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Research article

Extremal bi-Wiener indices of unbranched catacondensed benzenoids and polyphenyl hexagonal chains

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Abstract: The bi-Wiener index is a recently introduced distance-based invariant for connected bipartite graphs. Let G be a connected bipartite graph with bipartition $V(G) = X \cup Y$. The bi-Wiener index of G is defined by

$$W_b(G) = \sum_{(u,v)\in X\times Y} d_G(u, v),$$

where $d_G(u, v)$ is the distance between u and v in G. In this paper, we study extremal bi-Wiener indices of two families of hexagon-based molecular chains. The first family considered here is the family of unbranched catacondensed benzenoids, also called hexagonal chains, in which consecutive hexagons share an edge. If $F_n \in \mathcal{U}_n$ is an unbranched catacondensed benzenoid with n hexagons, then

$$\frac{4n^3 + 36n^2 - 10n + 15}{3} \leq W_b(F_n) \leq \frac{8n^3 + 18n^2 + 16n + 3}{3}.$$

For $n \geq 3$, the lower bound is attained uniquely by the helicene chain, and the upper bound is attained uniquely by the linear chain. The second family is the family of polyphenyl hexagonal chains, in which consecutive hexagons are joined by a cut edge. If $G_n \in \mathcal{P}_n$ is a polyphenyl hexagonal chain with internal configuration sequence $\ell_2, \ell_3, \ldots, \ell_{n-1} \in \{1, 2, 3\}$, then

$$W_b(G_n) = 3n^3 + 27n^2 - 15n + 18\sum_{k=2}^{n-1} \ell_k(k-1)(n-k),$$

where the sum is empty if $n \leq 2$. Consequently, among all polyphenyl hexagonal chains with n hexagons, the ortho-chain has the minimum bi-Wiener index and the para-chain has the maximum bi-Wiener index.

Keywords: bi-Wiener index; Wiener index; unbranched catacondensed benzenoid; hexagonal chain; polyphenyl hexagonal chain; linear chain; helicene chain; extremal graph
Mathematics Subject Classification: 05C12, 05C35, 05C92

1. Introduction

All graphs considered in this paper are finite, simple, undirected, and connected. For notation or terminology not explicitly defined here, refer to [1]. For a graph G, let $V(G)$ and $E(G)$ denote its vertex set and edge set, respectively. The distance between two vertices u and v in G is denoted by $d_G(u, v)$, or simply by $d(u, v)$ if no confusion can arise.

Distance-based topological indices are important graph invariants in chemical graph theory. The Wiener index, introduced by Wiener in the study of paraffin boiling points, is defined by

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v).$$

It is one of the earliest and most extensively studied molecular descriptors based on graph distances [2, 3]. Other classical molecular descriptors, such as the Hosoya index, have also played an important role in mathematical chemistry [4].

Recently, Chen et al. introduced and studied the bi-Wiener index for connected bipartite graphs [5]. Let G be a connected bipartite graph with bipartition $V(G) = X \cup Y$. By considering only the distances between vertices belonging to different bipartition classes, the bi-Wiener index is defined as

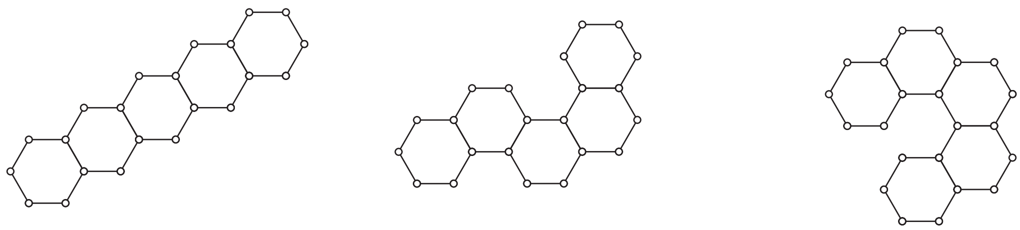
$$W_b(G) = \sum_{(u,v)\in X\times Y} d_G(u, v). \tag{1.1}$$

The notation $X \times Y$ fixes one endpoint in each bipartition class; equivalently, every unordered vertex pair with endpoints in different classes is counted exactly once. No pair whose two endpoints lie in the same bipartition class is included in (1.1). This invariant is a natural bipartite counterpart of the Wiener index. The definition in (1.1) is not merely a formal restriction of the Wiener sum. In a bipartite graph, distances between vertices in different bipartition classes are odd, while distances between vertices in the same bipartition class are even. Thus, the bi-Wiener index is precisely the odd-distance part of the distance matrix of a bipartite graph, and it satisfies $W_b(G) \leq W(G)$; see [5]. Consequently, $W_b(G)$ records the distance interaction between the two color classes and gives a parity-sensitive refinement of the ordinary Wiener index.

The introduction of the bi-Wiener index is also motivated by applications in chemical graph theory. The ordinary Wiener index summarizes all pairwise distances, but in some bipartite cyclic molecular graphs the even-distance and odd-distance contributions may behave differently. Chen et al. observed examples involving cyclohexane, methylcyclohexane, and corresponding substituted cyclobutyl isomers in which the bi-Wiener index is consistent with trends in physical properties such as boiling point and density [5]. Hence, the bi-Wiener index can be regarded as a complementary molecular descriptor: it preserves the distance-based nature of the Wiener index while emphasizing the bipartite structure of the molecular graph.

The practical relevance of this viewpoint is that bipartite molecular graphs naturally separate vertices into two alternating classes, and the bi-Wiener index measures the odd-distance interaction between these classes. For cyclic bipartite molecular graphs, this odd-distance part may change differently from the full Wiener sum when local hexagon connections are modified. Determining exact extremal values therefore gives benchmark structures with the smallest and largest possible cross-class distance interactions within a fixed molecular family. Although the present paper is theoretical and does not build a quantitative structure–property regression model, such closed formulas are useful as baseline descriptors for later comparative or data-driven studies of bipartite molecular systems.

The present paper is motivated by this viewpoint and by the natural problem of extending the study of the bi-Wiener index from trees to cyclic bipartite molecular graphs. The first family considered here is the family of unbranched catacondensed benzenoids, also known as hexagonal chains. These graphs are among the most basic and most important classes of benzenoid systems; each of them is obtained by arranging hexagons in a linear sequence so that consecutive hexagons share one edge and no vertex belongs to more than two hexagons [6]. See Figure 1.

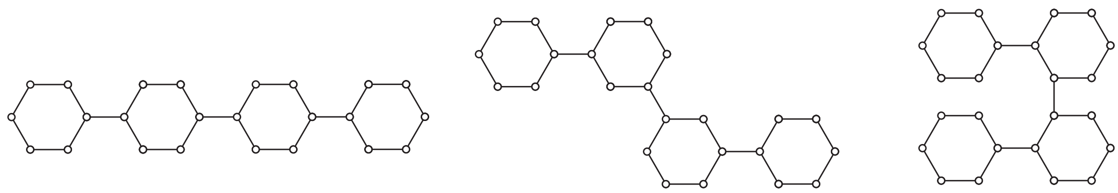


(a) (b) (c)

Figure 1. Three unbranched catacondensed benzenoids, where (a) is a linear chain and (c) is a helicene chain.

Previous work on unbranched catacondensed benzenoids has addressed their extremal properties [7], the anti-forcing number [8], the Wiener and eccentric connectivity indices [9, 10], the Padmakar–Ivan index [11], the Merrifield–Simmons and related matching indices [12, 13], Hosoya-type indices and polynomials [14, 15], and the Mostar index [6, 16].

The second family considered here is the family of polyphenyl hexagonal chains, where consecutive hexagons are not fused but are connected by cut edges. See Figure 2.



(a) (b) (c)

Figure 2. Three polyphenyl hexagonal chains, where (a) is a para-chain, (b) is a meta-chain, and (c) is an ortho-chain.

Related work on polyphenyl and spiro hexagonal chains includes the Hosoya and Merrifield–Simmons indices [17, 18], the Wiener and Kirchhoff indices [19, 20], subtree enumeration [21], comparative analyses of random chains [22], and the Mostar index [23]. In this paper, we first determine the extremal bi-Wiener index of unbranched catacondensed benzenoids with a fixed number of hexagons. We then determine an exact formula and extremal values for polyphenyl hexagonal chains. The two results show that the extremal behavior of the bi-Wiener index depends strongly on how adjacent hexagons are connected: for edge-fused chains the helicene chain is minimal and the linear chain is maximal, whereas for cut-edge polyphenyl chains the ortho-chain is minimal and the para-chain is maximal.

The contribution of the paper is threefold. First, it extends the study of the bi-Wiener index from trees to cyclic bipartite molecular graphs, where parity and block structure interact in a nontrivial way. Second, for unbranched catacondensed benzenoids, we introduce terminal-edge distance sums that separate ordinary endpoint-distance information from the bipartition-restricted bi-Wiener sum; this gives a concise recursive method for handling the odd-distance contribution. Third, by treating both edge-fused and cut-edge hexagonal chains, the paper provides a comparison showing that the same index can have different extremal configurations under different local connection mechanisms. These features also indicate that the method can be adapted to other even-cycle molecular block chains.

2. Definitions and main results

2.1. Unbranched catacondensed benzenoids

We first give the standard graph-theoretic definition of the main class studied in this paper. This class is often called the class of hexagonal chains, but in the present paper we use the more chemical name *unbranched catacondensed benzenoids*.

Definition 2.1 (Unbranched catacondensed benzenoid)**.** *An* unbranched catacondensed benzenoid F_n *with n hexagons is a graph consisting of n hexagons* $C_1, C_2, \ldots, C_n$ *arranged in a sequence such that*

(i) *for every* $1 \leq i \leq n-1$*, the intersection* $C_i \cap C_{i+1}$ *is exactly one edge;*

(ii) *if* $|i-j| > 1$*, then* $V(C_i) \cap V(C_j) = \emptyset$*;*

(iii) *no vertex belongs to more than two hexagons.*

Equivalently, consecutive hexagons are fused along exactly one common edge and nonconsecutive hexagons are vertex-disjoint. See Figure 1. Let $\mathcal{U}_n$ *denote the family of all unbranched catacondensed benzenoids with n hexagons. Under these assumptions, after the first hexagon each additional hexagon contributes four new vertices and five new edges; hence, every graph in* $\mathcal{U}_n$ *has* $4n+2$ *vertices and* $5n+1$ *edges, and every vertex has degree* 2 *or* 3*. For* $F_n \in \mathcal{U}_n$*, let*

$$V_3(F_n) = \{v \in V(F_n) : d_{F_n}(v) = 3\}.$$

Let $F_n \in \mathcal{U}_n$ and let $C_1, C_2, \ldots, C_n$ be its hexagons in the order of the chain. For $1 \leq i \leq n-1$, write

$$e_i = E(C_i) \cap E(C_{i+1})$$

for the common edge of the consecutive hexagons C_i and C_{i+1}. For an internal hexagon C_i, $2 \leq i \leq n-1$, the two common edges e_{i-1} and e_i are disjoint; otherwise a vertex would belong to three hexagons. If the vertices of C_i are written cyclically as $au_1u_2u_3u_4ba$, where $e_{i-1} = ab$, then e_i is one of u_1u_2, u_2u_3, and u_3u_4. Following the standard terminology, these three cases are the α-, β-, and γ-types. The β-type is the linear case, since the two common edges are opposite in the hexagon, while the α- and γ-types are angular cases.

Definition 2.2 (Linear chain and helicene chain)**.** *For $n \geq 2$, the* linear chain L_n *is the unbranched catacondensed benzenoid satisfying*

$$\mathsf{L}_n[V_3(\mathsf{L}_n)] \cong (n-1)K_2.$$

See Figure 1(a). Equivalently, every internal hexagon of L_n is of β-type; for $n = 1$, put $\mathsf{L}_1 = C_6$. For $n \geq 2$, the helicene chain H_n *is the unbranched catacondensed benzenoid such that $\mathsf{H}_n[V_3(\mathsf{H}_n)]$ is the comb of order $2n-2$, that is, the graph obtained from the path P_{n-1} by attaching one pendant vertex to each vertex of the path. Equivalently, up to reflection, the helicene chain is obtained by making consecutive angular extensions in the same direction; for $n = 1$, put $\mathsf{H}_1 = C_6$. See Figure 1(c).*

Theorem 2.3 (Unbranched catacondensed benzenoids)**.** *Let $F_n \in \mathcal{U}_n$ be an unbranched catacondensed benzenoid with n hexagons. Then,*

$$\frac{4n^3 + 36n^2 - 10n + 15}{3} \leq W_b(F_n) \leq \frac{8n^3 + 18n^2 + 16n + 3}{3}. \tag{2.1}$$

For $n \geq 3$, equality on the left holds if and only if $F_n \cong \mathsf{H}_n$, and equality on the right holds if and only if $F_n \cong \mathsf{L}_n$. Equivalently,

$$W_b(\mathsf{H}_n) = \frac{4n^3 + 36n^2 - 10n + 15}{3}, \qquad W_b(\mathsf{L}_n) = \frac{8n^3 + 18n^2 + 16n + 3}{3}. \tag{2.2}$$

For $n = 1, 2$, all unbranched catacondensed benzenoids with n hexagons are isomorphic, and both bounds coincide.

For example, when $n = 3$, Theorem 2.3 gives

$$W_b(\mathsf{H}_3) = 139, \qquad W_b(\mathsf{L}_3) = 143.$$

Thus, the bi-Wiener index of an unbranched catacondensed benzenoid is minimized by the helicene chain and maximized by the linear chain.

2.2. Polyphenyl hexagonal chains

We now introduce the second class considered in the paper. Unlike unbranched catacondensed benzenoids, consecutive hexagons in this class are not fused along an edge; instead, they are connected by a cut edge.

Definition 2.4 (Polyphenyl hexagonal chain)**.** *A* polyphenyl hexagonal chain *with n hexagons is a graph obtained from n pairwise disjoint copies $Q_1, Q_2, \ldots, Q_n$ of the cycle C_6 by adding one cut edge between Q_i and Q_{i+1} for every $1 \leq i \leq n-1$, and by adding no other edges. Equivalently, it is a cactus graph whose blocks are edges or hexagons, in which consecutive hexagons are connected by cut edges. See Figure 2. Let $\mathcal{P}_n$ denote the family of all polyphenyl hexagonal chains with n hexagons. Every graph in $\mathcal{P}_n$ has $6n$ vertices and $7n-1$ edges. The hexagons Q_1 and Q_n are called terminal hexagons, while $Q_2, \ldots, Q_{n-1}$ are called internal hexagons when $n \geq 3$.*

For an internal hexagon Q_k, $2 \le k \le n-1$, let a_k be the vertex of Q_k incident with the cut edge joining Q_{k-1} to Q_k, and let b_k be the vertex of Q_k incident with the cut edge joining Q_k to Q_{k+1}. Put

$$\ell_k = d_{Q_k}(a_k, b_k). \tag{2.3}$$

Since $Q_k \cong C_6$, one has $\ell_k \in \{1, 2, 3\}$. The three cases $\ell_k = 1, 2, 3$ are called the ortho-, meta-, and para-configurations, respectively. A chain is called the *ortho-chain* O_n, the *meta-chain* M_n, or the *para-chain* P_n if all of its internal hexagons are respectively ortho-, meta-, or para-configured. See Figures 2(c), 2(b), and 2(a), respectively. If $n = 1$ or $n = 2$, there is no internal hexagon and all chains in $\mathcal{P}_n$ are isomorphic; in this case the symbols O_n, M_n, and P_n all denote this unique chain up to isomorphism.

Theorem 2.5 (Polyphenyl hexagonal chains)**.** *Let $G_n \in \mathcal{P}_n$ be a polyphenyl hexagonal chain with internal configuration sequence $\ell_2, \ell_3, \ldots, \ell_{n-1} \in \{1, 2, 3\}$. Then,*

$$W_b(G_n) = 3n^3 + 27n^2 - 15n + 18 \sum_{k=2}^{n-1} \ell_k (k-1)(n-k), \tag{2.4}$$

where the sum is empty if $n \le 2$. Consequently,

$$6n^3 + 18n^2 - 9n \le W_b(G_n) \le 12n^3 + 3n. \tag{2.5}$$

For $n \ge 3$, equality on the left holds if and only if $G_n \cong \mathsf{O}_n$, and equality on the right holds if and only if $G_n \cong \mathsf{P}_n$. Moreover,

$$W_b(\mathsf{O}_n) = 6n^3 + 18n^2 - 9n, \qquad W_b(\mathsf{M}_n) = 9n^3 + 9n^2 - 3n, \qquad W_b(\mathsf{P}_n) = 12n^3 + 3n.$$

For example, when $n = 3$, Theorem 2.5 gives

$$W_b(\mathsf{O}_3) = 297, \qquad W_b(\mathsf{M}_3) = 315, \qquad W_b(\mathsf{P}_3) = 333.$$

Thus, for polyphenyl hexagonal chains, the bi-Wiener index increases when the internal connection changes from ortho to meta and then to para.

3. Proof for unbranched catacondensed benzenoids

3.1. Terminal edges and auxiliary sums

The proof of Theorem 2.3 uses two different kinds of sums. All sums denoted by W_b are bi-Wiener sums and therefore count only pairs whose two endpoints belong to different bipartition classes. In contrast, the terminal-edge sums introduced below are ordinary distance sums from all vertices to one or two fixed terminal vertices. They are auxiliary quantities only; they are not bi-Wiener sums.

In a partial unbranched catacondensed benzenoid G_i obtained from the first i hexagons of a chain, a *terminal edge* means an outer edge of the last hexagon that is used, or may be used, as the common edge for attaching the next hexagon. When such an edge is written as ab, it is regarded as an *oriented terminal edge*: the orientation only orders its two endpoints. Reversing the orientation interchanges the two endpoint sums A and B, but does not change their sum D. Thus, in the induction below, the notation $D(G_i, ab)$ is attached to the current ordered attachment edge, while the value of D itself is independent of the orientation.

Let G be an unbranched catacondensed benzenoid with an oriented terminal edge ab. For any subset $S \subseteq V(G)$, define the partial terminal sums

$$A_S(G, ab) = \sum_{z \in S} d_G(z, a), \qquad B_S(G, ab) = \sum_{z \in S} d_G(z, b).$$

When a bipartition $V(G) = X \cup Y$ is being used, the four quantities A_X, A_Y, B_X, B_Y record the two color-class contributions separately. The full terminal sums are

$$A(G, ab) = A_{V(G)}(G, ab) = \sum_{z \in V(G)} d_G(z, a), \qquad B(G, ab) = B_{V(G)}(G, ab) = \sum_{z \in V(G)} d_G(z, b),$$

and

$$D(G, ab) = A(G, ab) + B(G, ab).$$

Thus, $D(G, ab)$ is the total distance from all vertices of G to the two endpoints of the terminal edge ab. The labels A and B refer only to the endpoint labels a and b; they do not refer to the bipartition classes and they do not impose any opposite-class restriction. The opposite-class restriction is imposed explicitly only when a contribution to W_b is computed.

Suppose that a new hexagon is attached to G along the terminal edge ab. Write the new hexagon as

$$ax_1x_2x_3x_4ba,$$

so the new vertices are x_1, x_2, x_3, x_4. Denote the resulting graph by G^+. If $|V(G)| = N$, then $|V(G^+)| = N + 4$. The next terminal edge of G^+, if another hexagon is to be attached, must be one of x_1x_2, x_2x_3, and x_3x_4. These correspond respectively to an α-, β-, and γ-extension.

We shall repeatedly use the following elementary observation. Since every graph considered here is bipartite and a and b are adjacent, for every old vertex $z \in V(G)$ one has

$$|d_G(z, a) - d_G(z, b)| = 1.$$

Consequently, after the new hexagon is attached,

$$\begin{aligned} d_{G^+}(z, x_1) &= d_G(z, a) + 1, \qquad & d_{G^+}(z, x_2) &= d_G(z, a) + 2, \\ d_{G^+}(z, x_3) &= d_G(z, b) + 2, \qquad & d_{G^+}(z, x_4) &= d_G(z, b) + 1. \end{aligned} \tag{3.1}$$

For instance, a shortest path from z to x_2 may go through a, giving length $d_G(z, a)+2$; any route through b is no shorter because it has length at least $d_G(z, b) + 3 \geq d_G(z, a) + 2$. The other three identities are proved in the same way.

Lemma 3.1. *For a single hexagon C_6, one has $W_b(C_6) = 15$.*

Proof. Fix one bipartition class of C_6. From each of its three vertices, the distances to the three vertices in the other bipartition class are $1, 1, 3$. Therefore,

$$W_b(C_6) = 3(1 + 1 + 3) = 15.$$

□

Lemma 3.2. *With the notation above,*

$$W_b(G^+) = W_b(G) + D(G, ab) + 3N + 6. \tag{3.2}$$

Proof. Let $V(G) = X \cup Y$ be a bipartition chosen so that $a \in X$ and $b \in Y$. Then, G^+ has bipartition

$$X^+ = X \cup \{x_2, x_4\}, \qquad Y^+ = Y \cup \{x_1, x_3\}.$$

The bi-Wiener increment consists of two parts: cross-class pairs with one old and one new vertex, and cross-class pairs with two new vertices. No same-class pair is counted.

For an old vertex $z \in X$, the new vertices in the opposite class are x_1 and x_3. Using (3.1),

$$d_{G^+}(z, x_1) + d_{G^+}(z, x_3) = d_G(z, a) + 1 + d_G(z, b) + 2.$$

For an old vertex $z \in Y$, the new vertices in the opposite class are x_2 and x_4. Again using (3.1),

$$d_{G^+}(z, x_2) + d_{G^+}(z, x_4) = d_G(z, a) + 2 + d_G(z, b) + 1.$$

Therefore, the old–new contribution to the bi-Wiener index is

$$\begin{aligned}
&\sum_{z\in X}(d_{G^+}(z, x_1) + d_{G^+}(z, x_3)) + \sum_{z\in Y}(d_{G^+}(z, x_2) + d_{G^+}(z, x_4)) \\
&= \sum_{z\in X}(d_G(z, a) + d_G(z, b) + 3) + \sum_{z\in Y}(d_G(z, a) + d_G(z, b) + 3) \\
&= A_X(G, ab) + B_X(G, ab) + A_Y(G, ab) + B_Y(G, ab) + 3(|X| + |Y|) \\
&= D(G, ab) + 3N.
\end{aligned}$$

This is the step in which the bi-Wiener restriction is used: the summation is first separated according to the two bipartition classes, and only after that separation are the ordinary terminal sums A and B recombined.

The cross-class pairs among the four new vertices are, up to order,

$$(x_1, x_2), \quad (x_1, x_4), \quad (x_3, x_2), \quad (x_3, x_4),$$

and their distances are respectively $1, 3, 1, 1$. Thus, their contribution is 6. Finally, distances between old vertices are not changed by attaching the new hexagon, because the only additional route between the old attachment vertices a and b goes around the new part and is longer than the existing edge ab. Combining these three observations gives (3.2). □

Lemma 3.3. *With the notation above, the following recurrences hold. Here, $A(G^+, uv)$ and $B(G^+, uv)$ are again full terminal sums over all vertices of G^+, with respect to the first and second endpoints of the oriented edge uv. They are not bi-Wiener sums.*

(i) *If the next terminal edge is the linear edge x_2x_3, oriented as x_2x_3, then*

$$A(G^+, x_2x_3) = A(G, ab) + 2N + 4, \qquad B(G^+, x_2x_3) = B(G, ab) + 2N + 4,$$

and therefore

$$D(G^+, x_2x_3) = D(G, ab) + 4N + 8.$$

(ii) *If the next terminal edge is the angular edge x_1x_2, oriented as x_1x_2, then*

$$A(G^+, x_1x_2) = A(G, ab) + N + 6, \qquad B(G^+, x_1x_2) = A(G, ab) + 2N + 4,$$

and therefore

$$D(G^+, x_1x_2) = 2A(G, ab) + 3N + 10.$$

(iii) *If the next terminal edge is the angular edge x_3x_4, oriented as x_3x_4, then*

$$A(G^+, x_3x_4) = B(G, ab) + 2N + 4, \qquad B(G^+, x_3x_4) = B(G, ab) + N + 6,$$

and therefore

$$D(G^+, x_3x_4) = 2B(G, ab) + 3N + 10.$$

Proof. We prove (i) and (ii); the proof of (iii) is symmetric. In (i), the old vertices contribute

$$\sum_{z\in V(G)} d_{G^+}(z, x_2) = \sum_{z\in V(G)} (d_G(z, a) + 2) = A(G, ab) + 2N$$

and

$$\sum_{z\in V(G)} d_{G^+}(z, x_3) = \sum_{z\in V(G)} (d_G(z, b) + 2) = B(G, ab) + 2N.$$

The four new vertices x_1, x_2, x_3, x_4 have total distance 4 from x_2 and also total distance 4 from x_3. This gives (i).

In (ii), the old vertices contribute

$$\sum_{z\in V(G)} d_{G^+}(z, x_1) = A(G, ab) + N, \qquad \sum_{z\in V(G)} d_{G^+}(z, x_2) = A(G, ab) + 2N.$$

The four new vertices have total distances

$$d(x_1, x_1) + d(x_2, x_1) + d(x_3, x_1) + d(x_4, x_1) = 0 + 1 + 2 + 3 = 6$$

from x_1, and

$$d(x_1, x_2) + d(x_2, x_2) + d(x_3, x_2) + d(x_4, x_2) = 1 + 0 + 1 + 2 = 4$$

from x_2. This gives (ii). □

3.2. Bounds for terminal sums

Lemma 3.4. *Let G_i be an unbranched catacondensed benzenoid with i hexagons and let ab be an oriented terminal edge of G_i. Then,*

$$2i^2 + 6i + 1 \le A(G_i, ab), B(G_i, ab) \le 4i^2 + 4i + 1, \tag{3.3}$$

and

$$4i^2 + 16i - 2 \le D(G_i, ab) \le 8i^2 + 8i + 2. \tag{3.4}$$

Moreover, in a recursive construction of a chain, equality in the upper bound of (3.4) *for all prefixes occurs exactly for the linear chain, and equality in the lower bound of* (3.4) *for all prefixes occurs exactly for the helicene chain.*

Proof. We use induction on i. For $i = 1$, the graph is C_6. For any oriented edge ab of C_6,

$$A(C_6, ab) = B(C_6, ab) = 0 + 1 + 1 + 2 + 2 + 3 = 9.$$

The bounds in (3.3) and (3.4) hold with equality when $i = 1$.

For completeness, and also for the equality discussion, we record the first nontrivial step $i = 2$. Let a second hexagon be attached to C_6, so $N = 6$. If the next terminal edge is the linear edge x_2x_3, then Lemma 3.3 gives

$$A(C_6^+, x_2x_3) = B(C_6^+, x_2x_3) = 9 + 2 \cdot 6 + 4 = 25,$$

and hence

$$D(C_6^+, x_2x_3) = 50 = 8 \cdot 2^2 + 8 \cdot 2 + 2.$$

Thus, the linear choice attains the upper bound for D when $i = 2$. If the next terminal edge is the angular edge x_1x_2, then

$$A(C_6^+, x_1x_2) = 9 + 6 + 6 = 21, \qquad B(C_6^+, x_1x_2) = 9 + 2 \cdot 6 + 4 = 25,$$

and

$$D(C_6^+, x_1x_2) = 46 = 4 \cdot 2^2 + 16 \cdot 2 - 2.$$

The angular edge x_3x_4 gives the symmetric pair of endpoint sums 25 and 21, and again gives $D = 46$. Therefore, the bounds and the two equality patterns are valid at $i = 2$.

Assume that the assertions hold for i. Let $|V(G_i)| = N = 4i + 2$ and attach a new hexagon along the terminal edge ab. There are three possible choices for the next terminal edge.

If the next terminal edge is the linear edge x_2x_3, Lemma 3.3 gives

$$D(G_{i+1}, x_2x_3) = D(G_i, ab) + 4N + 8 = D(G_i, ab) + 16i + 16.$$

By the induction hypothesis,

$$D(G_{i+1}, x_2x_3) \geq 4i^2 + 16i - 2 + 16i + 16 = 4i^2 + 32i + 14,$$

which is larger than

$$4(i + 1)^2 + 16(i + 1) - 2 = 4i^2 + 24i + 18$$

for every $i \geq 1$. Also,

$$D(G_{i+1}, x_2x_3) \leq 8i^2 + 8i + 2 + 16i + 16 = 8(i + 1)^2 + 8(i + 1) + 2.$$

Thus, a linear extension can preserve the upper equality, but it cannot preserve the lower equality. For the separate endpoint sums,

$$A(G_{i+1}, x_2x_3) = A(G_i, ab) + 8i + 8, \qquad B(G_{i+1}, x_2x_3) = B(G_i, ab) + 8i + 8,$$

and the bounds in (3.3) follow immediately from the induction hypothesis.

If the next terminal edge is the angular edge x_1x_2, Lemma 3.3 gives

$$D(G_{i+1}, x_1x_2) = 2A(G_i, ab) + 3N + 10.$$

Using (3.3), we obtain

$$D(G_{i+1}, x_1x_2) \geq 2(2i^2 + 6i + 1) + 3(4i + 2) + 10 = 4(i + 1)^2 + 16(i + 1) - 2,$$

and

$$D(G_{i+1}, x_1x_2) \leq 2(4i^2 + 4i + 1) + 3(4i + 2) + 10 = 8i^2 + 20i + 18 < 8(i + 1)^2 + 8(i + 1) + 2.$$

Thus, an angular extension can preserve the lower equality, but it cannot preserve the upper equality. For the separate endpoint sums, Lemma 3.3 gives

$$A(G_{i+1}, x_1x_2) = A(G_i, ab) + 4i + 8, \qquad B(G_{i+1}, x_1x_2) = A(G_i, ab) + 8i + 8,$$

which again satisfy the two-sided bounds in (3.3). The case of the angular edge x_3x_4 is symmetric, with $B(G_i, ab)$ in place of $A(G_i, ab)$.

It remains to record the equality cases. To have the upper equality for D at every prefix, every extension must be linear; this gives exactly L_n. Indeed, a linear extension preserves the upper equality whenever the previous prefix has the upper equality, while an angular extension gives a value strictly below the upper bound.

For the lower equality, put

$$m_i = 2i^2 + 6i + 1, \qquad q_i = 2i^2 + 10i - 3.$$

Then, $m_i + q_i = 4i^2 + 16i - 2$, the lower bound for $D(G_i, ab)$. If a prefix G_i with terminal edge ab attains this lower bound, then an angular extension through x_1x_2 preserves lower equality if and only if the endpoint a has the smaller endpoint sum, namely $A(G_i, ab) = m_i$. Symmetrically, an angular extension through x_3x_4 preserves lower equality if and only if $B(G_i, ab) = m_i$. A linear extension cannot preserve lower equality, since

$$D(G_{i+1}, x_2x_3) \geq 4i^2 + 32i + 14 = 4(i + 1)^2 + 16(i + 1) - 2 + (8i - 4),$$

and $8i - 4 > 0$ for every $i \geq 1$.

After the first angular extension, the new terminal edge has endpoint sums m_2 and q_2, with $q_2 > m_2$. Inductively, if the current terminal edge has endpoint sums m_i and q_i with $q_i > m_i$, then the angular extension using the endpoint with sum m_i produces new endpoint sums

$$m_i + 4i + 8 = m_{i+1}, \qquad m_i + 8i + 8 = q_{i+1},$$

and therefore preserves lower equality. The angular extension in the opposite direction uses the endpoint with sum $q_i > m_i$ and gives a value of D strictly larger than the lower bound. This gives the inductive criterion for lower equality: at each step one must choose the angular edge determined by the endpoint with the smaller current terminal sum. Geometrically, this is equivalent to making all angular extensions in the same direction. Consequently, lower equality is preserved at every prefix if and only if all angular extensions are made in the same direction. The two possible directions are mirror images, and this construction is exactly the helicene chain H_n. This completes the induction. □

3.3. Completion of the proof for unbranched chains

Proof of Theorem 2.3. Let $F_n \in \mathcal{U}_n$. Choose the natural order $C_1, C_2, \ldots, C_n$ of its hexagons, and let F_i be the subchain induced by the first i hexagons. For $1 \le i \le n-1$, let e_i be the oriented terminal edge of F_i along which C_{i+1} is attached, and put

$$D_i = D(F_i, e_i).$$

By Lemma 3.1, $W_b(C_6) = 15$. Repeated use of Lemma 3.2 gives

$$W_b(F_n) = 15 + \sum_{i=1}^{n-1}(D_i + 3(4i+2) + 6) = 15 + \sum_{i=1}^{n-1}(D_i + 12i + 12). \tag{3.5}$$

By Lemma 3.4,

$$4i^2 + 16i - 2 \le D_i \le 8i^2 + 8i + 2.$$

Substituting the lower bounds into (3.5), we get

$$\begin{aligned} W_b(F_n) &\ge 15 + \sum_{i=1}^{n-1}(4i^2 + 28i + 10) \\ &= \frac{4n^3 + 36n^2 - 10n + 15}{3}. \end{aligned}$$

Similarly, substituting the upper bounds gives

$$\begin{aligned} W_b(F_n) &\le 15 + \sum_{i=1}^{n-1}(8i^2 + 20i + 14) \\ &= \frac{8n^3 + 18n^2 + 16n + 3}{3}. \end{aligned}$$

Equality in the lower bound for $W_b(F_n)$ requires equality in the lower bound for every D_i, and equality in the upper bound for $W_b(F_n)$ requires equality in the upper bound for every D_i. The equality conditions in Lemma 3.4 therefore show that, for $n \ge 3$, the lower bound is attained exactly by the helicene chain H_n, and the upper bound is attained exactly by the linear chain L_n. For $n = 1, 2$, all unbranched catacondensed benzenoids with n hexagons are isomorphic, and the two bounds coincide. This completes the proof. □

4. Proof for polyphenyl hexagonal chains

4.1. Inter-hexagon bi-Wiener contributions

Let $G_n \in \mathcal{P}_n$ have bipartition $V(G_n) = X \cup Y$. For $1 \le i \le n$, write

$$X_i = X \cap V(Q_i), \qquad Y_i = Y \cap V(Q_i).$$

For $1 \le i < j \le n$, define the bi-Wiener contribution of pairs with one endpoint in Q_i and the other endpoint in Q_j by

$$W_b(Q_i, Q_j) = \sum_{u \in X_i,\, v \in Y_j} d_{G_n}(u, v) + \sum_{u \in Y_i,\, v \in X_j} d_{G_n}(u, v).$$

This definition already contains the bipartition restriction: only cross-class pairs are included, and no pair with both endpoints in the same bipartition class is counted. For $1 \leq i < j \leq n$, let t_{ij} be the length of a shortest inter-hexagon route from the attachment vertex of Q_i facing Q_j to the attachment vertex of Q_j facing Q_i, excluding any movement inside the two terminal hexagons Q_i and Q_j. Equivalently, along the unique block chain from Q_i to Q_j, each cut edge contributes 1 and each intermediate hexagon Q_k contributes the shortest internal distance ℓ_k between its two attachment vertices; hence,

$$t_{ij} = (j - i) + \sum_{k=i+1}^{j-1} \ell_k. \tag{4.1}$$

For adjacent hexagons, $t_{i,i+1} = 1$.

Lemma 4.1. *For any two distinct hexagons Q_i and Q_j of G_n with $i < j$,*

$$W_b(Q_i, Q_j) = 18t_{ij} + 54. \tag{4.2}$$

Proof. Let x be the attachment vertex of Q_i facing Q_j, and let y be the attachment vertex of Q_j facing Q_i. Every shortest path from a vertex of Q_i to a vertex of Q_j must leave Q_i through x, follow the unique block chain from Q_i to Q_j, and enter Q_j through y. Inside each intermediate hexagon, a shortest path uses the shorter of the two arcs between its two attachment vertices, whose length is the corresponding ℓ_k. Thus, for $u \in V(Q_i)$ and $v \in V(Q_j)$,

$$d_{G_n}(u, v) = d_{Q_i}(u, x) + t_{ij} + d_{Q_j}(y, v).$$

There are $3 \cdot 3 + 3 \cdot 3 = 18$ cross-class pairs counted in $W_b(Q_i, Q_j)$: the pairs from $X_i \times Y_j$ and the pairs from $Y_i \times X_j$. Hence, the inter-hexagon part contributes $18t_{ij}$.

It remains to calculate the endpoint contribution. In a 6-cycle, the sum of the distances from a fixed vertex to all six vertices is

$$0 + 1 + 1 + 2 + 2 + 3 = 9.$$

Each vertex of Q_i is paired with exactly three vertices of Q_j in the opposite bipartition class, and each vertex of Q_j is paired with exactly three vertices of Q_i in the opposite bipartition class. Thus, the two terminal hexagons contribute

$$3 \sum_{u \in V(Q_i)} d_{Q_i}(u, x) + 3 \sum_{v \in V(Q_j)} d_{Q_j}(y, v) = 3 \cdot 9 + 3 \cdot 9 = 54.$$

This proves (4.2). □

4.2. Summation and extremal polyphenyl chains

Proof of Theorem 2.5. By Lemma 3.1, the contribution of all cross-class vertex pairs lying in the same hexagon is $15n$. By Lemma 4.1, the contribution of all cross-class vertex pairs lying in two distinct hexagons is

$$\sum_{1 \leq i < j \leq n} (18t_{ij} + 54).$$

Thus,

$$W_b(G_n) = 15n + 54\binom{n}{2} + 18 \sum_{1\le i<j\le n} t_{ij}. \tag{4.3}$$

Using (4.1), we get

$$\begin{aligned}\sum_{1\le i<j\le n} t_{ij} &= \sum_{1\le i<j\le n} (j-i) + \sum_{1\le i<j\le n} \sum_{k=i+1}^{j-1} \ell_k \\ &= \sum_{d=1}^{n-1} d(n-d) + \sum_{k=2}^{n-1} \ell_k(k-1)(n-k).\end{aligned}$$

Indeed, ℓ_k appears exactly for those pairs (i, j) with $i < k < j$, and the number of such pairs is $(k-1)(n-k)$. Moreover,

$$\sum_{d=1}^{n-1} d(n-d) = \frac{n(n^2-1)}{6}.$$

Substituting this identity into (4.3) gives

$$\begin{aligned}W_b(G_n) &= 15n + 54\binom{n}{2} + 18 \cdot \frac{n(n^2-1)}{6} + 18\sum_{k=2}^{n-1} \ell_k(k-1)(n-k) \\ &= 3n^3 + 27n^2 - 15n + 18\sum_{k=2}^{n-1} \ell_k(k-1)(n-k),\end{aligned}$$

which proves (2.4).

For $n \ge 3$, every coefficient $(k-1)(n-k)$ is positive and every ℓ_k belongs to $\{1, 2, 3\}$. Therefore, the sum in (2.4) is minimized exactly when every $\ell_k = 1$, and maximized exactly when every $\ell_k = 3$. Hence, O_n is the unique minimizer and P_n is the unique maximizer. Finally,

$$\sum_{k=2}^{n-1} (k-1)(n-k) = \binom{n}{3}.$$

Substituting $\ell_k = 1, 2, 3$ in (2.4) gives

$$\begin{aligned}W_b(\mathsf{O}_n) &= 6n^3 + 18n^2 - 9n, \\ W_b(\mathsf{M}_n) &= 9n^3 + 9n^2 - 3n, \\ W_b(\mathsf{P}_n) &= 12n^3 + 3n.\end{aligned}$$

This proves (2.5) and completes the proof. □

5. Concluding remarks and further problems

Theorems 2.3 and 2.5 give complete extremal results for the bi-Wiener index on two natural classes of bipartite hexagonal-chain graphs. They also show that the extremal behavior depends on the manner in which consecutive hexagons are connected. For unbranched catacondensed benzenoids, the bi-Wiener index is minimized by the helicene chain and maximized by the linear chain. For polyphenyl hexagonal chains, the bi-Wiener index is minimized by the ortho-chain and maximized by the para-chain.

These conclusions emphasize that the bi-Wiener index is sensitive not only to the number of hexagons, but also to the local connection pattern between adjacent hexagons. In particular, the extremal chains for the edge-fused family and for the cut-edge family are governed by different local configurations. This supports the use of the bi-Wiener index as a parity-sensitive complement to the Wiener index in bipartite molecular graph models. The terminal-edge recurrence used in the proof for unbranched catacondensed benzenoids also provides a reusable way to handle other bipartite molecular chains in which new even cycles are added through prescribed attachment edges.

Problem 5.1 (Higher extremal chains)**.** *Determine the second, third, and, more generally, the r-th largest and smallest bi-Wiener indices among all unbranched catacondensed benzenoids in $\mathcal{U}_n$ and all polyphenyl hexagonal chains in $\mathcal{P}_n$. Characterize all chains attaining these values.*

Problem 5.2 (Random chains)**.** *Consider random unbranched catacondensed benzenoids in which the α-, β-, and γ-types occur with fixed probabilities, and random polyphenyl hexagonal chains in which the ortho-, meta-, and para-configurations occur with fixed probabilities. Determine the expectation, variance, and limiting distribution of the bi-Wiener index.*

Problem 5.3 (Broader bipartite molecular block chains)**.** *Extend the terminal-edge recurrence method to broader bipartite molecular block chains, for example, catacondensed benzenoids with branching or cactus chains whose blocks are even cycles of different lengths. Determine which local attachment configurations force the minimum and maximum bi-Wiener indices in these larger graph classes.*

Use of Generative-AI tools declaration

The author declares that no artificial intelligence (AI) tools were used in the creation of this article.

Conflict of interest

The author declares no conflict of interest.

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