality of Lemma 2.2 holds if every branching vertex of G has degree Δ. For the case when $\Delta = 3$, it is easy to see that every branching vertex has degree $\Delta = 3$. Hence, $b = l - 2$ when $\Delta = 3$ and this completes the proof.

3.2. Proof of Theorem 2.3

Let C_n be the graph of hexagonal cacti defined in Definition 1.1. We have $V(C_n) = 5n + 1$ and $E(C_n) = 6n$ where n represents number of hexagons in C_n. We have found the edge partition of C_n based on the degree of end vertices of each edge.

It can be observed that there are 3 types of edges in C_n which are $(2,2), (2,4)$ and $(4,4)$. For the type $(2,2)$, there are 4 such edges in each leaf hexagon, 2 such edges in each meta- or para-hexagon and 3 edges in each ortho-hexagon. Thus, the number of $(2,2)$ edges in C_n is $4l + 2(m + p) + 3o$. Similarly, the number if $(2,4)$ and $(4,4)$ edges in C_n are $2(l + o) + 4(m + p) + 6b$ and o, respectively. Table 1 concludes such partition for C_n. Moreover, we have 3 type of edges according to degrees.

Table 1. Edge partition of hexagonal cactus based on the degree of end vertices

$(d_u, d_v)\|uv \in E(G)$	**Number of edges**
(2,2)	$4l$+2(m+p)+3o
(2,4)	2(l+o)+4(m+p)+6b
(4,4)	o

Now, by using the edge partition given in Table 1, we can use formula of Randic index to compute this index for C_n.

$$\chi(C_n) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

This implies that,

$$\begin{aligned}\chi(C_n) = {} & (4l + 2(m + p) + 3o)\frac{1}{\sqrt{2 \times 2}} \\ & + (2(l + o) + 4(m + p) + 6b)\frac{1}{\sqrt{2 \times 4}} \\ & + o\frac{1}{\sqrt{4 \times 4}}.\end{aligned}$$

After an easy simplification, we can get

$$\chi(C_n) = (\frac{1 + 2\sqrt{2}}{\sqrt{2}})l + (\frac{4 + 7\sqrt{2}}{4\sqrt{2}})o + (1 + \sqrt{2})(m + p) + \frac{3b}{\sqrt{2}}.$$

Now, we apply formula of Atom-bond connectivity index for C_n. By using edge partition given in Table 1, we can compute this index for C_n. Since,

$$ABC(C_n) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

This implies that,

$$\begin{aligned} ABC\left(C_n\right) = & (4l+2(m+p)+3o)\sqrt{\frac{2+2-2}{2\times 2}} \\ & +(2(l+o)+4(m+p)+6b)\sqrt{\frac{2+4-2}{2\times 4}} \\ & +o\sqrt{\frac{4+4-2}{4\times 4}}. \end{aligned}$$

An easy simplification gives,

$$ABC(C_n) = 3\sqrt{2}(l+m+p+b) + \frac{10+\sqrt{3}}{2\sqrt{2}}(o).$$

Now, we apply formula of geometric arithmetic index for C_n. By using edge partition given in Table 1, we can compute this index for C_n. Since,

$$GA\left(C_n\right) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{(d_u+d_v)}.$$

This implies that,

$$\begin{aligned} GA\left(C_n\right) = & (4l+2(m+p)+3o)\frac{2\sqrt{2\times 2}}{(2+2)} \\ & +[2(l+o)+4(m+p)+6b]\frac{2\sqrt{2\times 4}}{(2+4)} \\ & +o\frac{2\sqrt{4\times 4}}{(4+4)}. \end{aligned}$$

An easy simplification gives,

$$GA(C_n) = (\frac{4\sqrt{2}}{3}+4)(l+o) + (\frac{8\sqrt{2}}{3}+2)(m+p) + 4\sqrt{2}b.$$

Now, we apply formula of second Zagreb index for C_n. By using edge partition given in Table 1, we can compute this index for C_n. Since,

$$ZG_2\left(G\right) = \sum_{uv\in E(G)} (d_u d_v).$$

This implies that,

$$\begin{aligned} ZG_2\left(C_n\right) = & [4l+2(m+p)+3o](2\times 2) + [2(l+o)+4(m+p)+6b](2\times 4) \\ & +o(4\times 4). \end{aligned}$$

An easy simplification gives,

$$ZG_2\left(C_n\right) = 32l + 40(m+p) + 44o + 48b.$$

Table 2. Edge partition of hexagonal cactus based on the degree sum of neighbors of end vertices

$(S_u, S_v)\|uv \in E(G)$	**Number of edges**
(4,4)	$2o + 2\tilde{l} + 2\bar{l}$
(4,6)	$o + 2m + 2\tilde{l} + \bar{l}$
(4,10)	o
(6,6)	$2p$
(6,8)	$4p + 2m + 2\tilde{l}$
(6,10)	$o + 2\bar{l}$
(8,8)	$6\tilde{b} + 4\bar{b} + 2m$
(8,10)	$2\bar{b}$
(10,10)	o

3.3. Proof of Theorem 2.4

Let C_n be the graph of hexagonal chain cacti. We have $V(C_n) = 5n+1$ and $E(C_n) = 6n$ where n represents number of hexagons in hexagonal chain cacti. Let the number of branches be b and $b = \tilde{b} + \bar{b}$ where $\tilde{b}$ number of branches that are not attached to ortho hexagons and $\bar{b}$ be tha branches attached to ortho hexagons. The number of leaves be $l = \tilde{l} + \bar{l}$ where $\tilde{l}$ number of leaves that are not attached to ortho hexagons and let $\bar{l}$ be the leaves attached to ortho-hexagon. We can use formula of ABC_4 index to compute this index for C_n. We have found the edge partition of C_n based on degree sum of neighbors of end vertices of each edge.

It can be observed that there are 9 types of edges in C_n which are $(4,4), (4,6), (4,10), (6,6), (6,8), (6,10), (8,8), (8,10)$ and $(10,10)$. Table 1 concludes such partition for C_n. Moreover, we have 3 type of edges according to degrees.

Table 2 explains such partition for C_n. Moreover, we have 9 type of edges according to degrees.As given in the table,

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that,

$$\begin{aligned}
ABC_4(C_n) = &\sqrt{\frac{4+4-2}{4 \times 4}}(2o + 2\tilde{l} + 2\bar{l}) \\
&+ \sqrt{\frac{4+6-2}{4 \times 6}}(o + 2m + 2\tilde{l} + 2\bar{l}) + \sqrt{\frac{4+10-2}{4 \times 10}}o \\
&+ \sqrt{\frac{6+6-2}{6 \times 6}}(2p) + \sqrt{\frac{6+8-2}{6 \times 8}}(4p + 2m + 2\tilde{l}) \\
&+ \sqrt{\frac{6+10-2}{6 \times 10}}(o + 2\bar{l}) + \sqrt{\frac{8+8-2}{8 \times 8}}(6\tilde{b} + 4\bar{b} + 2m) \\
&+ \sqrt{\frac{8+10-2}{8 \times 10}}(2\bar{b}) + \sqrt{\frac{10+10-2}{10 \times 10}}o
\end{aligned}$$

an easy simplification gives,

$$ABC_4(C_n) = (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)\tilde{l} + (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}})\bar{l}$$
$$+ (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})o + (\frac{\sqrt{10}}{3} + 2)p$$
$$+ (\frac{2}{\sqrt{3}} + 1 + \frac{\sqrt{14}}{4})m + (\frac{3\sqrt{14}}{4})\tilde{b} + (\frac{\sqrt{14}}{2} + \frac{2}{\sqrt{5}})\bar{b}.$$

Now, we apply formula of fifth geometric arithmetic index for C_n. By using edge partition given in Table 2, we can compute this index for C_n. Since,

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{(S_u + S_v)}$$

this implies that,

$$GA_5(C_n) = \frac{2\sqrt{4 \times 4}}{4+4}(2o + 2\tilde{l} + 2\bar{l})$$
$$+ \frac{2\sqrt{4 \times 6}}{4+6}(o + 2m + 2\tilde{l} + 2\bar{l}) + \frac{2\sqrt{4 \times 10}}{4+10}o$$
$$+ \frac{2\sqrt{6 \times 6}}{6+6}(2p) + \frac{2\sqrt{6 \times 8}}{6+8}(4p + 2m + 2\tilde{l})$$
$$+ \frac{2\sqrt{6 \times 10}}{6+10}(o + 2\bar{l}) + \frac{2\sqrt{8 \times 8}}{8+8}(6\tilde{b} + 4\bar{b} + 2m)$$
$$+ \frac{2\sqrt{8 \times 10}}{8+10}(2\bar{b}) + \frac{2\sqrt{10 \times 10}}{10+10}o$$

an easy simplification gives,

$$GA_5(C_n) = (3 + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{10}}{7} + \frac{\sqrt{15}}{4})o + (2 + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7})(\tilde{l} + m)$$
$$+ (2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{15}}{2})\bar{l} + (2 + \frac{16\sqrt{3}}{7})p + (4 + \frac{8\sqrt{5}}{9})\bar{b} + 6\tilde{b}.$$

3.4. Proof of Theorem 2.5

By Observation 2.1 we have:

$$n = b + h + l \tag{3.5}$$

We further construct a tree T from C_n where the set of vertices of T is the set of hexagons of C_n. Two vertices of T are adjacent if and only if the two corresponding hexagons share a common vertex. Clearly, T is a tree with n vertices having l leaves, b vertices of degree at least three and h vertices of degree two. Further, by the definition of C_n, T has maximum degree three. Thus, Lemma 2.2 gives that $b = l - 2$. This implies that $b = l - 2$ for the graph C_n too. By Equation (3.5), we have

$$n = h + 2b + 2$$

which gives

$$2b + h = n - 2. \tag{3.6}$$

We will use Equations (3.5) and (3.6) to find bounds for all the indices given below.

3.4.1. Bounds of Randic Index

We first prove the lower bound. By Equation (2.1), we have

$$\chi(C_n) = (\frac{1+2\sqrt{2}}{\sqrt{2}})l + (\frac{4+7\sqrt{2}}{4\sqrt{2}})o + (1+\sqrt{2})(m+p) + \frac{3b}{\sqrt{2}}.$$

Replacing l by $b+2$ and $2b+h$ by $n-2$ yield

$$\begin{aligned}
\chi(C_n) &= (\frac{1+2\sqrt{2}}{\sqrt{2}})(b+2) + (\frac{4+7\sqrt{2}}{4\sqrt{2}})o + (1+\sqrt{2})(m+p) + \frac{3b}{\sqrt{2}} \\
&= (\frac{4+2\sqrt{2}}{\sqrt{2}})b + \frac{2+4\sqrt{2}}{4\sqrt{2}} + (\frac{4+7\sqrt{2}}{4\sqrt{2}})o + (1+\sqrt{2})(m+p) \\
&\geq (\frac{4+2\sqrt{2}}{\sqrt{2}})b + \frac{2+4\sqrt{2}}{4\sqrt{2}} + (1+\sqrt{2})o + (1+\sqrt{2})(m+p) \\
&= (2+2\sqrt{2})b + \frac{2+4\sqrt{2}}{4\sqrt{2}} + (1+\sqrt{2})(m+p+o) \\
&= (1+\sqrt{2})(2b) + \frac{2+4\sqrt{2}}{4\sqrt{2}} + (1+\sqrt{2})h \\
&= (1+\sqrt{2})(2b+h) + \frac{2+4\sqrt{2}}{4\sqrt{2}} \\
&= (1+\sqrt{2})(n-2) + \frac{2+4\sqrt{2}}{4\sqrt{2}} \\
&= (1+\sqrt{2})n - 2 - 2\sqrt{2} + \sqrt{2} + 4 \\
&= (1+\sqrt{2})n + 2 - \sqrt{2}.
\end{aligned}$$

Thus,

$$\chi(C_n) \geq (1+\sqrt{2})n + 2 - \sqrt{2}. \tag{3.7}$$

It can be observed that, if the equality of Equation (3.7) holds, then $o = 0$. Thus, the cactus C_n satisfies $\chi(C_n) = (1+\sqrt{2})n + 2 - \sqrt{2}$ if all the inner hexagons are either meta or para.

Next, we prove the upper bound. We have by Equation (3.6) that

$$\begin{aligned}
\chi(C_n) &= (\frac{1+2\sqrt{2}}{\sqrt{2}})(b+2) + (\frac{4+7\sqrt{2}}{4\sqrt{2}})o + (1+\sqrt{2})(m+p) + \frac{3b}{\sqrt{2}} \\
&= (\frac{4+2\sqrt{2}}{\sqrt{2}})b + (\frac{4+7\sqrt{2}}{4\sqrt{2}})o + (1+\sqrt{2})(m+p) + \sqrt{2} + 4 \\
&\leq (\frac{4+2\sqrt{2}}{\sqrt{2}})b + (\frac{4+7\sqrt{2}}{4\sqrt{2}})o + (\frac{4+7\sqrt{2}}{4\sqrt{2}})(m+p) + \sqrt{2} + 4 \\
&= (2+2\sqrt{2})b + (\frac{4+7\sqrt{2}}{4\sqrt{2}})(m+p+o) + \sqrt{2} + 4 \\
&\leq (\frac{4+7\sqrt{2}}{4\sqrt{2}})(2b) + (\frac{4+7\sqrt{2}}{4\sqrt{2}})h + \sqrt{2} + 4 \\
&= (\frac{4+7\sqrt{2}}{4\sqrt{2}})(n-2) + \sqrt{2} + 4.
\end{aligned}$$

Thus,

$$\chi(C_n) \leq \frac{4+7\sqrt{2}}{4\sqrt{2}})(n-2) + \sqrt{2} + 4. \tag{3.8}$$

It can be observed that, if the equality of Equation (3.8) holds, then $b = m = p = 0$. Thus, the cactus C_n satisfies $\chi(C_n) = (\frac{4+7\sqrt{2}}{4\sqrt{2}})(n-2) + \sqrt{2} + 4$ if it is the ortho-hexagonal cactus chain of n hexagons.

3.4.2. Bounds of Atom Bond Connectivity Index

We first prove the lower bound. By Equations (2.2) and (3.6), we have

$$\begin{aligned}
ABC(C_n) &= 3\sqrt{2}(2b+2+m+p) + \frac{10+\sqrt{3}}{2\sqrt{2}}o \\
&= 6\sqrt{2}b + 6\sqrt{2} + 3\sqrt{2}(m+p) + \frac{10+\sqrt{3}}{2\sqrt{2}}o \\
&\geq 6\sqrt{2}b + 6\sqrt{2} + \frac{10+\sqrt{3}}{2\sqrt{2}}(m+p+o) \\
&\geq \frac{10+\sqrt{3}}{2\sqrt{2}}(2b) + 6\sqrt{2} + \frac{10+\sqrt{3}}{2\sqrt{2}}h \\
&= \frac{10+\sqrt{3}}{2\sqrt{2}}(2b+h) + 6\sqrt{2} \\
&= \frac{10+\sqrt{3}}{2\sqrt{2}}(n-2) + 6\sqrt{2}.
\end{aligned}$$

Thus,

$$ABC(C_n) \geq (\frac{10+\sqrt{3}}{2\sqrt{2}})(n-2) + 6\sqrt{2}. \tag{3.9}$$

It can be observed that, if the equality of Equation (3.9) holds, then $b = m = p = 0$.

Thus, the cactus C_n satisfies $ABC(C_n) = (\frac{10+\sqrt{3}}{2\sqrt{2}})(n-2)+6\sqrt{2}$ if it is the ortho-hexagonal cactus chain of n hexagons.

Next, we prove the upper bound.

$$ABC(C_n) = 3\sqrt{2}(l+m+p+b) + \frac{10+\sqrt{3}}{2\sqrt{2}}o.$$

Replacing l by $b+2$ and $2b+h$ by $n-2$ yield

$$\begin{aligned}
ABC(C_n) &= 3\sqrt{2}(2b+2+m+p) + \frac{10+\sqrt{3}}{2\sqrt{2}}o \\
&= 6\sqrt{2}b + 6\sqrt{2} + 3\sqrt{2}(m+p) + \frac{10+\sqrt{3}}{2\sqrt{2}}o \\
&\leq 6\sqrt{2}b + 6\sqrt{2} + 3\sqrt{2}(m+p+o) \\
&= 6\sqrt{2}b + 6\sqrt{2} + 3\sqrt{2}h \\
&\leq 3\sqrt{2}(2b+h) + 6\sqrt{2} \\
&= 3\sqrt{2}(n-2) + 6\sqrt{2} \\
&= 3\sqrt{2}n.
\end{aligned}$$

Thus,

$$ABC(C_n) \leq 3\sqrt{2}n. \tag{3.10}$$

It can be observed that, if equality of Equation (3.10) holds, then $o = 0$. Thus, the cactus C_n satisfies $ABC(C_n) = 3\sqrt{2}n$ if all the inner hexagons are either meta or para.

3.4.3. Bound of Geometric Arithmetic Index

We first prove the lower bound. By Equations (2.3) and (3.6), we have

$$\begin{aligned}
GA(C_n) &= (\frac{4\sqrt{2}}{3}+4)(b+2+o) + (\frac{8\sqrt{2}}{3}+2)(m+p) + 4\sqrt{2}b \\
&= (\frac{16\sqrt{2}+12}{3})b + (\frac{8\sqrt{2}}{3}+8) + (\frac{8\sqrt{2}}{3}+2)(m+p) \\
&\quad + (\frac{4\sqrt{2}}{3}+4)o \\
&\geq (\frac{8\sqrt{2}}{3}+2)(2b) + (\frac{8\sqrt{2}}{3}+8) + (\frac{8\sqrt{2}}{3}+2)(m+p+o) \\
&\geq (\frac{8\sqrt{2}}{3}+2)(2b) + (\frac{8\sqrt{2}}{3}+8) + (\frac{8\sqrt{2}}{3}+2)(m+p+o) \\
&= (\frac{8\sqrt{2}}{3}+2)(2b) + (\frac{8\sqrt{2}}{3}+8) + (\frac{8\sqrt{2}}{3}+2)h \\
&= (\frac{8\sqrt{2}}{3}+2)(2b+h) + (\frac{8\sqrt{2}}{3}+8) \\
&= (\frac{8\sqrt{2}}{3}+2)(n-2) + (\frac{8\sqrt{2}}{3}+8).
\end{aligned}$$

Thus,

$$GA(C_n) \geq (\frac{8\sqrt{2}}{3} + 2)(n-2) + (\frac{8\sqrt{2}}{3} + 8). \tag{3.11}$$

It can be observed that, if the equality of Equation (3.11) holds, then $o = 0$. Thus, the cactus C_n satisfies $GA(C_n) = (\frac{8\sqrt{2}}{3} + 2)(n-2) + (\frac{8\sqrt{2}}{3} + 8)$ if all the inner hexagons are either meta or para.

Next, we prove the upper bound.

$$GA(C_n) = (\frac{4\sqrt{2}}{3} + 4)(l + o) + (\frac{8\sqrt{2}}{3} + 2)(m + p) + 4\sqrt{2}b.$$

Replacing l by $b + 2$ and $2b + h$ by $n - 2$ yield

$$\begin{aligned}
GA(C_n) &= (\frac{4\sqrt{2}}{3} + 4)(b + 2 + o) + (\frac{8\sqrt{2}}{3} + 2)(m + p) + 4\sqrt{2}b \\
&= (\frac{16\sqrt{2} + 12}{3})b + (\frac{8\sqrt{2}}{3} + 8) + (\frac{8\sqrt{2}}{3} + 2)(m + p) \\
&+ (\frac{4\sqrt{2}}{3} + 4)o \\
&\leq (\frac{8\sqrt{2} + 6}{3})(2b) + (\frac{8\sqrt{2}}{3} + 8) + (\frac{4\sqrt{2}}{3} + 4)(m + p + o) \\
&= (\frac{8\sqrt{2} + 6}{3})(2b) + (\frac{8\sqrt{2}}{3} + 8) + (\frac{4\sqrt{2}}{3} + 4)h \\
&\leq (\frac{4\sqrt{2}}{3} + 4)(2b) + (\frac{8\sqrt{2}}{3} + 8) + (\frac{4\sqrt{2}}{3} + 4)h \\
&= (\frac{4\sqrt{2}}{3} + 4)(2b + h) + (\frac{8\sqrt{2}}{3} + 8) \\
&= (\frac{4\sqrt{2}}{3} + 4)(n - 2) + (\frac{8\sqrt{2}}{3} + 8) \\
&= (\frac{4\sqrt{2}}{3} + 4)n.
\end{aligned}$$

Thus,

$$GA(C_n) \leq (\frac{4\sqrt{2}}{3} + 4)n. \tag{3.12}$$

It can be observed that, if the equality of Equation (3.12) holds, then $b = m = p = 0$. Thus, the cactus C_n satisfies $GA(C_n) = (\frac{4\sqrt{2}}{3} + 4)n$ if it is the ortho-hexagonal cactus chain of n hexagons.

3.4.4. Bounds of Second Zagreb Index

We first prove the lower bound. By Equations (2.4), we have

$$ZG_2(C_n) = 32l + 40(m + p) + 44o + 48b.$$

Replacing l by $b+2$ and $2b+h$ by $n-2$ yield

$$\begin{aligned} ZG_2\left(C_n\right) &= 32(b+2)+40(m+p)+44o+48b \\ &= 80b+40(m+p)+44o+64 \\ &\geq 40(2b)+40(m+p+o)+64 \\ &= 40(2b)+40h+64 \\ &= 40(2b+h)+64 \\ &= 40(n-2)+64 \\ &= 40n-16. \end{aligned}$$

Thus,

$$ZG_2\left(C_n\right) \geq 40n-16. \tag{3.13}$$

It can be observed that, if the equality of Equation (3.13) holds, then $o=0$. Thus, the cactus C_n satisfies $ZG_2\left(C_n\right)=40n-16$ if all the inner hexagons are either meta or para.

Next, we prove the upper bound. We have that

$$\begin{aligned} ZG_2\left(C_n\right) &= 32(b+2)+40(m+p)+44o+48b \\ &= 80b+40(m+p)+44o+48b+64 \\ &\leq 40(2b)+44(m+p+o)+64 \\ &= 40(2b)+44h+64 \\ &\leq 44(2b+h)+64 \\ &= 44(n-2)+64 \\ &= 44n-24. \end{aligned}$$

Thus,

$$ZG_2\left(C_n\right) \leq 44n-24. \tag{3.14}$$

It can be observed that, if the equality of Equation (3.14) holds, then $b=m=p=0$. Thus, the cactus C_n satisfies $ZG_2\left(C_n\right)=44n-24$ if it is the ortho-hexagonal cactus (chain) of n hexagons.

3.5. Proof of Theorem 2.6

3.5.1. Bounds of Fourth Atom Bond Connectivity Index

We first prove the upper bound. By Equation (2.5), we have

$$\begin{aligned} ABC_4(C_n) = {} & (\sqrt{\frac{3}{2}}+\frac{2}{\sqrt{3}}+1)\tilde{l}+(\sqrt{\frac{3}{2}}+\frac{2}{\sqrt{3}}+2\frac{\sqrt{7}}{\sqrt{30}})\bar{l} \\ & +(\sqrt{\frac{3}{2}}+\frac{\sqrt{3}}{\sqrt{10}}+\frac{\sqrt{7}}{\sqrt{30}}+\frac{3\sqrt{2}}{10}+\frac{1}{\sqrt{3}})o \\ & +(\frac{\sqrt{10}}{3}+2)p+(\frac{2}{\sqrt{3}}+1+\frac{\sqrt{14}}{4})m \\ & +(\frac{3\sqrt{14}}{4})\tilde{b}+(\frac{\sqrt{14}}{2}+\frac{2}{\sqrt{5}})\bar{b}. \end{aligned}$$

Replacing the coefficients of p and m by the coefficient of o yield

$$\begin{aligned}ABC_4(C_n) \leq {} & (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)\tilde{l} + (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}})\bar{l} \\ & + (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})(m + p + o) \\ & + (\frac{3\sqrt{14}}{4})\tilde{b} + (\frac{\sqrt{14}}{2} + \frac{2}{\sqrt{5}})\bar{b}.\end{aligned}$$

The equality holds if $m = p = 0$. As all inner hexagons are ortho hexagons, $\tilde{b} = \tilde{l} = 0$. This implies $b = \bar{b}$ and $l = \bar{l}$. By Equations (3.5) and (3.6), we have

$$\begin{aligned}ABC_4(C_n) = {} & (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}})l + (\frac{\sqrt{14}}{2} + \frac{2}{\sqrt{5}})b \\ & + (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})h \\ = {} & (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}} + \frac{\sqrt{14}}{2} + \frac{2}{\sqrt{5}})b + 2(\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} \\ & + 2\frac{\sqrt{7}}{\sqrt{30}}) + (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})h \\ = {} & (\frac{\sqrt{3}}{2\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{\sqrt{14}}{4} + \frac{1}{\sqrt{5}})(2b) \\ & + 2(\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}}) \\ & + (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})h \\ \leq {} & (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})(2b + h) \\ & + 2(\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}}) \\ = {} & (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})(n - 2) \\ & + 2(\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}}) \\ = {} & (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})n \\ & - 2\sqrt{\frac{3}{10}} + 2\frac{\sqrt{7}}{\sqrt{30}} - 3\frac{\sqrt{2}}{5} + \frac{2}{\sqrt{3}}.\end{aligned}$$

Thus,

$$\begin{aligned} ABC_4(C_n) \leq (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})n \\ - 2\sqrt{\frac{3}{10}} + 2\frac{\sqrt{7}}{\sqrt{30}} - 3\frac{\sqrt{2}}{5} + \frac{2}{\sqrt{3}}. \end{aligned} \tag{3.15}$$

It can be observed that, if the equality of Equation (3.15) holds, then $b = m = p = 0$. Thus, the cactus C_n satisfies $ABC_4(C_n) = (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})n - 2\sqrt{\frac{3}{10}} + 2\frac{\sqrt{7}}{\sqrt{30}} - 3\frac{\sqrt{2}}{5} + \frac{2}{\sqrt{3}}$ if it is the ortho-hexagonal cactus chain of n hexagons.

Next, we prove the lower bound. By Equation (2.5), we have

$$\begin{aligned} ABC_4(C_n) &= (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)\tilde{l} + (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}})\bar{l} \\ &+ (\sqrt{\frac{3}{2}} + \frac{\sqrt{3}}{\sqrt{10}} + \frac{\sqrt{7}}{\sqrt{30}} + \frac{3\sqrt{2}}{10} + \frac{1}{\sqrt{3}})o \\ &+ (\frac{\sqrt{10}}{3} + 2)p + (\frac{2}{\sqrt{3}} + 1 + \frac{\sqrt{14}}{4})m \\ &+ (\frac{3\sqrt{14}}{4})\tilde{b} + (\frac{\sqrt{14}}{2} + \frac{2}{\sqrt{5}})\bar{b} \\ &\geq (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)\tilde{l} + (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 2\frac{\sqrt{7}}{\sqrt{30}})\bar{l} \\ &+ (\frac{\sqrt{10}}{3} + 2)(m + p + o) \\ &+ (\frac{3\sqrt{14}}{4})\tilde{b} + (\frac{\sqrt{14}}{2} + \frac{2}{\sqrt{5}})\bar{b}. \end{aligned}$$

Thus, the equality holds if $m = o = 0$. As all the inner hexagons are para hexagons, we have that $\bar{b} = \bar{l} = 0$. This implies $b = \tilde{b}$ and $l = \tilde{l}$. By Equations (3.5) and (3.6), we have that

$$\begin{aligned} ABC_4(C_n) &\geq (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)l + (\frac{\sqrt{10}}{3} + 2)(m + p + o) + (\frac{3\sqrt{14}}{4})b \\ &= (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)l + (\frac{\sqrt{10}}{3} + 2)h + (\frac{3\sqrt{14}}{4})b \\ &= (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)(b + 2) + (\frac{\sqrt{10}}{3} + 2)h + (\frac{3\sqrt{14}}{4})b \\ &= (\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1 + \frac{3\sqrt{14}}{4})b + (\frac{\sqrt{10}}{3} + 2)h \\ &+ 2(\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1) \end{aligned}$$

$$= (\sqrt{\frac{3}{8}} + \frac{1}{\sqrt{3}} + \frac{1}{2} + \frac{3\sqrt{14}}{8})(2b) + (\frac{\sqrt{10}}{3} + 2)h$$
$$+ 2(\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)$$
$$\geq (\frac{\sqrt{10}}{3} + 2)(2b + h) + 2(\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)$$
$$= (\frac{\sqrt{10}}{3} + 2)(n - 2) + 2(\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{3}} + 1)$$
$$= (\frac{\sqrt{10}}{3} + 2)n - 2\frac{\sqrt{10}}{3} + \sqrt{6} + \frac{4}{\sqrt{3}} - 2.$$

Therefore,

$$ABC_4(C_n) \geq (\frac{\sqrt{10}}{3} + 2)n - 2\frac{\sqrt{10}}{3} + \sqrt{6} + \frac{4}{\sqrt{3}} - 2. \tag{3.16}$$

It can be observed that, if the equality of Equation (3.16) holds, then $b = m = o = 0$. Thus, the cactus C_n satisfies $ABC_4(C_n) = (\frac{\sqrt{10}}{3} + 2)n - 2\frac{\sqrt{10}}{3} + \sqrt{6} + \frac{4}{\sqrt{3}} - 2$ if it is para-hexagonal cactus chain of n hexagons.

3.5.2. Bounds of Fifth Geometric Arithmetic Index

We first prove the upper bound. By Equation (2.6), we have

$$GA_5(C_n) = (3 + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{10}}{7} + \frac{\sqrt{15}}{4})o + (2 + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7})(\tilde{l} + m)$$
$$+ (2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{15}}{2})\bar{l} + (2 + \frac{16\sqrt{3}}{7})p + (4 + \frac{8\sqrt{5}}{9})\bar{b} + 6\tilde{b}.$$

Replacing the coefficients of o and m by the coefficient of p yield

$$GA_5(C_n) \leq (2 + \frac{16\sqrt{3}}{7})(m + p + o) + (2 + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7})(\tilde{l})$$
$$+ (2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{15}}{2})\bar{l} + (4 + \frac{8\sqrt{5}}{9})\bar{b} + 6\tilde{b}.$$

The equality holds if $m = o = 0$. As there is no ortho hexagon, we have that $\bar{b} = \bar{l} = 0$. This implies $b = \tilde{b}$ and $l = \tilde{l}$. By Equations (3.5) and (3.6), we have

$$GA_5(C_n) = (2 + \frac{16\sqrt{3}}{7})h + (2 + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7})l + 6b$$
$$= (2 + \frac{16\sqrt{3}}{7})h + (2 + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7})(b + 2) + 6b$$

$$
\begin{aligned}
&= (2+\frac{16\sqrt{3}}{7})h + (8+\frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7})b \\
&\quad + 2(2+\frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7}) \\
&= (2+\frac{16\sqrt{3}}{7})h + (4+\frac{2\sqrt{6}}{5}+\frac{4\sqrt{3}}{7})(2b) \\
&\quad + 2(2+\frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7}) \\
&\leq (4+\frac{2\sqrt{6}}{5}+\frac{4\sqrt{3}}{7})(2b+h) + 2(2+\frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7}) \\
&= (4+\frac{2\sqrt{6}}{5}+\frac{4\sqrt{3}}{7})(n-2) + 2(2+\frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7}) \\
&= (4+\frac{2\sqrt{6}}{5}+\frac{4\sqrt{3}}{7})n - 4 + \frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7}.
\end{aligned}
$$

Thus,

$$
GA_5(C_n) \leq (4+\frac{2\sqrt{6}}{5}+\frac{4\sqrt{3}}{7})n - 4 + \frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7}. \tag{3.17}
$$

It can be observed that, if the equality of Equation (3.17) holds, then $h = 0$. Thus, the cactus C_n satisfies $GA_5(C_n) = (4+\frac{2\sqrt{6}}{5}+\frac{4\sqrt{3}}{7})n - 4 + \frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7}$ if it is a cactus of n hexagons having only branching hexagons and leaf hexagons.

Next, we prove the lower bound. By Equation (2.6), we have

$$
\begin{aligned}
GA_5(C_n) &= (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})o + (2+\frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7})(\tilde{l}+m) \\
&\quad + (2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{15}}{2})\bar{l} + (2+\frac{16\sqrt{3}}{7})p + (4+\frac{8\sqrt{5}}{9})\bar{b} + 6\tilde{b} \\
&\geq (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})(o+m+p) + (2+\frac{4\sqrt{6}}{5} \\
&\quad + \frac{8\sqrt{3}}{7})\tilde{l} + (2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{15}}{2})\bar{l} + (4+\frac{8\sqrt{5}}{9})\bar{b} + 6\tilde{b}.
\end{aligned}
$$

Thus, the equality holds if $m = p = 0$. That is all the inner hexagons are ortho hexagons. So, $\tilde{b} = \tilde{l} = 0$. This implies $b = \bar{b}$ and $l = \bar{l}$. By Equations (3.5) and (3.6), we have

$$
\begin{aligned}
GA_5(C_n) &= (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})h + (2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{15}}{2})l \\
&\quad + (4+\frac{8\sqrt{5}}{9})b \\
&= (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})h + (2+\frac{4\sqrt{6}}{5} \\
&\quad + \frac{\sqrt{15}}{2})(b+2) + (4+\frac{8\sqrt{5}}{9})b
\end{aligned}
$$

$$
\begin{aligned}
&= (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})h+(6+\frac{4\sqrt{6}}{5}\\
&\quad+\frac{\sqrt{15}}{2}+\frac{8\sqrt{5}}{9})b+2(2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{15}}{2})\\
&= (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})h+(3+\frac{2\sqrt{6}}{5}\\
&\quad+\frac{\sqrt{15}}{4}+\frac{4\sqrt{5}}{9})(2b)+2(2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{15}}{2})\\
&\geq (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})(2b+h)\\
&\quad+2(2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{15}}{2})\\
&= (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})(n-2)+2(2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{15}}{2})\\
&= (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})n+2+\frac{4\sqrt{6}}{5}-\frac{4\sqrt{10}}{7}+\frac{\sqrt{15}}{2}
\end{aligned}
$$

$$
GA_5\left(C_n\right) \geq (3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})n+2+\frac{4\sqrt{6}}{5}-\frac{4\sqrt{10}}{7}+\frac{\sqrt{15}}{2}. \tag{3.18}
$$

It can be observed that, if the equality of Equation (3.18) holds, then $b=m=p=0$. Thus, the cactus C_n satisfies $GA_5\left(C_n\right)=(3+\frac{2\sqrt{6}}{5}+\frac{2\sqrt{10}}{7}+\frac{\sqrt{15}}{4})n+2+\frac{4\sqrt{6}}{5}-\frac{4\sqrt{10}}{7}+\frac{\sqrt{15}}{2}$ if it is the ortho-hexagonal cactus chain of n hexagons.

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