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

Andrey A. DOBRYNIN

Institute of Mathematics, Russian Academy of Sciences, Siberian Branch, Novosibirsk 630090, Russia

(Received: July 1996)

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]. Itohaya 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 $S \subseteq S'$. Suppose that $S$ is isomorphic to the linear polycene 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 polycene. 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 $G$, $2 \leq l(S) \leq h(G)$.

![Diagram of a hexagonal chain](image)

**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 $n > 1$. 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 $C_n$ 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

$$W(G) = \frac{1}{3} \sum_{i=1}^{n} (16l_i^3 + 36l_i^2 + 26l_i - 78) + 27$$

$$+ 16 \sum_{i=1}^{n} \left( (l_i - 1) \sum_{k=i+1}^{n} \left[ (l_i + l_k + 1)(l_k - 1) + (2l_k - 3 + z_k) \sum_{j=k+1}^{n} (l_j - 1) \right] \right).$$

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 $D(u \mid G) - D(v \mid G) = n_u(G) - n_v(G)$ 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](image-url)
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

$$
W(F) = W(G) + W(H) + (p_G - 2)D(v \mid H) + (p_H - 2)D(u \mid G) \\
+ 2[n_{u_1}(G) + n_{v_1}(H) - n_{u_1}(G)n_{v_1}(H)] - (p_G + p_H) + 1. \quad (1)
$$

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

$$
W(F) = W(G) + W(H) + 4h(G)D(v \mid H) + 4h(H)D(u \mid G) - 4h(G) \\
- (12h(H) + 1). \quad (2)
$$

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

![Diagram](image-url)
Applying eq. (2), we have

$$W(G_1) = W(G_2) + W(H_1)$$
$$+ 4h(G_2)(D(v_1 | H_1) - 1) + 4h(H_1)D(v_1 | G_2) - 12h(H_1) - 1.$$  

**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

$$W(G_2) = W(G_3) + W(H_2)$$
$$+ 4h(G_3)(D(v_2 | H_2) - 1) + 4h(H_2)D(v_2 | G_3) - 12h(H_2) - 1,$$
\[ W(G_i) = W(G_{i+1}) + W(H_i) \]
\[ + 4h(G_{i+1})(D(v_i | H_i) - 1) + 4h(H_i)D(v_i | G_{i+1}) - 12h(H_i) - 1, \]

\[ W(G_n) = W(G_{n+1}) + W(H_n) \]
\[ + 4h(G_{n+1})(D(v_n | H_n) - 1) + 4h(H_n)D(v_n | G_{n+1}) - 12h(H_n) - 1, \]

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

As a final result we obtain

\[ W(G_1) = W(G_{n+1}) + \sum_{i=1}^{n} W(H_i) \]
\[ + 4 \sum_{i=1}^{n} h(G_{i+1})(D(v_i | H_i) - 1) + 4 \sum_{i=1}^{n} h(H_i)D(v_i | G_{i+1}) \]
\[ - 12 \sum_{i=1}^{n} h(H_i) - n, \quad (3) \]

where \( h_t = h(G_t) \).

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

\[ W(G_1) = 27 + \frac{1}{3} \sum_{i=1}^{n} [16(l_i - 1)^3 + 36(l_i - 1)^2 + 26(l_i - 1) + 3] \]
\[ + 16 \sum_{i=1}^{n} l_i(l_i - 1)h_{i+1} + 4 \sum_{i=1}^{n} (l_i - 1)D(v_i | G_{i+1}) \]
\[ - 12 \sum_{i=1}^{n} (l_i - 1) - n. \quad (4) \]
It easy to see that
\[ h_i = h(G_i) = \sum_{k=i+1}^{n} (l_k - 1) + 1. \]

Simplifying eq. (4), we have
\[
W(G_1) = \frac{1}{3} \sum_{i=1}^{n} (16l_i^3 + 36l_i^2 - 82l_i + 30) + 27 + 16 \sum_{i=1}^{n} (l_i(l_i - 1)) \sum_{k=i+1}^{n} (l_k - 1) + 4 \sum_{i=1}^{n} (l_i - 1) D(v_i \mid G_{i+1}). \tag{5}
\]

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),
\[
D(v_i \mid G_{i+1}) = D(v_{i+1} \mid G_{i+2}) + f(l_{i+1}, h_{i+2}),
\]
\[
D(v'_i \mid G_{i+1}) = D(v_{i+1} \mid G_{i+2}) + f(l_{i+1}, h_{i+2}) + 4(h_{i+2} - 1),
\]
where \( f(l_{i+1}, h_{i+2}) = 4h_{i+2}(2l_{i+1} - 3) + (l_{i+1} - 1)^2 + 1 \).

**Proof.** Since \( V(G_i) = (V(G_{i+1}) \cup V(H_i)) \setminus \{v_i, w\} \), we have
\[
D(v_i \mid G_{i+1}) = \sum_{u \in V(H_{i+1})} d_{G_{i+1}}(v_i, u) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} d_{G_{i+2}}(v_i, u)
\]
\[
= D(v_i \mid H_{i+1}) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} [d_{G_{i+1}}(v_i, v_{i+1}) + d_{G_{i+1}}(v_{i+1}, u)]
\]
\[
= D(v_i \mid H_{i+1}) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} [d_{H_{i+1}}(v_i, v_{i+1}) + d_{G_{i+2}}(v_{i+1}, u)].
\]

It is not hard to calculate that \( D(v_i \mid H_{i+1}) = 4(l_{i+1} - 1)^2 + 5 \) and \( d_{H_{m}}(v_{i+1}, v_1) = 2(l_{m} - 1) - 1 \). Then
\[
D(v_i \mid G_{i+1}) = 4h_{i+2}[2(l_{i+1} - 1) - 1] + 4(l_{i+1} - 1)^2 + 5
\]
\[
+ \sum_{u \in V(G_{i+2})} d_{G_{i+2}}(v_{i+1}, u) - d_{G_{i+2}}(v_{i+1}, u)
\]
\[
= D(v_{i+1} \mid G_{i+2}) + 4h_{i+2}(2l_{i+1} - 3) + (l_{i+1} - 1)^2 + 1. \]
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

\[
D(v'_i \mid G_{i+1}) = \sum_{u \in V(H_{i+1})} d_{G_{i+1}}(v'_i, u) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} d_{G_{i+2}}(v'_i, u) \\
= D(v'_i \mid H_{i+1}) + \sum_{u \in V(G_{i+2}) \setminus \{v_{i+1}, w\}} [d_{H_{i+1}}(v'_i, w) + d_{G_{i+2}}(w, u)] \\
= D(w \mid G_{i+2}) + f(l_{i+1}, h_{i+2}).
\]

Since the vertices \( w \) and \( v_{i+1} \) are adjacent in the bipartite graph \( G_{i+2} \),

\[
D(v'_i \mid G_{i+2}) = n_{v_{i+1}}(G_{i+2}) - n_w(G_{i+2}) = (p(G_{i+2}) - 3) - 3 = 4(h_{i+2} - 1). \text{ Then}
\]

\[
D(v'_i \mid G_{i+1}) = D(v_{i+1} \mid G_{i+2}) + f(l_{i+1}, h_{i+2}) + 4(h_{i+2} - 1).
\]

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. \( \Box \)

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

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

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

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

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 $h(G_1) = l_1 + l_2 - 1$.

![Hexagonal chain with two segments](image)

**FIGURE 5.** A hexagonal chain with two segments.

By the Theorem, we have

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

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 $L(G_2) = (l_1, h(G_2) - l_1 - l_3 + 2, l_3)$, $Z(G_2) = (0, 0, 0)$.
Then we have

\[ W(G_1) = \frac{1}{3} \sum_{i=1}^{3} (16l_i^3 + 36l_i^2 + 26l_i - 78) + 27 \]
\[ + 16(l_1 - 1) \sum_{k=2}^{3} \left[ (l_1 + l_k + 1)(l_k - 1) + (2l_k - 3 + z) \sum_{i=k+1}^{3} (l_j - 1) \right] \]
\[ + 16(l_2 - 1)(l_2 + l_3 + 1)(l_3 - 1) \]
\[ = \frac{1}{3} [16h^3 + 36h^2 - 2h(12l_1 + 12l_3 - 37)] + 8[(l_1 - 1)^2 + (l_3 - 1)^2 + l_1l_3] - 7. \]

For the graph \(G_2\),

\[ W(G_2) = \frac{1}{3} [16h^3 + 36h^2 - 2h(12l_1 + 12l_3 - 37)] + 8(h_2^2 + l_3^2 - l_1l_3) - 7. \]

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

\[ W(G_1) = \frac{1}{3} (16h^3 + 28h^2 + 42h - 5), \]
\[ W(G_2) = \frac{1}{9} (48h^3 + 68h^2 + 158h - 31). \]
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 $W(G_1) \equiv W(G_2) \pmod{8}$ 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

$$W(G_1) \equiv W(G_2) \pmod{16}.$$ 

**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

$$W(G_1) \equiv W(G_2) \pmod{16k^2}.$$ 

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 $l_i = kc_i + 1$ for all $i = 1, 2, \ldots, n$ ($k \geq 1, c_i \geq 1$). Suppose that all $l_i$ and $k$ are odd. Then

$$W(G_1) \equiv W(G_2) \pmod{64k^2}.$$ 

**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 $kc_i$ 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 \(c_1 = c_3 = 2\) \((l_1 = l_3 = 2k + 1)\).

Acknowledgement. The author would like to thank the referee for many helpful suggestions.

References


