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On the Szeged Index of Unbranched Catacondensed Benzenoid Molecules

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The Szeged index (*Sz*) of unbranched catacondensed benzenoid (UBCB) hydrocarbons is examined. An efficient method for the calculations of their *Sz* is put forward. Among the UBCB molecules with a fixed number of hexagons, the linear polyacene has a maximal and the helicene a minimal *Sz*.

INTRODUCTION

In this paper, we are concerned with the Szeged index of unbranched catacondensed benzenoid (UBCB) hydrocarbons.[1] The Szeged index is a recently proposed[2] structural descriptor, based on the distances between the vertices of the molecular graph.[3,4]

The molecular graphs of UBCB hydrocarbons (which we will call »unbranched catacondensed benzenoid graphs«, UBCB graphs) are composed of hexagons. Two hexagons have either one common edge (and are then said to be adjacent) or have no common vertices at all (in which case they are not adjacent). 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. A UBCB system has exactly two terminal hexagons.

The above defined UBCB graphs correspond not only to geometrically planar, but also to non-planar, helicenic benzenoid hydrocarbons. (We mention in passing that not only the helicenes,[5] but a significant number of other known benzenoid hydrocarbons exist in highly nonplanar, even chiral conformations[6]).

The set of all UBCB graphs with h rings is denoted by C_h. It is easy to see that every graph U from C_h has $p(U) = 4h + 2$ vertices and $q(U) = 5h + 1$ edges.

In order to introduce the concept of the novel Szeged index, and to see its conceptual relation to the long-known Wiener index, consider an arbitrary connected graph G. If u and v are vertices of G, then the number of edges in the shortest path connecting them is said to be their distance and is denoted by $d(u,v)$.

Let $e = (u,v)$ be an edge of graph G. Denote by $n_u = n_u(e)$ and $n_v = n_v(e)$ the number of elements of the vertex sets $B_u(e) = \{w \mid d(w,u) < d(w,v)\}$ and $B_v(e) = \{w \mid d(w,v) < d(w,u)\}$, respectively. Recall that $n_u(e)$ is the number of the vertices of G which lie closer to one endpoint of the edge e (namely to vertex u) than to its other endpoint (namely to vertex v). Analogously, $n_v(e)$ counts the vertices that lie closer to v than to u.

The sum $W(G)$ of distances between all pairs of vertices of graph G is the Wiener index (Wiener number), one of the oldest and best studied topological descriptors of molecular structure.[3,4,7,8] A classical result in the theory of the Wiener index[4,7–9] states that

$$W(G) = \sum_e n_u n_v \qquad (1)$$

where the summation goes over all edges $e = (u,v)$ of G. Formula (1) holds only for trees (= connected acyclic graphs) and is, in a general case, violated when G is cyclic. (The cyclic graphs for which Eq. (1) is obeyed have been recently characterized.[10] These graphs are of little relevance for the chemical graph theory).

The obvious advantage of formula (1) is that it provides a decomposition of the Wiener index into bond-contributions. Indeed, the natural interpretation of the quantity ${}_u n_v$ is that it is the increment associated with the chemical bond, represented by edge e.

Finding the bond-contributions to the Wiener index of cyclic molecules is a much more difficult task which was approached only recently.[11,12] The expressions obtained for the respective increments are, however, quite cumbersome and not easy to be used in practice.[13]

A different and somewhat unorthodox way out of this difficulty was proposed by one of the authors.[2] Namely, Wiener's formula (1) served as a motivation for introduction of a new distance-based graph invariant, called »Szeged index«,[14] defined as

$$Sz(G) = \sum_e {}_u n_v \qquad (2)$$

where G is now any connected graph. Evidently, Sz and W coincide in the case of trees. It was eventually established[2,10,15–18] that Sz possesses a number of interesting properties. For example, the equality $Sz(G) = W(G)$ holds if and only if every block of G is a complete graph.[10] In cyclic bipartite graphs, $Sz(G)$ is always greater than $W(G)$.[2] In the general case (of cyclic molecular graphs), the behaviour of Sz and W seem to be quite dissimilar.

However, for certain classes of benzenoid molecules, remarkable analogies between the properties for Sz and W were discovered.[15,17] In this paper, we make one more step in this direction by showing that, in the class of UBCB hydrocarbons, the Szeged index achieves its maximal and minimal value for linear polyacenes and helicenes, respectively. These are precisely the same UBCB species for which the Wiener index is maximal and minimal.[19]

In order to find the UBCB systems that are extreme with respect to the Szeged index, some preparations are needed.

SOME MORE DEFINITIONS

Let $e = (x,y)$ be an arbitrary, but fixed, edge of a graph U from the class C_h. We define for every edge $e = (x,y)$ the set $E_1(e) = E_1(e) \mid U) = \{(u,v) \mid u \in B_z(e)$ and $v \in B_y(e)\}$. It is clear that if $(u,v) \in E_1(e)$, then $d(v,y) = d(u,x)$. Note that $x,y)$ belongs to $E_1(e)$. With every edge $e = (x,y)$ of U in C_h, we associate three subgraphs: R_x, R_y and R_{xy}, also consisting of hexagons. R_{xy} is spanned by the vertices belonging to those hexagons of U whose some (two) edges are from $E_1(e)$. Consequently, R_{xy} belongs to the class $C_{h_{xy}}$, where $h_{xy} = |E_1(e)| - 1$. The subgraph R_x is spanned by those vertices of U which lie closer to x than to y. Similarly, R_y is spanned by the vertices of U whose distance to y is smaller than the distance to x. Note that the vertex sets of R_{xy} and R_x, as well as of R_{xy} and R_y, have non-empty intersections, *i.e.*, some vertices of U belong simultaneously to R_x and R_{xy} or to R_y and R_{xy}. The vertex sets of R_x and R_y are, of course, disjoint. Besides, R_x and R_y may be disconnected. Let h_x and h_y be the number of hexagons of R_x and R_y, respectively. Then, $h_x + h_y + h_{xy} = h$. In Figure 1, examples are given for graphs

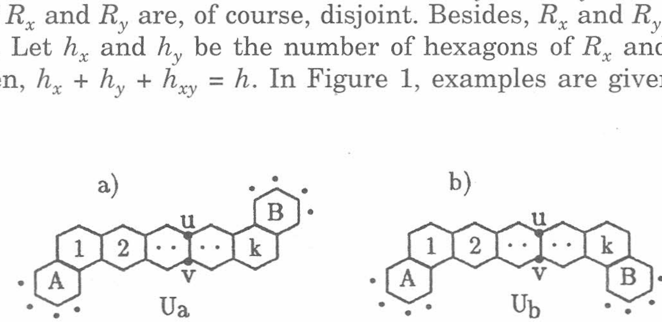

Figure 1. Two unbranched catacondensed benzenoid systems used to illustrate the concept of subgraphs R_x, R_y and R_{xy}; for details see text.

from C_h (two possible configurations). Here, A and B stand for arbitrary fragments; in particular, they may be absent. In both cases, the subgraph R_{uv} consists of the hexagons numbered 1 to k. In case (a), $R_v = A$ and $R_u = B$. In case (b), R_v consists of fragments A and B (and is disconnected) whereas R_u is empty (*i.e.*, R_u is without vertices).

A subgraph R_{xy} is said to be a segment of U if $h_{xy} \geq 2$. Then, h_{xy} is called the length of the segment. Therefore, a segment of U is isomorphic to the linear polyacene having at least two hexagons. Every segment shares a hexagon with its neighbouring segment. The terminal segment has only one neighbouring segment.

CALCULATION OF THE SZEGED INDEX FROM VERTEX DISTANCES

The distance of a vertex v in a (connected) graph G, $d(v) = d(v|G)$, is the sum of distances between vertex v and all other vertices of G. We need the following simple lemma.

LEMMA 1. Let G be a connected bipartite graph and u and v be its adjacent vertices. Then, $d(u|G) - d(v|G) = n_v - n_u$, and $n_v + n_u = p(G)$. Further, if G is a UBCB graph, then $d(u|G) - d(v|G) = 4(h_v - h_u)$.

Proof. Let $e = (u,v) \in E(G$. Then, $d(u|G) = \Sigma_{\omega \in B_\upsilon(\varepsilon)} d(w,u) + \Sigma_{\omega \in B_\upsilon(\varepsilon)} d(w,u)$ $= \Sigma_{\omega \in B_\upsilon(\varepsilon)} (d(w,v) - 1) + \Sigma_{\omega \in B_\upsilon(\varepsilon)} (d(w,v) + 1) = d(v|G) - n_u + n_v$. Since G has no cycles of odd length, $n_v + n_u = p(G)$. If G belongs to C_h, then $d(u|G) - d(v|G) = n_v - n_u = (p(R_{uv})/2 + 4h_v) - (p(R_{uv})/2 + 4h_u) = 4(h_v - h_u)$.

It was shown[18] that, in a bipartite graph, the Szeged index can be expressed through distances of the vertices. This allows us to present Sz of a UBCB graph by a polynomial depending only on the number of hexagons of some of its subgraphs.

LEMMA 2. Let U be a UBCB graph with p vertices and q edges. Then

$$Sz(U) = \frac{1}{4}\left(p^2(U)q(U) - \sum_{(u,v)\in E(U)} (d(u|U) - d(v|U))^2\right) = \qquad (3)$$

$$= (2h + 1)^2(5h + 1) - 4 \sum_{(u,v)\in E(U)} (h_v - h_u)^2 .$$

Proof. From Lemma 1, we have $n_u = (p(U) + d(v|U) - d(u|U))/2$ and $n_v = (p(U) - d(v|U) + d(u|U))/2$. Formula (3) is obtained by combining the above relations with definition (2) of the Szeged index.

Eq. (3) implies that, in order to obtain the extreme values of $Sz(U)$ for UBCB graphs with a given number of hexagons, we need to get the maximal and the minimal values of the auxiliary function:

$$\sum_{(u,v)\in E(U)} f(u,v) = \sum_{(u,v)\in E(U)} (h_v - h_u)^2 .$$

In the subsequent section, we describe in detail the possible values of $f(u,v)$.

UBCB SYSTEMS EXTREMAL WITH RESPECT TO THE SZEGED INDEX

The edge set $E(U)$ of a UBCB graphs can be divided into two disjoint subsets,

$$E(U) = E_t(U) \cup E_m(U),$$

where $E_t(U) = \{e = (u,v) : |E_1(e|U)| = 2\}$ and $E_m(U) = \{e = (u,v) : |E_1(e|U)| > 2\}$, $|E(U)| = |E_t(U)| + |E_m(U)|$. Note that $|E_1(e|U)| > 2$ if and only if a subgraph R_{uv} forms a segment. The case $|E_1(e|U)| = 2$ corresponds to R_{uv} with only one hexagonal ring.

We first calculate $f(u,v)$ for the edges belonging to $E_t(U)$. Suppose that the hexagons of U are numbered consecutively from 1 to h.

PROPOSITION 1. Let $U \in C_h$. If $e = (u,v) \in E_t(U)$ and e belongs to the i-th hexagon of U, then

$$f(u,v) = ((h - i) - i - 1))^2 = (h - 2i + 1)^2 .$$

Proof. Let $e = (u,v) \in E_t(U)$. It is clear that $E_1(e|U)$ is an edge cut of U, *i.e.* after deleting all edges of $E_1(e|U)$ from U, we obtain two disconnected components. One of these components has $i - 1$ hexagons and the other has $h - i$ hexagons.

Below we establish the extreme values of $f(u,v)$ when (u,v) is any edge of a UBCB graph. In order to do this, we simply substitute $i = 1, 2, ..., h$ into the formula of Propostion 1.

COROLLARY 1. If $e = (u,v) \in E_t(U)$, then

(a) max $f(u,v) = (h - 1)^2$, if and only if e belongs to a terminal hexagons of U;

(b) max $f(u,v) = (h - 3)^2$, otherwise.

(c) min $f(u,v) = 0$, if and only if h_U is odd and e belongs only to the central hexagon of U;

(d) min $f(u,v) = 1$, otherwise.

Every UBCB graph has exactly two terminal hexagons, *i.e.*, it has 8 edges pertaining to case (a). Every such graph with odd h_U was exactly one central ring, *i.e.*, it has 2 or 4 edges for which $f(u,v)$ has the value given under (c).

Consider now the edges of $E_m(U)$. Let $e \in E_m(U)$. Recall that for every edge $e' \in E_1(e)$, $E_1(e) = E_1(e')$. Then, we can associate $E_1(e)$ with the corresponding segment S . Denote this set by $E_m(S)$. Hence, the set $E_m(U)$ is presented as the union of mutually disjoint subsets.

$$E_m(U) = \cup E_m(S),$$

where the union goes over all segments of the UBCB graph U.

PROPOSITION 2. If $e = (u,v) \in E_i(U)$, then

$$f(u,v) = \begin{cases} (h_A - h_B)^2, & \text{if } S \text{ belongs to } U_a \text{ (see Figure 1);} \\ (h_A + h_B)^2, & \text{if } S \text{ belongs to } U_b \text{ (see Figure 1).} \end{cases}$$

This immediately implies

COROLLARY 2. Let $e = (u,v) \in E_m(\mathrm{S})$. Then

(a) $\max f(u,v) = h - 2)^2$. This value is achieved on every segment with $k = 2$ hexagons, provided U is of type Ub (see Figure 1).

(b) $\min f(u,v) = 0$. This value is only achieved on a segment with $k - h_U$.

We are now ready to find the UBCB graph with the maximal (minimal) value of Sz. Let $e = (u,v) \in E_m(U)$, $e' = (u',v') \in E_t(U)$, and let e' not belong to a terminal hexagon of U. By Propositions 1 and 2, we have

$$\max f(u',v') = (h - 3)^2 < \max f(u,v) = (h - 2)^2 \ .$$

If h_U is odd, we require that e' does not belong to the central ring. Then,

$$\min f(u,v) - 0 < \min f(u',v') = 1$$

Hence, we are interested in a UBCB graph for which

$$|E_t(U)| - |E_m(U)| \to \max \text{ (min)} \tag{4}$$

Every nonterminal segment with k hexagons has $4k - 4$ edges from E_t and $k + 1$ edges from E_m. Every terminal segment with k hexagons has $4k - 2$ edges from E_t and $k + 1$ edges from E_m. We thus arrive at:

PROPOSITION 3. Among UBCB graphs with a fixed number of hexagons the helicene graph has the minimal value of (4). The linear polyacene graph has the maximal value of (4).

THEOREM. Among the UBCB hydrocarbons with a fixed number of hexagons, helicene has the minimal value of the Szeged index and the linear polyacene has the maximal value of the Szeged index. These benzenoid systems are unique.

EXTREMAL VALUES FOR THE SZEGED INDEX

From the results obtained in the preceding section, it is easy to calculate Sz for the extremal UBCB graphs.

By direct counting, we establish that the linear polyacene Lpa_h with h hexagons has $h + 1$ edges from $E_m(Lpa_h$ and $4h$ edges from $E_t(Lpa_h)$. Therefore,

$$Sz(Lpa_h) = (2h + 1)^2(5h + 1) - 4 \sum_{i=1}^{h} (h - 2i + 1)^2 .$$

Simplifying this expression, we obtain the maximal value of Sz as a cubic polynomial in h:

$$Sz(Lpa_h) = (44h^3 + 72h^2 + 43h +3)/3.$$

The helicene Hel_h with h hexagons has $2(h - 2)$ edges from E_t for hexagons $i = 2, 3, \dots h - 1$ and 8 edges from E_t for the terminal hexagons. Hence, all other $3h - 3$ edges belong to E_m. Then,

$$Sz(Hel_h) = (2h + 1)^2(5h + 1) - 4(3h - 3)(h - 2)^2 - \\ - 4 \cdot 2 \sum_{i=2}^{h-1} (h - 2i + 1)^2 - 4 \cdot 8(h - 1)^2 .$$

Then, the minimal value of Sz is

$$Sz(Hel_h) = (16h^3 + 204h^2 - 157h + 99)/3.$$

CALCULATING THE SZEGED INDEX FOR AN ARBITRARY UBCB GRAPH

The previous analysis provides us with a simple way to calculate the Szeged index of an arbitrary graph from C_h. We derive a formula depending on the number and type of segments.

Let $U \in C_h$ have n segments. Define the vector of segments' lengths $L(U) = (l_1, l_2, ..., l_n)$, where $l_i \geq 2$ is the number of hexagons in the i-th segment S_i, $i = 1, 2, ... n$. The second vector $M(U) = (m_1, m_2, ..., m_n)$ describes the mutual relation of the segments. A label $m_i = (S_i)$, either 0 or 1, is assigned to every segment S_i. We first choose $m_1 = m_2 = 0$. Consider the segment S_i and draw a line through the centres of the hexagons of S_{i-1}. Then, $m_i = m_{i-2}$ if S_i and S_{i-2} lie on the same side of the line, and $m_i \neq m_{i-2}$ otherwise. For example, the segments marked A and B in Figure 1 have distinct labels in U_a and the same lables in U_b.

In order to make our notation compact, we further assume that $m_0 = m_2$ and $m_{n+1} = m_{n-1}$.

Suppose now that L and M are arbitrary integer and binary n-dimensional vectors, respectively, and $l_i \geq 2$ for all i. It is clear that they uniquely determine a graph from C_h for some $h \geq 2$. Then, of course, L and M completely determine also the Szeged index of the corresponding graph.

PROPOSITION 4. The Szeged index of a UBCB system U is computed from the respective vectors L and M in the following manner:

$$Sz(U) = (2h+1)^2(5h+1) - 4\sum_{i=1}^{n}(l_i+1)(A_i+(-1)^{k_i}B_i)^2 - \tag{5}$$

$$-4\sum_{i=1}^{n}\left(4\sum_{r=2}^{l_i-1}(h-2r+1-2A_i)^2 + 2(h-2l_i+1-2A_i)^2\right) - 24(h-1)^2$$

where $h = \sum_{i=1}^{n} l_i - n + 1$, $k_i = m_{i-1} + m_{i1}$ and $A_i = \sum_{j=1}^{i-1} l_j - i + 1$, $B_i = \sum_{j=i+1}^{n} l_j - i + 1$.

Proof. We first observe that U has $\sum_{i=1}^{n} l_i - n + 1$ hexagons. Denote by A_i and B_i the number of hexagons in the graphs that are obtained after deleting the edges of segment S_i (the edges belong only to S_i).

Based on our previous results we can write

$$\sum_{(u,v)\in E(U)} f(u,v) = \sum_{i=1}^{n} \sum_{(u,v)\in E_m(S_i)} f(u,v) + \sum_{(u,v)\in E_t(U)} f(u,v)\,.$$

Let $(u,v) \in E_m(S_i)$. Applying Proposition 2, we have

$$\sum_{(u,v)\in E(U)} f(u,v) = (l_i+1)(A_i+(-1)^{m_{i-1}+m_{i+1}}B_i)^2\,.$$

Let $(u,v) \in E_t(U)$. Segment S_i has the hexagons labeled by $A_i + 1$, $A_i + 2$, ..., $A_i + l_i$. Since $|E_t(S_{i+1}) \cap E_m(S_i)| = 2$ (provided $n > 1$), we use for the calculation the sets $E'_t(S_l) = E_t(S_l)$ and $E'_t(S_{i+1}) = E_t(S_{i+1}) / E_m(S_i)$ for $1 \le i \le n - 1$. Then,

$$\sum_{(u,v)\in E_t(U)} f(u,v) = \sum_{i=1}^{n} \sum_{(u,v)\in E_t'(S_i)} f(u,v) =$$

$$= \sum_{i=1}^{n} \left(4 \sum_{r=2}^{l_i-1} (h - 2(A_i + r) + 1)^2 + 2(h - 2(A_i + l_i) + 1)^2 \right) + 6(h - 1)^2 .$$

The latter term corresponds to the edges of $E_t(U)$ from the terminal hexagons.

As an illustration, we apply formula (5) to calculate the Szeged index of the UBCB system U with two segments. Let the lengths of the segments be h_1 and h_2 (see Figure 2).

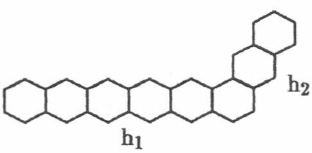

Figure 2. An unbranched catacondensed benzenoid system with two segments.

In this case, $L(U) = (h_1,h_2)$ amd $M(U) = (0,0)$. Hence, $h = h_1 + h_2 - 1$, $A = (A_1,A_2) = (0, h_1 - 1)$ and $B = (B_1,B_2) = (h_2 - 1, 0)$. Substituting these values back into (5), we have

$$Sz(U) = (2h + 1)^2(5h + 1) - 4((h_1 + 1)(h_2 - 1)^2 + (h_2 + 1)(h_1 - 1)^2) -$$
$$- 4(4 \sum_{r=2}^{h_1-1} (h - 2r + 1)^2 + 2(h - 2h_1 + 1)^2) -$$
$$- 4(4 \sum_{r=2}^{h_1-1} (h - 2r - 2h_1 + 3)^2 + 2(h - 2h_1 - 2h_2 + 3)^2) - 24(h - 1)^2$$

from which it straightforwardly follows:

$$Sz(U) = (44(h_1^3 + h_2^3) + 120h_1h_2)(h_1 + h_2) - 48(h_1^2 + h_2^2) -$$
$$- 120h_1h_2 + 43(h_1 + h_2) - 36)/3 .$$

UBCB GRAPHS WITH COINCIDING SZEGED AND WIENER INDICES

In this section, we answer in the affirmative the following question: Are there pairs of UBCB graphs such that the Szeged index of one coincides with the Wiener index of the other?

It was shown[2] that for a (cyclic) graph G, $Sz(G) > W(G)$. (For UBCB graphs we could have established this strict inequality by direct comparison of the extremal values of Sz and W). Because of this, if $Sz(U_1) = W(U_2)$ then U_1 and U_2 cannot be isomers, *i.e.* they must have different numbers of hexagons.

In class C_h, the graphs Lpa_h and Hel_h have also extremal Wiener indices, the W values of both Lpa and Hel are cubic polynomials in h.

PROPOSITION 5.[19] The extremal values of the Wiener index for the graphs from C_h are equal to $W_{min}(h) = W(Hel) = (8h^3 + 72h^2 - 26h + 27)/3$ and $W_{max}(h) = W(Lpa_h) = (16h^3 + 36h^2 + 26h + 3)/3$.

The following useful result determines the possible values of the Szeged indices of UBCB graphs.[15] The analogous property of W has been known for some time.[19]

PROPOSITION 6.[15,19] Let $U_1, U_2 \in C_h$. Then, $Sz(U_1) \equiv Sz(U_2) \pmod 8$ and $W(U_1) \equiv W(U_2) \pmod 8$.

In view of Proposition 6, we define the following two sets: $_{Sz}(h) = \{Sz_{\min}(h) + 8k \mid k = 0,1...., (Sz_{\max}(h) - Sz_{\min}(h))/8\}$ and $E_W(h) = \{W_{\min}(h) + 8k \mid k = 0,1,..., (W_{\max}(h) - W_{\min}(h))/8\}$. It is clear that the necessary conditions for coinciding indices are $E_W(h_1) \cap E_{Sz}(h_2) \neq 0$ and $W_{\min}(h_1) \equiv Sz_{\mathrm{nmin}}(h_2) \pmod 8$.

We have to distinguish between three cases:

(a) $W_{\min}(h_1) \leq Sz_{\min}(h_2) \leq W_{\max}(h_1) \leq Sz_{\max}(h_2)$

(b) $Sz_{\min}(h_2) \leq W_{\min}(h_1) \leq SZ_{\max}(h_2) \leq W_{\max}(h_1)$

(c) $Sz_{\min}(h_2) \leq W_{\min}(h_1) \leq W_{\max}(h_1) \leq Sz_{\max}(h_2)$.

Table I shows the first few admissible values of parameters h_1 and h_2 for each of the cases (a), (b) and (c).

TABLE I

Number of hexagons of the UBCB systems with coinciding Szeged and Wiener indicecs; for details see text.

(a)	$h_1(W)$	13	19	20	21	26	27	28	29	33	34
	$h_2(Sz)$	10	14	16	18	20	22	24	26	26	28
(b)	$h_1(W)$	12	18	23	24	29	30	31	35	36	37
	$h_2(Sz)$	8	12	14	16	18	20	22	22	24	26
(c)	$h_1(W)$	25	32	38	44	45	50	51	56	57	58
	$h_2(Sz)$	18	24	28	32	34	36	38	40	42	44

TABLE II

UBCB systems with given values of Sz and W.

value $Sz = W$	N_{Sz} $h = 8$	N_W $h = 12$	value $Sz = W$	N_{Sz} $h = 8$	N_W $h = 12$
7969	2	1	8537	2	1
8121	2	1	8553	2	2
8225	2	1	8585	1	4
8377	1	3	8633	1	5
7401	3	1	8697	2	4
8449	2	2	8721	1	5
8457	4	2	8897	1	14
8481	6	1	9161	1	32
8505	2	3	–	–	–

Table II contains a more detailed information on graphs with given values of the indices and the minimal number of hexagons. Here, N_{Sz} and N_W denote the number of elements of degeneracy classes for Sz and W, respectively.

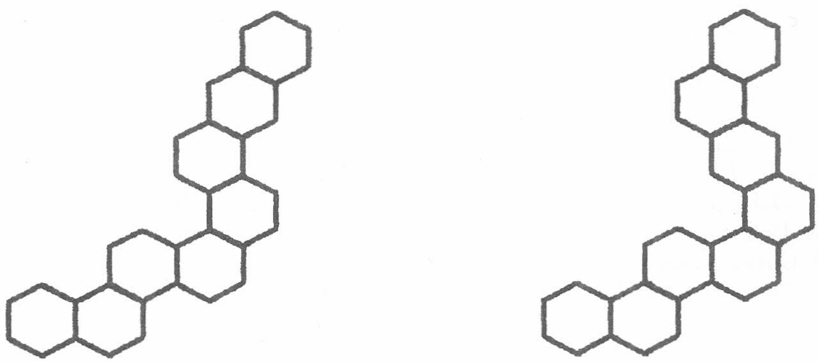

Figure 3. Two unbranched catacondensed benzenoid systems with 8 haxagons, having equal Szeged indices (Sz = 7969); this is the same value as the Wiener index of [12]helicene.

Two UBCB systems with h = 8 and Sz = 7969 are depicted in Figure 3. This value of the Szeged index is equal to othe Wiener index of the helicene with h = 12, *i.e.*, $W)Hel_{12}) = W_{\min}(12) = 7969$.

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SAŽETAK

O Szegedskom indeksu nerazgrananih katakondenziranih benzenoidnih molekula

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Ispitivan je Szegedski indeks (*Sz*) nerazgrananih katakondenziranih benzenoidnih (UBCB) ugljikovodika. Predložena je efikasna metoda za računanje *Sz* za te sustave. Među UBCB molekulama s fiksiranim brojem šesterokuta, linearni poliacen ima najveću, a helicen najmanju vrijednost *Sz*.