Research Article

On-Bond Incident Degree Indices of Square-Hexagonal Chains

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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 $v \in V(G)$, its degree is denoted by $d_v(G)$ (or simply by $d_v$ 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:

$$M_1(G) = \sum_{uv \in E(G)} (d_u)_2,$$

$$M_2(G) = \sum_{uv \in E(G)} d_ud_v. \quad (1)$$

It is known that $\sum_{uv \in E(G)} (d_u)_2 = \sum_{uv \in E(G)} (d_u + d_v)$. 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:

$$\text{BID}(G) = \sum_{uv \in E(G)} f(d_u, d_v) = \sum_{1 \leq a < b \leq \Delta(G)} m_{a,b}(G) \theta_{a,b}, \quad (2)$$

where is the degree of the vertex $u$, $f$ is a real-valued function such that $f(d_u, d_v) = f(d_u, d_v)$, $uv$ 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 $\theta_{a,b} = ab$ or $\theta_{a,b} = ab$, then the corresponding BID index is $M_1$ or $M_2$, respectively.
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 \( M_4 \) 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 (non-terminal, 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 \( T_2 \): A nonterminal square containing a vertex of degree two and adjacent to two squares (see Figure 2(a));
3. Kinks of type \( T_2 \): 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 \( T_2 \): 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 \( \delta_{R_n} \) 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.

\[
\mu(S_i) = \begin{cases} 
1, & \text{if } S_i \text{ is an internal segment consisting of a hexagon and a square and contains} \\
0, & \text{otherwise}.
\end{cases}
\]

\[
v(S_i) = \begin{cases} 
1, & \text{if } S_i \text{ is an internal segment of length three and contains an edge} \\
0, & \text{otherwise.}
\end{cases}
\]
Moreover, \( \mu(S_1) = \mu(S_s) = \nu(S_1) = \nu(S_s) = 0. \)

Moreover, \( \mu(S_i) = \mu(S_i) = v(S_i) = v(S_i) = 0. \)

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.

\[
m_{2,2}(R_n) = 2\delta_{R_n} + \alpha_1 + 2, \\
m_{2,3}(R_n) = 4n - 4d + 4 + 2\alpha_{2,1} + \alpha_{2,2} - 4\delta_{R_n} - 2\alpha_1 - \tau(S_1) - \tau(S_s) - \sum_{i=2}^{s-1} (2\tau(S_i) - \mu(S_i)), \\
m_{3,3}(R_n) = n + 2d - 5 + 2\delta_{R_n} + \alpha_1 - 6\alpha_{2,1} - 5\alpha_{2,2} - 4\alpha_{2,3} + \tau(S_1) + \tau(S_s) + \sum_{i=2}^{s-1} (3\tau(S_i) - \mu(S_i) + v(S_i)), \\
m_{2,4}(R_n) = \alpha_{2,2} + 2\alpha_{2,3} + \tau(S_1) + \tau(S_s) + \sum_{i=2}^{s-1} (2\tau(S_i) - \mu(S_i)), \\
m_{3,4}(R_n) = 4\alpha_{2,1} + 3\alpha_{2,2} + 2\alpha_{2,3} - \tau(S_1) - \tau(S_s) - \sum_{i=2}^{s-1} (4\tau(S_i) - \mu(S_i) + 2v(S_i)), \\
m_{4,4}(R_n) = \sum_{i=2}^{s-1} (\tau(S_i) + v(S_i)).
\]

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

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 \( \alpha_j \) kinks of type \( T_1 \) and \( \alpha_{2,j} \) kinks of type \( T_{2,j} \) for \( j = 1, 2, 3. \) Then,
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 \( A_i = E(C_i) \setminus E(C_{i-1}) \), for \( i = 2, \ldots, s-1 \). Also, we set \( B_1 = E(S_1) \setminus E(C_1) \), \( B_i = E(S_i) \setminus E(C_{i-1}) \), and \( B_j = E(S_j) \setminus E(C_{j+1}) \cup E(C_j) \), for \( j = 2, \ldots, s-1 \).

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

First, we calculate \( m_{22}(R_n) \). We have \( q_{22}^{(i)} = 0 \) and \( m_{22}(R_n) = \sum_{i=1}^{s-1} p_{22}^{(i)} + \sum_{j=1}^{s-1} q_{22}^{(j)} \).

To calculate \( m_{44}(R_n) \), note that a segment \( S_i \) contains an edge joining vertices of degree 2 if and only if it is of type \( T_1 \). Hence, \( m_{22} = 2\delta_{R_1} + \alpha_1 + 2 \).

Next, we calculate \( m_{24}(R_n) \). Vertices of degree 4 appear only in kinks of types \( T_{2,1}, T_{2,2} \), and \( T_{3,2} \). In fact, \( p_{24}^{(i)} = \tau(S_i) \), \( p_{24}^{(i-1)} = \tau(S_{i-1}) \), and for \( 2 \leq i \leq s-2 \), \( p_{24}^{(i)} = \tau(S_i) + \tau(S_{i+1}) \) if \( C_i \) is a kink of type \( T_{2,1}, T_{2,2} \), or \( T_{3,2} \), and \( p_{24}^{(i)} = 0 \) otherwise. Hence, \( \sum_{i=1}^{s-1} p_{24}^{(i)} = 2 \sum_{i=1}^{s-1} \tau(S_i) \). Also, \( \sum_{i=1}^{s-1} q_{24}^{(i)} = 2 \alpha_2 + 2 \alpha_3 + \tau(S_1) + \tau(S_s) - \sum_{i=2}^{s-1} \mu(S_i) \). Thus,

\[
m_{24}(R_n) = \alpha_2 + 2 \alpha_3 + \tau(S_1) + \tau(S_s) + \tau(S_1) = \sum_{i=2}^{s-1} (2\tau(S_i) - \mu(S_i)). \tag{6}
\]

Now, each kink of types \( T_{2,1}, T_{2,2} \), or \( T_{3,2} \) contains exactly one vertex of degree 4, and so the number of vertices of degree 4 is \( \alpha_2 + \alpha_3 \). Therefore,\n
\[
m_{24}(R_n) + m_{44}(R_n) + 2m_{44}(R_n) = 4(\alpha_2 + \alpha_2 + \alpha_2).
\tag{7}
\]

Substituting the values of \( m_{24}(R_n) \) and \( m_{44}(R_n) \) in (7) and solving the resulting equation for \( m_{34}(R_n) \) yield the following:

\[
m_{34}(R_n) = 4(\alpha_2 + \alpha_2 + \alpha_2) - \alpha_2 - 2\alpha_2 - \tau(S_1) + \tau(S_1) + \sum_{i=2}^{s-1} (2\tau(S_i) - \mu(S_i)) \]

\[
- \alpha_2 - 2\alpha_2 - \tau(S_1) - \tau(S_1) - \sum_{i=2}^{s-1} (2\tau(S_i) - \mu(S_i)) \]

\[
- 4\alpha_2 - 3\alpha_2 - 2\alpha_2 + \tau(S_1) + \tau(S_1) + \sum_{i=2}^{s-1} (4\tau(S_i) - \mu(S_i) + 2\nu(S_i)) \]

\[
- \sum_{i=2}^{s-1} (\tau(S_i) + \nu(S_i)) \]

\[
= n + 2d - 5 + 2\delta_{R_1} + \alpha_1 - 6\delta_{R_2} - 5\delta_{R_2} - 4\alpha_2 + \tau(S_1) + \tau(S_s) + \sum_{i=2}^{s-1} (3\tau(S_i) - \mu(S_i) + \nu(S_i)).
\]

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 \( T_{3,2} \). 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 \( 2n - 2d + 4 + \alpha_2 + \alpha_2 + \alpha_2 \). Hence, \( 2m_{22}(R_n) + m_{23}(R_n) + m_{24}(R_n) = 2(n - 2d + 4 + \alpha_2 + \alpha_2 + \alpha_2) \).

Therefore,

\[
m_{23}(R_n) = 2(n - 2d + 4 + \alpha_2 + \alpha_2 + \alpha_2) - \sum_{i=2}^{s-1} (2\tau(S_i) - \mu(S_i)) \]

\[
- \sum_{i=2}^{s-1} (2\tau(S_i) - \mu(S_i)) = 4n - 4d + 4 \]

\[
+ 2\alpha_2 + 2\alpha_2 - 2\alpha_1 - \tau(S_1) - \tau(S_s) \]

\[
- \sum_{i=2}^{s-1} (2\tau(S_i) - \mu(S_i)).
\]

\[
= n + 2d - 5 + 2\delta_{R_1} + \alpha_1 - 6\delta_{R_2} - 5\delta_{R_2} - 4\alpha_2 + \tau(S_1) + \tau(S_s) + \sum_{i=2}^{s-1} (3\tau(S_i) - \mu(S_i) + \nu(S_i)).
\]

The total number of edges in \( R_n \) is \( n + 1 + 2d + 4(n - d) = 5n - 2d + 1 \), and so
The following results are a direct consequence of Theorem 1.

\[ BID(R_n) = \sum_{2a \leq n \leq 4} m_{a,b}(R_n)\theta_{ab} \]
\[ = (4\theta_{2,3} + \theta_{3,3})n + (2\theta_{3,3} - 4\theta_{2,3})d + (2\theta_{2,2} + 4\theta_{2,3} - 5\theta_{3,3}) + (2\theta_{2,2} - 2\theta_{2,3} + 3\theta_{3,3})\delta_{\text{R}_n} \]
\[ + (\theta_{2,3} - 2\theta_{2,3} + 3\theta_{3,3})\theta_{4,4} + (\theta_{3,3} - 2\theta_{2,3} + 4\theta_{4,4} + 6\theta_{2,2})\sum_{i=1}^{n-1} \tau(S_i) \]
\[ + (\theta_{2,2} - \delta_{\text{R}_n} + \theta_{4,4})\sum_{i=2}^{n-2} \tau(S_i) \]

(11)

**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 \( \alpha_i \) kinks of type \( T_1 \) and \( \alpha_{2,j} \) kinks of type \( T_{2,j} \), for \( j = 1, 2, 3 \). Then,

**Theorem 2**

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

(1) \( BID(L_n) \) is minimum if and only if \( L_n \equiv L_n^0 \);

(2) \( BID(L_n) \) is maximum if and only if \( L_n \equiv L_n^1 \).

(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 \( d + \delta_{\text{R}_n} \geq 2 \) and \( \delta_{\text{R}_n} \geq 0 \), we obtain the following:

\[ BID(L_n) = (4\theta_{2,3} + \theta_{3,3})n + (2\theta_{3,3} - 4\theta_{2,3})(d + \delta_{\text{R}_n}) + (2\theta_{2,2} + 4\theta_{2,3} - 5\theta_{3,3}) + 2\theta_{2,2}\delta_{\text{R}_n} \]
\[ \geq (4\theta_{2,3} + \theta_{3,3})n + 2(2\theta_{3,3} - 4\theta_{2,3}) + (2\theta_{2,2} + 4\theta_{2,3} - 5\theta_{3,3}) \]
\[ = (4\theta_{2,3} + \theta_{3,3})n + 2\theta_{2,2} - 4\theta_{2,3} - 3\theta_{3,3} = BID(L_n^0). \]

The equality holds if and only if \( \delta_{\text{R}_n} = 0 \) and \( d = 2 \) equivalently \( L_n \equiv L_n^0 \).

Also, we have \( d + \delta_{\text{R}_n} \leq n \). Therefore,

\[ BID(L_n) \]
\[ = (4\theta_{2,3} + \theta_{3,3})n + (2\theta_{3,3} - 4\theta_{2,3})d + (2\theta_{2,2} + 4\theta_{2,3} - 5\theta_{3,3}) + (2\theta_{2,2} - 2\theta_{2,3} + 2\theta_{3,3})\delta_{\text{R}_n} \]
\[ = (4\theta_{2,3} + \theta_{3,3})n + (2\theta_{3,3} - 4\theta_{2,3})(d + \delta_{\text{R}_n}) + (2\theta_{2,2} + 4\theta_{2,3} - 5\theta_{3,3}) + 2\theta_{2,2}\delta_{\text{R}_n} \]
\[ \leq (4\theta_{2,3} + \theta_{3,3})n + (2\theta_{3,3} - 4\theta_{2,3})n + 4\theta_{2,3} - 5\theta_{3,3} + 6\theta_{2,2} \]
\[ = 3\theta_{2,3}n - 5\theta_{3,3} + 4\theta_{2,3} + 6\theta_{2,2} = BID(L_n^1). \]

(15)
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 $M_1(LP_n) = 18n-2$, $M_1(H_n) = 26n-2$, $M_1(LP_n) = 27n-13$, and $M_2(ZH_n) = 34n-11$. Let $R_n$ be a square-hexagonal chain with $d$ squares, $s$ segments $S_1, \ldots, S_s$, $\alpha_i$ kinks of type $T_1$, and $\alpha_{2,j}$ kinks of type $T_{2,j}$, $j = 1, 2, 3$.

By (d) we have

\[
M_2(R_n) = 33n - 6d + 2\delta_{R_n} - 13 + \alpha_1 + 6\alpha_{2,1} + 5\alpha_{2,2} + 4\alpha_{2,3} - \sum_{i=1}^{s} (\tau(S_i) - \mu(S_i) - \nu(S_i)).
\]

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 $\alpha_{2,1} \geq 1$, then $6\alpha_{2,1} - \sum_{i=1}^{s} \tau(S_i) \geq 5$, and hence $M_2(R_n) > 27n - 13 = M_1(LP_n)$. If $\alpha_{2,1} = 0$, then $\sum_{i=1}^{s} \tau(S_i) = 0$, and then $R_n \equiv LP_n$.

(d) We have the following:

\[
M_2(R_n) = 33n - 6d + 2\delta_{R_n} - 13 + \alpha_1 + 6\alpha_{2,1} + 5\alpha_{2,2} + 4\alpha_{2,3} - \sum_{i=1}^{s} (\tau(S_i) - \mu(S_i) - \nu(S_i))
\]

\[
\leq 33n - 13 + 2\delta_{R_n} - 6\left(d - \alpha_{2,1} - \alpha_{2,2} - \alpha_{2,3} - \sum_{i=1}^{s} \nu(S_i)\right)
\]

\[
- \left(\alpha_{2,2} + \alpha_{2,3} - \sum_{i=1}^{s} \mu(S_i)\right) + \alpha_1 - \alpha_{2,3} - 5\sum_{i=1}^{s} \nu(S_i).
\]
If, for some \( i \), \( \mu(S_i) \neq 0 \), then one of the terminal polygons of \( S_i \) is a kink of type \( T_2 \) or type \( T_3 \). 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, \( d \geq \alpha_{2,3} + \alpha_{2,2} + \alpha_{2,1} + \sum_{i=1}^{s} \nu(S_i) \). 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 \( R_n \equiv ZH_n \). \( \square \)

**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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