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Research Article

On-Bond Incident Degree Indices of Square-Hexagonal Chains

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For a graph G, its bond incident degree (BID) index is defined as the sum of the contributions $f(d_u, d_v)$ over all edges uv of G, where d_w denotes the degree of a vertex w of G and f is a real-valued symmetric function. If $f(d_u, d_v) = d_u + d_v$ or $d_u d_v$, then the corresponding BID index is known as the first Zagreb index M_1 or the second Zagreb index M_2, respectively. The class of square-hexagonal chains is a subclass of the class of molecular graphs of minimum degree 2. (Formal definition of a square-hexagonal chain is given in the Introduction section). The present study is motivated from the paper (C. Xiao, H. Chen, Discrete Math. **339** (2016) 506–510) concerning square-hexagonal chains. In the present paper, a general expression for calculating any BID index of square-hexagonal chains is derived. The chains attaining the maximum or minimum values of M_1 and M_2 are also characterized from the class of all square-hexagonal chains having a fixed number of polygons.

1. Introduction

Those (chemical) graph-theoretical terminologies and notations adopted in the current paper that are not defined here in this paper can be found in some standard (chemical) graph-theoretical books; for example, [1–3]. All the graphs to be considered in the current paper are finite and connected.

In what follows, it is assumed that G is a graph. The edge set and vertex set of G are denoted by $E(G)$ and $V(G)$, respectively. For a vertex $w \in V(G)$, its degree is denoted by $d_w(G)$ (or simply by d_w whenever there is only one graph under consideration).

In chemical graph theory, those graph invariants that have some chemical applicability are often referred to as topological indices. The first and second Zagreb indices [4], appeared in the first half of 1970s (see for example [4, 5]), belong to the most-studied topological indices (especially in chemical graph theory); they are usually denoted by M_1 and M_2, respectively, and for G, they are defined as follows:

$$\begin{aligned} M_1(G) &= \sum_{u\in V(G)} (d_u)^2, \\ M_2(G) &= \sum_{uv\in E(G)} d_u d_v. \end{aligned} \tag{1}$$

It is known that $\sum_{u\in V(G)} (d_u)^2 = \sum_{uv\in E(G)} (d_u + d_v)$. Most of their known properties can be found in the review paper [4] and in the related references included therein.

For G, its bond incident degree (BID) index is defined as follows:

$$\mathrm{BID}(G) = \sum_{uv\in E(G)} f(d_u, d_v) = \sum_{1\le a\le b\le \Delta(G)} m_{a,b}(G)\theta_{a,b}, \tag{2}$$

where is the degree of the vertex u, f is a real-valued function such that $f(d_u, d_v) = f(d_v, d_u)$, uv is the edge d_u with end vertices u and v of G, $\Delta(G)$ is the maximum degree in G, $\theta_{a,b} = f(a,b)$ and $m_{a,b}(G)$ is the number of those edges of G whose one end vertex has the degree a and the other end vertex has the degree b. We note here that if $\theta_{a,b} = a + b$ or $\theta_{a,b} = ab$, then the corresponding BID index is M_1 or M_2, respectively. Details about some mathematical aspects of the BID indices can be found in the papers [6–8] as well as in the related references listed therein.

A square-hexagonal system is a connected geometric figure formed by concatenating congruent regular squares and/or hexagons side to side in a plane in such a way that the figure divides the plane into one infinite (external) region and a number of finite (internal) regions, and all internal regions must be congruent regular squares and/or hexagons. In a square-hexagonal system, two polygons having a common side are known as adjacent polygons. By inner dual of a square-hexagonal system, we mean a graph ID whose vertices are the polygons of the considered square-hexagonal system, while there is an edge between two vertices of ID if and only if the corresponding polygons share a side. A square-hexagonal system is said to be a square-hexagonal chain if its inner dual is the path graph. It should be noted that different square-hexagonal chains may be obtained depending on the polygons' type and depending on the way how polygons are concatenated. $R_n$refers to a square-hexagonal chain consisting of n polygons. If all polygons in R_n are hexagons, then we say that R_n is a hexagonal chain (see, for instance, [9]) and if all the polygons are squares, then R_n is known as a polyomino chain (see, for instance, [10]). Also, if squares and hexagons are concatenated alternately in R_n, then we say that R_n is a phenylene chain (see [11]).

Every square-hexagonal chain can be considered as a graph in which the edges represent the sides of the polygons and the vertices represent the points where two sides of a polygon intersect. In the rest of the present paper, by the terminology "square-hexagonal chain(s)" we mean the graph(s) corresponding to the considered square-hexagonal chain(s).

Analogous to the definition of square-hexagonal chains, one may give a definition of triangular/square/pentagonal chains. BID indices of triangular/square/pentagonal chains were studied in [10, 12]. The present study can be considered as a continuation of the research conducted in [10, 12] and it is motivated from the paper [13–15] concerning square-hexagonal chains. In the current paper, a general expression for calculating any BID index of square-hexagonal chains is derived. The chains attaining the maximum or minimum values of M_1 and M_2 are also characterized from the class of all square-hexagonal chains having a fixed number of polygons.

2. Main Results

In order to obtain the main results, we require some terminology concerning square-hexagonal chains. In a square-hexagonal chain, a polygon adjacent with only one (two, respectively) other polygon is known as a terminal (nonterminal, respectively) polygon. A nonterminal polygon in the chain is called a kink if its center is not collinear with centers of the two adjacent polygons. In other words, a nonterminal hexagon is a kink if and only if it contains two adjacent vertices of degree two (Figure 1) and a nonterminal square is a kink if and only if it contains a vertex of degree two (Figure 2). Following [15], we will consider square-hexagonal chains that contain the following types of kinks:

(1) Kinks of type T_1: A nonterminal hexagon having exactly two adjacent vertices of degree two (see Figure 1);

(2) Kinks of type $T_{2,1}$: A nonterminal square containing a vertex of degree two and adjacent to two squares (see Figure 2(a));

(3) Kinks of type $T_{2,2}$: A nonterminal square containing a vertex of degree two and adjacent to a square and a hexagon (see Figure 2(b));

(4) Kinks of type $T_{2,3}$: A nonterminal square containing a vertex of degree two and adjacent to two hexagons (see Figure 2(c));

A square-hexagonal chain is called linear if it has no kinks and it is called a zigzag chain if every nonterminal polygon is a kink. A segment is a maximal linear chain in a square-hexagonal chain, including kinks and/or terminal polygons at its ends.

The length $l(S)$ of a segment S is its number of polygons. $E(S)$ refers to the set of all edges of a segment S. A segment that contains a terminal polygon is known as an external segment. A segment that contains only nonterminal polygons is known as an internal segment. Clearly, a square-hexagonal chain consists of s segments if and only if it contains exactly $s-1$ kinks.

For a square-hexagonal R_n, we define the value δ_{R_n} to be the number of terminal hexagons in R_n. We also define the following values for segments $S_1, \ldots, S_s$ of R_n: see Figures 3 and 4.

$$
\begin{aligned}
\mu(S_i) &= \begin{cases} 1, & \text{if } S_i \text{ is an internal segment consisting of a hexagon and a square and contains} \\ & \text{only one edge connecting vertices of degree 3,} \\ 0, & \text{otherwise.} \end{cases} \\
\nu(S_i) &= \begin{cases} 1, & \text{if } S_i \text{ is an internal segment of length three and contains an edge} \\ & \text{connecting vertices of degree 3,} \\ 0, & \text{otherwise.} \end{cases}
\end{aligned}
\tag{3}
$$

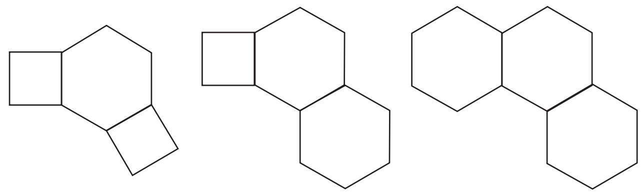

Figure 1: Kinks of type T_1.

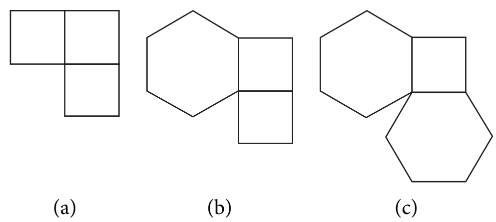

Figure 2: (a) Kinks of type $T_{2,1}$; (b) Kinks of type $T_{2,2}$; (c) Kinks of type $T_{2,3}$.

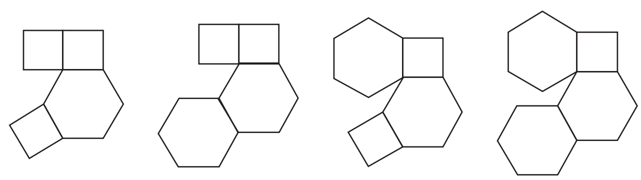

Figure 3: Internal segment consisting of a hexagon and a square and contains an edge connecting vertices of degree 3.

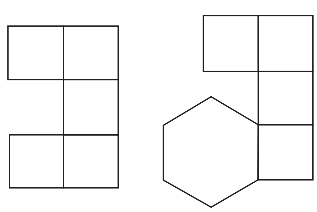

Figure 4: Internal segment of length three containing an edge connecting vertices of degree 3.

Moreover, $\mu(S_1) = \mu(S_s) = \nu(S_1) = \nu(S_s) = 0$.

$$\tau(S_i) = \begin{cases} 1, & \text{if } S_i \text{ consists of two squares,} \\ 0, & \text{otherwise.} \end{cases} \tag{4}$$

Now, we are ready to establish the general expression for calculating the BID indices of square-hexagonal chains.

Theorem 1. *Let R_n be square-hexagonal chain containing d squares and $n-d$ hexagons. Suppose that R_n consists of s segments $S_1, \ldots, S_s$ and contains α_1 kinks of type T_1 and $\alpha_{2,j}$ kinks of type $T_{2,j}$, for $j = 1, 2, 3$. Then,*

$$\begin{aligned}
m_{2,2}(R_n) &= 2\delta_{R_n} + \alpha_1 + 2, \\
m_{2,3}(R_n) &= 4n - 4d + 4 + 2\alpha_{2,1} + \alpha_{2,2} - 4\delta_{R_n} - 2\alpha_1 - \tau(S_1) - \tau(S_s) - \sum_{i=2}^{s-1}\left(2\tau(S_i) - \mu(S_i)\right), \\
m_{3,3}(R_n) &= n + 2d - 5 + 2\delta_{R_n} + \alpha_1 - 6\alpha_{2,1} - 5\alpha_{2,2} - 4\alpha_{2,3} + \tau(S_1) + \tau(S_s) + \sum_{i=2}^{s-1}\left(3\tau(S_i) - \mu(S_i) + \nu(S_i)\right), \\
m_{2,4}(R_n) &= \alpha_{2,2} + 2\alpha_{2,3} + \tau(S_1) + \tau(S_s) + \sum_{i=2}^{s-1}\left(2\tau(S_i) - \mu(S_i)\right), \\
m_{3,4}(R_n) &= 4\alpha_{2,1} + 3\alpha_{2,2} + 2\alpha_{2,3} - \tau(S_1) - \tau(S_s) - \sum_{i=2}^{s-1}\left(4\tau(S_i) - \mu(S_i) + 2\nu(S_i)\right), \\
m_{4,4}(R_n) &= \sum_{i=2}^{s-1}\left(\tau(S_i) + \nu(S_i)\right).
\end{aligned} \tag{5}$$

Proof. Let $C_1, \ldots, C_{s-1}$ be the kinks of R_n such that C_i joins segments S_i and S_{i+1}.

Let $A_1 = E(C_1)$, and $A_i = E(C_i)\backslash E(C_{i-1})$, for $i = 2, \ldots, s-1$. Also, we set $B_1 = E(S_1)\backslash E(C_1)$, $B_s = E(S_s)\backslash E(C_{s-1})$, and $B_j = E(S_j)\backslash (E(C_{j-1}) \cup E(C_j))$, for $j = 2, \ldots, s-1$.

Clearly, the collection $\{A_1, \ldots, A_{s-1}, B_1, \ldots, B_s\}$ forms a partition for $E(R_n)$. For $2 \leq a \leq b \leq 4$, $i = 1, \ldots, s-1$, $j = 1, \ldots, s$, let $p_{a,b}^{(i)}$ be the number of edges in A_i that connects vertices of degrees a and b and $q_{a,b}^{(j)}$ be the number of edges in B_j that connect vertices of degrees a and b. Then, we get $m_{a,b}(R_n) = \sum_{i=1}^{s-1} p_{a,b}^{(i)} + \sum_{j=1}^{s} q_{a,b}^{(j)}$.

First, we calculate $m_{2,2}(R_n)$. We have $q_{2,2}^{(1)} + q_{2,2}^{(s)} = 2(\delta_{R_n} + 1)$, and for $j = 2, \ldots, s-1$, we have $q_{2,2}^{(j)} = 0$. Also, a kink contains an edge joining vertices of degree 2 if and only if it is of type T_1. Hence, $m_{2,2} = 2\delta_{R_n} + \alpha_1 + 2$.

To calculate $m_{4,4}(R_n)$, note that a segment S_i contains an edge joining vertex of degree 4 if and only if S_i is an internal segment and $\tau(S_i) = 1$ or $\nu(S_i) = 1$. Thus, $m_{4,4}(R_n) = \sum_{i=2}^{s-1}(\tau(S_i) + \nu(S_i))$.

Next, we calculate $m_{2,4}(R_n)$. Vertices of degree 4 appear only in kinks of type $T_{2,1}, T_{2,2}$, and $T_{2,3}$. In fact, $p_{2,4}^{(1)} = \tau(S_2)$, $p_{2,4}^{(s-1)} = \tau(S_{s-1})$, and for $2 \leq i \leq s-2$, $p_{2,4}^{(i)} = \tau(S_i) + \tau(S_{i+1})$ if C_i is a kink of type $T_{2,1}, T_{2,2}$, or $T_{2,3}$, and $p_{2,4}^{(i)} = 0$ otherwise. Hence, $\sum_{i=1}^{s-1} p_{a,b}^{(i)} = 2\sum_{i=2}^{s-1}\tau(S_i)$. Also, $\sum_{i=1}^{s} q_{a,b}^{(i)} = \alpha_{2,2} + 2\alpha_{2,3} + \tau(S_1) + \tau(S_s) - \sum_{i=2}^{s-1}\mu(S_i)$. Thus,

$$m_{2,4}(R_n) = \alpha_{2,2} + 2\alpha_{2,3} + \tau(S_1) + \tau(S_s) + \sum_{i=2}^{s-1}(2\tau(S_i) - \mu(S_i)). \tag{6}$$

Now, each kink of types $T_{2,1}, T_{2,2}$, or $T_{2,3}$ contains exactly one vertex of degree 4, and so the number of vertices of degree 4 is $\alpha_{2,1} + \alpha_{2,2} + \alpha_{2,3}$. Therefore,

$$m_{2,4}(R_n) + m_{3,4}(R_n) + 2m_{4,4}(R_n) = 4(\alpha_{2,1} + \alpha_{2,2} + \alpha_{2,3}). \tag{7}$$

Substituting the values of $m_{2,4}(R_n)$ and $m_{4,4}(R_n)$ in (7) and solving the resulting equation for $m_{3,4}(R_n)$ yield the following:

$$\begin{aligned} m_{3,4}(R_n) &= 4(\alpha_{2,1} + \alpha_{2,2} + \alpha_{2,3}) - \alpha_{2,2} - 2\alpha_{2,3} - \tau(S_1) \\ &\quad - \tau(S_s) - \sum_{i=2}^{s-1}(2\tau(S_i) - \mu(S_i)) \\ &\quad - 2\sum_{i=2}^{s-1}(\tau(S_i) + \nu(S_i)) = 4\alpha_{2,1} + 3\alpha_{2,2} + 2\alpha_{2,3} \\ &\quad - \tau(S_1) - \tau(S_s) - \sum_{i=2}^{s-1}(4\tau(S_i) - \mu(S_i) + 2\nu(S_i)). \end{aligned} \tag{8}$$

Similarly, every nonterminal hexagon contains exactly two vertices of degree 2, and a nonterminal square contains a vertex of degree 2 if and only if it is a kink of type $T_{2,1}, T_{2,2}$, or $T_{2,3}$. Now, adding number of vertices of degree 2 in the terminal polygons, we see that the number of vertices of degree 2 in R_n is $2n - 2\mathrm{d} + 4 + \alpha_{2,1} + \alpha_{2,2} + \alpha_{2,3}$. Hence, $2m_{2,2}(R_n) + m_{2,3}(R_n) + m_{2,4}(R_n) = 2(2n - 2\,d + 4 + \alpha_{2,1} + \alpha_{2,2} + \alpha_{2,3})$. Therefore,

$$\begin{aligned} m_{2,3}(R_n) &= 2(2n - 2\mathrm{d} + 4 + \alpha_{2,1} + \alpha_{2,2} + \alpha_{2,3}) \\ &\quad - 2(2\delta_{R_n} + \alpha_1 + 2) - \alpha_{2,2} - 2\alpha_{2,3} - \tau(S_1) - \tau(S_s) \\ &\quad - \sum_{i=2}^{s-1}(2\tau(S_i) - \mu(S_i)) = 4n - 4d + 4 \\ &\quad + 2\alpha_{2,1} + \alpha_{2,2} - 4\delta_{R_n} - 2\alpha_1 - \tau(S_1) - \tau(S_s) \\ &\quad - \sum_{i=2}^{s-1}(2\tau(S_i) - \mu(S_i)). \end{aligned} \tag{9}$$

The total number of edges in R_n is $n + 1 + 2\,d + 4(n-d) = 5n - 2\,d + 1$, and so

$$\begin{aligned} m_{3,3}(R_n) &= 5n - 2d + 1 - 2\delta_{R_n} - 2 - \alpha_1 - 4n + 4d - 4 - 2\alpha_{2,1} - \alpha_{2,2} + 4\delta_{R_n} + 2\alpha_1 \\ &\quad + \tau(S_1) + \tau(S_s) + \sum_{i=2}^{s-1}(2\tau(S_i) - \mu(S_i)) \\ &\quad - \alpha_{2,2} - 2\alpha_{2,3} - \tau(S_1) - \tau(S_s) - \sum_{i=2}^{s-1}(2\tau(S_i) - \mu(S_i)) \\ &\quad - 4\alpha_{2,1} - 3\alpha_{2,2} - 2\alpha_{2,3} + \tau(S_1) + \tau(S_s) + \sum_{i=2}^{s-1}(4\tau(S_i) - \mu(S_i) + 2\nu(S_i)) \\ &\quad - \sum_{i=2}^{s-1}(\tau(S_i) + \nu(S_i)) \\ &= n + 2\,d - 5 + 2\delta_{R_n} + \alpha_1 - 6\alpha_{2,1} - 5\alpha_{2,2} - 4\alpha_{2,3} + \tau(S_1) + \tau(S_s) \\ &\quad + \sum_{i=2}^{s-1}(3\tau(S_i) - \mu(S_i) + \nu(S_i)). \end{aligned} \tag{10}$$

The following results are a direct consequence of Theorem 1. □

Corollary 1. *Let R_n be a square-hexagonal chain containing d squares and $n-d$ hexagons. Suppose that R_n consists of s segments $S_1,\ldots,S_s$ and contains α_1 kinks of type T_1 and $\alpha_{2,j}$ kinks of type $T_{2,j}$, for $j=1,2,3$. Then,*

$$\begin{aligned}
BID(R_n) &= \sum_{2\le a\le b\le 4} m_{a,b}(R_n)\theta_{a,b}\\
&= (4\theta_{2,3}+\theta_{3,3})n + (2\theta_{3,3}-4\theta_{2,3})d + (2\theta_{2,2}+4\theta_{2,3}-5\theta_{3,3})\\
&\quad + (2\theta_{2,2}-4\theta_{2,3}+2\theta_{3,3})\delta_{R_n} + (\theta_{2,2}-2\theta_{2,3}+\theta_{3,3})\alpha_1\\
&\quad + (2\theta_{2,3}-6\theta_{3,3}+4\theta_{3,4})\alpha_{2,1} + (\theta_{2,3}-5\theta_{3,3}+\theta_{2,4}+3\theta_{3,4})\alpha_{2,2}\\
&\quad + (2\theta_{2,4}-4\theta_{3,3}+2\theta_{3,4})\alpha_{2,3} + (\theta_{3,3}-\theta_{2,3}+\theta_{2,4}-\theta_{3,4})(\tau(S_1)+\tau(S_s))\\
&\quad + (3\theta_{3,3}-2\theta_{2,3}+2\theta_{2,4}-4\theta_{3,4}+\theta_{4,4})\sum_{i=2}^{s-1}\tau(S_i)\\
&\quad + (\theta_{2,3}-\theta_{3,3}-\theta_{2,4}+\theta_{3,4})\sum_{i=2}^{s-1}\mu(S_i) + (\theta_{3,3}-2\theta_{3,4}+\theta_{4,4})\sum_{i=2}^{s-1}\nu(S_i).
\end{aligned} \tag{11}$$

Corollary 2. *If L_n is a linear square-hexagonal chain with d squares and $n-d$ hexagons, then*

$$\begin{aligned}
\mathrm{BID}(L_n) &= (4\theta_{2,3}+\theta_{3,3})n + (2\theta_{3,3}-4\theta_{2,3})d\\
&\quad + (2\theta_{2,2}+4\theta_{2,3}-5\theta_{3,3}) + (2\theta_{2,2}-4\theta_{2,3}+2\theta_{3,3})\delta_{L_n}.
\end{aligned} \tag{12}$$

L_n^0 (resp. L_n^1) denotes the linear square-hexagonal chain with n polygons where the terminal polygons are squares (resp. hexagons) and all nonterminal polygons are hexagons (resp. squares). Then,

$$\begin{aligned}
\mathrm{BID}(L_n^0) &= (4\theta_{2,3}+\theta_{3,3})n + 2\theta_{2,2} - 4\theta_{2,3} - \theta_{3,3},\\
\mathrm{BID}(L_n^1) &= 3\theta_{3,3}n + 6\theta_{2,2} + 4\theta_{2,3} - 5\theta_{3,3}.
\end{aligned} \tag{13}$$

The next theorem gives the extreme values of BID indices for the class of linear square-hexagonal chains.

Theorem 2

(a) If $\theta_{3,3}-2\theta_{2,3}>0$, then

(1) $BID(L_n)$ is minimum if and only if $L_n \cong L_n^0$;
(2) $BID(L_n)$ is maximum if and only if $L_n \cong L_n^1$.

(b) If $\theta_{3,3}-2\theta_{2,3}<0$, then

(1) $BID(L_n)$ is minimum if and only if L_n is linear polyomino chain;
(2) $BID(L_n)$ is maximum if and only if L_n is linear hexagonal chain.

Proof. (a) Suppose that $\theta_{3,3}-2\theta_{2,3}>0$. Let L_n be a linear square-hexagonal chain with d squares. Since $d+\delta_{R_n}\ge 2$ and $\delta_{R_n}\ge 0$, we obtain the following:

$$\begin{aligned}
\mathrm{BID}(L_n) &= (4\theta_{2,3}+\theta_{3,3})n + (2\theta_{3,3}-4\theta_{2,3})(d+\delta_{L_n}) + (2\theta_{2,2}+4\theta_{2,3}-5\theta_{3,3}) + 2\theta_{2,2}\delta_{L_n}\\
&\ge (4\theta_{2,3}+\theta_{3,3})n + 2(2\theta_{3,3}-4\theta_{2,3}) + (2\theta_{2,2}+4\theta_{2,3}-5\theta_{3,3})\\
&= (4\theta_{2,3}+\theta_{3,3})n + 2\theta_{2,2} - 4\theta_{2,3} - \theta_{3,3} = \mathrm{BID}(L_n^0).
\end{aligned} \tag{14}$$

The equality holds if and only if $\delta_{L_n}=0$ and $d=2$ equivalently $L_n \cong L_n^0$.

Also, we have $d+\delta_{L_n}\le n$. Therefore,

$$\begin{aligned}
\mathrm{BID}(L_n) &= (4\theta_{2,3}+\theta_{3,3})n + (2\theta_{3,3}-4\theta_{2,3})d + (2\theta_{2,2}+4\theta_{2,3}-5\theta_{3,3}) + (2\theta_{2,2}-4\theta_{2,3}+2\theta_{3,3})\delta_{L_n}\\
&= (4\theta_{2,3}+\theta_{3,3})n + (2\theta_{3,3}-4\theta_{2,3})(d+\delta_{L_n}) + (2\theta_{2,2}+4\theta_{2,3}-5\theta_{3,3}) + 2\theta_{2,2}\delta_{L_n}\\
&\le (4\theta_{2,3}+\theta_{3,3})n + (2\theta_{3,3}-4\theta_{2,3})n + 4\theta_{2,3} - 5\theta_{3,3} + 6\theta_{2,2}\\
&= 3\theta_{3,3}n - 5\theta_{3,3} + 4\theta_{2,3} + 6\theta_{2,2} = \mathrm{BID}(L_n^1).
\end{aligned} \tag{15}$$

The equality holds if and only if $\delta_{L_n} = 2$ and $d = n-2$ equivalently $L_n \cong L_n^1$.

(b) is similar to the proof of part (a).

Now, we focus on the special cases of the first Zagreb index M_1 ($\theta_{a,b} = a+b$) and the second Zagreb index M_2 ($\theta_{a,b} = ab$) of square-hexagonal chains. □

Corollary 3. *If R_n is a square-hexagonal chain with d squares, s segments $S_1, \ldots, S_s$, α_1 kinks of type T_1, and $\alpha_{2,j}$ kinks of type $T_{2,j}$, $j = 1,2,3$, then*

$$\begin{aligned} M_1(R_n) &= 26n - 8d + 2\alpha_{2,1} + 2\alpha_{2,2} + 2\alpha_{2,3} - 2,\\ M_2(R_n) &= 33n - 6d + 2\delta_{R_n} - 13 + \alpha_1 + 6\alpha_{2,1} + 5\alpha_{2,2} + 4\alpha_{2,3} - \sum_{i=1}^{s}\left(\tau(S_i) - \mu(S_i) - \nu(S_i)\right). \end{aligned} \tag{16}$$

The next result gives the extreme values of the first and second Zagreb indices for the class of square-hexagonal chains.

Theorem 3

(a) $M_1(R_n)$ is minimum if and only if R_n is a linear polyomino chain.

(b) $M_1(R_n)$ is maximum if and only if R_n is a hexagonal chain.

(c) $M_2(R_n)$ is minimum if and only if R_n is a linear polyomino chain.

(d) $M_2(R_n)$ is maximum if and only if R_n is a zigzag hexagonal chain.

Proof. Let LP_n denote the linear polyomino chain with n squares, H_n denote a hexagonal chain with n hexagons, and ZH_n denote the zigzag hexagonal chain with n squares and $n-2$ kinks of type T_1. Then, by Corollary 3, we have $M_1(LP_n) = 18n - 2$, $M_1(H_n) = 26n - 2$, $M_2(LP_n) = 27n - 13$, and $M_2(ZH_n) = 34n - 11$. Let R_n be a square-hexagonal chain with d squares, s segments $S_1, \ldots, S_s$, and α_1 kinks of type T_1, $\alpha_{2,j}$ kinks of type $T_{2,j}$, $j = 1,2,3$.

(a) Since $d \le n$ and $\alpha_{2,j} \ge 0$ for $j = 1,2,3$, we have the following:

$$\begin{aligned} M_1(R_n) &= 26n - 8d + 2\alpha_{2,1} + 2\alpha_{2,2} + 2\alpha_{2,3}\\ &\quad - 2 \ge 18n - 2 = M_1(LP_n), \end{aligned} \tag{17}$$

with equality holds if and only $d = n$ and $\alpha_{2,1} = \alpha_{2,2} = \alpha_{2,3} = 0$.

(b) Since all kinks of type $T_{2,j}$, $j = 1,2,3$ are squares, we clearly see that $d \ge \alpha_{2,1} + \alpha_{2,2} + \alpha_{2,3}$. Hence,

$$\begin{aligned} M_1(R_n) &= 26n - 2\left(4d - \alpha_{2,1} - \alpha_{2,2} - \alpha_{2,3}\right) - 2\\ &\le 26n - 2 = M_1(H_n), \end{aligned} \tag{18}$$

and equality holds if and only if $d = 0$.

(c) If S_i is an internal segment and $\tau(S_i) = 1$, then each terminal polygon of S_i is a kink of type $T_{2,1}$ or type $T_{2,2}$. This implies that $\sum_{i=1}^{s}\tau(S_i) \le \alpha_{2,1} + \alpha_{2,2} + 1$. Therefore,

$$\begin{aligned} M_2(R_n) &= 33n - 6d + 2\delta_{R_n} - 13 + \alpha_1 + 6\alpha_{2,1} + 5\alpha_{2,2} + 4\alpha_{2,3} - \sum_{i=1}^{s}\left(\tau(S_i) - \mu(S_i) - \nu(S_i)\right)\\ &\ge 27n - 13 + 6\alpha_{2,1} + 5\alpha_{2,2} - \sum_{i=1}^{s}\tau(S_i). \end{aligned} \tag{19}$$

Equality holds if and only if $d = n$ (consequently $\alpha_{2,2} = 0$), $\delta_{R_n} = 0$, and $\alpha_{2,3} = \sum_{i=1}^{s}\mu(S_i) = \sum_{i=1}^{s}\nu(S_i) = 0$. Now, if $\alpha_{2,1} \ge 1$, then $6\alpha_{2,1} - \sum_{i=1}^{s}\tau(S_i) \ge 5$, and hence $M_2(R_n) > 27n - 13 = M_2(LP_n)$. If $\alpha_{2,1} = 0$, then $\sum_{i=1}^{s}\tau(S_i) = 0$, and then $R_n \cong LP_n$.

(d) We have the following:

$$\begin{aligned} M_2(R_n) &= 33n - 6d + 2\delta_{R_n} - 13 + \alpha_1 + 6\alpha_{2,1} + 5\alpha_{2,2} + 4\alpha_{2,3} - \sum_{i=1}^{s}\left(\tau(S_i) - \mu(S_i) - \nu(S_i)\right)\\ &\le 33n - 13 + 2\delta_{R_n} - 6\left(d - \alpha_{2,1} - \alpha_{2,2} - \alpha_{2,3} - \sum_{i=1}^{s}\nu(S_i)\right)\\ &\quad - \left(\alpha_{2,2} + \alpha_{2,3} - \sum_{i=1}^{s}\mu(S_i)\right) + \alpha_1 - \alpha_{2,3} - 5\sum_{i=1}^{s}\nu(S_i). \end{aligned} \tag{20}$$

If, for some i, $\mu(S_i) \neq 0$, then one of the terminal polygons of S_i is a kink of type $T_{2,2}$ or type $T_{2,3}$. This implies that $\sum_{i=1}^{s} \mu(S_i) \leq \alpha_{2,2} + \alpha_{2,3}$. Moreover, if $\nu(S_i) \neq 0$, then S_i contains a square that is not a kink, and hence, $d \geq \alpha_{2,3} + \alpha_{2,2} + \alpha_{2,3} + \sum_{i=1}^{s} \nu(S_i)$. On the other hand, we know that $\delta_{R_n} \leq 2$ and $\alpha_1 \leq n - 2$. Thus, we have the following:

$$M_2(R_n) \leq 34n - 11 = M_2(ZH_n). \tag{21}$$

Now, if one of the values d, $\alpha_{2,1}$, $\alpha_{2,2}$, $\alpha_{2,3}$, $\sum_{i=1}^{s} \nu(S_i)$, and $\sum_{i=1}^{s} \mu(S_i)$ is nonzero, then $\delta_{R_n} \leq 1$ or $\alpha_1 < n - 2$, and so $M_2(R_n) < 34n - 11 = M_2(ZH_n)$. Therefore, equality in (21) holds if and only if $\delta_{R_n} = 2$ and $\alpha_1 = n - 2$ equivalently $R_n \cong ZH_n$. □

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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