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THE SZEGED INDEX FOR COMPLEMENTS OF HEXAGONAL CHAINS

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Abstract

The Szeged index (Sz) is the extension of the Wiener formula (H.Wiener, 1947) on cyclic graphs. Namely, $Sz(G) = \sum_{(u,v)} n_u n_v$, where the summation goes over all edges (u,v) in an arbitrary graph G, $n_u = |\{w \mid d(w,u) < d(w,v)\}|$, $n_v = |\{w \mid d(w,v) < d(w,u)\}|$, and the distance $d(u,v)$ is the number of edges in a shortest path connecting vertices v, u in G. It is shown that if G_1 and G_2 are complements of hexagonal chains H_1 and H_2, then $Sz(G_1) = Sz(G_2)$ if and only if the angular numbers of H_1 and H_2 coincide (the angular number counts angularly connected hexagons in a hexagonal chain). The congruence relation $Sz(G_1) \equiv Sz(G_2)$ $(mod\ 3)$ is also established and the extremal graphs are found.

1. Introduction

In his classical work, H.Wiener introduced a new topological index (graph invariant) and established correlations between this index and physico-chemical properties of alkanes [23, 24, 25]. Molecular graphs of alkanes are finite connected trees. If u and v are vertices of a tree G, then the number of edges in a shortest path connecting them is said to be their distance and is denoted $d(u,v)$. Then the Wiener's invariant may be presented by the formula

$$W(G) = \sum_{(u,v)} n_u n_v ,$$

where the summation goes over all edges (u, v) in a tree G and $n_u = |\{w \mid d(w, u) < d(w, v)\}|$, $n_v = |\{w \mid d(w, v) < d(w, u)\}|$. The most well known extension of W for cyclic graphs was put forward by Hosoya [15]. He defined W in terms of distances between vertices in an arbitrary graph. According to his considerations, the *Wiener index (or the Wiener number)* of a graph G is the sum of distances between all pairs of vertices and it may be written as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v).$$

This graph invariant has been intensively investigated by many mathematicians and chemists and numerous remarkable properties of W have been discovered (see monographs [3, 4, 10, 22] and reviews [2, 13, 18, 19, 20, 21]). A new generalization of the Wiener index for cyclic graphs was proposed recently by Gutman [14]. This topological index is now referred to as the *Szeged index* and the corresponding formula for Sz has the similar form:

$$Sz(G) = \sum_{(u,v)} n_u n_v,$$

where G is an arbitrary graph. Conditions for coinciding W and Sz was established in [6, 7]. Namely, $W(G) = Sz(G)$ if and only if every block of G is a complete graph. It could be shown [6, 8, 9, 11, 16, 17] that certain properties of the Wiener and the Szeged index are the same and the other properties are quite different. For instance, values of every index congruent by modulo 8 for molecular graphs of catacondensed benzenoid hydrocarbons having the same numbers of rings [11, 16]. For these graphs, $Sz(G) \equiv q(G)$ $(mod\ 8)$, where $q(G)$ is the number of edges in G. However the later property is not valid for the Wiener index.

In this note we study new properties of the Szeged index for graphs with small diameter, which are obtained from hexagonal chains by complement graph operation. We demonstrate significant difference between Sz and W for complements of hexagonal chains.

2. Hexagonal chains

Hexagonal chains are composed exclusively of six-membered cycles (hexagonal rings or hexagons). We assume that a chain contains at least two hexagons. Any two hexagons either have one common edge (and are then said to be adjacent) or have no common vertices. No three hexagons share a common vertex. Each hexagon is adjacent to two other hexagons, with the exception of the *terminal hexagons* to which a single hexagon is adjacent. The considered hexagonal chains have exactly two terminal hexagons. Evidently, all hexagonal chains are planar graphs. These graphs include molecular graphs of unbranched catacondensed hydrocarbons [12]. If all hexagons are regular, then the above defined graphs contain non-planar molecular graphs corresponding to helicenic benzenoid hydrocarbons. The set of all hexagonal chains with h hexagons is denoted by $\mathcal{H}_h$. It is easy to see that every graph H from $\mathcal{H}_h$ has $p(H) = 4h+2$ vertices and $q(H) = 5h + 1$ edges.

A hexagon of a hexagonal chain is in a mode [12]. A mode of fixed hexagon depends on the number of its neighbor hexagons and their mutual position (see Fig. 1). Angularly connected hexagons have mode A; linearly connected and terminal hexagons are in mode L. The number of hexagons of mode A is said *the angular number* of a graph and is denoted by $a(H)$. If $a(H) = 0$, then H is called the *linear polyacene*.

A graph G is the *complement* of a graph H, $G = \overline{H}$, if $V(G) = V(H)$, and $(u, v) \in E(G)$ if and only if $(u, v) \notin E(H)$ and $u \neq v$. Denote by $\mathcal{G}_h$ the set of complements for all graphs of $\mathcal{H}_h$, *i.e.*, $\mathcal{G}_h = \{G \mid G = \overline{H},\ H \in \mathcal{H}_h\}$. Throughout this paper, we assume that G always denotes the complement of some hexagonal chain H.

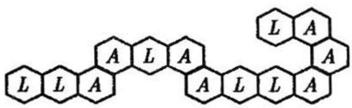

FIGURE 1. Modes of hexagons in a hexagonal chain.

3. Calculation formula for Sz

Let $[u, v]$ be a pair of nonadjacent vertices u and v of $H \in \mathcal{H}_h$. The neighborhood of a vertex v is defined as $N(v) = \{u \mid (v, u) \in E(H)\}$. Let $m_{uv}(H) = N(u) \cap N(v)$ for a nonedge $[u, v]$. Since the minimal cycle in H is of length 6, $m_{uv} \in \{0, 1\}$. It is easy to see that $m_{uv} = 1$ if and only if $d(u, v) = 2$; $m_{uv} = 0$, otherwise. The sum of all distances between a vertex v and other vertices of G, $D(v|G) = \sum_u d(u, v)$, is called the ***distance sum*** of v. By diameter of a graph H we mean $diam(H) = max\{d(u, v) \mid u, v \in V(H)\}$.

Since $diam(H) \geq 5$ for $H \in \mathcal{H}_h$ $(h \geq 2)$, every graph $G \in \mathcal{G}_h$ is connected and $diam(G) = 2$. This immediately implies

Proposition 1. *For every* $G \in \mathcal{G}_h$, $W(G) = 8h^2 + 11h + 2$.

Proof. For an arbitrary vertex $v \in V(G)$, we have $D(v|G) = deg_G(v) + 2(p - 1 - deg_G(v)) = 2p - deg_G(v) - 2$. Then $W(G) = \frac{1}{2}\sum_v (2p - deg_G(v) - 2) = p^2 - q(G) - p = p^2 - [p(p-1)/2 - q(H)] - p = (4h+2)^2 - (4h+2)(4h+1)/2 + (5h+1) - (4h+2) = 8h^2 + 11h + 2$. □

Consider the fragment of the graph H shown in Fig. 2. Every nonedge $[u, v]$ of H forms the edge (u, v) in $G = \overline{H}$. It is easy to see that $n_u(G) = deg_H(v) + 1 - m_{uv}(H)$ and $n_v(G) = deg_H(u) + 1 - m_{uv}(H)$. Therefore

$$Sz(G) = \sum_{[u,v] \in H} (deg_H(v) + 1 - m_{uv})(deg_H(u) + 1 - m_{uv}), \tag{1}$$

where summation goes over all nonedges in H.

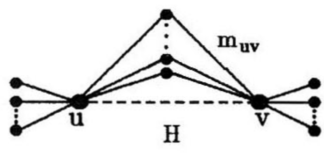

FIGURE 2.

Let v be fixed and denote $D^*(v|H) = \sum_{[v,u]\in H}(deg_H(v)+1-m_{uv})(deg_H(u)+1-m_{uv})$. Then we can rewrite (1) in the form

$$\begin{aligned} Sz(G) &= \frac{1}{2}\sum_{v\in V(H)} D^*(v|H) \qquad (2)\\ &= \frac{1}{2}\sum_{v\in V(H)}\sum_{[v,u]\in H}(deg_H(v)+1-m_{uv})(deg_H(u)+1-m_{uv}). \end{aligned}$$

For a vertex $v \in V(H)$, we define the numbers of vertices of v-spheres in H as $s_2(v) = |\{u \mid d(v,u) = 2, deg(u) = 2\}|$ and $s_3(v) = |\{u \mid d(v,u) = 2, deg(u) = 3\}|$; the numbers of vertices of v-balls as $b_2(v) = |\{u \mid d(v,u) \le 2, deg(u) = 2\}|$ and $b_3(v) = |\{u \mid d(v,u) \le 2, deg(u) = 3\}|$; the numbers of vertices of v-exteriors as $e_2(v) = |\{u \mid d(v,u) > 2, deg(u) = 2\}|$ and $e_3(v) = |\{u \mid d(v,u) > 2, deg(u) = 3\}|$.

If $deg_H(v) = 3$, then we can write $D^*(v|H) = 6s_2+9s_3+12e_2+16e_3$; if $deg_H(v) = 2$, then $D^*(v|H) = 4s_2+6s_3+9e_2+12e_3$. Let $V_2(H) = \{u \mid deg(u) = 2\}$ and $V_3(H) = \{u \mid deg(u) = 3\}$. Therefore equation (2) may be presented as follows

$$Sz(G) = \frac{1}{2}[\sum_{v\in V_2(H)}(4s_2+6s_3+9e_2+12e_3) \;+\; \sum_{v\in V_3(H)}(6s_2+9s_3+12e_2+16e_3)].$$

Let $N_2 = |V_2| = 2(h+2)$ and $N_3 = |V_3| = 2(h-1)$. Hence $e_2(v) = N_2 - b_2(v)$ and $e_3(v) = N_3 - b_3(v)$. Then we have the final formula for the calculation of Sz:

$$\begin{aligned} Sz(G) &= \frac{1}{2}\left(\sum_{v\in V_2(H)}[4s_2+6s_3+9(N_2-1-b_2)+12(N_3-b_3)]\right. \qquad (3)\\ &\quad\left. + \sum_{v\in V_3(H)}[6s_2+9s_3+12(N_2-b_2)+16(N_3-1-b_3)]\right). \end{aligned}$$

The obtained formula shows that in order to calculate the Szeged index of $G \in \mathcal{G}_h$ it is sufficient to take into account only the numbers of vertices in v-spheres and v-balls of the corresponding hexagonal chain.

4. Congruence relation for Sz

Let G_1, G_2 be arbitrary graphs of $\mathcal{G}_h$ and H_1, H_2 be the corresponding graphs of $\mathcal{H}_h$. There is a simple relationship between the Szeged index of G_1, G_2 and angular numbers of H_1, H_2.

Proposition 2. *If $a(H_2) = a(H_1) + 1$, then $Sz(G_2) = Sz(G_1) - 3$.*

Proof. In order to calculate the Szeged index, we apply formula (3). Consider the fragments of graphs H_1 and H_2 as illustrated in Fig. 3. Subgraphs A and B have the same structure, *i.e.*, H_1 and H_2 have only different subgraph C. Note that degrees of the vertices v_1, v_2, v_3 and v_4 are the same in graphs H_1 and H_2. Therefore, without loss of generality we assume that these degrees are equal to 2. By definition, we have $D^*(v|H_1) = D^*(v|H_2)$ for every $v \in V(A) \cup V(B)$. This implies

$$Sz(G_1) - Sz(G_2) = \frac{1}{2}\left(\sum_{v\in C(H_1)} D^*(v|H_1) \quad - \sum_{v\in C(H_2)} D^*(v|H_2)\right). \tag{4}$$

Consider the graph H_1. Vertices of $A \cup B$ contribute equal quantities into (4). For the marked vertices of C, we have

$$D^*(v_1|H_1) = 4(1+...) + 6(1+...) + 9(N_2 - 1 - 1 + ...) + 12(N_3 - 2 + ...) = -32 + ...;$$
$$D^*(v_5|H_1) = 4(2+...) + 6(2+...) + 9(N_2 - 1 - 2 + ...) + 12(N_3 - 4 + ...) = -55 + ...;$$
$$D^*(u_1|H_1) = 6(2+...) + 9(1+...) + 12(N_2 - 4 + ...) + 16(N_3 - 1 - 2 + ...) = -75 + ...$$

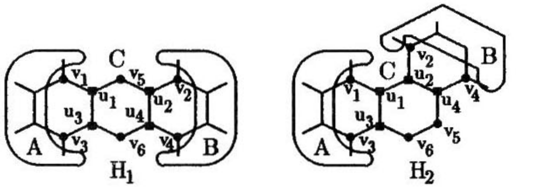

FIGURE 3.

Here and further the dots in formulae mean values that are the same in H_1 and H_2. By symmetry, all calculations are similar for the vertices v_2, v_3, v_4, v_6 and u_2, u_3, u_4. Therefore

$$\sum_{v\in C(H_1)} D^*(v|H_1) = -538 + \ldots .$$

Now consider the graph H_2. It is easy to calculate the corresponding values for marked vertices of C:

$$D^*(v_1|H_2) = 4(0+\ldots)+6(2+\ldots)+9(N_2-1-0+\ldots)+12(N_3-3+\ldots) = -33+\ldots;$$
$$D^*(v_3|H_2) = 4(1+\ldots)+6(1+\ldots)+9(N_2-1-1+\ldots)+12(N_3-2+\ldots) = -32+\ldots;$$
$$D^*(v_5|H_2) = 4(1+\ldots)+6(2+\ldots)+9(N_2-1-2+\ldots)+12(N_3-3+\ldots) = -47+\ldots;$$
$$D^*(u_1|H_2) = 6(3+\ldots)+9(1+\ldots)+12(N_2-4+\ldots)+16(N_3-1-3+\ldots) = -85+\ldots;$$
$$D^*(u_3|H_2) = 6(2+\ldots)+9(1+\ldots)+12(N_2-4+\ldots)+16(N_3-1-2+\ldots) = -75+\ldots .$$

For the vertices v_2, v_4, v_6 and u_2, u_4, we have analogous values. Then

$$\sum_{v\in C(H_2)} D^*(v|H_2) = -544 + \ldots .$$

Substituting all necessary terms into (4), we have $Sz(G_1) - Sz(G_2) = 3$. □

The obtained result shows that the change of the Szeged index does not depend on location of hexagon of mode A in a graph. It is clear that every hexagonal chain may be constructed from the linear polyacene by changing modes of the corresponding hexagons from L to A. Applying Proposition 2 to every hexagon of mode A, we get

Corollary 1. *If $a(H_2) = a(H_1) + n$, then $Sz(G_2) = Sz(G_1) - 3n$.*

Corollary 2. *For arbitrary graphs $G_1, G_2 \in \mathcal{G}_h$, $Sz(G_1) \equiv Sz(G_2)$ (mod 3).*

Corollary 3. *Let $G_1, G_2 \in \mathcal{G}_h$. Then $Sz(G_1) = Sz(G_2)$ if and only if $a(H_1) = a(H_2)$ for the corresponding hexagonal chains $H_1, H_2 \in \mathcal{H}_h$.*

Obviously the minimal angular number is equal to 0, and the maximal angular number is equal to $h-2$.

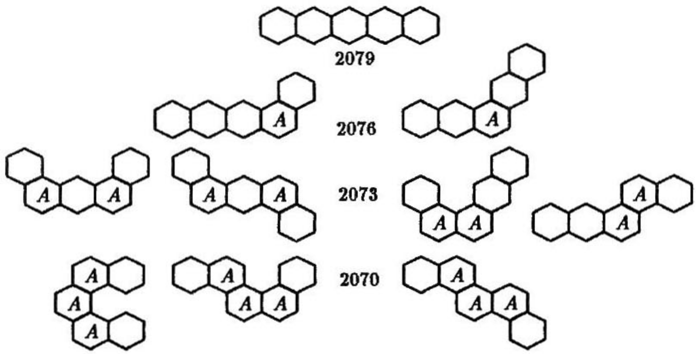

FIGURE 4. All hexagonal chains with $h = 5$ and Sz of their complements.

Corollary 4. *The complement of linear polyacene has the maximal value of the Szeged index and this graph is unique. A graph $G \in \mathcal{G}_h$ has the minimal value of Sz if and only if $a(H) = h - 2$ for the corresponding hexagonal chain $H \in \mathcal{H}_h$.*

As an illustration of the above corollaries all graphs with $h = 5$ and Sz of their complements are shown in Fig. 4.

5. Graphs with extremal Sz

In this section we calculate the Szeged index for the complements of two extremal hexagonal chains. First consider the graph H_1 depicted in Fig. 5, where some nonedges are shown by dotted lines. In order to calculate $Sz(\overline{H}_1)$, we again apply formula (3). All vertices of degree 3 in H_1 may be divided into two classes with respect to vertex degrees in its spheres and balls. We have four vertices of type w_1 and $2(h-3)$ vertices of type w_2 (see Fig. 5). Therefore

$D^*(w_1|H_1) = 6 \cdot 3 + 9 \cdot 1 + 12(N_2 - 5) + 16(N_3 - 1 - 2) = 56h - 65;$

$D^*(w_2|H_1) = 6 \cdot 2 + 9 \cdot 2 + 12(N_2 - 4) + 16(N_3 - 1 - 3) = 56h - 66.$

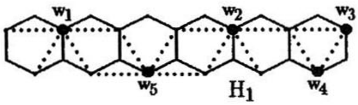

FIGURE 5.

All vertices of degree 2 may be divided into three classes: four vertices of type w_3, four vertices of type w_4 and $2(h-2)$ vertices of type w_5. Then we can write

$$D^*(w_3|H_1) = 4\cdot 1 + 6\cdot 1 + 9(N_2 - 1 - 3) + 12(N_3 - 1) = 42h - 26;$$
$$D^*(w_4|H_1) = 4\cdot 2 + 6\cdot 1 + 9(N_2 - 1 - 3) + 12(N_3 - 2) = 42h - 34;$$
$$D^*(w_5|H_1) = 4\cdot 2 + 6\cdot 2 + 9(N_2 - 1 - 2) + 12(N_3 - 4) = 42h - 43.$$

Summing all necessary terms, we obtain

$$Sz(G_1) = Sz(\overline{H}_1) = 98h^2 - 81h + 34.$$

Consider the graph H_2 shown in Fig. 6. It is easy to recognize in H_2 the vertices are of types w_1 (2 vertices), w_2 ($h-3$ vertices), w_3 (4 vertices), and w_4 (2 vertices) as above. Other vertices of degree 3 we divide into three new classes: $h-5$ vertices of type w_7, 2 vertices of type w_8 and 2 vertices of type w_9. For the vertices of new types, we have

$$D^*(w_7|H_2) = 6\cdot 2 + 9\cdot 4 + 12(N_2 - 2) + 16(N_3 - 1 - 7) = 56h - 88;$$
$$D^*(w_8|H_2) = 6\cdot 3 + 9\cdot 3 + 12(N_2 - 3) + 16(N_3 - 1 - 6) = 56h - 87;$$
$$D^*(w_9|H_2) = 6\cdot 3 + 9\cdot 2 + 12(N_2 - 4) + 16(N_3 - 1 - 4) = 56h - 76.$$

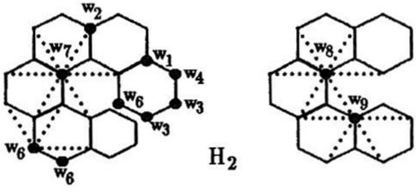

FIGURE 6.

Other $2(h-1)$ vertices of degree 2 are of type w_6. In this case, we have

$D^*(w_6|H_2) = 4 \cdot 1 + 6 \cdot 2 + 9(N_2 - 1 - 2) + 12(N_3 - 3) = 42h - 35.$

Summing all corresponding terms, we arrive at

$$Sz(G_2) = Sz(\overline{H}_2) = 98h^2 - 84h + 40.$$

As a result we can formulate

Proposition 3. *The extremal values of the Szeged index for complements of hexagonal chains with h hexagons are $Sz_{min}(h) = 98h^2-84h+40$ and $Sz_{max}(h) = 98h^2-81h+34$.*

6. Degeneracy classes for Sz

The previous results demonstrate that every admissible integer is realized as the Szeged index of the complement of a hexagonal chain. Calculated degeneracy classes of Sz for graphs of $\mathcal{G}_h$, $3 \le h \le 10$, are presented in Table 1. Here N is the number of graphs with the same Szeged index. For two graphs of $\mathcal{G}_3$, $Sz \in \{673, 670\}$.

Table 1. Degeneracy classes for Sz.

h=4		h=5		h=6		h=7		h=8		h=9		h=10	
Sz	N	Sz	N	Sz	N	Sz	N	Sz	N	Sz	N	Sz	N
1272	2	2070	3	3064	6	4254	10	5640	20	7222	36	9000	72
1275	1	2073	4	3067	8	4257	22	5643	48	7225	116	9003	256
1278	1	2076	2	3070	8	4260	22	5646	66	7228	174	9006	464
-	-	2079	1	3073	2	4263	12	5649	40	7231	146	9009	448
-	-	-	-	3076	1	4266	3	5652	18	7234	73	9012	292
-	-	-	-	-	-	4269	1	5655	3	7237	24	9015	112
-	-	-	-	-	-	-	-	5658	1	7240	4	9018	32
-	-	-	-	-	-	-	-	-	-	7243	1	9021	4
-	-	-	-	-	-	-	-	-	-	-	-	9024	1

In order to count numbers of graphs in $\mathcal{G}_h$ having the same Szeged index, we can examine graphs of $\mathcal{H}_h$ with coinciding angular numbers. It is well known the number of graphs in $\mathcal{H}_h$ [1]. Let $N(h,a)$ be the number of hexagonal chains of $\mathcal{H}_h$ with $a \ge 1$.

By simple considerations, we derive the following formulae:

if h is even, then

$$N(h,a)=\begin{cases} 2^{a-2}\binom{h-2}{a}+2^{(a-2)/2}\binom{(h-2)/2}{a/2}, & \text{if } a \text{ is even}\\ 2^{a-2}\binom{h-2}{a}, & \text{if } a \text{ is odd;}\end{cases}$$

if h is odd, then

$$N(h,a)=\begin{cases} 2^{a-2}\binom{h-2}{a}+2^{(a-2)/2}\binom{(h-3)/2}{a/2}, & \text{if } a \text{ is even}\\ 2^{a-2}\binom{h-2}{a}+2^{(a-3)/2}\binom{(h-3)/2}{(a-1)/2}, & \text{if } a \text{ is odd.}\end{cases}$$

Recall that the linear polyacene is the unique hexagonal chain having the angular number $a = 0$ for every h.

7. Graphs with the same Sz and W

In this section we find hexagonal chains H such that $W(H) = Sz(\overline{H})$. The well known result from theory of the Wiener index states

Proposition 4 [11]. *1) The extremal values of the Wiener index for graphs of $\mathcal{H}_h$ are equal to $W_{min}(h) = (8h^3+72h^2-26h+27)/3$ and $W_{max}(h) = (16h^3+36h^2+26h+3)/3$. The maximal value achieves on the linear polyacene.*

2) If $H_1, H_2 \in \mathcal{H}_h$, then $W(H_1) \equiv W(H_2)$ (mod 8).

Let $I(\mathcal{G}_h) = \{Sz_{min}(h) + 3n \mid n = 0, 1, ..., \frac{1}{3}(Sz_{max}(h) - Sz_{min}(h))\}$ be the discrete interval of Sz-values, $|I(\mathcal{G}_h)| = (h-2)+1 = h-1$. Every element $k \in I(\mathcal{G}_h)$ is realized by graphs having the angular number $(k - Sz_{min}(h))/3$. Denote the values interval for the Wiener index as $I(\mathcal{H}_h) = \{W_{min}(h) + 8n \mid n = 0, 1, ..., \frac{1}{8}(W_{max}(h) - W_{min}(h))\}$.

A graph $H \in \mathcal{H}_h$ is called the *double realization* of integer k if $W(H) = Sz(G) = k$, where $G = \overline{H}$. The obvious necessary conditions for existence a double realization is

$I(\mathcal{H}_h) \cap I(\mathcal{G}_h) \neq \oslash$. Hence if $k \in I(\mathcal{H}_h) \cap I(\mathcal{G}_h)$, then $W_{min}(h) \equiv k \ (mod\ 8)$ and $Sz_{min}(h) \equiv k \ (mod\ 3)$ simultaneously. By direct calculation, we establish

Proposition 5. *If a double realization exists, then* $h \in \{16, 17, 18, ..., 25\}$.

For the corresponding classes of graphs, we have $I(\mathcal{H}_{16}) \cap I(\mathcal{G}_{16}) = \{23793,\ 23817\}$, $I(\mathcal{H}_{17}) \cap I(\mathcal{G}_{17}) = \{26955, 26979\}$, $I(\mathcal{H}_{18}) \cap I(\mathcal{G}_{18}) = \{30301, 30325\}$, $I(\mathcal{H}_{19}) \cap I(\mathcal{G}_{19}) = \{33831, 33855\}$, $I(\mathcal{H}_{20}) \cap I(\mathcal{G}_{20}) = \{37569, 37593\}$, $I(\mathcal{H}_{21}) \cap I(\mathcal{G}_{21}) = \{41515, 41539\}$, $I(\mathcal{H}_{22}) \cap I(\mathcal{G}_{22}) = \{45645, 45669\}$, $I(\mathcal{H}_{23}) \cap I(\mathcal{G}_{23}) = \{49959, 49983,\ 50007\}$, $I(\mathcal{H}_{24}) \cap I(\mathcal{G}_{24}) = \{54481, 54505, 54529\}$, $I(\mathcal{H}_{25}) \cap I(\mathcal{G}_{25}) = \{59211, 59235,\ 59259\}$. Bounds of the indices for considered intervals are shown in Table 2.

Table 2. Bounds of the indices.

h	$W_{min}(h)$	$Sz_{min}(h)$	$Sz_{max}(h)$	$W_{max}(h)$
16	16937	23784	23826	25057
17	19899	26934	26979	29819
18	23181	30280	30328	35149
19	26799	33822	33873	41079
20	30769	37560	37614	47641
21	35107	41494	41551	54867
22	39829	45624	45684	62789
23	44951	49950	50013	71439
24	50489	54472	54538	80849
25	56459	59190	59259	91051

Consider the value intervals for $h = 16, 17$. Denote $\mathcal{H}_h(W)$ the subset of graphs in $\mathcal{H}_h$ with the Wiener index W. Then $|\mathcal{H}_{16}(23793)| = 932$ and $|\mathcal{H}_{16}(23817)| = 599$ [5]. There does not exist a double realization for $W = 23793$. All double realizations for $W = 23817$ are shown in Fig. 7 (their angular number is equal to 3). For $h = 17$, we note that $26979 = Sz_{max}(17)$, *i.e.*, H must be the linear polyacene. However, $W_{max}(17) = 29819$. There are many double realizations among $|\mathcal{H}_{17}(26955)| = 8295$ graphs of $\mathcal{H}_{17}$. Two such graphs are presented in Fig. 8 (their angular number is equal to 8).

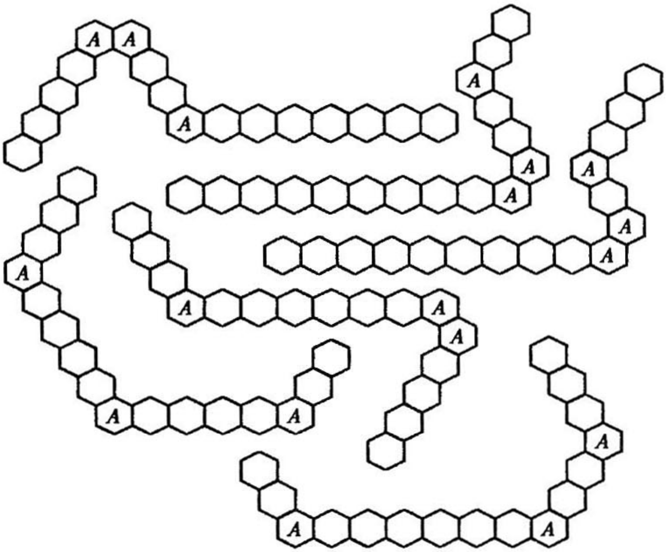

FIGURE 7. All double realizations for $h = 16$.

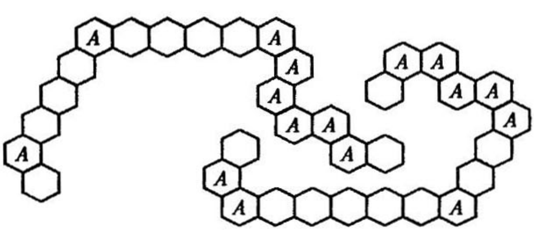

FIGURE 8. An example of double realization for $h = 17$.

8. Sz for complements of branched hexagonal chains

Every nonterminal hexagon in a branched hexagonal chain may be adjacent with two other hexagons (no three hexagons share a common vertex). Such hexagon is in mode B and is said the *branched* hexagon. Let $\mathcal{H}_{h,b}$ be the set of all branched hexagonal chains having b hexagons of mode B. Graphs of $\mathcal{H}_{h,b}$ include molecular graphs of branched catacondensed hydrocarbons [12]. A graph of $\mathcal{H}_{h,b}$ has exactly $b+2$ terminal hexagons. It is clear that Proposition 2 is also valid for complements of graphs of $\mathcal{H}_{h,b}$, *i.e.*, $Sz(G_1) \equiv Sz(G_2)\ (mod\,3)$ for $G_1 = \overline{H}_1$ and $G_2 = \overline{H}_2$, where $H_1, H_2 \in \mathcal{H}_{h,b}$. For the angular number of a hexagonal chain of $\mathcal{H}_{h,b}$, the inequalities $0 \le a(H) \le h - 2b(H) - 2$ hold. Applying formulae from the previous points to graphs of $\mathcal{H}_{h,b}$, we obtain

Proposition 6. *Let $H \in \mathcal{H}_{h,b}$. If H has the angular number a, then $Sz(\overline{H}) = Sz_{max}(h,0) - 9b - 3a$. The extremal values of the Szeged index for complements of branched hexagonal chains of $\mathcal{H}_{h,b}$ are $Sz_{min}(h,b) = Sz_{min}(h,0) - 3b$ and $Sz_{max}(h,b) = Sz_{max}(h,0) - 9b$.*

For complements of the top graphs shown in Fig. 9, the Szeged index is maximal among all graphs of $\mathcal{H}_{10,2}$. Complements of the other graphs have the minimal value of Sz.

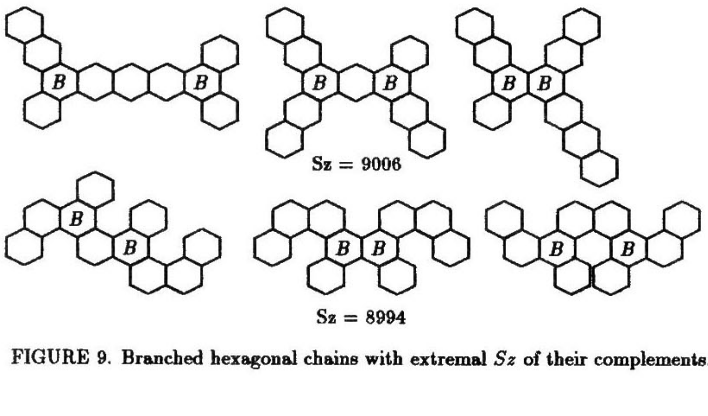

FIGURE 9. Branched hexagonal chains with extremal Sz of their complements.

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