

Hexagonal Systems with Minimal Number of Inlets

Roberto Cruz¹, Frank Duque², Juan Rada¹

¹*Instituto de Matemáticas, Universidad de Antioquia
Medellín, Colombia*

²*Departamento de Matemáticas, Cinvestav
D. F., México*

(Received February 10, 2016)

Abstract

Let \mathcal{HS}_h denote the set of hexagonal systems with h hexagons. If $U \in \mathcal{HS}_h$ then the number of inlets of U is denoted by $r(U)$. In this paper we show that $r(U) \geq \lceil \sqrt{3(h-1)} \rceil$ for every $U \in \mathcal{HS}_h$. Moreover, for every $h \geq 4$ we construct hexagonal systems $B_h \in \mathcal{HS}_h$ such that $r(B_h) = \lceil \sqrt{3(h-1)} \rceil$.

1 Introduction

We consider in this paper the class of hexagonal systems, graph representations of benzenoid hydrocarbons which are of great importance in chemistry. A hexagonal system is a finite connected plane graph without cut vertices, in which all interior regions are mutually congruent regular hexagons (we exclude the hollow coronoid species from the class of hexagonal systems). More details on these graphs can be found in [5].

We can associate to each path u_1, \dots, u_k of a hexagonal system H , the vertex degree sequence $(d_{u_1}, \dots, d_{u_k})$. If one goes along the perimeter of H , then a fissure, bay, cove and fjord, are respectively paths of degree sequences

$$(2, 3, 2), (2, 3, 3, 2), (2, 3, 3, 3, 2) \text{ and } (2, 3, 3, 3, 3, 2)$$

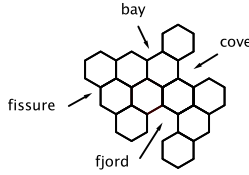


Figure 1: Features lying in the perimeter of a hexagonal system

(see Figure 1). The number of fissures, bays, coves and fjords are denoted respectively by $f(H)$, $B(H)$, $C(H)$ and $F(H)$. An important parameter associated to a hexagonal system is the so-called bay regions of H , denoted by $b = b(H)$, and defined as

$$b(H) = B(H) + 2C(H) + 3F(H).$$

which counts the number of edges on the perimeter, connecting two vertices of degree 3. If $b(H) = 0$ then we say that H is a convex hexagonal system [3]. Another parameter associated to a hexagonal system was introduced in [8], called the number of inlets of H , and defined as

$$r(H) = f(H) + B(H) + C(H) + F(H)$$

Hexagonal systems for which the number of inlets r is extremal (maximal or minimal) were considered in the papers ([1], [2], [3], [4]) in connection to the problem of extremal values of vertex-degree based topological indices. It was shown in [3, Lemma 6] that the linear hexagonal chain L_h has the maximal number of inlets in \mathcal{HS}_h , the set of all hexagonal systems with h hexagons. The minimality of r over \mathcal{HS}_h was considered for convex hexagonal systems, but the following question remained open [3, Problem 7]:

Which hexagonal systems in \mathcal{HS}_h have minimal number of inlets? (1)

In this paper we show that $r(H) \geq \lceil \sqrt{3(h-1)} \rceil$ for every $H \in \mathcal{HS}_h$ (see Theorem 3.2). Moreover, for every $h \geq 4$ we construct hexagonal systems $B_h \in \mathcal{HS}_h$ such that $r(B_h) = \lceil \sqrt{3(h-1)} \rceil$ (see Theorem 3.4).

2 Inlet-increasing hexagonal systems

For each $H \in \mathcal{HS}_h$, consider the set $\mathcal{A}(H)$ of all hexagonal systems with $h + 1$ hexagons that contains H :

$$\mathcal{A}(H) = \{H' \in \mathcal{HS}_{h+1} : H \subset H'\}.$$

Definition 2.1 Let $H \in \mathcal{HS}_h$. We say that H is an inlet-increasing hexagonal system if $r(H) < r(H')$ for every $H' \in \mathcal{A}(H)$.

The hexagonal system H_1 in Figure 2 is inlet-increasing since $\mathcal{A}(H_1) = \{H'_1, H''_1\}$, $r(H_1) = 3$ and $r(H'_1) = r(H''_1) = 4$. On the other hand, the hexagonal system H_2 in the same figure is not inlet-increasing since $H'_2 \in \mathcal{A}(H_2)$ and $r(H_2) > r(H'_2)$.

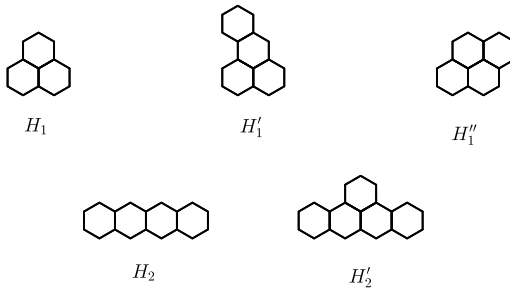


Figure 2: Inlet-increasing and not inlet-increasing hexagonal systems.

Let $a(H)$ be the number of adjacent inlets of H (i.e. pair of inlets that have a common vertex of degree 2) introduced in [7]. Next we describe the inlets of an inlet-increasing hexagonal system.

Proposition 2.2 Let H be an inlet-increasing hexagonal system. Then H has no fjords and $a(H) = 0$.

Proof. Let H be an inlet-increasing hexagonal system with h hexagons and r inlets.

1. Suppose H has a fjord formed by the perimetral path $a, x_1, x_2, x_3, x_4, x_5, x_6, b$ with degree sequence $(d_a, 2, 3, 3, 3, 3, 2, d_b)$ where d_a and d_b are the degrees of the vertices a and b respectively. Adding the edge x_1x_6 we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = d_b = 2$, or $r(H') = r - 1$ if $d_a \neq d_b$ or $r(H') = r - 2$ if $d_a = d_b = 3$ (see Figure 3). Since H is inlet-increasing we get a contradiction.
2. Suppose $a(H) > 0$. Since H has no fjords, we have to consider the following cases:

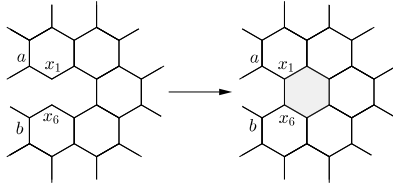


Figure 3: Figure used in the proof of Proposition 2.2 part 1.

Case 1: H has two adjacent fissures with a common vertex u . Then H has a perimetral path a, x_1, x_2, u, y_1, y_2 with degree sequence $(d_a, 2, 3, 2, 3, 2)$. Adding a hexagon with edges x_1x_2 and x_2u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 4). This contradicts the fact that H is inlet-increasing.

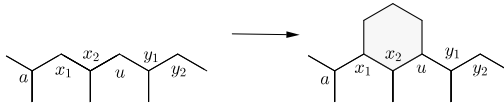


Figure 4: Figure used in the proof of Proposition 2.2 part 2, Case 1.

Case 2: A fissure and a bay of H are adjacent with a common vertex u . Then H has a perimetral path $a, x_1, x_2, u, y_1, y_2, y_3$ with degree sequence $(d_a, 2, 3, 2, 3, 3, 2)$. Adding a hexagon with edges x_1x_2 and x_2u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 5). This contradicts the fact that H is inlet-increasing.

Case 3: A fissure and a cove of H are adjacent with a common vertex u . Then H has a perimetral path $a, x_1, x_2, u, y_1, y_2, y_3, y_4$ with degree sequence $(d_a, 2, 3, 2, 3, 3, 3, 2)$. Adding a hexagon with edges x_1x_2 and x_2u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 6). This contradicts the fact that H is inlet-increasing.

Case 4: H has two adjacent bays with a common vertex u . Then H has a perimetral

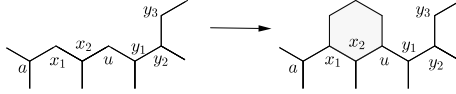


Figure 5: Figure used in the proof of Proposition 2.2 part 2, Case 2.

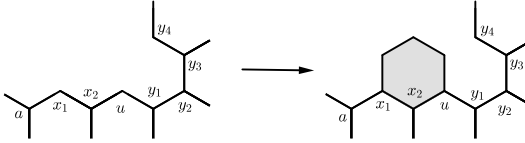


Figure 6: Figure used in the proof of Proposition 2.2 part 2, Case 3.

path $a, x_1, x_2, x_3, u, y_1, y_2, y_3$ with degree sequence $(d_a, 2, 3, 3, 2, 3, 3, 2)$. Adding a hexagon with edges x_1x_2, x_2x_3 and x_3u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 6). This contradicts the fact that H is inlet-increasing.

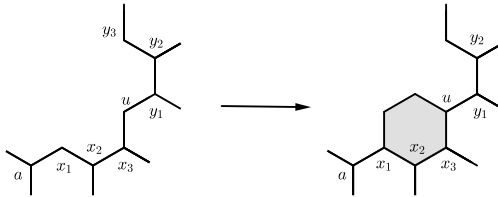


Figure 7: Figure used in the proof of Proposition 2.2 part 2, Case 4.

Case 5: A bay and a cove of H are adjacent with a common vertex u . Then H has a perimetral path $a, x_1, x_2, x_3, u, y_1, y_2, y_3, y_4$ with degree sequence $(d_a, 2, 3, 3, 2, 3, 3, 3, 2)$. Adding a hexagon with edges x_1x_2, x_2x_3 and x_3u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 8). This contradicts the fact that H is inlet-increasing.

Case 6: H has two adjacent coves with a common vertex u . Then H has a perimetral path $a, x_1, x_2, x_3, x_4, u, y_1, y_2, y_3, y_4$ with degree sequence $(d_a, 2, 3, 3, 3, 2, 3, 3, 3, 2)$.

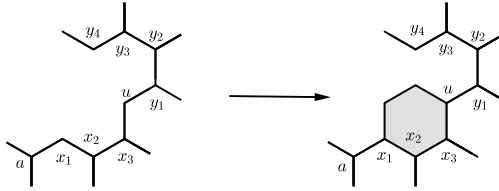


Figure 8: Figure used in the proof of Proposition 2.2 part 2, Case 5.

Adding a hexagon with edges x_1x_2 , x_2x_3 , x_3x_4 and x_4u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 9). This contradicts the fact that H is inlet-increasing.

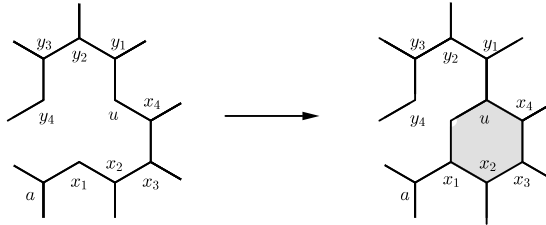


Figure 9: Figure used in the proof of Proposition 2.2 part 2, Case 6.



Proposition 2.3 *Let H be an inlet-increasing hexagonal system with h hexagons and r inlets. Then there exists a convex hexagonal system H' that contains H such that*

$$r' = r(H') \leq 2r \tag{2}$$

$$h' = h(H') = h + r' - r \tag{3}$$

Proof. By Proposition 2.2, the inlets of the maximal hexagonal system H are fissures, bays and coves and there are no adjacent inlets. We construct a new hexagonal system H' in the following way:

To each bay in H , with perimetral path a, x_1, x_2, x_3, x_4, b and degree sequence $(2, 2, 3, 3, 2, 2)$ we add a hexagon with edges x_1x_2, x_2x_3, x_3x_4 (see Figure 10).

To each cove in H , with perimetral path $a, x_1, x_2, x_3, x_4, x_5, b$ and degree sequence $(2, 2, 3, 3, 3, 2, 2)$ we add a hexagon with edges $x_1x_2, x_2x_3, x_3x_4, x_4x_5$ (see Figure 10).

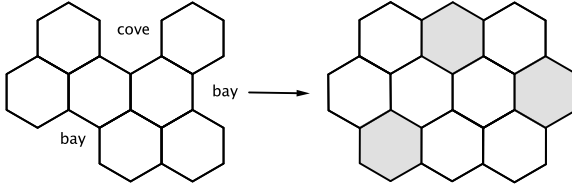


Figure 10: A inlet-increasing hexagonal system and its corresponding convex hexagonal system.

Note that the obtained hexagonal system H' has no bay regions so it is a convex hexagonal system. Moreover, for each bay and each cove we add one hexagon and obtain two fissures in H' , then

$$r' = f(H) + 2B(H) + 2C(H) = r + B(H) + C(H) \leq 2r$$

$$h' = h + B(H) + C(H) = h + r + B(H) + C(H) - r = h + r' - r$$

■

A convex hexagonal system H' can be described as $H' = H'(a_1, a_2, a_3, a_4, a_5, a_6)$ for non-negative integers $a_1, a_2, a_3, a_4, a_5, a_6$ (see Figure 11).

In [3] it was shown that H' is completely determined by the parameters a_1, a_2, a_3, a_4 since the following relations holds

$$a_5 = a_1 + a_2 - a_4$$

$$a_6 = a_3 + a_4 - a - a_1$$

The number h' of hexagons and the number r' of inlets in H' , can be also described in terms of parameters a_1, a_2, a_3, a_4 as follows (see Theorem 2 in [3]):

$$h' = a_1a_3 + a_1a_4 + a_2a_3 + a_2a_4 - a_2 - a_3 - \frac{1}{2}a_1(a_1 + 1) - \frac{1}{2}a_4(a_4 + 1) + 1 \tag{4}$$

$$r' = a_1 + 2a_2 + 2a_3 + a_4 - 6 \tag{5}$$

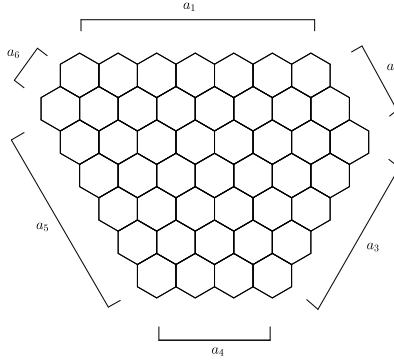


Figure 11: A convex hexagonal system.

Next we find the lower bound on the number of inlets for the inlet-increasing hexagonal systems.

Proposition 2.4 *Let H be an inlet-increasing hexagonal system with h hexagons and r inlets. Then*

$$r \geq \left\lceil \sqrt{3(h-1)} \right\rceil$$

Proof. Let H be an inlet-increasing hexagonal system with h hexagons and r inlets. Let $H' = H'(a_1, a_2, a_3, a_4)$ be a convex hexagonal system obtained from H as described in Proposition 2.3. We use the method of Lagrange multipliers to find the maximal value of the function $h'(a_1, a_2, a_3, a_4)$, determined by equation (4), imposing the condition (5).

The maximal value of the function $h'(a_1, a_2, a_3, a_4)$ is attained for

$$a_1 = a_2 = a_3 = a_4 = \frac{r'}{6} + 1$$

and

$$h'_{\max} = 3 \left(\frac{r'}{6} + 1 \right) \left(\frac{r'}{6} \right) + 1.$$

Using relations (2) and (3) in Proposition 2.3 we obtain:

$$\begin{aligned} h &= h' - r' + r \leq h'_{\max} - r' + r \\ &= 3 \left(\frac{r'}{6} + 1 \right) \left(\frac{r'}{6} \right) + 1 - r' + r = \frac{r'}{12} (r' - 6) + 1 + r \\ &\leq \frac{r^2}{3} + 1 \end{aligned}$$

which implies

$$r \geq \left\lceil \sqrt{3(h-1)} \right\rceil.$$

■

3 Hexagonal systems with minimal number of inlets

In this section we present our main results. In order to extend Proposition 2.4 for general hexagonal systems we need the following lemma.

Lemma 3.1 *Let $H \subset H_1 \subset H_2 \subset \dots \subset H_i \subset \dots$ be a sequence of hexagonal systems such that $H \in \mathcal{HS}_h$, $H_i \in \mathcal{HS}_{h_i}$ for all $i = 1, 2, 3, \dots$ and $h < h_1 < h_2 < \dots < h_i < \dots$.*

Then

$$\lim_{i \rightarrow \infty} r(H_i) = +\infty.$$

Proof. Let $H \in \mathcal{HS}_h$ with n_2^* (resp. n_3^*) external vertices of degree 2 (resp. 3) . It is well known [5] that

$$\begin{aligned} n_2^* &= 2h + 4 - n_i \\ n_3^* &= 2h - 2 - n_i \end{aligned}$$

where n_i is the number of internal vertices. It follows that

$$\begin{aligned} n_2^* &\geq \left\lceil \sqrt{12h-3} \right\rceil + 3 \\ n_3^* &\geq \left\lceil \sqrt{12h-3} \right\rceil - 3 \end{aligned}$$

since $n_i \leq 2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil$ [6]. Hence the number of external vertices of degree 2 and 3 in the perimeter of a hexagonal system approaches infinity as h approaches infinity. Since there are at most four consecutive vertices of degree 2 in the perimeter, the number $r = 2m_{23}$ [8], where m_{23} is the number of edges connecting vertices of degree 2 and 3, also approaches infinity. ■

Theorem 3.2 *Let H be a hexagonal system with h hexagons and r inlets. Then*

$$r \geq \left\lceil \sqrt{3(h-1)} \right\rceil.$$

Proof. If H is an inlet-increasing hexagonal system, by Proposition 2.4 we are done. Otherwise we will show that there exists an inlet-increasing hexagonal system $H_s \in \mathcal{HS}_{h+s}$ such that $r = r(H) \geq r(H_s)$.

In fact, if H is not inlet-increasing there exists $H_1 \in \mathcal{A}(H)$ such that $r \geq r(H_1)$. If H_1 is not inlet-increasing there exists $H_2 \in \mathcal{A}(H_1)$ such that $r \geq r(H_1) \geq r(H_2)$.

Continuing this process we construct a sequence

$$H = H_0 \subset H_1 \subset H_2 \subset \dots \subset H_i \subset \dots$$

such that $H_i \in \mathcal{A}(H_{i-1})$ and

$$r = r(H) \geq r(H_1) \geq r(H_2) \geq \dots \geq r(H_i) \geq \dots$$

Note that the sequence $\{r(H_i)\}_i$ is bounded by r . Consequently by Lemma 3.1, the sequence is finite. In other words, there exists $H_s \in \mathcal{A}(H_{s-1})$ such that H_s is inlet-increasing and $r = r(H) \geq r(H_1) \geq \dots \geq r(H_s)$. Hence, by Proposition 2.4

$$r = r(H) \geq r(H_s) \geq \sqrt{3(h+s-1)} \geq \sqrt{3(h-1)}$$

which implies

$$r \geq \left\lceil \sqrt{3(h-1)} \right\rceil.$$

■

Recall that Harary and Harboth [6] constructed the spiral hexagonal system as depicted in Figure 12.

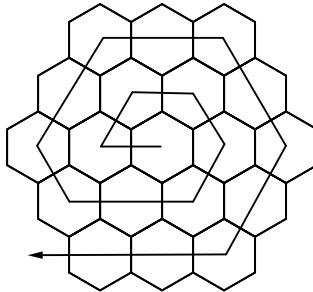


Figure 12: Spiral hexagonal system

Let $S_{h'}$ be the spiral hexagonal system with h' hexagons. It is known that $S_{h'}$ is the hexagonal system in $\mathcal{HS}_{h'}$ with maximal number of internal vertices. The number of internal vertices $n'_i = n_i(S_{h'})$, the number of bay regions $b' = (S_{h'})$ and the number of inlets $r' = r(S_{h'})$ satisfy the following relations:

$$n'_i = n'_i(S_{h'}) = 2h' + 1 + \left\lceil \sqrt{12h' - 3} \right\rceil \quad (6)$$

$$b' = b'(S_{h'}) \in \{0, 1\} \quad (7)$$

$$r' = r'(S_{h'}) = \left\lceil \sqrt{12h' - 3} \right\rceil - 3 - b' \quad (8)$$

Now we introduce a parametrization of the spiral hexagonal system $S_{h'}$ that will be useful in the sequel. Let $h' \geq 7$ and k be the greatest integer such that $3k(k-1) + 1 \leq h' < 3k(k+1) + 1$. Since $0 \leq h' - 3k(k-1) - 1 < 6k$, let

$$\begin{aligned} q' &= \left\lfloor \frac{h' - 3k(k-1) - 1}{k} \right\rfloor \\ l' &= h' - 3k(k-1) - 1 - q'k. \end{aligned}$$

Then h' has a unique representation of the form

$$h' = h'(k, q', l') = 3k(k-1) + 1 + q'k + l' \quad (9)$$

where $k = 2, 3, \dots$, $q' \in \{0, 1, 2, 3, 4, 5\}$ and $l' = 0, 1, \dots, k-1$. From the construction of $S_{h'}$ we conclude that k is the number of complete loops in $S_{h'}$, q' is the side of the spiral to which belongs the last hexagon in $S_{h'}$ and l' is the number of the last hexagon in the side q' . In Figure 13 the spiral system $S_{h'}$ for every value of $h' = h'(2, q', l')$ are depicted.

Next we obtain the number of bay regions, the number of inlets and the number of hexagons in the perimeter of $S_{h'}$ in terms of the introduced parameters k, q' and l' .

Proposition 3.3 *Let $h' = h'(k, q', l')$ of the form (9) and h'_e be the number of hexagons in the perimeter of $S_{h'}$. Then*

$$\begin{aligned} b' = b'(S_{h'}) &= \begin{cases} 0 & \text{if } l' = 0, & q' = 0 \\ 0 & \text{if } l' = k-1, & q' < 5 \\ 1 & \text{otherwise} \end{cases} \\ r' = r'(S_{h'}) &= \begin{cases} 6k-6 & \text{if } l' = 0, & q' = 0 \\ 6k-5+q' & \text{if } l' = k-1, & q' < 5 \\ 6k-6+q' & \text{otherwise} \end{cases} \\ h'_e = h'_e(S_{h'}) &= \begin{cases} 6k-6 & \text{if } l' = 0, & q' = 0 \\ 6k-5+q' & \text{otherwise} \end{cases} \end{aligned}$$

Proof. Since

$$12h' - 3 = 36k^2 - 36k + 12q'k + 12l' + 9$$

we have:

If $q' = 0$ and $l' = 0$ then $12h' - 3 = (6k - 3)^2$. Consequently, $\left\lceil \sqrt{12h' - 3} \right\rceil = 6k - 3$.

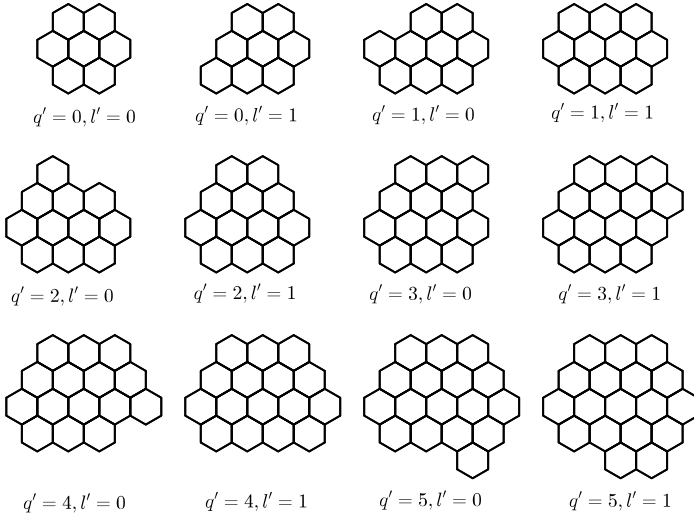


Figure 13: Spiral systems $S_{h'}$ for every value of $h' = h'(2, q', l')$.

If $q' = 0$ and $0 < l' \leq k - 1$ we have

$$12h' - 3 > (6k - 3)^2,$$

$$12h' - 3 \leq 36k^2 - 24k - 3 < (6k - 2)^2.$$

Consequently, $\lceil \sqrt{12h' - 3} \rceil = 6k - 3$.

If $0 < q' \leq 5$ and $0 \leq l' \leq k - 1$ we have

$$12h' - 3 \geq 36k^2 - 36k + 12q'k + 9 = (6k - 3 + q')^2 + 9 - (3 - q')^2 > (6k - 3 + q')^2,$$

$$12h' - 3 \leq 36k^2 - 36k + 12q'k + 12k - 3 < (6k - 2 + q')^2.$$

Consequently, $\lceil \sqrt{12h' - 3} \rceil = 6k - 2 + q'$.

It follows that

$$\lceil \sqrt{12h' - 3} \rceil = \begin{cases} 6k - 3 & \text{if } l' = 0, q' = 0 \\ 6k - 2 + q' & \text{otherwise} \end{cases} \quad (10)$$

Note that $b' = b(S_{h'}) = 0$ if and only if $n_i(S_{h'+1}) = n_i(S_{h'}) + 1$. From (6) this fact occurs if and only if

$$\lceil \sqrt{12h' - 3} \rceil + 1 = \lceil \sqrt{12(h' + 1) - 3} \rceil.$$

From (10) we obtain the expression for b' in terms of k and q' . From (8) and the fact that $h'_e = r' + b'$ we obtain the expressions for r' and h'_e in terms of k and q' . ■

Theorem 3.4 For any $h \geq 4$ there exists a hexagonal system B_h such that $r(B_h) = \lceil \sqrt{3(h-1)} \rceil$.

Proof. Let $h \geq 4$ and k be the greatest integer such that $3(k-1)^2 + 1 \leq h < 3k^2 + 1$. Since $0 \leq h' - 3(k-1)^2 - 1 < 3(2k-1)$, let

$$\begin{aligned} q &= \left\lfloor \frac{h' - 3(k-1)^2 - 1}{2k-1} \right\rfloor \\ l &= h - 3(k-1)^2 - 1 - q(2k-1). \end{aligned}$$

Then h has a unique representation of the form

$$h = h(k, q, l) = 3(k-1)^2 + 1 + q(2k-1) + l \tag{11}$$

where $k = 3, 4, \dots$, $q \in \{0, 1, 2\}$ and $l = 0, 1, \dots, 2k-2$.

In order to construct a system B_h with minimal number of inlets for each $h \geq 4$, we take the spiral system $S_{h'}$, with an appropriate value of $h' = h'(k, q', l')$ of the form (9), and remove alternately $\lfloor h'_e/2 \rfloor$ hexagons from the perimeter of $S_{h'}$, starting from the last hexagon and moving in opposite direction with respect to the construction of the spiral systems described in Figure 12. Consider the following cases:

- $h = h(k, 0, 0) = 3(k-1)^2 + 1$.

Let $h' = h'(k, 0, 0) = 3k(k-1) + 1$. By Proposition 3.3, $h'_e = r' = 6k - 6$ and $S_{h'}$ has no bay regions. Note that when we remove from $S_{h'}$ each one of the $3k - 3$ hexagons, we reduce by one the number of inlets of $S_{h'}$. Note that

$$\begin{aligned} h'(k, 0, 0) - \left\lfloor \frac{h'_e}{2} \right\rfloor &= 3(k-1)^2 + 1 = h(k, 0, 0) \\ r &= \frac{r'}{2} = 3(k-1) \end{aligned}$$

- $h = h(k, q, l)$ where $(q, l) \neq (0, 0)$, $q \in \{0, 1, 2\}$ and $l = 0, \dots, k-2$.

Let $h' = h'(k, q', l')$ where $q' = 2q$ and $l' = l$. By Proposition 3.3, $h'_e = 6k - 5 + 2q$ and $S_{h'}$ has one bay region next to the last hexagon in $S_{h'}$. When we remove the last hexagon in $S_{h'}$, the number of inlets does not change, while when we remove each one of the remained $\left\lfloor \frac{h'_e}{2} \right\rfloor - 1$ hexagons, the number of inlets of $S_{h'}$ reduces by one. Note that

$$\begin{aligned} h'(k, q', l') - \left\lfloor \frac{h'_e}{2} \right\rfloor &= 3k(k-1) + 2qk + l - [3(k-1) + q] \\ &= 3(k-1)^2 + 1 + q(2k-1) + l = h(k, q, l) \\ r &= r' - \left(\left\lfloor \frac{h'_e}{2} \right\rfloor - 1 \right) = 6k - 6 + 2q + 1 - [3(k-1) + q] \\ &= 3k - 2 + q \end{aligned}$$

- $h = h(k, q, l)$ where $q \in \{0, 1, 2\}$ and $l = k - 1, \dots, 2k - 3$.

Let $h' = h'(k, q', l')$ where $q' = 2q + 1$ and $l' = l - k + 1$. By Proposition 3.3, $h'_e = 6k - 4 + 2q$ and $S_{h'}$ has one bay region next to the last hexagon in S_h . When we remove the last hexagon in $S_{h'}$ the number of inlets does not change, while when we remove each one of the remained $\frac{h'_e}{2} - 1$ hexagons, the number of inlets of $S_{h'}$ reduces by one. Note that

$$\begin{aligned} h'(k, q', l') - \frac{h'_e}{2} &= 3k(k-1) + 1 + (2q+1)k + l - k + 1 - [3k - 2 + q] \\ &= 3(k-1)^2 + 1 + q(2k-1) + l = h(k, q, l) \\ r &= r' - \left(\frac{h'_e}{2} - 1\right) = 6k - 6 + (2q+1) + 1 - [3k - 2 + q] \\ &= 3k - 2 + q \end{aligned}$$

- $h = h(k, q, l)$ where $q \in \{0, 1, 2\}$ and $l = 2k - 2$.

Let $h' = h'(k, q', l')$ where $q' = 2q + 1$ and $l' = k - 1$. By Proposition 3.3, $h'_e = 6k - 4 + 2q$. Note that

$$\begin{aligned} h'(k, q', l') - \frac{h'_e}{2} &= 3k(k-1) + 1 + (2q+1)k + k - 1 - [3k - 2 + q] \\ &= 3(k-1)^2 + 1 + q(2k-1) + l = h(k, q, l) \end{aligned}$$

If $q' = 2q + 1 = 5$ then $S_{h'}$ has one bay region next to the last hexagon in S_h . When we remove the last hexagon in $S_{h'}$ the number of inlets does not change, while when we remove each one of the remained $\frac{h'_e}{2} - 1$ hexagons, the number of inlets of $S_{h'}$ reduces by one. Then

$$\begin{aligned} r &= r' - \left(\frac{h'_e}{2} - 1\right) = 6k - 6 + 2q + 1 + 1 - [3k - 2 + q] \\ &= 3k - 2 + q \end{aligned}$$

If $q' = 2q + 1 < 5$ then $S_{h'}$ has no bay regions. When we remove each one of the $\frac{h'_e}{2}$ hexagons, the number of inlets of $S_{h'}$ reduces by one. Then

$$\begin{aligned} r &= r' - \frac{h'_e}{2} = 6k - 5 + 2q + 1 - [3k - 2 + q] \\ &= 3k - 2 + q \end{aligned}$$

In both cases we obtain $r = 3k - 2 + q$.

For each value of $h = h(k, q, l)$ we constructed a hexagonal system B_h such that $r = r(B_h) = 3k - 3$ if $(q, l) = (0, 0)$ and $r = r(B_h) = 3k - 2 + q$ otherwise. In Figure

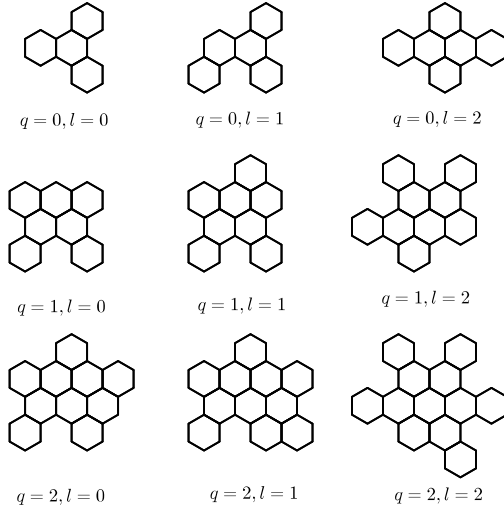


Figure 14: Hexagonal systems B_h for every value of $h = h(2, q, l)$.

14 the hexagonal systems B_h for every value of $h = h(2, q, l)$ are depicted. Now we show that $r = \left\lceil \sqrt{3(h-1)} \right\rceil$.

If $(q, l) = (0, 0)$ we have $3(h-1) = 9(k-1)^2$ and $\sqrt{3(h-1)} = 3(k-1) = r$.

If $(q, l) \neq (0, 0)$, since $l \leq 2k-2$ and $q \in \{0, 1, 2\}$ we have

$$\begin{aligned} 3(h-1) &= 9(k-1)^2 + 3q(2k-1) + 3l \leq 9k^2 - 6k(2-q) + 3 - 3q \\ &= (3k-2+q)^2 + 3 - (2-q)^2 - 3q < (3k-2+q)^2. \end{aligned}$$

On the other hand, if $q = 0$ then $l > 0$ and

$$3(h-1) = 9(k-1)^2 + 3l > 9(k-1)^2.$$

If $q \neq 0$ then $l \geq 0$ and

$$\begin{aligned} 3(h-1) &= 9(k-1)^2 + 3q(2k-1) + 3l \geq 9k^2 - 6k(3-q) + 9 - 3q \\ &= (3k-3+q)^2 + 9 - (3-q)^2 - 3q > (3k-3+q)^2. \end{aligned}$$

It means that if $(q, l) \neq (0, 0)$ then

$$(3k-3+q)^2 < 3(h-1) < (3k-2+q)^2.$$

We conclude that

$$\left\lceil \sqrt{3(h-1)} \right\rceil = 3k-2+q = r.$$



Note that the hexagonal systems B_h , when $h = h(p-1, 0, 0)$ where p is an even integer such that $p \geq 4$, coincide with the systems $B_{p,p-2}$ obtained in [4].

From Theorems 3.2 and 3.4 we obtain the following result.

Corollary 3.5 *The system B_h is a hexagonal system with minimal number of inlets in \mathcal{HS}_h for every value of $h \geq 4$.*

References

- [1] L. Berrocal, A. Olivieri, J. Rada, Extremal values of vertex-degree-based topological indices over hexagonal systems with fixed number of vertices, *Appl. Math. Comput.* **243** (2014) 176–183.
- [2] R. Cruz, H. Giraldo, J. Rada, Extremal values of vertex-degree topological indices over hexagonal systems, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 501–512.
- [3] R. Cruz, I. Gutman, J. Rada, Convex hexagonal systems and their topological indices, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 97–108.
- [4] R. Cruz, I. Gutman, J. Rada, On benzenoid systems with minimal number of inlets, *J. Serb. Chem. Soc.* **78** (2013) 1351–1357.
- [5] I. Gutman, S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer-Verlag, Berlin, 1989.
- [6] F. Harary, H. Harboth, Extremal animals, *J. Comb. Inf. Syst. Sci.* **1** (1976) 1–8.
- [7] J. Rada, Second order Randić index of benzenoid systems, *Ars Comb.* **72** (2004) 77–88.
- [8] J. Rada, O. Araujo, I. Gutman, Randić index of benzenoid systems and phenylenes, *Croat. Chem. Acta.* **74** (2001) 225–235.