Extremal hexagonal chains

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Dedicated to Frank Harary, teacher, inspirer and friend, pioneer, champion and proprietor of graph theory, on the occasion of his 70th birthday.

Some extremal properties of the linear chain L_h of h hexagons are pointed out. In the class of all hexagonal chains with h hexagons, L_h has minimum K, Z and x_1 values, as well as maximum W and σ values; K = number of perfect matchings, Z = number of independent edge sets (Hosoya index), x_1 = largest graph eigenvalue, W = Wiener index, σ = number of independent vertex sets (Merrifield–Simmons index). The extremality of L_h with respect to Z, σ and x_1 is demonstrated here for the first time.

1. Introduction

Frank Harary was the first to realize that hexagonal systems (or, as he named them: "hexagonal animals") are very attractive objectives for graph-theoretical studies and the first to initiate their serious mathematical investigations [1,2]*. In a seminal paper [3], Harary and Harborth examined extremal hexagonal (and other) systems, e.g. systems which for a given number of hexagons have as few as possible or as many as possible vertices.

In this work, we report some results on extremal hexagonal chains. A hexagonal chain is a hexagonal system with the properties that (a) it has no vertex belonging to three hexagons, and (b) it has no hexagon with more than two adjacent hexagons. The ten distinct hexagonal chains with five hexagons are depicted in fig. 1.

Hexagonal chains are extremal in the Harary–Harborth sense: they possess a maximum number of vertices and a maximum number of edges for a given number of hexagons.

Hexagonal systems are of great importance for theoretical chemistry because they are the natural graph representations of benzenoid hydrocarbons [4]. A considerable amount of research in mathematical chemistry has been devoted to

*The prize of "$100 in United States currency" offered by Harary [2] for the enumeration of hexagonal (and other) animals has not yet been collected.

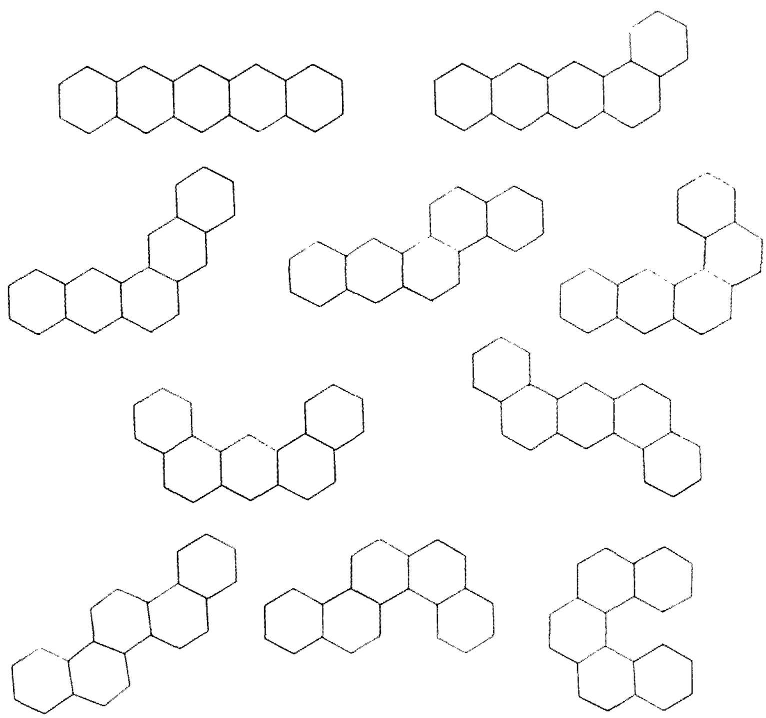


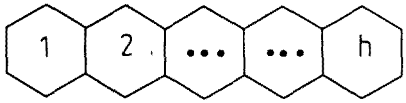
Fig. 1.

hexagonal systems/benzenoid hydrocarbons [4–6]. Hexagonal chains are the graph representations of an important subclass of benzenoid molecules, namely of the so-called unbranched catacondensed benzenoids. The structure of these graphs is apparently the simplest among all hexagonal systems. Therefore, it is not surprising that a great deal of mathematical and mathematico-chemical results known in the theory of hexagonal systems apply, in fact, only to hexagonal chains [4–6]. In particular, the enumeration of hexagonal chains was accomplished by Balaban and Harary [2,7].

The following notation and terminology willl be used throughout this paper. First of all, in full harmony with Harary's original definition of a hexagonal animal (see, in particular, refs. [7,8]), the hexagonal chains considered by us include both geometrically planar and geometrically non-planar (helicenic) species.

The number of hexagons in a hexagonal chain C is denoted by h. All hexagonal chains with h hexagons have $4h + 2$ vertices and $5h + 1$ edges [4]. The set of all hexagonal chains with h hexagons will be denoted by $\mathcal{C}_h$. For example, the elements of $\mathcal{C}_5$ are just the ten graphs depicted in fig. 1.

The chain whose h hexagons are arranged in a linear manner is denoted by L_h; the respective benzenoid hydrocarbons form the linear polyacene homologous series (benzene, naphthalene, anthracene, naphthacene, pentacene, . . .). Observe that $\mathcal{C}_1 = \{L_1\}$ and $\mathcal{C}_2 = \{L_2\}$.



L_h

The aim of this paper is to point out a few extremal properties of the systems L_h. As a matter of fact, at least two such results are already known. We formulate them in theorems 1 and 2.

THEOREM 1 [9, 10]

Denote by $K(G)$ the number of perfect matchings of the graph G. Then for all $C \in \mathcal{C}_h$ and for all $h \geq 1$,

$$K(L_h) \leq K(C)$$

with equality holding only if $C = L_h$. Furthermore, $K(L_h) = h + 1$.

THEOREM 2 [11]

Denote by $W(G)$ the Wiener index (= sum of the distances of all pairs of vertices) of the graph G. Then for all $C \in \mathcal{C}_h$ and for all $h \geq 1$,

$$W(L_h) \geq W(C)$$

with equality holding only if $C = L_h$. Furthermore, $W(L_h) = \frac{1}{3}(16h^3 + 36h^2 + 26h + 3)$.

2. The main results

In this paper, we offer three more results on extremal properties of L_h, summarized in theorems 3–5.

THEOREM 3

Denote by $Z(G)$ the number of independent edge sets of the graph G (= the Hosoya index). Then for all $C \in \mathcal{C}_h$ and for all $h \geq 1$,

$$Z(L_h) \leq Z(C)$$

with equality holding only if $C = L_h$.

THEOREM 4

Denote by $\sigma(G)$ the number of independent vertex sets of the graph G (= the Merrifield–Simmons index). Then for all $C \in \mathcal{C}_h$ and for all $h \geq 1$,

$$\sigma(L_h) \geq \sigma(C)$$

with equality holding only if $C = L_h$.

THEOREM 5

Denote by $x_1(G)$ the largest eigenvalue of the graph G. Then for all $C \in \mathcal{C}_h$ and for all $h \geq 1$,

$$x_1(L_h) \leq x_1(C)$$

with equality holding only if $C = L_h$.

3. Proof of theorem 3

Two edges of a graph G are said to be independent if they are not incident. Let $E(G)$ be the edge set of G. Any subset of $E(G)$ containing no two mutually incident edges is called an independent edge set. The total number of independent edge sets of G is denoted by $Z(G)$. In 1971, Hosoya [12] proposed this graph-theoretical invariant for quantifying certain structural features of organic molecules. Since then, numerous studies of Z have been undertaken (see, for example, ref. [13], pp. 127–134); Z is nowadays commonly called "the Hosoya index".

The Hosoya index conforms to the following two basic recurrence relations [12,13]:

$$Z(G) = Z(G-e) + Z(G-u-v), \tag{1}$$

where e denotes an edge of the graph G, connecting the vertices u and v, and

$$Z(G_1 \cup G_2) = Z(G_1)Z(G_2), \tag{2}$$

where $G_1 \cup G_2$ denotes the graph composed of disconnected components G_1 and G_2. An immediate consequence of (1) is [12]

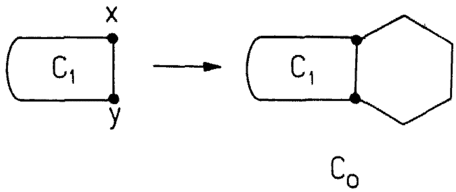
$$Z(G) = Z(G-u) + Z(G-u-v) + \sum_i Z(G-u-w_i^G) \tag{3}$$

with the right-hand side summation going over all vertices w_i^G of the graph G, which are adjacent to u, but which differ from the vertex v. Consequently,

$$Z(G) - Z(G-u) - Z(G-u-v) \geq 0 \tag{4}$$

with equality only if v is the unique neighbor of u.

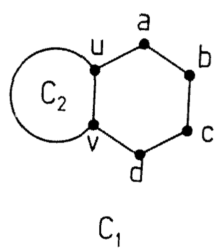
Any element C_0 of $\mathcal{C}_h$ can be obtained from an appropriately chosen graph $C_1 \in \mathcal{C}_{h-1}$ by attaching to it a new hexagon:



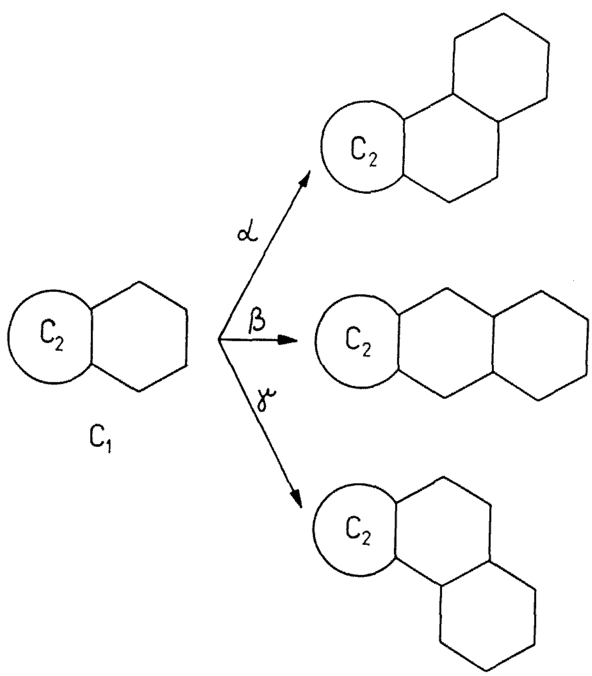
Using formulas (1) and (2), we easily deduce

$$Z(C_0) = 5Z(C_1) + 3[Z(C_1 - x) + Z(C_1 - y)] + 2Z(C_1 - x - y). \tag{5}$$

The relevant features of the structure of the graph C_1 are represented by the diagram below, in which $C_2 \in \mathcal{C}_{h-2}$.



Accordingly, the construction $C_1 \to C_0$ can be realized in three different ways, denoted by α, β and γ.



Note that in the case α, $x \equiv a$, $y \equiv b$, in the case β, $x \equiv b$, $y \equiv c$, whereas in the case γ, $x \equiv c$, $y \equiv d$. A repeated annelation of mode β produces a linear system, whereas the result of the modes α and γ are angularly annelated chains.

Application of relations (1) and (2) straightforwardly leads to

$$[Z(C_1 - x) + Z(C_1 - y)]_\alpha$$
$$= 5Z(C_2) + 2Z(C_2 - u) + 3Z(C_2 - v) + Z(C_2 - u - v), \tag{6a}$$

$$[Z(C_1 - x) + Z(C_1 - y)]_\beta$$
$$= 4Z(C_2) + 3Z(C_2 - u) + 3Z(C_2 - v) + 2Z(C_2 - u - v), \tag{6b}$$

$$[Z(C_1 - x) + Z(C_1 - y)]_\gamma$$
$$= 5Z(C_2) + 3Z(C_2 - u) + 2Z(C_2 - v) + Z(C_2 - u - v) \tag{6c}$$

and

$$[Z(C_1 - x - y)]_\alpha = 2Z(C_2) + Z(C_1 - v), \tag{7a}$$

$$[Z(C_1 - x - y)]_\beta = Z(C_2) + Z(C_2 - u) + Z(C_2 - v) + Z(C_2 - u - v), \tag{7b}$$

$$[Z(C_1 - x - y)]_\alpha = 2Z(C_2) + Z(C_2 - u). \tag{7c}$$

The subscripts in the left-hand side terms in eqs. (6) and (7) indicate the respective annelation modes.

We now verify that

$$[Z(C_0)]_\alpha > [Z(C_0)]_\beta, \tag{8}$$

$$[Z(C_0)]_\gamma > [Z(C_0)]_\beta. \tag{9}$$

Bearing eq. (5) in mind, for the proof of (8) it is sufficient to demonstrate the simultaneous validity of

$$[Z(C_2 - x) + Z(C_1 - y)]_\alpha > [Z(C_1 - x) + Z(C_1 - y)]_\beta \tag{10}$$

and

$$[Z(C_1 - x - y)]_\alpha > [Z(C_1 - x - y)]_\beta. \tag{11}$$

Indeed, by comparing (6a) with (6b) and (7a) with (7b), we arrive at

$$[Z(C_1 - x) + Z(C_1 - y)]_\alpha$$
$$= [Z(C_1 - x) + Z(C_1 - y)]_\beta + Z(C_2) - Z(C_2 - u) - Z(C_2 - u - v)$$

and

$$[Z(C_1 - x - y)]_\alpha = [Z(C_1 - x - y)]_\beta + Z(C_2) - Z(C_2 - u) - Z(C_2 - u - v).$$

On the other hand, the fact that the expression $Z(C_2) - Z(C_2 - u) - Z(C_2 - u - v)$ is strictly positive is a special case of the inequality (4). This implies (10) and (11), and the inequality (8) follows.

The inequality (9) can be deduced in a fully analogous manner.

The relations (8) and (9) mean that linear annelation of a hexagon always results in a hexagonal chain having a smaller Hosoya index than the respective chain obtained by angular annelation. Evidently, L_h is the unique hexagonal chain (β). Theorem 3 follows. □

We mention in passing that [14]

$$Z(L_h) = v_1(t_1)^h + v_2(t_2)^h + v_2(t_3)^h,$$

where

$$t_1 = 3 + (80/3)^{1/2} \cos\lambda,$$

$$t_2 = 3 + (80/3)^{1/2} \cos(\lambda - 2\pi/3),$$

$$t_3 = 3 + (80/3)^{1/2} \cos(\lambda + 2\pi/3),$$

$$v_1 = [148 - 18(t_2 + t_3) + 2t_2t_3]/[(t_1 - t_2)(t_1 - t_3)],$$

$$v_2 = [148 - 18(t_3 + t_1) + 2t_3t_1]/[(t_2 - t_3)(t_2 - t_1)],$$

$$v_3 = [148 - 18(t_1 + t_2) + 2t_1t_2]/[(t_3 - t_1)(t_3 - t_2)]$$

and

$$\lambda = (1/3)\arccos[(7803/8000)^{1/2}].$$

4. Proof of theorem 4

Two vertices in a graph G are said to be independent if they are not adjacent. Let $V(G)$ be the vertex set of G. Any subset of $V(G)$ containing no two mutually adjacent vertices is called an independent vertex set. The total number of independent vertex sets of G is denoted by $\sigma(G)$.

Merrifield and Simmons recently developed a topological approach to structural chemistry [15,16]. The cardinality of the topological space in their theory turns out to be equal to the number of independent vertex sets of the respective molecular graph [15,16]. Because the same authors also established the basic mathematical properties of the graph invariant $\sigma(G)$ [16,17], we find it justified to name this quantity the "Merrifield–Simmons index".

The Merrifield–Simmons and the Hosoya indices conform to similar, but not identical recurrence relations. Thus, in analogy to eq. (1) one has [16]

$$\sigma(G) = \sigma(G - u) + \sigma(G - N_u), \tag{12}$$

where N_u is the subset of the vertex set $V(G)$, which contains the vertex u and its first neighbors. The formula analogous to eq. (2) reads

$$\sigma(G_1 \cup G_2) = \sigma(G_1)\sigma(G_2). \tag{13}$$

Our proof of theorem 4 follows a similar pattern of reasoning as the proof of theorem 3, and will be outlined in an abbreviated form.

If u and v are adjacent vertices of the graph G then, evidently, $\sigma(G - N_u) \le \sigma(G - u - v)$. From eq. (12), we therefore deduce

$$\sigma(G) - \sigma(G - u) - \sigma(G - u - v) \le 0 \tag{14}$$

with equality only if v is the unique neighbor of u. This relation should be compared with (4).

Using eqs. (12) and (13) and by adopting the same notation as in the previous section, we arrive at

$$\sigma(C_0) = 3\sigma(C_1) + 2[\sigma(C_1 - x) + \sigma(C_1 - y)] + \sigma(C_1 - x - y), \tag{15}$$

as well as

$$[\sigma(C_1 - x) + \sigma(C_1 - y)]_\alpha$$
$$= 5\sigma(C_2) + 2\sigma(C_2 - u) + 3\sigma(C_2 - v) + \sigma(C_2 - u - v), \tag{16a}$$

$$[\sigma(C_1 - x) + \sigma(C_1 - y)]_\beta$$
$$= 4\sigma(C_2) + 3\sigma(C_2 - u) + 3\sigma(C_2 - v) + 2\sigma(C_2 - u - v), \tag{16b}$$

$$[\sigma(C_1 - x) + \sigma(C_1 - y)]_\gamma$$
$$= 5\sigma(C_2) + 3\sigma(C_2 - u) + 2\sigma(C_2 - v) + \sigma(C_2 - u - v) \tag{16c}$$

and

$$[\sigma(C_1 - x - y)]_\alpha = 2\sigma(C_2) + \sigma(C_2 - v), \tag{17a}$$

$$[\sigma(C_1 - x - y)]_\beta = \sigma(C_2) + \sigma(C_2 - u) + \sigma(C_2 - v) + \sigma(C_2 - u - v), \tag{17b}$$

$$[\sigma(C_1 - x - y)]_\gamma = 2\sigma(C_2) + \sigma(C_2 - u). \tag{17c}$$

There is a complete analogy between the above formulas and eqs. (5), (6) and (7).

Bearing in mind eqs. (16) and (17), the proof of the inequalities

$$[\sigma(C_0)]_\alpha < [\sigma(C_0)]_\beta, \tag{18}$$

$$[\sigma(C_0)]_\gamma < [\sigma(C_0)]_\beta \tag{19}$$

is now straightforward. In order to obtain (18), we have first to observe that

$$[\sigma(C_1 - x) + \sigma(C_1 - y)]_\alpha$$
$$= [\sigma(C_1 - x) + \sigma(C_1 - y)]_\beta + \sigma(C_2) - \sigma(C_2 - u) - \sigma(C_2 - u - v),$$

$$[\sigma(C_1 - x - y)]_\alpha = [\sigma(C_1 - x - y)]_\beta + \sigma(C_2) - \sigma(C_2 - u) - \sigma(C_2 - u - v)$$

and to take into account the inequality (14). Then the relation (18) follows from eq. (15).

The verification of (19) is analogous.

From (18) and (19), theorem 4 follows straightforwardly. □

The explicit combinatorial expression for the Merrifield–Simmons index of L_h has recently been found [18]. It reads:

$$\sigma(L_h) = \frac{3}{R}\, 2^{-(h+1)}[(R+5)(7+R)^h + (R-5)(7-R)^h], \quad R = \sqrt{33}.$$

5. Proof of theorem 5

Denote the characteristic polynomial [13,19] of a graph G by $\phi(G) = \phi(G, x)$ and recall that the largest eigenvalue of G is just the largest root of the equation $\phi(G, x) = 0$. Therefore,

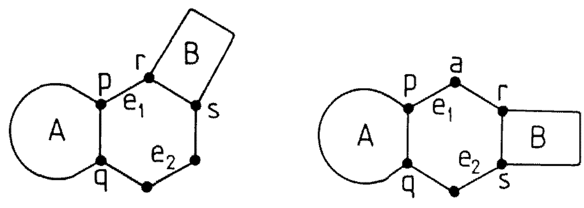
$$\phi(G, x) > 0 \quad \text{for all} \quad x > x_1(G). \tag{20}$$

As an immediate consequence of (20), we have the following elementary statement.

LEMMA 6

Let F and H be two graphs and let $\Delta(x) = \phi(F, x) - \phi(H, x)$. If for $x = x_1(H)$, $\Delta(x) < 0$, then $x_1(F) > x_1(H)$.

Instead of theorem 5, we prove a somewhat stronger result, namely lemma 7. Let F and H be graphs of the following form:



F H

LEMMA 7

If either $\phi(A-p) \equiv \phi(A-q)$ or $\phi(B-r) \equiv \phi(B-s)$ (or both), then $x_1(F) > x_1(H)$.

Proof of lemma 7

Let e be an edge of the graph G, connecting the vertices u and v. Then the characteristic polynomial of G obeys the following recurrence relations [13, 19, 20]:

$$\phi(G) = \phi(G-e) - \phi(G-u-v) - 2\sum_j \phi(G - Z_j^G), \tag{21}$$

where Z_j^G is a circuit of G and the summation embraces all circuits containing the edge e. Further,

$$\phi(G) = x\phi(G-u) - \phi(G-u-v) - \sum_i \phi(G-u-w_i^G) - 2\sum_j \phi(G-Z_j^G) \tag{22}$$

with the second summation going over all circuits of G containing the vertex u. As before (cf. eq. (3)), the first summation on the right-hand side of (22) runs over all the vertices w_i^G which are adjacent to the vertex u, but which differ from v.

The summation on the right-hand side of (21) vanishes if the edge e does not belong to any circuit:

$$\phi(G) = \phi(G-e) - \phi(G-u-v). \tag{23}$$

A special case of eq. (22) of interest to us is [20]

$$\phi(G) = x\phi(G-u) - \phi(G-u-v), \tag{24}$$

which holds if the vertex v is the unique neighbor of u.

In what follows, we also need the identity [13, 19, 20]

$$\phi(G_1 \cup G_2) = \phi(G_1)\phi(G_2), \tag{25}$$

in which the same notation is used as in eqs. (2) and (13).

Applying (21) to the edges of F and H, labeled by e_1, we obtain

$$\phi(F) = \phi(F - e_1) - \phi(F - p - r) - 2\sum_j \phi(G - Z_j^F),$$

$$\phi(H) = \phi(H - e_1) - \phi(H - p - a) - 2\sum_j \phi(H - Z_j^H).$$

It is easy to see that F and H possess equal numbers of circuits. Furthermore, the circuits of F and H, containing the edge e_1, can be labeled so that the subgraphs $F - Z_j^F$ and $H - Z_j^H$ are isomorphic and, consequently, $\phi(F - Z_j^F) \equiv \phi(H - Z_j^H)$ for all values of j. Then

$$\Delta(x) = \phi(F - e_1) - \phi(F - p - r) - \phi(H - e_1) + \phi(H - p - a). \tag{26}$$

In all the four subgraphs which appear on the right-hand side of (26), the edge e_2 does not belong to any circuit. Therefore, a repeated application of (23), (24) and (25) yields

$$\phi(F - e_1) = [x\phi(A) - \phi(A - q)][x\phi(B) - \phi(B - s)] - \phi(A)\phi(B),$$

$$\phi(F - p - r) = [x\phi(A - p) - \phi(A - p - q)][x\phi(B - r) - \phi(B - r - s)]$$
$$- \phi(A - p)\phi(B - r),$$

$$\phi(H - e_1) = [x\phi(A) - \phi(A - q)][x\phi(B) - \phi(B - r)]$$
$$- \phi(A)[x\phi(B - s) - \phi(B - r - s)]$$

$$\phi(H - p - a) = [x\phi(A - p) - \phi(A - p - q)]\phi(B) - \phi(A - p)\phi(B - s).$$

When the above relations are substituted back into (26) and when either $\phi(A - p) \equiv \phi(A - q)$ or $\phi(B - r) \equiv \phi(B - s)$, then $\Delta(x)$ is simplified to

$$\Delta(x) = -[\phi(A) - x\phi(A - p) + \phi(A - p - q)][\phi(B) - x\phi(B - r) + \phi(B - r - s)]. \tag{27}$$

Because of (22),

$$\phi(A) - x\phi(A - p) + \phi(A - p - q) = -\sum_i \phi(A - p - w_i^A) - 2\sum_j \phi(A - Z_j^A), \tag{28}$$

$$\phi(B) - x\phi(B - r) + \phi(B - r - s) = -\sum_i \phi(B - r - w_i^B) - 2\sum_j \phi(B - Z_j^B). \tag{29}$$

Now, according to a well-known result of graph-spectral theory [19,21], the largest eigenvalue of a connected graph is (strictly) greater than the largest eigenvalue of any of its proper subgraphs. This, in turn, implies $x_1(H) > x_1(A) > x_1(A - p - w_i^A)$, $x_1(A - Z_j^A)$ and $x_1(H) > x_1(B) > x_1(B - r - w_i^B)$, $x_1(B - Z_j^B)$. Consequently, for all vertices w_i^A, w_i^B and for all circuits Z_j^A, Z_j^B, the characteristic polynomials of the subgraphs $A - p - w_i^A$, $B - r - w_i^B$, $A - Z_j^A$, $B - Z_j^B$ are all positive-valued for $x = x_1(H)$. Consequently, for $x = x_1(H)$, the right-hand sides of both (28) and (29) are negative-valued. Consequently, for $x = x_1(H)$ the right-hand side of eq. (27) is also negative-valued.

Lemma 7 follows now from lemma 6. □

The statement of theorem 5 holds in a trivial manner for $h = 1$ and $h = 2$. We may therefore assume that $h \geq 3$.

Consider a hexagonal chain $C \in C_h$ and label its hexagons consecutively by $\rho_1, \rho_2, \ldots, \rho_h$. Thus, the hexagons ρ_1 and ρ_h are terminal and for $i = 1, 2, \ldots, h-1$, the hexagons ρ_i and ρ_{i+1} are adjacent.

Suppose that $C \neq L_h$. Then C possesses angularly annelated hexagons. Let ρ_j be the first angularly annelated hexagon of C, i.e. the hexagons $\rho_1, \rho_2, \ldots, \rho_{j-1}$ are assumed to be not angularly annelated. Let C^* be the hexagonal chain differing from C only at the hexagon ρ_j, i.e. the hexagon ρ_j in C^* is assumed to be linearly annelated. Then C and C^* can be viewed as special cases of the graphs F, H from lemma 7. Furthermore, the hexagons $\rho_1, \rho_2, \ldots, \rho_{j-1}$ induce a linear chain L_{j-1} corresponding to the fragment A in lemma 7. Since L_{j-1} is symmetric, the condition $\phi(A - p) \equiv \phi(A - q)$ is evidently fulfilled. Then lemma 7 is applicable and $x_1(C) > x_1(C^*)$. Whence, by "linearizing" the hexagon ρ_j, we reduce the largest graph eigenvalue.

Repeating the above transformation to all angularly annelated hexagons of C, we ultimately arrive at L_h which therefore has the smallest largest eigenvalue in the set C_h.

The proof of theorem 5 has thus been completed. □

The analytical expression for the largest eigenvalue of L_h is long known [22]:

$$x_1(L_h) = \tfrac{1}{2}\{1 + \{9 + 8\cos[\pi/(h+1)]\}^{1/2}\}.$$

6. Concluding remarks

A question which naturally arises from theorems 1–5 is which member(s) of the class C_h have maximum values for K, Z and x_1 and minimum values for W and σ. In the case of the Wiener index, the respective hexagonal chain has been identified [11] and shown to be the helicene graph. It is also long known [23–25] that all fully-angularly annelated hexagonal chains (with a given h) have equal and maximal K-values.

From the proofs of theorems 3–5, it is evident that the member (or members) of C_h having largest Z, smallest σ and largest x_1 must be fully-angularly annelated.

However, whereas the linear annelation is unique (mode β), there are two distinct modes of angular annelation (α and γ). As a consequence of this, by means of the analysis outlined in the preceding sections, we are not able to completely characterize the oppositely-extremal hexagonal chain(s).

We have recently made extensive numerical studies of the graph invariants Z, σ and x_1 of hexagonal chains [26,27]. Based upon these findings, we offer the following hypotheses which (if true) complement theorems 3, 4 and 5.

CONJECTURE 3*

The element of the class C_h with the largest Hosoya index is unique and is the zig-zag polyphene graph.

CONJECTURE 4*

The element of the class C_n with the smallest Merrifield–Simmons index is unique and is the zig-zag polyphene graph.

CONJECTURE 5*

The element of the class C_h with the largest largest eigenvalue is unique and is the helicene graph.

Acknowledgement

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