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A NEW FORMULA FOR THE CALCULATION OF THE WIENER INDEX OF HEXAGONAL CHAINS

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Abstract

The Wiener index (W) of hexagonal chains (*i.e.*, the molecular graphs of unbranched cata-condensed benzenoid hydrocarbons) is examined. The index W is a graph invariant defined as the sum of distances between all pairs of vertices in a graph. An efficient calculation formula for W is put forward. This formula is based on simple structural parameters of a graph and does not include distances between the vertices of the graph.

1. Introduction

Fifty years ago the first method for the calculation of the Wiener index (or Wiener number) for trees was put forward [1]. Hosoya reformulated the Wiener index in terms of distances between vertices in an arbitrary graph [2]. He defined W as the sum of distances between all pairs of vertices of the respective graph G,

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

where $d(u, v)$ is the number of edges in a shortest path connecting the vertices u and v.

Up to the present, the distance matrix is a basic tool for computing the Wiener index and related topological indices. Design and applications of topological indices based on distances in molecular graphs are described in detail in [4–12]. Numerous articles in the chemical and mathematical literature are devoted to the Wiener index (see monographs [4, 6, 11] and reviews [7, 9, 12, 13]). Various methods for calculation of W were discussed in [13, 15–23].

In this paper we derive a new formula for calculation of W for some classes of graphs which include molecular graphs of unbranched catacondensed benzenoid hydrocarbons. This formula depends on simple structural parameters of a graph and does not include distances between the vertices of the graph.

2. Hexagonal chains

In this section we define a class of graphs which are called the *hexagonal chains*. Hexagonal chains are exclusively composed of hexagons. Two hexagons have either 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 hexagonal chains have exactly two terminal hexagons. Hexagonal chains include the molecular graphs of unbranched catacondensed benzenoid hydrocarbons [23].

The set of all hexagonal chains with h hexagons is denoted by C_h. It is easy to see that every graph G from C_h has $p_G = 4h + 2$ vertices and $q_G = 5h + 1$ edges.

Let S and S' be arbitrary subgraphs of a hexagonal chain G such that they are themselves hexagonal chains and $S \subset S'$. Suppose that S is isomorphic to the linear polyacene and $h(S') = h(S) + 1$. It is evident that if S does not contain the terminal hexagon, then S' may be chosen by two ways. The subgraph S is called the *segment* of a hexagonal chain G if every S' is not isomorphic to the linear polyacene. In other words, a segment is a subgraph between neighboring kinks of G.

The hexagonal chain G shown in Fig. 1 has seven segments. Every segment is marked by a straight line. The number of hexagons in a segment S is called its length and is denoted by $l(S)$. For a segment of a hexagonal chain G, $2 \leq l(S) \leq h(G)$.

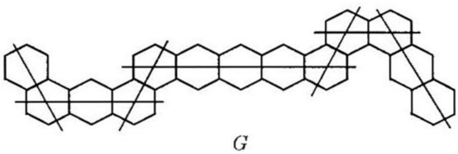

FIGURE 1. Segments of a hexagonal chain.

A hexagonal chain consists of a set of segments $S_1, S_2, \ldots, S_n$ with lengths $l(S_i) = l_i$ for some $n \geq 1$. Since two neighboring segments have always one hexagon in common, $h(G) = l_1 + l_2 + \ldots + l_n - n + 1$. Denote the vector of segments' lengths by $L(G) = (l_1, l_2, \ldots, l_n)$. The second vector $Z(G) = (z_1, z_2, \ldots, z_n)$ describes the mutual relation of the segments. An entry $z_i = z(S_i)$, either 0 or 1, is assigned to every segment S_i. We first choose $z_1 = z_n = 0$. Note that three segments S_{i-1}, S_i, S_{i+1}, $i = 2, \ldots, n-1$, induce a hexagonal chain. Suppose that this chain is embedded into the regular hexagonal lattice in the plane. Consider the segment S_i and draw a line through the centers of the hexagons of S_i. Then $z_i = 0$ if S_{i-1} and S_{i+1} lie on the same side of the line, and $z_i = 1$ otherwise. If $z_i = 1$, then the segments S_{i-1}, S_i, S_{i+1} form a "zigzag fragment" in the corresponding graph. Therefore we will call S_i the *zigzag* segment. The graph G in Fig. 1 has three zigzag segments and $L = (2,3,2,5,2,2,3)$, $Z = (0,0,1,1,1,0,0)$.

Suppose now that L and Z are an arbitrary integer and an arbitrary binary n-dimensional vector, respectively, and let $l_i \geq 2$ for all i. It is clear that they uniquely determine a graph having n segments. We show that L and Z completely determine also the Wiener index of the corresponding graph.

3. The main result

Let G be an arbitrary graph from C_h with $L(G) = (l_1, l_2, \ldots, l_n)$ and $Z(G) = (z_1, z_2, \ldots, z_n)$. Then the Wiener index of G may be calculated from these structural parameters of G.

Theorem. *The Wiener index of a hexagonal chain G is computed from the vectors $L(G)$ and $Z(G)$ as follows*

$$\begin{aligned} W(G) &= \frac{1}{3}\sum_{i=1}^{n}(16l_i^3 + 36l_i^2 + 26l_i - 78) + 27 \\ &+ 16\sum_{i=1}^{n}\left((l_i - 1)\sum_{k=i+1}^{n}\left[(l_i + l_k + 1)(l_k - 1) + (2l_k - 3 + z_k)\sum_{j=k+1}^{n}(l_j - 1)\right]\right). \end{aligned}$$

Note that the above formula does not contain distances between vertices of G. Therefore it enables a very easy calculation of the Wiener index of hexagonal chains.

4. Proof of Theorem

For an arbitrary edge $e = (v, u)$ of a hexagonal chain G, we define two disjoint vertex subsets $B_u(G) = \{w \mid d(w,u) < d(w,v)\}$ and $B_v(G) = \{w \mid d(w,v) < d(w,u)\}$. Let $n_u(G) = |B_u(G)|$ and $n_v(G) = |B_v(G)|$. By $D(v \mid G)$ we denote the *distance* of a vertex v, $D(v \mid G) = \sum_u d(u,v)$. It is easy to see that $D(u \mid G) - D(v \mid G) = n_v(G) - n_u(G)$ for arbitrary adjacent vertices of a bipartite graph.

Let G and H be hexagonal chains. Suppose that F is obtained from these graphs by identifying its edges $(u, v) \in E(G)$ and $(u_1, v_1) \in E(H)$ as depicted in Fig. 2.

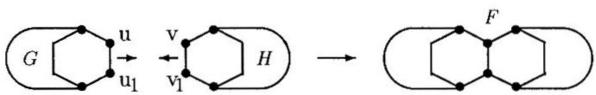

FIGURE 2.

It was shown that the Wiener index of the graph F may be calculated from the Wiener indices of its subgraphs G and H [24, 25].

Proposition 4 [25]. *For the graph F, we have*

$$\begin{aligned} W(F) &= W(G) + W(H) + (p_G - 2)D(v \mid H) + (p_H - 2)D(u \mid G) \\ &+ 2[n_{u_1}(G) + n_{v_1}(H) - n_{u_1}(G)n_{v_1}(H)] - (p_G + p_H) + 1 \,. \end{aligned} \tag{1}$$

Suppose that the graph F consists of the segments $S_1, S_2, \ldots, S_n$. The growth of F may be understood as a sequential attachment of linear polyacenes H_i with $h(H_i) = l(S_i) - 1 = l_i - 1$ hexagons. If H is the linear polyacene, then eq. (1) may be simplified (see Fig. 3). Indeed, in both cases $n_{u_1}(G) = 3$ and $n_{v_1}(H) = p_H/2 = 2h(H) + 1$. Then

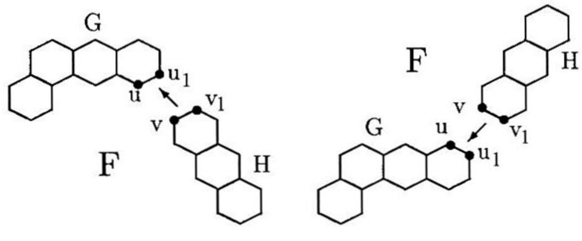

FIGURE 3.

$$\begin{aligned} W(F) &= W(G) + W(H) + 4h(G)D(v \mid H) + 4h(H)D(u \mid G) - 4h(G) \\ &- (12h(H) + 1) \,. \end{aligned} \tag{2}$$

Consider the graph G_1 in Fig. 4. Then G_1 is obtained by attaching H_1 to G_2.

Applying eq. (2), we have

$$\begin{aligned} W(G_1) &= W(G_2) + W(H_1) \\ &+ 4h(G_2)(D(v_1 \mid H_1) - 1) + 4h(H_1)D(v_1 \mid G_2) - 12h(H_1) - 1\,. \end{aligned}$$

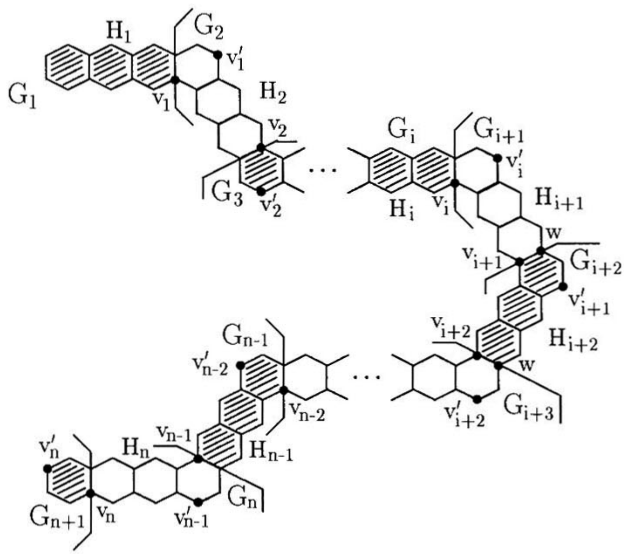

FIGURE 4. The sequential growth of G_1.

The graph $W(G_i)$ may be expressed in terms of $W(G_{i+1})$ in the same manner. Then

$$\begin{aligned} W(G_2) &= W(G_3) + W(H_2) \\ &+ 4h(G_3)(D(v_2 \mid H_2) - 1) + 4h(H_2)D(v_2 \mid G_3) - 12h(H_2) - 1\,, \end{aligned}$$

$$\cdots\cdots\cdots$$

$$
\begin{aligned}
W(G_i) &= W(G_{i+1}) + W(H_i) \\
&+ 4h(G_{i+1})(D(v_i \mid H_i) - 1) + 4h(H_i)D(v_i \mid G_{i+1}) - 12h(H_i) - 1\,,
\end{aligned}
$$

. . . .

$$
\begin{aligned}
W(G_n) &= W(G_{n+1}) + W(H_n) \\
&+ 4h(G_{n+1})(D(v_n \mid H_n) - 1) + 4h(H_n)D(v_n \mid G_{n+1}) - 12h(H_n) - 1\,,
\end{aligned}
$$

where G_{n+1} denotes the hexagonal chain with a single hexagon.

As a final result we obtain

$$
\begin{aligned}
W(G_1) &= W(G_{n+1}) + \sum_{i=1}^{n} W(H_i) \\
&+ 4\sum_{i=1}^{n} h(G_{i+1})(D(v_i \mid H_i) - 1) + 4\sum_{i=1}^{n} h(H_i)D(v_i \mid G_{i+1}) \\
&- 12\sum_{i=1}^{n} h(H_i) - n\,,
\end{aligned} \tag{3}
$$

where $h_i = h(G_i)$.

It is well known that the Wiener index of the linear polyacene with h hexagons is equal to

$$
W(H) = \frac{1}{3}(16h^3 + 36h^2 + 16h + 3)
$$

and for the considered vertex of the linear polyacene, $D(v|H) = 4h^2 + 4h + 1$ [26, 27]. In particular, for a single hexagon $W(H) = 27$ and $d(v|H) = 9$. Then we rewrite eq. (3) as follows

$$
\begin{aligned}
W(G_1) &= 27 + \frac{1}{3}\sum_{i=1}^{n}[16(l_i - 1)^3 + 36(l_i - 1)^2 + 26(l_i - 1) + 3] \\
&+ 16\sum_{i=1}^{n} l_i(l_i - 1)h_{i+1} + 4\sum_{i=1}^{n}(l_i - 1)D(v_i \mid G_{i+1}) \\
&- 12\sum_{i=1}^{n}(l_i - 1) - n\,.
\end{aligned} \tag{4}
$$

It easy to see that

$$h_i = h(G_i) = \sum_{k=i+1}^{n} (l_k - 1) + 1 \,.$$

Simplifying eq. (4), we have

$$\begin{aligned} W(G_1) &= \frac{1}{3}\sum_{i=1}^{n}(16l_i^3 + 36l_i^2 - 82l_i + 30) + 27 \\ &+ 16\sum_{i=1}^{n}\left(l_i(l_i-1)\sum_{k=i+1}^{n}(l_k - 1)\right) + 4\sum_{i=1}^{n}(l_i - 1)D(v_i \mid G_{i+1}) \,. \qquad (5) \end{aligned}$$

In order to complete the proof we need to determine the vertex distances from the above equation. The following result allows to compute these distances recursively.

Lemma. *For the vertices v_i and v_i' of the graph G_{i+1} (see Fig. 4),*

$$\begin{aligned} D(v_i \mid G_{i+1}) &= D(v_{i+1} \mid G_{i+2}) + f(l_{i+1}, h_{i+2}), \\ D(v_i' \mid G_{i+1}) &= D(v_{i+1} \mid G_{i+2}) + f(l_{i+1}, h_{i+2}) + 4(h_{i+2} - 1) \,, \end{aligned}$$

where $f(l_{i+1}, h_{i+2}) = 4[h_{i+2}(2l_{i+1} - 3) + (l_{i+1} - 1)^2 + 1]$.

Proof. Since $V(G_i) = (V(G_{i+1}) \cup V(H_i)) \setminus \{v_i, w\}$, we have

$$\begin{aligned} D(v_i \mid G_{i+1}) &= \sum_{u \in V(H_{i+1})} d_{G_{i+1}}(v_i, u) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} d_{G_{i+1}}(v_i, u) \\ &= D(v_i \mid H_{i+1}) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} [d_{G_{i+1}}(v_i, v_{i+1}) + d_{G_{i+1}}(v_{i+1}, u)] \\ &= D(v_i \mid H_{i+1}) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} [d_{H_{i+1}}(v_i, v_{i+1}) + d_{G_{i+2}}(v_{i+1}, u)] \,. \end{aligned}$$

It is not hard to calculate that $D(v_i \mid H_{i+1}) = 4(l_{i+1} - 1)^2 + 5$ and $d_{H_m}(v_a, v_1) = 2(l_m - 1) - 1$. Then

$$\begin{aligned} D(v_i \mid G_{i+1}) &= 4h_{i+2}[2(l_{i+1} - 1) - 1] + 4(l_{i+1} - 1)^2 + 5 \\ &+ \sum_{u \in V(G_{i+2})} d_{G_{i+2}}(v_{i+1}, u) - d_{G_{i+2}}(v_{i+1}, w) \\ &= D(v_{i+1} \mid G_{i+2}) + 4[h_{i+2}(2l_{i+1} - 3) + (l_{i+1} - 1)^2 + 1] \,. \end{aligned}$$

Next we present the distance of the vertex v_i' in G_{i+1} through the distance of w in G_{i+2} as follows

$$\begin{aligned} D(v_i' \mid G_{i+1}) &= \sum_{u \in V(H_{i+1})} d_{G_{i+1}}(v_i', u) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} d_{G_{i+1}}(v_i', u) \\ &= D(v_i' \mid H_{i+1}) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} [d_{H_{i+1}}(v_i', w) + d_{G_{i+2}}(w, u)] \\ &= D(w \mid G_{i+2}) + f(l_{i+1}, h_{i+2}) . \end{aligned}$$

Since the vertices w and v_{i+1} are adjacent in the bipartite graph G_{i+2} , $D(w \mid G_{i+2}) - D(v_{i+1} \mid G_{i+2}) = n_{v_{i+1}}(G_{i+2}) - n_w(G_{i+2}) = (p(G_{i+2}) - 3) - 3 = 4(h_{i+2} - 1)$. Then

$$D(v_i' \mid G_{i+1}) = D(v_{i+1} \mid G_{i+2}) + f(l_{i+1}, h_{i+2}) + 4(h_{i+2} - 1) .$$

Note that the distances of v_{n-1} and v_{n-1}' must be equal for $i = n - 1$. Indeed, in this case $h_{i+2} - 1 = h_{n+1} - 1 = 0$. This completes the proof. □

Applying the above Lemma, we derive the final expression for the distance of the vertex v_i.

Corollary 2. *Let G_i be obtained from G_{i+1} by attachment of H_i to the vertex v_i. Then*

$$D(v_i \mid G_{i+1}) = D(v|G_{n+1}) + \sum_{k=i+1}^{n} f(l_k, h_{k+1}) + 4 \sum_{k=i+1}^{n} z_k(h_{k+1} - 1) ,$$

Further we rewrite the distance $D(v_i \mid G_{i+1})$ in terms of the vectors $L(G_{i+1})$ and $Z(G_{i+1})$.

Corollary 3. *Let G_i be obtained from G_{i+1} by attachment of H_i to the vertex v_i. Then*

$$D(v_i \mid G_{i+1}) = 4 \sum_{k=i+1}^{n} \left[(l_k + 1)(l_k - 1) + (2l_k - 3 + z_k) \sum_{j=k+1}^{n} (l_j - 1) \right] + 9 .$$

Substituting the corresponding expression for $D(v_i \mid G_{i+1})$ back into eq. (5), we obtain

$$\begin{aligned} W(G_1) &= \frac{1}{3}\sum_{i=1}^{n}(16l_i^3+36l_i^2-82l_i+30)+27+16\sum_{i=1}^{n}\left(l_i(l_i-1)\sum_{k=i+1}^{n}(l_k-1)\right) \\ &+ 16\sum_{i=1}^{n}\left((l_i-1)\sum_{k=i+1}^{n}\left[(l_i+l_k+1)(l_k-1)+(2l_k-3+z_k)\sum_{j=k+1}^{n}(l_j-1)\right]\right) \\ &+ 36\sum_{i=1}^{n}(l_i-1)\,. \end{aligned}$$

The proof follows now by direct calculation. □

6. Examples

As an illustration we apply Theorem to calculate the Wiener index of three simple hexagonal chains. Consider the graph G_1 in Fig.5. For this graph, $L(G_1) = (l_1, l_2)$, $Z(G_1) = (0,0)$ and $h(G_1) = l_1 + l_2 - 1$.

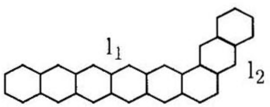

FIGURE 5. A hexagonal chain with two segments.

By the Theorem, we have

$$\begin{aligned} W(G_1) &= \frac{1}{3}(16l_1^3+36l_1^2+26l_1-78)+\frac{1}{3}(16l_2^3+36l_2^2+26l_2-78)+27 \\ &+ 16(l_1-1)[(l_1+l_2+1)(l_2-1)+(2l_2-3)(l_2-1)] \\ &= \frac{1}{3}[16h^3+36h^2-2h(12l_1-25)+3(8l_1^2-8l_1+1)]\,. \end{aligned}$$

If $l_1 = l_2$ or $l_1 = l_2 - 1$, then we arrive at

$$W(G_1) = \frac{1}{3}(16h^3+30h^2+38h)+(-1)^h,$$

a result obtained previously by Gutman and Polansky [28].

Consider the graphs G_1 and G_2 shown in Fig.6. In this case $L(G_1) = (l_1, h(G_1) - l_1 - l_3 + 2, l_3)$, $Z(G_1) = (0,1,0)$ and $L(G_2) = (l_1, h(G_2) - l_1 - l_3 + 2, l_3)$, $Z(G_2) = (0,0,0)$.

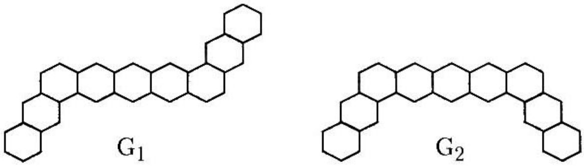

FIGURE 6. Hexagonal chains with three segments.

Then we have

$$\begin{aligned} W(G_1) &= \frac{1}{3}\sum_{i=1}^{3}(16l_i^3 + 36l_i^2 + 26l_i - 78) + 27 \\ &+ 16(l_1 - 1)\sum_{k=2}^{3}\left[(l_1 + l_k + 1)(l_k - 1) + (2l_k - 3 + z_k)\sum_{j=k+1}^{3}(l_j - 1)\right] \\ &+ 16(l_2 - 1)(l_2 + l_3 + 1)(l_3 - 1) \\ &= \frac{1}{3}[16h^3 + 36h^2 - 2h(12l_1 + 12l_3 - 37)] + 8[(l_1 - 1)^2 + (l_3 - 1)^2 + l_1 l_3] - 7\,. \end{aligned}$$

For the graph G_2,

$$W(G_2) = \frac{1}{3}[16h^3 + 36h^2 - 2h(12l_1 + 12l_3 - 37)] + 8(l_1^2 + l_3^2 - l_1 l_3) - 7\,.$$

Suppose that all segments of G_1 and G_2 are of equal size, *i.e.*, $l_1 = l_2 = l_3 = (h+2)/3$. Then

$$\begin{aligned} W(G_1) &= \frac{1}{3}(16h^3 + 28h^2 + 42h - 5), \\ W(G_2) &= \frac{1}{9}(48h^3 + 68h^2 + 158h - 31)\,. \end{aligned}$$

6. Congruence relations for the Wiener index

Let G_1 and G_2 be hexagonal chains with equal number of hexagons. A classical result in the theory of the Wiener index states that $W(G_1) \equiv W(G_2)$ $(mod\ 8)$ for every pair of hexagonal chains G_1 and G_2, *i.e.*, the difference $W(G_1) - W(G_2)$ is divisible by 8 [26, 27]. New congruence relations for some classes of hexagonal chains were recently established [29]. In the previous sections we dealt with the ordered sequence of segments lengths. Now we consider an unordered sequence $\{l_1, l_2, \ldots, l_n\}$ which is called the *set of segments lengths*.

Proposition 1. [29] *If graphs G_1 and G_2 have coinciding sets of segments lengths, then*

$$W(G_1) \equiv W(G_2) \quad (mod\ 16)\,.$$

Proposition 2. [29] *If graphs G_1 and G_2 have coinciding sets of segments lengths $\{l_1, l_2, \ldots, l_n\}$ and $l_i = kc_i + 1$ for all $i = 1, 2, \ldots, n$ $(k \geq 1, c_i \geq 1)$, then*

$$W(G_1) \equiv W(G_2) \quad (mod\ 16k^2)\,.$$

It is easy to see that these relations immediately follows from the Theorem. By making use of Theorem, we can establish an additional congruence relation for some subclasses of C_h.

Proposition 3. *Let G_1 and G_2 have coinciding sets of segments lengths $\{l_1, l_2, \ldots, l_n\}$ and $l_i = k\ c_i + 1$ for all $i = 1, 2, \ldots, n$ $(k \geq 1, c_i \geq 1)$. Suppose that all l_i and k are odd. Then*

$$W(G_1) \equiv W(G_2) \quad (mod\ 64k^2)\,.$$

Proof. Let $G_1, G_2 \in C_h$. Let all segments of the graphs have odd length l_i, $l_i = kc_i + 1$. This implies that $k\,c_i$ is even for every i. Since k is odd, all coefficients c_i must be even.

Therefore every term $(l_i - 1) = k\,c_i$ is divisible by $2k$. Applying the Theorem, we conclude that the difference $W(G_1) - W(G_2)$ is divisible by $64k^2$. □

Consider again the graphs G_1 and G_2 shown in Fig. 6. Suppose that $L(G_1) = L(G_2)$. Then

$$W(G_1) - W(G_2) = 16(l_1 l_3 - l_1 - l_3 + 1) = 16k^2 c_1 c_3 .$$

This example provides pairs of graphs with smallest possible nonzero difference between their Wiener indices for every $k \geq 1$. Indeed, if these graphs have coinciding sets of segments lengths, then $W(G_1) - W(G_2) = 16k^2$ at $c_1 = c_3 = 1$ $(l_1 = l_3 = k + 1)$. If all segments are of odd lengths and k is also odd, then $W(G_1) - W(G_2) = 64k^2$ at $c_1 = c_3 = 2$ $(l_1 = l_3 = 2k + 1)$.

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