Fully Angular Hexagonal Chains Extremal with regard to the Largest Eigenvalue*

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Abstract

Let G be a molecular graph with characteristic polynomial $\phi(G,x)$ its . The leading eigenvalue of G is the largest root of the equation $\phi(G,x) = 0$. In this paper, the hexagonal chain (unbranched catacondensed benzenoids molecule) with minimum leading eigenvalue among fully angular hexagonal chains having a given number of hexagons is determined.

Keywords : fully angular hexagonal chain, zig-zag hexagonal chain, eigenvalue.

AMS 2000 MSC : 05C10, 05C70, 05C90

1 Introduction

A *hexagonal system* is a 2-connected plane graph whose interior faces are regular hexagons. Hexagonal systems are very attractive for graph-theoretical studies and are of great importance to theoretical chemistry because they are the natural graph representations of benzenoid hydrocarbons. Much research in mathematical chemistry has been devoted to hexagonal systems and benzenoid hydrocarbons [1–4].

A *hexagonal chain* is a hexagonal system with the properties that (a) no vertex is incident with three hexagons, and (b) no hexagon is adjacent to more than two hexagons. Suppose H is a hexagonal system. Denote by H_C the graph whose vertex set is the set of the centers of hexagons in H, and edge set is the set of lines connecting the centers of any two adjacent hexagons. A hexagonal system H is a hexagonal chain if the graph H_C is a path. In this paper, we consider both geometrically planar and non-planar (helicenic) hexagonal chains. This means that H_C may be a helix. Hexagonal chains are the graph representations of an important subclass of benzenoid

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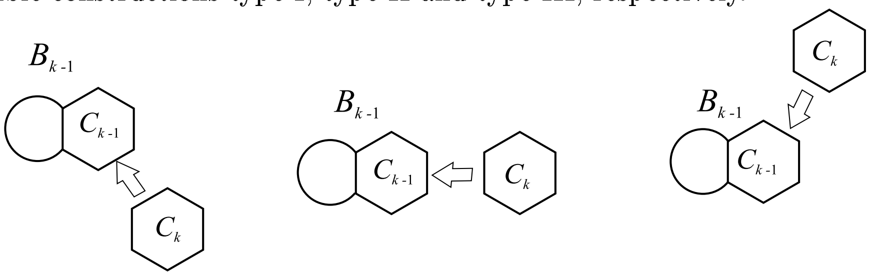
molecules, unbranched catacondensed benzenoids molecules, which play a distinguished role in the theoretical chemistry of benzenoid hydrocarbons. The extremal graphs with respect to some useful topological indices in chemical applications have been extensively studied, and many results concerning this topic can be found in [5–15].

Put $\mathscr{B}_n = \{B_n \mid B_n \text{ is a hexagonal chain with } n \text{ hexagons}\}$. We write $B_n = C_1C_2\cdots C_n$ if $C_1, C_2, \ldots, C_n$ are the n hexagons of B_n, where C_i and C_{i+1} are adjacent for $i = 1, 2, \ldots, n-1$. A hexagonal chain B_n, where $n \geq 3$, can be obtained from a hexagon by a stepwise addition of terminal hexagons. At each step $k = 2, 3, \ldots, n$, a type of addition is selected from the three possible constructions $B_{k-1} \to B_k^{(i)} := B_k$, for $i = 1, 2$ or 3, as depicts in Figure 1. We shall call the three possible constructions type I, type II and type III, respectively.

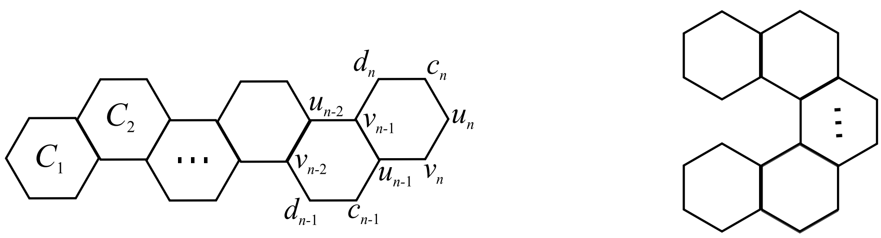


$B_k^{(1)}$ $B_k^{(2)}$ $B_k^{(3)}$

Figure 1.

A hexagonal chain B_n is said to be *linear* if each mode of attachment of the hexagons is realized with type II construction. A hexagonal chain B_n is *fully angular* if each mode of attachment of the hexagons is realized with either a type I construction or a type III construction. A fully angular hexagonal chain with n hexagons is called a *zig-zag hexagonal chain*, denoted by Z_n, if each mode of attachment of the hexagons is realized alternately with a type I construction and a type III construction. It is called a *helicene hexagonal chain*, denoted by H_n, if all mode of attachment of the hexagons is realized with type I, or symmetrically, type III constructions. The two special fully angular hexagonal chains are illustrated in Figure 2.

Denote by $\mathscr{A}_n$ the set of fully angular hexagonal chains with n hexagons. Note that for $n = 1$ or 2, $\mathscr{B}_n = \mathscr{A}_n$, and both sets contain exactly one element. So in the following, we always suppose that $n \geq 3$.



(a) Z_n (b) H_n

Figure 2.

Some topological indices of the fully angular hexagonal chains depend only on the number of hexagons. For example, fully angular hexagonal chains with equal number of hexagons have equal K-values [16–18], where K is the number of Kekule structures (perfect matchings). Recently, Dobrynin and Gutman [11] demonstrated the following property of fully angular hexagonal chains with the same number of hexagons: the sum of their Wiener indices is divisible by the number of chains.

The two special fully angular hexagonal chains Z_n and H_n have many extremal properties with respect to topological indices. In the class $\mathscr{B}_n$, Z_n has maximal Hosoya index (i.e., the numbers of matchings), minimal Merrifield-Simmons index (i.e., the number of independence sets) [6] and maximal total π-energy [10], and H_n has maximal largest eigenvalue [7]. Furthermore, Z_n has maximal number of k-matchings and minimal number of k-independence sets, for each $k = 1, 2, \ldots$ [12]. Moreover, Shiu, Lam and Zhang [15] proved that $H_n \in \mathscr{A}_n$ has minimal Hosoya index and maximal Merrifield-Simmons index. In this paper, we shall determine the extremal chains of $\mathscr{A}_n$ with respect to the *leading* or the largest eigenvalue. We shall show that Z_n has the minimum leading eigenvalues among all hexagonal chains in $\mathscr{A}_n$.

2 Preliminary Results

The leading eigenvalue of molecular graphs is one of the useful topological indices in chemical applications. Denote the characteristic polynomial of a graph G by $\phi(G) = \phi(G, x)$ and recall that the leading eigenvalue of G, denoted by $\lambda_1(G)$, is the largest root of the equation $\phi(G) = 0$. The leading eigenvalue is an important molecular structure-descriptor. Cvetković and Gutman [19] claimed that $\lambda_1(G)$ is a measure of branching of the molecular graph. Recently, Gutman and Vidović [20] showed some relationship between $\lambda_1(G)$ and χ, the connectivity index (or branching index) of a molecular graph [21]. More information and references about the leading eigenvalue can be found in [20]. It was known that $\lambda_1(G) \geq 1$ [22, Theorem 0.13].

The following properties of $\phi(G)$ will be useful [22, 23].

Claim 2.1. *Let G be a graph consisting of two components G_1 and G_2. Then*

$$\phi(G) = \phi(G_1)\phi(G_2). \tag{1}$$

Claim 2.2. *Let $e = uv$ be an edge of G. Then*

(a) $\phi(G) = \phi(G - uv) - \phi(G - u - v) - 2\sum_j \phi(G - W_j^G)$, (2)
where the summation runs over all cycles W_j^G containing the edge e.

(b) $\phi(G) = x\phi(G - u) - \phi(G - u - v) - \sum_i \phi(G - u - w_i^G) - 2\sum_j \phi(G - W_j^G)$, (3)
where the first summation runs over all the vertices w_i^G which are adjacent to u, but different from v; and the second summation runs over all cycles W_j^G containing the vertex u.

If the edge $e = uv$ does not belong to any cycle, then the summation on the right-hand side of (2) will vanish and

$$\phi(G) = \phi(G - uv) - \phi(G - u - v). \tag{4}$$

Similarly, if v is the unique neighbor of u, then (3) becomes

$$\phi(G) = x\phi(G - u) - \phi(G - u - v). \tag{5}$$

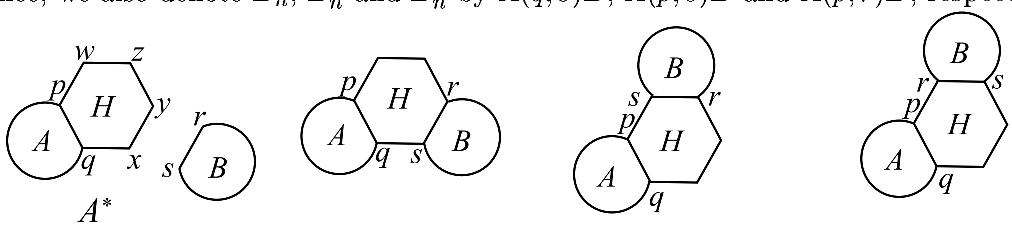
Claim 2.3 [5]. *Let F, H be two graphs and let $\Delta(F, H, x) = \phi(F, x) - \phi(H, x)$. If for $x = \lambda_1(H)$, $\Delta(F, H, x) < 0$, then $\lambda_1(F) > \lambda_1(H)$.*

According to a well-known result of graph-spectral theory [22], the leading eigenvalue of a connected graph is (strictly) greater than the leading eigenvalue of any of its proper subgraphs. Note that $\phi(G) > 0$ for all $x > \lambda_1(G)$. Applying of formula (3), we obtain:

Claim 2.4. *Let H be a subgraph of G and uv an edge of H. If v is not the unique neighbor of u, then for $x = \lambda_1(G)$,*

$$\phi(H) - x\phi(H - u) + \phi(H - u - v) < 0. \tag{6}$$

Suppose that A^* and B are two fully angular hexagonal chains with i and $n - i$ hexagons, respectively. Denote by A the hexagonal chains induced by the former $i - 1$ hexagons of A^*. Some relevant vertices of A^* and B are labelled as indicated in Fig 3(a). Denote by B_n, B'_n and B''_n the hexagonal chains with n hexagons obtained from A^* and B by identifying the vertices s and x with two out of four vertices x, y, w and z as in Figures 3(b), 3(c) and 3(d), respectively. For convenience, we also denote B_n, B'_n and B''_n by $A(q, s)B$, $A(p, s)B$ and $A(p, r)B$, respectively.



(a) A^* and B (b) $B_n = A(q, s)B$ (c) $B'_n = A(p, s)B$ (d) $B''_n = A(p, r)B$

Figure 3.

Lemma 2.1 *Let B_n, B'_n and B''_n be three fully angular hexagonal chains.*

(a) If for $x = \lambda_1(B_n)$, $\phi(A - p) < \phi(A - q)$ and $\phi(B - r) \geq \phi(B - s)$, then $\lambda_1(B_n) > \lambda_1(B'_n)$.

(b) If for $x = \lambda_1(B_n)$, $\phi(A - p) < \phi(A - q)$ and $\phi(B - r) \leq \phi(B - s)$, then $\lambda_1(B_n) > \lambda_1(B''_n)$.

Proof: (a) By Claim 2.3, it suffices to show that for $x = \lambda_1(B_n)$,

$$\Delta(B_n, B'_n, x) = \phi(B_n) - \phi(B'_n) < 0.$$

Applying (2) to B_n' and B_n, we get

$$\phi(B_n) = \phi(B_n - qs) - \phi(B_n - q - s) - 2\sum_j \phi(B_n - W_j^{B_n}),$$

$$\phi(B_n') = \phi(B_n' - ps) - \phi(B_n' - p - s) - 2\sum_j \phi(B_n' - W_j^{B_n'}).$$

Similar to the proof in [5], we have $\phi(B_n - W_j^{B_n}) \equiv \phi(B_n' - W_j^{B_n'})$ for all values of j. Therefore

$$\Delta(B_n, B_n', x) = \phi(B_n - qs) - \phi(B_n - q - s) - \phi(B_n' - ps) + \phi(B_n' - p - s).$$

A repeated application of (1), (4) and (5) yields

$$\phi(B_n - qs) = \{x\phi(A) - \phi(A - p)\}\{x\phi(B) - \phi(B - r)\} - \phi(A)\phi(B), \tag{7}$$

$$\begin{aligned}\phi(B_n - q - s) = {} & \{x\phi(A - q) - \phi(A - p - q)\}\{x\phi(B - s) - \phi(B - s - r)\} \\ & - \phi(A - q)\phi(B - s),\end{aligned} \tag{8}$$

$$\phi(B_n' - ps) = \{x\phi(A) - \phi(A - q)\}\{x\phi(B) - \phi(B - r)\} - \phi(A)\phi(B), \tag{9}$$

and

$$\begin{aligned}\phi(B_n' - p - s) = {} & \{x\phi(A - p) - \phi(A - p - q)\}\{x\phi(B - s) - \phi(B - r - s)\} \\ & - \phi(A - p)\phi(B - s).\end{aligned} \tag{10}$$

By (7)–(10), $\Delta(B_n, B_n', x)$ may be simplified to

$$\begin{aligned}\Delta(B_n, B_n', x) \quad = \quad & \{x\phi(B) - x^2\phi(B - s) - \phi(B - r) + \phi(B - s) + x\phi(B - r - s)\} \\ & \{\phi(A - q) - \phi(A - p)\}.\end{aligned}$$

Note that $\lambda_1(B_n) \geq 1$. For $x = \lambda_1(B_n)$, by the hypotheses of (a) we have

$$\Delta(B_n, B_n', x) \leq x\{\phi(B) - x\phi(B - s) + \phi(B - r - s)\}\{\phi(A - q) - \phi(A - p)\}.$$

By (6) we have that $\Delta(B_n, B_n', x) < 0$.

(b) By Claim 2.3, we only need to show that for $x = \lambda_1(B_n)$,

$$\Delta(B_n, B_n'', x) = \phi(B_n) - \phi(B_n'') < 0.$$

Similarly, we have

$$\Delta(B_n, B_n'', x) = \phi(B_n - qs) - \phi(B_n - q - s) - \phi(B_n'' - pr) + \phi(B_n'' - p - r).$$

A repeated application of (1), (4) and (5) yields

$$\phi(B_n'' - pr) = \{x\phi(A) - \phi(A - q)\}\{x\phi(B) - \phi(B - s)\} - \phi(A)\phi(B) \tag{11}$$

and

$$\phi(B''_n - p - r) = \{x\phi(A-p) - \phi(A-p-q)\}\{x\phi(B-r) - \phi(B-r-s)\} \\ - \phi(A-p)\phi(B-r). \tag{12}$$

Therefore by (9)-(12), $\Delta(B_n, B''_n, x)$ is simplified to

$$\begin{aligned}\Delta(B_n, B''_n, x) &= x\{\phi(A) - x\phi(A-q) + \phi(A-p-q)\}\{\phi(B-r) - \phi(B-s)\} \\ &\quad + x\{\phi(B) - x\phi(B-r) + \phi(B-r-s)\}\{\phi(A-q) - \phi(A-p)\}.\end{aligned}$$

By (6) and the hypotheses of (b), we have that for $x = \lambda_1(B_n)$, $\Delta(B_n, B''_n, x) < 0$. □

3 Main Result and its Proof

Suppose $C_1, C_2, \ldots, C_n$ are n hexagons of the hexagonal chain Z_n. For $k \leq n$, we also write $Z_k = C_1C_2\cdots C_k$. We label the common edge of C_1 and C_2 as v_1u_1; and for each k, $2 \leq k \leq n$, we label the vertices of $V(C_k)\setminus V(C_{k-1})$ as v_k, u_k, c_k and d_k such that $u_{k-1}v_k, v_ku_k, u_kc_k, c_kd_k$ and d_kv_{k-1} are edges in Z_n (see Figure 2(a)).

Lemma 3.1 *Let $B_n = C_1C_2\cdots C_n$ be a hexagonal chain and $Z_k = C_1C_2\cdots C_k$ be a zig-zag hexagonal sub-chain of B_n. Then for $x = \lambda_1(B_n)$, $\phi(Z_1 - v_1) = \phi(Z_1 - u_1)$ and $\phi(Z_i - v_i) > \phi(Z_i - u_i)$, $2 \leq i \leq k$.*

Proof: Obviously, $\phi(Z_1 - v_1) = \phi(Z_1 - u_1)$ for $x = \lambda_1(B_n)$. Now we suppose that $k \geq 2$. Applying (5) to $Z_k - v_k$ and $Z_k - u_k$, we get

$$\begin{aligned}\phi(Z_k - v_k) &= x\phi(Z_k - v_k - u_k) - \phi(Z_k - v_k - u_k - c_k) \\ &= x\{x\phi(Z_k - v_k - u_k - c_k) - \phi(Z_{k-1})\} \\ &\quad -\{x\phi(Z_{k-1}) - \phi(Z_{k-1} - v_{k-1})\} \\ &= x^2\{x\phi(Z_{k-1}) - \phi(Z_{k-1} - v_{k-1})\} - 2x\phi(Z_{k-1}) + \phi(Z_{k-1} - v_{k-1}) \\ &= (x^3 - 2x)\phi(Z_{k-1}) + (1 - x^2)\phi(Z_{k-1} - v_{k-1})\end{aligned}$$

and

$$\begin{aligned}\phi(Z_k - u_k) &= x\phi(Z_k - u_k - c_k) - \phi(Z_k - u_k - c_k - d_k) \\ &= x\{x\phi(Z_k - u_k - c_k - v_k) - \phi(Z_k - u_k - c_k - v_k - u_{k-1})\} \\ &\quad -\{x\phi(Z_{k-1}) - \phi(Z_{k-1} - u_{k-1})\} \\ &= x^2\{x\phi(Z_{k-1}) - \phi(Z_{k-1} - v_{k-1})\} - x\phi(Z_k - u_k - c_k - v_k - u_{k-1}) \\ &\quad -x\phi(Z_{k-1}) + \phi(Z_{k-1} - u_{k-1}),\end{aligned}$$

respectively. Note that $Z_k - u_k - c_k - v_k - u_{k-1}$ is isomorphic to $Z_{k-1} - c_{k-1}u_{k-1}$. (When $k = 2$, c_0 is the vertex adjacent to u_1 in Z_1 with $c_0 \neq v_1$).

Applying (5) to $Z_{k-1} - c_{k-1}u_{k-1}$, we get

$$\phi(Z_{k-1} - c_{k-1}u_{k-1}) = x\phi(Z_{k-1} - u_{k-1}) - \phi(Z_{k-1} - v_{k-1} - u_{k-1}).$$

Therefore

$$\begin{aligned}\phi(Z_k - v_k) - \phi(Z_k - u_k) &= \{\phi(Z_{k-1} - v_{k-1}) - \phi(Z_{k-1} - u_{k-1})\} \\ &\quad -x\{\phi(Z_{k-1}) - x\phi(Z_{k-1} - u_{k-1}) \\ &\quad +\phi(Z_{k-1} - v_{k-1} - u_{k-1})\}.\end{aligned}$$

Note that $\lambda_1(B_n) \geq 1$. By Claim 2.4, we get that for $x = \lambda_1(B_n)$,

$$\phi(Z_k - v_k) - \phi(Z_k - u_k) > \phi(Z_{k-1} - v_{k-1}) - \phi(Z_{k-1} - u_{k-1}).$$

Since $x = \lambda_1(B_n)$, $\phi(Z_1 - v_1) - \phi(Z_1 - u_1) = 0$. Consequently $\phi(Z_i - v_i) > \phi(Z_i - u_i)$ for $2 \leq i \leq k$. $\square$

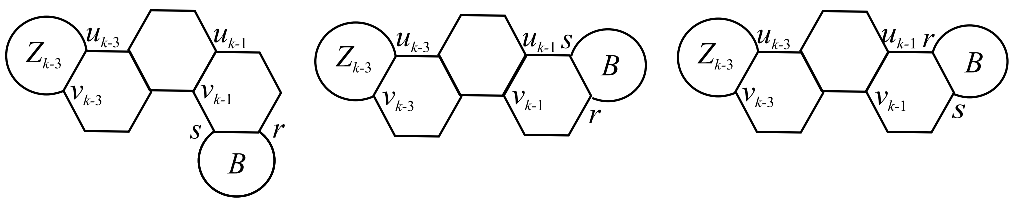
Theorem 3.2 *For $n \geq 1$ and $B_n \in \mathscr{A}_n$, if $B_n \neq Z_n$, then $\lambda_1(Z_n) < \lambda_1(B_n)$.*

Proof: Let $A_n = C_1C_2 \cdots C_n \in \mathscr{A}_n$ such that for any $B_n \in \mathscr{A}_n$, $\lambda_1(A_n) \leq \lambda_1(B_n)$. We will show that $A_n = Z_n$. Since $\mathscr{A}_1 = \{Z_1\}, \mathscr{A}_2 = \{Z_2\}$ and $\mathscr{A}_3 = \{Z_3\}$, we assume that $n \geq 4$.

Assume that $A_n \neq Z_n$. Then there must be a k with $3 \leq k \leq n-1$ such that the hexagonal sub-chain $C_1C_2 \cdots C_k$ of A_n is a zig-zag hexagonal chain and the hexagonal sub-chain $C_1C_2 \cdots C_kC_{k+1}$ is not a zig-zag hexagonal chain.

Set $A = Z_{k-1} = C_1C_2 \cdots C_{k-1}$, $p = u_{k-1}$, $q = v_{k-1}$, $B = C_{k+1}C_{k+2} \cdots C_n$ and $A_n = A(q, s)B$ illustrated in Figure 4.

By Lemma 3.1, for $x = \lambda_1(A_n)$, we have $\phi(A - p) < \phi(A - q)$. If $\phi(B - r) \geq \phi(B - s)$, then by Lemma 2.1(a) we have that $\lambda_1(A_n) > \lambda_1(B'_n)$, where $B'_n = A(p, s)B$. This contradicts the minimality of $\lambda_1(A_n)$. If $\phi(B-r) \leq \phi(B-s)$, then by Lemma 2.1(b) we have that $\lambda_1(A_n) > \lambda_1(B''_n)$, where $B''_n = A(p, r)B$. This also contradicts the minimality of $\lambda_1(A_n)$ again. So $A_n = Z_n$. $\square$



(a) A_n (b) $Z_{k-1}(u_{k-1}, s)B$ (c) $Z_{k-1}(u_{k-1}, r)B$

Figure 4.

4 Remark

The degree of any vertex of a hexagonal chain B_n ie either 2 or 3. Denote $V_2 = V_2(B_n)$ and $V_3 = V_3(B_n)$ the sets of the vertices in G with degrees 2 and 3, respectively. The subgraphs of B_n induced by V_2 and V_3 are denoted by $B_n[V_2]$ and $B_n[V_3]$, respectively. Note that for any hexagonal chain B_n, the induced subgraph $B_n[V_3]$ has a perfect matching, consisting of the common edges of any two adjacent hexagons in B_n.

A hexagonal chain B_n is fully angular if and only if $B_n[V_3]$ is a tree (i.e., connected acyclic graph) with a perfect matching. A hexagonal chain B_n is a zig-zag or helicenic if and only if $B_n[V_3]$ is a path or a comb obtained by adding a pendant edge to each vertex of the path of order $\frac{n}{2}$, respectively. It is well known that paths and combs possess many extremal properties in the sets of trees with a perfect matching. For instance, among order n trees with perfect matchings, a path has the maximal total π-electron energy $E(T)$ [24]. Moreover, among order n trees with perfect matchings and maximum degree 3; the comb has the minimal total π-electron energy.

On the other hand, from known results and the result of this paper, we can see that Z_n and H_n, having as subgraphs induced by V_3 a path and a comb respectively, also play extremal role in $\mathscr{A}_n$ and $\mathscr{B}_n$, respectively. It will be of interest if there is some inherent connection between the two.

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