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WIENER INDEX DECOMPOSITION BASED ON VERTEX DEGREES OF CATACONDENSED BENZENOID GRAPHS

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Abstract

The Wiener index is a distance-based structural descriptor of organic molecules defined as the sum of distances between all vertices of a molecular graph. A Wiener index decomposition based on vertex degrees of catacondensed benzenoid graphs is studied. It is shown that terms of the decomposition can be computed through the Wiener index.

1. Introduction

The Wiener index (or Wiener number) is a topological index based on distances between vertices of molecular graphs. The Wiener index was introduced as structural descriptor for characterization of alkanes [1]. A conventional definition of the Wiener index for an arbitrary molecular graph H is due to Hosoya [2]:

$$W(H) = \frac{1}{2} \sum_{u,v \in V(G)} d(u,v),$$

where $d(u,v)$ is the standard distance of the graph H, *i.e.*, the number of edges in a shortest path connecting the vertices u and v in H. Mathematical properties and chemical applications of the Wiener index have been intensively studied in the last thirty years (see books [3–5] and selected reviews [6–10]).

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We consider a class of graphs which include molecular graphs of catacondensed benzenoid hydrocarbons [11]. *Benzenoid graphs* are composed of six-membered cycles (hexagonal rings). We assume that such a graph contains at least two hexagonal rings. Any two rings either have one common edge (and are then said to be adjacent) or have no common vertices. No three rings share a common vertex.

Each hexagonal ring is adjacent to two or three other rings, with the exception of the terminal rings to which a single ring is adjacent. The inner dual graph of a given benzenoid graph consists of vertices corresponding to hexagonal rings of the graph; two vertices are adjacent if and only if the corresponding rings share an edge. A benzenoid graph is called *catacondensed* if its inner dual graph is a tree. Denote by L_h the linear polyacene with h rings. It is known that L_h has maximum W among all graphs of this class having h rings [12].

By construction, a benzenoid graph H has $4h+2$ vertices and every vertex has degree 2 or 3. The vertex set of H can be divided into two disjoint subsets with respect to vertex degrees: $V(H) = V_2(H) \cup V_3(H)$, where $V_k(H)$ contains all vertices of degree k, $|V_2(H)| = 2h+4$ and $|V_3(H)| = 2h-2$. The Wiener index of H can be decomposed into three terms in the following manner:

$$W(H) = \frac{1}{2}(W_{22}(H) + 2W_{23}(H) + W_{33}(H)), \tag{1}$$

where $W_{km}(H) = \sum_{u \in V_k(H)} \sum_{v \in V_m(H)} d(u,v)$ for $k, m \in \{2,3\}$.

For instance, for the linear polyacene we have $W_{22}(L_h) = 2(4h^3 + 27h^2 + 38h + 12)/3$, $W_{23}(L_h) = 2(4h^3 + 9h^2 - 7h - 6)/3$ and $W_{33}(L_h) = 2(4h^3 - 9h^2 + 2h + 3)/3$.

In this paper we show that the quantities $W_{22}(H)$, $W_{23}(H)$ and $W_{33}(H)$ can be computed through $W(H)$ and $W(L_h)$ by the similar way.

2. Main result

Let H be an arbitrary catacondensed benzenoid graph with h rings and $\Delta(H) = W(L_h) - W(H)$. Then the differences between the corresponding parts of decompositions of $W(H)$ and $W(L_h)$ coincide.

Theorem. *For the terms of the Wiener index decomposition (1),*

$$W_{22}(L_h) - W_{22}(H) = W_{23}(L_h) - W_{23}(H) = W_{33}(L_h) - W_{33}(H) = \Delta(H)/2.$$

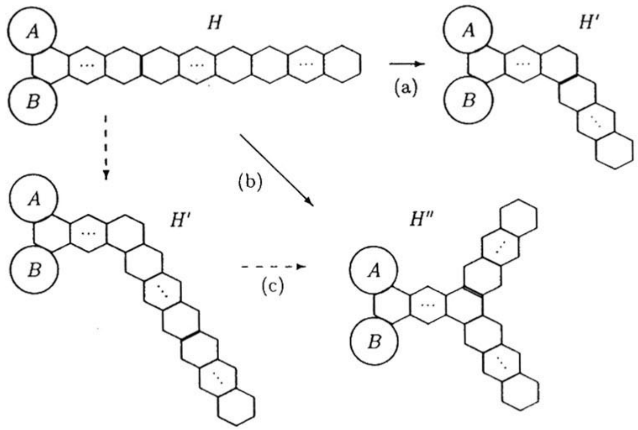

Figure 1. Kink transformations of catacondensed benzenoid graphs.

The Theorem implies numerous properties of the Wiener index for catacondensed benzenoid graphs that are outlined elsewhere [13]. Among them we mention the following: the discriminating ability of the Wiener index and the quantities W_{22}, W_{33} and W_{23} is the same (this proves an earlier stated conjecture [14,15]); the Wiener index can be calculated through the number of rings in a graph and any of the sums W_{22}, W_{33} or W_{23}. This approach has been previously applied for decomposition of the Wiener index into two terms with respect to vertex degree (sums of vertex distances for $v \in V_2$ and $v \in V_3$) [17].

3. Kink transformations of benzenoid graphs

Consider two graph operations of a catacondensed benzenoid graph H that consists of transforming a linear terminal part of H into new parts as shown in Figure 1 (see solid arrows). In other words, a terminal part of H is displaced from its initial location to another one making a new kink or branch in the resulting graph H'. Such operations are called *kink transformations*. Here and further, A and B stand for arbitrary fragments; in particular, they may be absent. Every transformation of type (b) can be decomposed into two transformations of type (a) and (c) as depicted in Figure 1 by dotted arrows.

Let H be arbitrary catacondensed benzenoid graph with h rings. It was shown that H

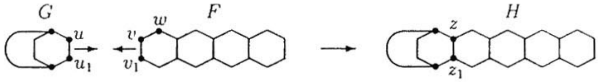

Figure 2.

can always be obtained from the linear polyacene L_h by a sequence of kink transformations [16]. Suppose that H is obtained from L_h in such a way. We shall evaluate the change of W_{22} for neighboring graphs from the corresponding sequence of kink transformations.

4. Distance of vertices of degree 2 under graph attachment

For an edge (v, v_1) of a graph H, define $V_2(v, v_1|H) = \{u \in V_2(H) \mid d(u,v) \le d(u,v_1)\}$, $D_2(v|H) = \sum_{u\in V_2(H)} d(v,u)$ and $D_2(v,v_1|H) = \sum_{u\in V_2(v,v_1|H)} d(v,u)$. It is clear that $V_2(H) = V_2(v,v_1|H) \cup V_2(v_1,v|H)$ and $D_2(v|H) - D_2(v_1|H) = |V_2(v_1,v|H)| - |V_2(v,v_1|H)|$. For vertices of the linear polyacene (see F in Figure 2), $D_2(v|L_h) = (2h+1)(h+2)$ and $D_2(v,v_1|L_h) = h(h+2)$.

Let H be obtained from the catacondensed benzenoid graph G and the linear polyacene F by identifying the edges (u,u_1) in G and (v,v_1) in F as depicted in Figure 2. Then the sum of vertex distances $W_{22}(H)$ can be expressed using the analogous sums of its subgraphs G and F.

Proposition 1. *For the graphs H, G and F shown in Figure 2, we have*

$$\begin{aligned} W_{22}(H) &= W_{22}(G) + W_{22}(F) + h_F(D_2(u|G) + D_2(u_1|G)) \\ &+ 2h_F(D_2(u,u_1|G) + D_2(u_1,u|G)) + \phi(h_G, h_F). \end{aligned}$$

where $\phi(h_G, h_F)$ is some polynomial in the variables h_G and h_F.

Proof. Let H be obtained from G and F as depicted in Figure 2. Then the vertex set $V_2(H)$ can be decomposed as follows $V_2(H) = (V_2(G) \cup V_2(F)) \setminus \{u,u_1,v,v_1\} = (V_2(u,u_1|G) \cup V_2(u_1,u|G) \cup V_2(v,v_1|F) \cup V_2(v_1,v|F)) \setminus \{u,u_1,v,v_1\}$. Vertices of these subsets will be examined.

a). Let $w \in V_2(u,u_1|G)$. It is clear that

$$\begin{aligned} D_2(w|H) &= \sum_{x\in V_2(G)\setminus\{u,u_1\}} d_G(w,x) + \sum_{x\in V_2(F)\setminus\{v,v_1\}} (d_G(w,u) + d_F(v,x)) \\ &= D_2(w|G) - d(w,u) - d(w,u_1) + (|V_2(F)| - 4)d_G(w,u) + D_2(v|F) - 1 \\ &= D_2(w|G) + 2h_F d_G(w,u) + D_2(v|F) - 2. \end{aligned}$$

Summing the above equality for all vertices of $V_2(u,u_1|G)\setminus\{u\}$, we obtain

$$\sum_{w\in V_2(u,u_1|G)\setminus\{u\}} D_2(w|H) = \sum_{w\in V_2(u,u_1|G)\setminus\{u\}} D_2(w|G) + 2h_F D_2(u,u_1|G) + (|V_2(u,u_1|G)|-1)(D_2(v|F)-2). \quad (2)$$

b). Let $w \in V_2(u_1,u|G)$. By symmetry of u and u_1,

$$D_2(w|H) = D_2(w|G) + 2h_F\, d_G(w,u_1) + D_2(v_1|F) - 2.$$

For all vertices of $V_2(u_1,u|G)\setminus\{u_1\}$, we have

$$\sum_{w\in V_2(u_1,u|G)\setminus\{u_1\}} D_2(w|H) = \sum_{w\in V_2(u_1,u|G)\setminus\{u_1\}} D_2(w|G) + 2h_F D_2(u_1,u|G) + (|V_2(u_1,u|G)|-1)(D_2(v_1|F)-2). \quad (3)$$

Summing the both parts of (2) and (3), we arrive at

$$\sum_{w\in V_2(G)\setminus\{u,u_1\}} D_2(w|H) = W_{22}(G) - D_2(u|G) - D_2(u_1|G) + 2h_F(D_2(u,u_1|G) + D_2(u_1,u|G)) + (|V_2(G)|-2)(D_2(v|F)-2). \quad (4)$$

c). Let $w \in V_2(v,v_1|F)$. Then

$$\begin{aligned} D_2(w|H) &= D_2(w|F) + \sum_{x\in V(G)\setminus\{u,u_1\}} (d_F(w,v) + d_G(u,x)) \\ &= D_2(w|F) + 2h_G\, d_F(w,v) + D_2(u|G) - 2. \end{aligned}$$

Let $w \in V_2(v_1,v|F)$. By symmetry of v and v_1, we get

$$D_2(w|H) = D_2(w|F) + 2h_G\, d_F(w,v_1) + D_2(u_1|G) - 2.$$

Using similar reasoning as in the case of the graph G, we have

$$\begin{aligned} &\sum_{w\in V_2(F)\setminus\{v,v_1\}} D_2(w|H) = \\ &= W_{22}(F) - D_2(v|F) - D_2(v_1|F) + 2h_G(D_2(v,v_1|F) + D_2(v_1,v|F)) \\ &+ (|V_2(v,v_1|F)|-1)(D_2(u|G) + D_2(u_1|G) - 4) \\ &= W_{22}(F) + 2h_G(D_2(v,v_1|F) + D_2(v_1,v|F)) - D_2(v|F) - D_2(v_1|F) \\ &+ (h_F+1)(D_2(u|G) + D_2(u_1|G)) - 4(|V_2(v,v_1|F)|-1). \quad (5) \end{aligned}$$

Finally, summing (4) and (5), we obtain

$$\begin{aligned}W_{22}(H) &= W_{22}(G)+W_{22}(F)\\ &+ h_F(D_2(u|G)+D_2(u_1|G))+2h_F(D_2(u,u_1|G)+D_2(u_1,u|G))\\ &+ 2h_G D_2(v|F)+4h_G D_2(v,v_1|F)-4h_G-4h_F-8.\end{aligned}$$

The proof of Proposition 1 is complete. □

5. Change of vertex distances under kink transformations

Consider the first type of kink transformation. Let the graph H' be obtained from H as shown in Figure 1. In order to calculate W, we decompose these graphs into two subgraphs as shown in Figure 3.

Proposition 2. $W_{22}(H)-W_{22}(H')=4(k+l)(2h_B+m-1)$.

Proof. Using Proposition 1 for H and H', we can write

$$\begin{aligned}W_{22}(H) &= W_{22}(G)+W_{22}(F)+(k+l)(D_2(u|G)+D_2(u_1|G))\\ &+ 2(k+l)(D_2(u,u_1|G)+D_2(u_1,u|G))+\phi(h_G,h_F),\end{aligned}$$

$$\begin{aligned}W_{22}(H') &= W_{22}(G)+W_{22}(F)+(k+l)(D_2(w|G)+D_2(u_1|G))\\ &+ 2(k+l)(D_2(w,u_1|G)+D_2(u_1,w|G))+\phi(h_G,h_F).\end{aligned}$$

Then

$$\begin{aligned}&W_{22}(H)-W_{22}(H')=(k+l)(D_2(u|G)-D_2(w|G))\\ &+\ 2(k+l)(D_2(u,u_1|G)+D_2(u_1,u|G)-D_2(w,u_1|G)-D_2(u_1,w|G)).\end{aligned} \qquad (6)$$

Now we compute every difference of distances in (6).

Consider subgraphs G_1 and G_2 of G shown in Figure 4a. It is easy to see that $D_2(u|G)-D_2(w|G)=2(m-2+|V_2(B)|-2)+4-6=2(2h_B+m-1)$. Since $V_2(u_1,w|G)=\{u_1,u,x\}$ (see Figure 4b), $D_2(u_1,w|G)=d(u_1,u)+d(u_1,x)=3$.

The quantity $D_2(w,u_1|G)$ can be divided into two parts (see the edge (w,u_1) in Figure 4b and graphs G_1, G_2 in Figure 4a):

$$D_2(w,u_1|G)=P(G_1)+P(G_2)=\sum_{z\in V_2(w,u_1|G)\cap V_2(G_1)} d(w,z)+\sum_{z\in V_2(w,u_1|G)\cap V_2(G_2)} d(w,z).$$

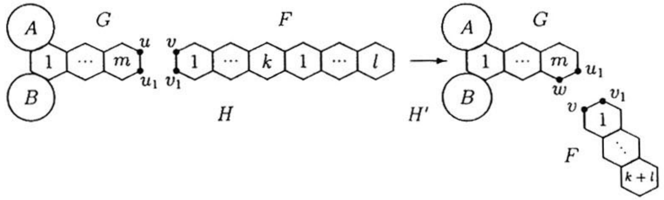

Figure 3. The first type of graph decomposition.

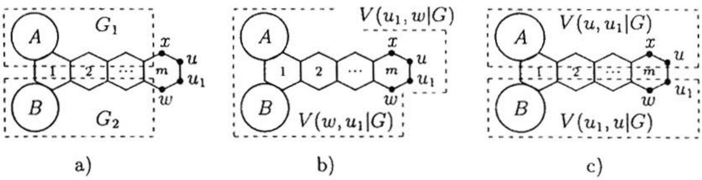

Figure 4. Vertex sets associated with edges.

Then we can write (the sets $V(u, u_1|G)$ and $V(u_1, u|G)$ are depicted in Figure 4c)

$$\begin{aligned} D_2(u_1, u|G) - P(G_2) &= (1 + 3 + ... + (2m - 3)) - (2 + 4 + ... + (2m - 4)) \\ &+ |V_2(B)| - 2 = 2h_B + m + 1, \\ D_2(u, u_1|G) - P(G_1) &= d(u, x) = 1. \end{aligned}$$

Substituting all necessary terms back into (6), we obtain

$$\begin{aligned} D_2(H) - D_2(H') &= 2(k + l)(2h_B + m - 1) + 2(k + l)(2h_B + m + 1 + 1 - 3) \\ &= 4(k + l)(2h_B + m - 1). \end{aligned}$$

The proof of Proposition 2 is complete. □

Consider now the second type of kink transformation. Let the graph H'' be obtained from H as shown in Figure 1. Because of Proposition 2, it is sufficient to examine a transformation of type (c) (see Figure 1). The corresponding graphs H' and H'' we present as depicted in Figure 5.

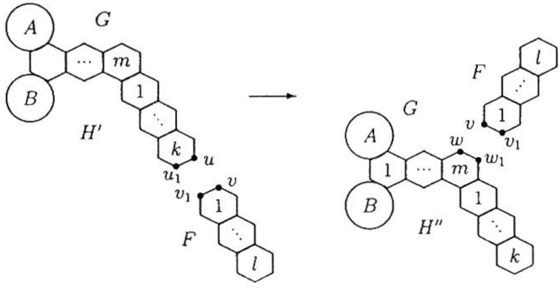

Figure 5. The second type of graph decomposition.

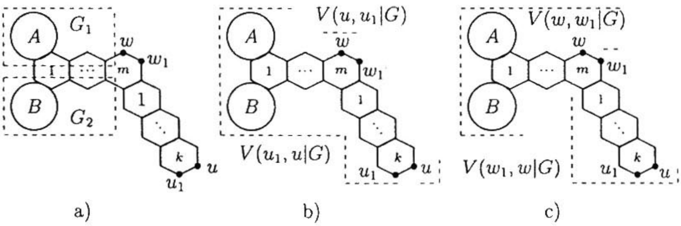

Figure 6. Vertex sets associated with edges.

Proposition 3. $W_{22}(H') - W_{22}(H'') = 16kl(h_A + h_B + m - 1) + 8l(h_A - h_B) + 4kl$.

Proof. Using Proposition 1 for the vertices of degree 2, we have

$$W_{22}(H') - W_{22}(H'') = l(D_2(u|G) - D_2(w|G) + D_2(u_1|G) - D_2(w_1|G))$$
$$+ \;\; 2l(D_2(u, u_1|G) - D_2(w_1, w|G) + D_2(u_1, u|G) - D_2(w, w_1|G)). \qquad (7)$$

Consider subgraphs G_1 and G_2 of G shown in Figure 6a. It is not hard to verify that

$$\begin{aligned} D_2(u|G) - D_2(w|G) &= (2(k+2) - 2)|V_2(G_1)| + (2(k+1) + 1 - 3)|V_2(G_2)| \\ &- (2k+2) - (2k+3) + 3 \\ &= 2(k+1)(2h_A + m - 1) + 2k(2h_B + m - 1), \end{aligned}$$

$$\begin{aligned} D_2(u_1|G) - D_2(w_1|G) &= (2(k+1) + 1 - 3)|V_2(G_1)| + (2(k+1) - 4)|V_2(G_2)| \\ &+ D_2(u_1|L_{k+1}) - D_2(w_1|L_{k+1}) - (2k+1) - (2k+2) + 5 \\ &= 2k(2h_A + m - 1) + 2(k-1)(2h_B + m - 1) + 2k. \end{aligned}$$

Consider the edges (u, u_1), (w, w_1) and the vertex sets $V_2(u, u_1|G)$, $V_2(u_1, u|G)$ and $V_2(w, w_1|G)$, $V_2(w_1, w|G)$ shown in Figures 5b,c. By direct calculation, we have

$$\begin{aligned} D_2(u, u_1|G) - D_2(w_1, w|G) &= (1 + 3 + ... + (2k + 1) + (2k + 2)) \\ &- (2 + 4 + ... + 2k + (2k + 2)) - (3 + 5 + ... + (2k + 1) + (2k + 2)) \\ &= -k(k + 3), \\ D_2(u_1, u|G) - D_2(w, w_1|G) &= (2(k + 1) + 1 - 2)(|V_2(A)| - 2 + m - 2) \\ &+ (2(k + 1) - 3)(|V_2(B)| - 2 + m - 2) + (1 + 3 + ... + (2k - 1)) \\ &= (2k + 1)(2h_A + m) + (2k - 1)(2h_B + m) + k^2. \end{aligned}$$

Substituting the above terms into (7), we obtain

$$\begin{aligned} W_{22}(H') - W_{22}(H'') &= l[2(k + 1)(2h_A + m - 1) + 2k(2h_B + m - 1) \\ &+ 2k(2h_A + m - 1) + 2(k - 1)(2h_B + m - 1) + 2k] \\ &+ 2l[2(k + 1)(2h_A + m) + 2(k - 1)(2h_B + m) + k^2 - k(k + 3)] \\ &= 16kl(h_A + h_B + m - 1) + 8l(h_A - h_B) + 4kl. \end{aligned}$$

The proof of Proposition 3 is complete. □

6. Proof of Theorem

Let H be an arbitrary catacondensed benzenoid graph with h rings. Then this graph can be obtained from the linear polyacene L_h by a sequence of kink transformations:

$$L_h = H_1 \to H_2 \to ... \to H_{m-1} \to H_m = H.$$

Using Propositions 2 and 3 for the neighboring graphs of the sequence, we can write $W_{22}(H_i) = W_{22}(H_{i+1}) + \Delta'_i$ for $i = 1, 2, ..., m - 1$. Therefore, $W_{22}(H) = W_{22}(L_h) - \Delta'(H)$, where $\Delta'(H) = \Delta'_1 + \Delta'_2 + \cdots + \Delta'_{m-1}$.

Let $W_2(H) = W_{22}(H) + W_{23}(H)$ and $W_3(H) = W_{33}(H) + W_{23}(H)$. It has been recently demonstrated that $W_2(H) = W_2(L_h) - \Delta(H)$ and $W_3(H) = W_3(L_h) - \Delta(H)$, where $\Delta(H) = W(L_h) - W(H)$ [17]. Comparing $\Delta'(H)$ and $\Delta(H)$, one recognizes the following unexpected result: $\Delta'(H) = \Delta(H)/2$. These properties immediately prove the Theorem.

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