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DISCRIMINATING POWER OF THE SCHULTZ INDEX FOR CATACONDENSED BENZENOID GRAPHS

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Abstract

The Schultz index (or molecular topological index, MTI) is a topological index based on distances between vertices of chemical graphs. This index is examined for isomeric benzenoid graphs (*i.e.*, molecular graphs of benzenoid hydrocarbons). It is shown that the Schultz index and the Wiener index (W) have the same discriminating power, *i.e.*, $MTI(G_1) = MTI(G_2)$ if and only if $W(G_1) = W(G_2)$ for arbitrary catacondensed benzenoid graphs G_1 and G_2.

1. Introduction

The Schultz index and the Wiener index (or Wiener number) are topological indices based on distances between vertices of molecular graphs. The Wiener index was introduced as structural descriptor for characterization of alkanes [1]. The first generalization of W for an arbitrary molecular graph G is due to Hosoya [2]. Now his formula is a conventional definition of the Wiener index:

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

where $d(u,v)$ is the standard distance of the graph G, *i.e.*, the number of edges in a shortest path connecting the vertices u and v in G. Mathematical properties and chemical applications of the Wiener index have been intensively studied in the last twenty five years (see books [3–5] and reviews [6–8]).

The Schultz index of a chemical graph G was also put forward as a topological index of alkanes [9]. Nowadays, it is usually referred to as the molecular topological index, $MTI(G)$, and it may be presented as

$$MTI(G) = \sum_{u\in V(G)} \sum_{v\in(G)} deg(u)[a_{uv} + d(u,v)],$$

where $deg(v)$ is the degree (valence) of vertex v in G and a_{uv} is the element of the adjacency matrix for G. Namely, an entry a_{uv} is equal to unity if vertices u and v are adjacent and zero otherwise. The molecular topological index has found interesting chemical applications [10–13]. A number of mathematical properties of MTI were also discovered [14–18]. It has been demonstrated that MTI and W are closely mutually related for certain classes of molecular graphs [15,16].

Discriminating power of a topological index reflects its ability to distinguish between isomers. Discriminating power of the Wiener index has been investigated for various classes of molecular graphs (see selected articles [19–21]). In this paper we shall study discriminating power of MTI for benzenoid graphs.

2. Benzenoid graphs

In this section we define a class of graphs which include molecular graphs of catacondensed benzenoid hydrocarbons [22]. *Benzenoid graphs* are composed of six-membered cycles (hexagonal rings). We assume that 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 *characteristic 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 characteristic graph is a tree. By construction, every vertex of a benzenoid graph has degree 2 or 3. An example of a catacondensed benzenoid graph and its characteristic graph is shown in Figure 1. The set of all catacondensed benzenoid graphs with h rings is denoted by $\mathcal{H}_h$. Every graph H from $\mathcal{H}_h$ has $p_H = 4h + 2$ vertices and $q_H = 5h + 1$ edges.

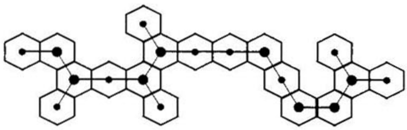

Figure 1. A catacondensed benzenoid graph and its characteristc graph.

3. Main result

There is a simple relation between the Wiener index and the Schultz molecular topological index of graphs in $\mathcal{H}_h$.

Theorem. *Let H and H' be arbitrary catacondensed benzenoid graphs in $\mathcal{H}_h$. Then*

$$MTI(H) - MTI(H') = 5(W(H) - W(H')).$$

This result shows that W and MTI have the same discriminating power among isomeric catacondensed benzenoid graphs.

Corollary 1. *Let $H, H' \in \mathcal{H}_h$. Then $MTI(H) = MTI(H')$ if and only if $W(H) = W(H')$.*

Properties of the Wiener index provide also the similar properties of MTI. For instance, it is a well-known fact that $W(H) \equiv W(H') \ (mod\ 8)$ for arbitrary $H, H' \in \mathcal{H}_h$ [23,24]. This implies the following regularity among values of MTI.

Corollary 2. *Let $H, H' \in \mathcal{H}_h$. Then $MTI(H) \equiv MTI(H') \ (mod\ 40)$, i.e. the difference $MTI(H) - MTI(H')$ is divisible by 40.*

Other regularities of W-values for catacondensed benzenoid graphs can be found in [23–27]. An explicit relation between MTI and W will be reported elsewhere [28].

4. Decomposition of vertex distances

Let $V(H)$ be the vertex set of a graph H. By $D(v \mid H)$ we denote the *distance* of a vertex v which is equal to the sum of distances from v to all vertices in H, $D(v \mid H) = \sum_{u \in V(H)} d(u,v)$. The vertex set of H may be divided into two disjoint subsets with respect of vertex degree: $V(H) = V_2(H) \cup V_3(H)$, where $V_n(H) = \{v \in V(H) \mid deg(v) = n\}$, $n = 2,3$. For every graph $H \in \mathcal{H}_h$, $|V_2(H)| = 2h + 4$ and $|V_3(H)| = 2h - 2$. The Wiener index may be presented by the same way: $2W(H) = D_2(H) + D_3(H)$, where

$D_n(H) = \sum_{deg(v)=n} D(v|H)$, $n = 2, 3$. The linear polyacene, L_h, has maximum W among all graphs of $\mathcal{H}_h$ [23].

The proof of Theorem is based on the following decomposition of sums of vertex distances D_2 and D_3.

Proposition 1. *Let H be arbitrary catacondensed benzenoid graph in $\mathcal{H}_h$. Then $D_2(H) = D_2(L_h) - \Delta$ and $D_3(H) = D_3(L_h) - \Delta$, where $\Delta = \Delta(H) > 0$.*

Proposition 1 will be proven in the subsequent sections. It should be noted that the similar statement was formulated as conjecture in [29,30].

Corollary 3. *Let $H, H' \in \mathcal{H}_h$ and the sums D_2, D_3 of vertex distances of these graphs be decomposed with Δ and Δ', respectively. Then $W(H) - W(H') = \Delta' - \Delta$.*

Corollary 3 immediately follows from the equation $W(H) = (D_2(H) + D_3(H))/2$ and Proposition 1.

Corollary 4. *Let $H, H' \in \mathcal{H}_h$ and the sums D_2, D_3 of vertex distances of these graphs be decomposed with Δ and Δ', respectively. Then $MTI(H) - MTI(H') = 5(\Delta' - \Delta)$.*

It has been recently demonstrated that $MTI(H) - MTI(H') = 4(W(H) - W(H')) + D_3(H) - D_3(H')$ holds for any catacondensed benzenoid graphs H and H' [18]. This equality and Proposition 1 lead to Corollary 4.

The above corollaries imply Theorem.

5. Kink transformations of graphs

Hexagonal rings of a catacondensed benzenoid graph may be angularly or linearly connected. Each angularly connected ring is said to correspond to a "kink" in a graph. As an illustration consider the graph shown in Figure 1. Big vertices of its characteristic graph correspond to angularly connected rings. Kinks of a graph define a convenient method to construct a benzenoid graph from the linear polyacene.

Consider two graph operations of a catacondensed benzenoid graph H that consist of transforming a linear terminal part of H into new parts as shown in Figure 2 (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* [27]. Here and further, A and B stand for arbitrary fragments; in particular, they may be absent. Every transformation of type (b) may be decomposed into two transformations of type (a) and (c) as depicted in Figure 2 by dotted arrows.

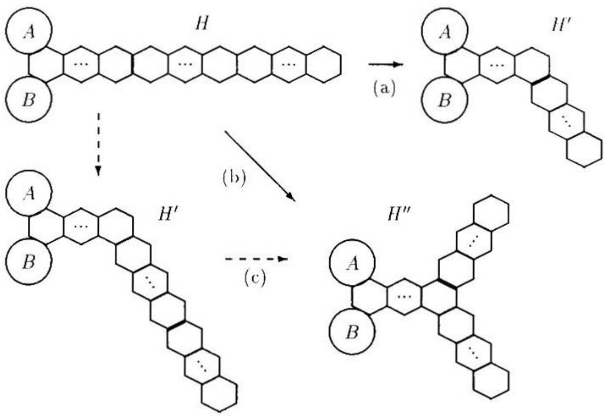

Figure 2. Kink transformations of catacondensed benzenoid graphs.

Proposition 2. [27] *Let H be arbitrary catacondensed benzenoid graph in $\mathcal{H}_h$. Then H can always be obtained from the linear polyacene L_h by a sequence of kink transformations.*

Suppose that $H \in \mathcal{H}_h$ is obtained from L_h in such a way. Based on the above result, we try to evaluate the change of distance sums D_2 and D_3 for neighboring graphs from the corresponding sequence of kink transformations.

6. Formula for sums of vertex distances

In order to examine properties of D_2 and D_3 in detail, we define a number of additional notations taking into account vertex degree $n \in \{2, 3\}$. Let (v, v_1) be an arbitrary edge of a graph H. Then

$$\begin{aligned} V((v, v_1)|H) &= \{u \in V(H) \mid d(u, v) < d(u, v_1)\}, \\ V_n((v, v_1)|H) &= \{u \in V((v, v_1)|H) \mid deg(u) = n\}, \\ D_n(v|H) &= \sum_{u \in V_n((v, v_1)|H)} d(v, u), \\ D_n(v_1|H) &= \sum_{u \in V_n((v_1, v)|H)} d(v_1, u). \end{aligned}$$

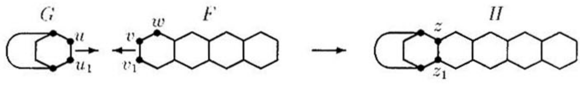

Figure 3.

It is clear that

$$
\begin{aligned}
V_n(H) &= V_n((v,v_1)|H) \cup V_n((v_1,v)|H), \\
V((v,v_1)|H) &= V_2((v,v_1)|H) \cup V_3((v,v_1)|H), \\
V(H) &= V((v,v_1)|H) \cup V((v_1,v)|H), \\
D(v|H) &= D_2(v|H) + D_3(v|H) + \sum_{u \in V((v_1,v)|H)} [d(v,v_1) + d(v_1,u)] + d(v,v_1) \\
&= D_2(v|H) + D_3(v|H) + D_2(v_1|H) + D_3(v_1|H) + |V((v_1,v)|H)| + 1.
\end{aligned}
$$

It is easy to verify that $D(v|H) - D(v_1|H) = |V((v_1,v)|H)| - |V((v,v_1)|H)|$. Further we need the above parameters of the linear polyacene L_h (see the edge (v,v_1) of $F \cong L_h$ in Figure 3):

1. $|V_2((v,v_1)|L_h)| = h+2$ and $|V_3((v,v_1)|L_h)| = h-1$.
2. $D_2(v|L_h) = h(h+2)$ and $D_3(v|L_h) = h(h-1)$,
3. $D(v|L_h) = 4h^2+4h+1$ and $D(w|L_h) = 4h^2+5$.

Let $H \in \mathcal{H}_h$ and 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 3. Then the sum of vertex distances of the graph H can be expressed using the analogous sums of its subgraphs G and F.

Proposition 3. *For the graphs H, G and F shown in Figure 3, we have*

$$
\begin{aligned}
D_n(H) &= D_n(G) + D_n(F) + h_F(D(u|G) + D(u_1|G)) \\
&+ 4h_F(D_n(u|G) + D_n(u_1|G)) + \phi_n(h_G,h_F).
\end{aligned}
$$

where $\phi_n(h_G,h_F)$ is some polynomial, $n = 2,3$.

Proof. Let H be obtained from G and F as depicted in Figure 3. Then the vertex sets $V_2(H)$ and $V_3(H)$ may be decomposed as follows

$$
\begin{aligned}
V_2(H) &= (V_2(G) \cup V_2(F)) \setminus \{u,u_1,v,v_1\} \\
&= (V_2((u,u_1)|G) \cup V_2((u_1,u)|G) \cup V_2((v,v_1)|F) \cup V_2((v_1,v)|F)) \setminus \{u,u_1,v,v_1\},
\end{aligned}
$$

$$\begin{aligned} V_3(H) &= V_3(G) \cup V_3(F) \cup \{z, z_1\} \\ &= V_3((u,u_1)|G) \cup V_3((u_1,u)|G) \cup V_3((v,v_1)|F) \cup V_3((v_1,v)|F) \cup \{z, z_1\}. \end{aligned}$$

First the vertices of degree 2 will be examined.

a1). Let $w \in V_2((u,u_1)|G)$. It is clear that

$$\begin{aligned} D(w|H) &= D(w|G) + \sum_{x \in V(F)\setminus\{v,v_1\}} (d(w,u) + d(v,x)) \\ &= D(w|G) + (p_F - 2)d(w,u) + D(v|F) - 1. \end{aligned}$$

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

$$\begin{aligned} \sum_{w \in V_2((u,u_1)|G)\setminus\{u\}} D(w|H) &= \sum_{w \in V_2((u,u_1)|G)\setminus\{u\}} D(w|G) + (p_F - 2)D_2(u|G) \\ &+ (|V_2((u,u_1)|G)| - 1)(D(v|F) - 1). \end{aligned} \tag{1}$$

a2). Let $w \in V_2((u_1,u)|G)$. In this case

$$D(w|H) = D(w|G) + (p_F - 2)d(w,u_1) + D(v_1|F) - 1.$$

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

$$\begin{aligned} \sum_{w \in V_2((u_1,u)|G)\setminus\{u_1\}} D(w|H) &= \sum_{w \in V_2((u_1,u)|G)\setminus\{u_1\}} D(w|G) + (p_F - 2)D_2(u_1|G) \\ &+ (|V_2((u_1,u)|G)| - 1)(D(v_1|F) - 1). \end{aligned} \tag{2}$$

Summing the both parts of (1) and (2), we arrive at

$$\begin{aligned} \sum_{w \in V_2(G)\setminus\{u,u_1\}} D(w|H) &= D_2(G) - D(u|G) - D(u_1|G) + 4h_F(D_2(u|G) + D_2(u_1|G)) \\ &+ 8h_F(h_F + 1)(h_G + 1). \end{aligned} \tag{3}$$

a3). Let $w \in V_2((v,v_1)|F)$. Then

$$\begin{aligned} D(w|H) &= D(w|F) + \sum_{x \in V(G)\setminus\{u,u_1\}} (d(w,v) + d(u,x)) \\ &= D(w|F) + (p_G - 2)d(w,v) + D(u|F) - 1. \end{aligned}$$

a4). Let $w \in V_2((v_1,v)|F)$. By symmetry of v and v_1, we get

$$D(w|H) = D(w|F) + (p_G - 2)d(w,v_1) + D(u_1|F) - 1.$$

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

$$\begin{aligned}\sum_{u\in V_2(F)\setminus\{v,v_1\}} D(w|H) &= D_2(F) - D(v|F) - D(v_1|F)\\ &+ 4h_G(D_2(v|F) + D_2(v_1|F)) + (|V_2((v,v_1)|F)| - 1)(D(u|G) - 1)\\ &+ (|V_2((v_1,v)|F)| - 1)(D(u_1|G) - 1)\\ &= D_2(F) + (h_F + 1)(D(u|G) + D(u_1|G)) + \phi_1(h_G, h_F) \qquad (4)\end{aligned}$$

Finally, summing (3) and (4), we obtain

$$\begin{aligned}D_2(H) &= D_2(G) + D_2(F) + h_F(D(u|G) + D(u_1|G))\\ &+ 4h_F(D_2(u|G) + D_2(u_1|G)) + \phi_2(h_G, h_F).\end{aligned}$$

In order to derive a formula for $D_3(H)$ we can apply analogous considerations for vertices of $V_3(H)$. In this case we arrive at

$$\begin{aligned}D_3(H) &= D_3(G) + D_3(F) + (|V_3((v,v_1)|F)| + 1)(D(u|G) + D(u_1|G))\\ &+ 4h_F(D_3(u|G) + D_3(u_1|G)) + \phi_3(h_G, h_F).\end{aligned}$$

The proof of Proposition 3 is complete. □

7. Change of vertex distances under kink transformations

Consider the first type of kink transformation.

Proposition 4. *Let the graph H' be obtained from H as shown in Figure 2. Then $D_2(H) - D_2(H') = D_3(H) - D_3(H')$.*

Proof. First consider vertices of degree 2 in the graphs H and H'. In order to calculate W, we decompose these graphs into two subgraphs as shown in Figure 4. Using Proposition 3 for H and H', we can write

$$\begin{aligned}D_2(H) &= D_2(G) + D_2(F) + (k+l)(D(u|G) + D(u_1|G))\\ &+ 4(k+l)(D_2(u|G) + D_2(u_1|G)) + \phi_2(h_G, h_F).\end{aligned}$$

$$\begin{aligned}D_2(H') &= D_2(G) + D_2(F) + (k+l)(D(w|G) + D(u_1|G))\\ &+ 4(k+l)(D_2(w|G) + D_2'(u_1|G)) + \phi_2(h_G, h_F).\end{aligned}$$

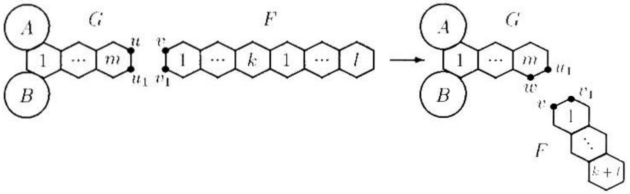

Figure 4. The first type of graph decomposition.

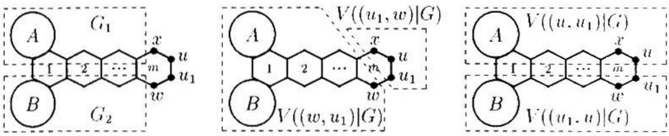

Figure 5. Vertex sets associated with edges.

Since $D_2(u_1|G)$ may be associated with two edges (u_1, u) and (u_1, w), in the above equations this term is denoted by $D_2(u_1|G)$ and $D_2'(u_1|G)$, respectively. Then

$$\begin{aligned} D_2(H) - D_2(H') &= (k+l)(D(u|G) - D(w|G)) - 4(k+l)D_2'(u_1|G) \\ &+ 4(k+l)(D_2(u|G) + D_2(u_1|G) - D_2(w|G)). \end{aligned} \tag{5}$$

Now we compute every difference of distances in (5).

Consider subgraphs G_1 and G_2 of G shown in Figure 5a. It is easy to see that $D(u|G) - D(w|G) = 2p_{G_2} - 2 = 4(2h_B + m - 1)$. Since $V_2((u_1, w)|G) = \{u_1, u, x\}$ (see Figure 5b), $D_2'(u_1|G) = d(u_1, u) + d(u_1, x) = 3$.

The quantity $D_2(w|G)$ may be divided into two parts (see the edge (w, u_1) in Figure 5b and graphs G_1, G_2 in Figure 5a):

$$D_2(w|G) = P(G_1) + P(G_2) = \sum_{\substack{z \in V((w,u_1)|G) \cap V(G_1) \\ deg(z)=2}} d(w, z) + \sum_{\substack{z \in V((w,u_1)|G) \cap V(G_2) \\ deg(z)=2}} d(w, z).$$

Then we can write (the sets $V((u, u_1)|G)$ and $V((u_1, u)|G)$ are depicted in Figure 5c)

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

Substituting all necessary terms back into (5), we obtain

$$D_2(H) - D_2(H') = 8(k+l)(2h_B + m - 1).$$

Using Proposition 3 for the vertices of degree 3 in H and H', we have

$$\begin{aligned} D_3(H) - D_3(H') &= (k+l)(D(u|G) - D(w|G)) - 4(k+l)D_3'(u_1|G) \\ &+ 4(k+l)(D_3(u|G) + D_3(u_1|G) - D_3(w|G)). \qquad (6) \end{aligned}$$

Since $V_3((u_1, w)|G) = \emptyset$ (see Figure 5b), $D_3'(u_1|G) = 0$. By analogy with the case of vertices of degree 2, $D_3(w|G)$ may be also divided into two parts $P(G_1)$ and $P(G_2)$. Then

$$\begin{aligned} D_3(u_1|G) - P(G_2) &= |V_3(B)| + 2 + (m-1) = 2h_B + m - 1, \\ D_3(u|G) - P(G_1) &= 0. \end{aligned}$$

Substituting all necessary terms into (6), we have

$$D_3(H) - D_3(H') = 8(k+l)(2h_B + m - 1).$$

The proof of Proposition 4 is complete. □

Let us consider the second type of kink transformation.

Proposition 5. *Let the graph H'' be obtained from H as shown in Figure 2. Then $D_2(H) - D_2(H'') = D_3(H) - D_3(H'')$.*

Proof. Because of Proposition 4, it is sufficient to examine a transformation of type (c) shown in Figure 2. The corresponding graphs H' and H'' we present as depicted in Figure 6. Using Proposition 3 for the vertices of degree 2, we have

$$\begin{aligned} D_2(H') - D_2(H'') &= l(D(u|G) - D(w|G)) + l(D(u_1|G) - D(w_1|G)) \\ &+ 4l(D_2(u|G) - D_2(w_1|G)) + 4l(D_2(u_1|G) - D_2(w|G)). \qquad (7) \end{aligned}$$

Consider subgraphs G_1 and G_2 of G shown in Figure 7a. It is not hard to verify that

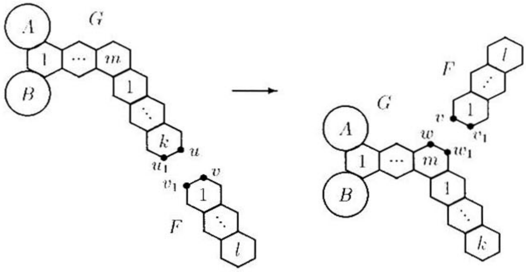

Figure 6. The second type of graph decomposition.

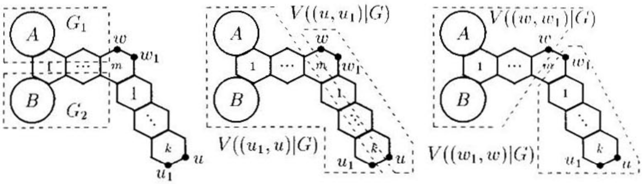

Figure 7. Vertex sets associated with edges.

$$\begin{aligned}
D(u|G) - D(w|G) &= (2(k+2)-2)(p_{G_1}-1) + (2(k+1)+1-3)(p_{G_2}-1) \\
&= 4(k+1)(2h_A+m-1) + 4k(2h_B+m-1),
\end{aligned}$$

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

Consider the edges (u,u_1), (w,w_1) and the vertex sets $V((u,u_1)|G)$, $V((u_1,u)|G)$ and $V((w,w_1)|G)$, $V((w_1,w)|G)$ shown in Figures 7b,c. By direct calculation, we have

$$D_2(u|G) - D_2(w_1|G) = (k+1)(k+3) - (2k^2+7k+3) = -k(k+3),$$

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

Substituting the above terms into (7), we obtain

$$D_2(H') - D_2(H'') = 32kl(h_A + h_B + m - 1) + 16l(h_A - h_B) + 8kl.$$

Applying Proposition 3 to the vertices of degree 3 of H and H', we can write

$$\begin{aligned} D_3(H') - D_3(H'') &= l(D(u|G) - D(w|G)) + l(D(u_1|G) - D(w_1|G)) \\ &+ 4l(D_3(u|G) - D_3(w_1|G)) + 4l(D_3(u_1|G) - D_3(w|G)). \end{aligned} \quad (8)$$

For vertices of the edges (u, u_1) and (w, w_1) (see Figures 7b,c), we have

$$D_3(u|G) - D_3(w_1|G) = k(k+1) - (k(k+1) + k^2) = -k^2.$$

Consider again the graphs G_1 and G_2 in Figure 7a. Then

$$\begin{aligned} D_3(u_1|G) - D_3(w|G) &= (2(k+1) - 1)|V_3(G_1)| + ((2k+1) - 3)|V_3(G_2)| \\ &+ D_3(u_1|L_k) + 2k \\ &= (2k+1)(2h_A + m - 1) + (2k-1)(2h_B + m - 1) \\ &+ k(k+1). \end{aligned}$$

Finally, substituting all necessary terms into (8), we arrive at

$$D_3(H') - D_3(H'') = 32kl(h_A + h_B + m - 1) + 16l(h_A - h_B) + 8kl.$$

The proof of Proposition 5 is complete. □

8. Proof of Proposition 1

Let H be an arbitrary catacondensed benzenoid graph in $\mathcal{H}_h$. By Proposition 2, H may be obtained from the linear polyacene L_h by a sequence of kink transformations:

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

Using Propositions 4 and 5 for the neighboring graphs of this sequences, we can write $D_2(H_i) = D_2(H_{i+1}) + \Delta_i$ and $D_3(H_i) = D_3(H_{i+1}) + \Delta_i$, $i = 1, 2, \dots, m-1$. Therefore, $D_2(H) = D_2(L_h) - \Delta$ and $D_3(H) = D_3(L_h) - \Delta$, where $\Delta = \Delta(H) = \Delta_1 + \Delta_2 + \dots + \Delta_{m-1}$.

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