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Hexagonal systems with extremal connectivity index

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Abstract

We find extremal values of the connectivity index in the class $\mathcal{HS}_h$ of hexagonal systems with h hexagons.

1 Introduction

The connectivity index ([17]) is one of the graph-based molecular structure descriptors most widely used in applications to physical and chemical properties ([6],[12],[13]). It is defined for a simple graph G with $n(G)$ vertices, as

$$\chi(G) = \sum_{1 \leq i \leq j \leq n(G)-1} \frac{m_{ij}(G)}{\sqrt{ij}}$$

where $m_{ij}(G)$ is the number of edges in G connecting a vertex of degree i with a vertex of degree j.

One of the main problems in the mathematical literature of the connectivity index is to determine extremal values of χ in significant classes of graphs ([1]-[5],[8]-[10]). 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 ([7]).

The hexagons of a hexagonal system can be classified according to the number and position of edges shared with the adjacent hexagons. Figure 1 shows the 12 different types of hexagons that can occur in a hexagonal system.

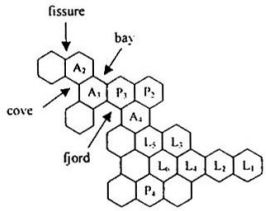


Figure 1: Different types of hexagons and inlets in a hexagonal system

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

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

(see Figure 1). The number of fissures, bays, coves and fjords are denoted respectively by $f(S), B(S), C(S)$ and $F(S)$. The parameter

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

was introduced in ([14]), called the number of inlets of S, and a simple relation with χ was established; namely

$$\chi(S) = \frac{n(S)}{2} - \alpha r(S) \tag{1}$$

where $\alpha = \frac{5-2\sqrt{6}}{6} > 0$.

If we restrict to catacondensed hexagonal systems, i.e. hexagonal systems with no internal vertices, then equation (1) can be used to determine the extremal values of χ over the class $\mathcal{CHS}_h$ of catacondensed hexagonal systems with h hexagons ([15]). Moreover, a complete description of the

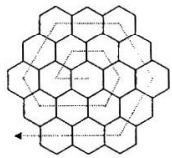
order relation induced by χ over $\mathcal{CHS}_h$ is given in ([16]). We now approach the problem of extremal values of χ in the class $\mathcal{HS}_h$ of hexagonal systems with h hexagons.

2 Hexagonal systems with minimal connectivity index

In this section we find minimal elements of $\mathcal{HS}_h$ with respect to the linear order induced by χ. We will strongly rely on a result of Harary and Harborth ([11]): for every $S \in \mathcal{HS}_h$

$$2h + 1 + u \leq n(S) \leq 4h + 2 \tag{2}$$

where $u = \left\{\sqrt{12h - 3}\right\}$ and $\{x\}$ denotes the smallest integer greater or equal to x. Moreover, this bound is reached in spiral hexagonal systems, which we will denote by T_h (see Figure 2).



T_h

Figure 2: Spiral hexagonal system

Let $b(S)$ denote the number of bay regions, i.e. $b(S) = B(S) + 2C(S) + 3F(S)$. Considering the well known relations ([7],[14])

$$\begin{aligned} 2r(S) &= m_{23}(S) = 4h - 4 - 2b(S) - 2n_i(S) \\ n(S) &= 4h + 2 - n_i(S) \end{aligned}$$

where $n_i(S)$ denotes the number of internal vertices of S, we easily deduce that

$$r(S) = n(S) - 2h - 4 - b(S)$$

and so by equation (1)

$$\chi(S) = \left(\frac{1}{2} - \alpha\right) n(S) + \alpha b(S) + \alpha(2h+4) \tag{3}$$

where $\frac{1}{2} - \alpha > 0$.

Note that if $S_0 \in \mathcal{HS}_h$ is such that

$$\left.\begin{array}{r} n(S_0) = 2h+1+u \\ b(S_0) = 0 \end{array}\right\} \tag{4}$$

then S_0 is a minimal element of $\mathcal{HS}_h$. In fact, by (2) and (3), if $S \in \mathcal{HS}_h$ then

$$\chi(S) - \chi(S_0) = \left(\frac{1}{2} - \alpha\right)(n(S) - (2h+1+u)) + \alpha b(S) \geq 0$$

In order to simplify relations (4), recall that the size of the perimeter of an hexagonal system $S \in \mathcal{HS}_h$, denoted by $p(S)$, is the number of external vertices which is known to conform the relation $p(S) = 4h + 2 - 2n_i(S)$. Since $n_i(S) = 4h + 2 - n(S)$ then

$$p(S) = 2n(S) - 4h - 2$$

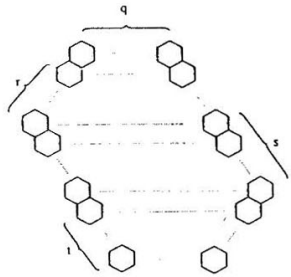
It follows that $n(S) = 2h + 1 + u$ if and only if $p(S) = 2u$, which implies that the set of relations given in (4) is equivalent to the set of relations

$$\left.\begin{array}{r} p(S_0) = 2u \\ b(S_0) = 0 \end{array}\right\} \tag{5}$$

We next give a precise description of hexagonal systems $S \in \mathcal{HS}_h$ such that $b(S) = 0$. For these systems, only hexagons of mode L_1, L_2, L_3, L_6, P_2 and P_4 occur (the modes L_1 or L_2 only occur in the linear hexagonal chain). Consequently, it is not difficult to see that there exists $(q, r, s, t) \in \mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$, where $\mathbb{N} = \{0, 1, 2, ...\}$ denotes the natural numbers and $\mathbb{N}^* = \mathbb{N} \setminus \{0\} = \{1, 2, ...\}$, such that S is isomorphic to the hexagonal system $S(q, r, s, t)$ shown in Figure 3.

Remark 2.1 *Given $S \in \mathcal{HS}_h$ such that $b(S) = 0$, the 4-tuple $(q, r, s, t) \in \mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$ satisfying $S \cong S(q, r, s, t)$ is not unique. For instance, the hexagonal systems S and S' shown in Figure 4 can be represented as*

$$\begin{aligned} S &\cong S(3,1,3,1) \cong S(4,1,2,1) \cong S(2,2,2,2) \\ S' &\cong S(2,3,1,1) \cong S(4,1,1,3) \end{aligned}$$



S(q,r,s,t)

Figure 3: Hexagonal system with no bay regions

Theorem 2.2 *Let h be a positive integer. The following conditions are equivalent:*

1. *There exists $S_0 \in \mathcal{HS}_h$ satisfying relations (5);*
2. *The system of equations*

$$\left.\begin{array}{c} rq + \frac{1}{2}(r-1)r + (s+t)(q+r) - \frac{1}{2}t(t+1) = h \\ 2q + 3r + 2s + t - 1 = u \end{array}\right\} \qquad (6)$$

has a solution $(q, r, s, t) \in \mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$.

If this occurs, then S_0 is a minimal element of $\mathcal{HS}_h$.

Proof. 1. $\Rightarrow$ 2. Suppose that there exists $S_0 \in \mathcal{HS}_h$ satisfying relations (5). Since $b(S_0) = 0$ then $S_0 = S(q, r, s, t)$, where $(q, r, s, t) \in \mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$. By a combinatoric argument we obtain

$$\begin{aligned} h &= h(S_0) = q + (q+1) + \cdots + (q+r-1) + s(q+r) + \\ &\quad (q+r-1) + \cdots + (q+r-t) \\ &= rq + \frac{1}{2}(r-1)r + s(q+r) + t(q+r) - \frac{1}{2}t(t+1) \\ &= rq + \frac{1}{2}(r-1)r + (s+t)(q+r) - \frac{1}{2}t(t+1) \end{aligned}$$

and

$$\begin{aligned} 2u &= p(S_0) = (2q+1) + 4(r-1) + 4(s+1) + 4(t-1) + 2(q+r-t) + 1 \\ &= 2(2q+3r+2s+t-1) \end{aligned}$$

Consequently, (q, r, s, t) is a solution of the system of equations (6).

2. $\Rightarrow$ 1. If the system of equations (6) has a solution (q, r, s, t) in $\mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$, consider the hexagonal system $S_0 = S(q, r, s, t)$. Then by the argument above,

$$h(S_0) = rq + \frac{1}{2}(r-1)r + (s+t)(q+r) - \frac{1}{2}t(t+1) = h$$

and so $S_0 \in \mathcal{HS}_h$. Furthermore,

$$p(S_0) = 2(2q+3r+2s+t-1) = 2u$$

and clearly by construction, $b(S_0) = 0$. Hence S_0 satisfies relations (5).

The last statement was shown above. ■

Remark 2.3 *Hexagonal systems verifying relations (5) (if they exist) are not necessarily unique. For example, the hexagonal systems S and S' depicted in Figure 4 are non-isomorphic hexagonal systems belonging to $\mathcal{HS}_{18}$ which satisfy relations (5). In particular, S and S' are minimal elements of $\mathcal{HS}_{18}$.*

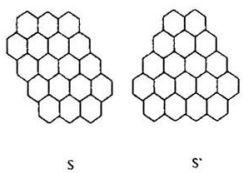


Figure 4: Minimal non-isomorphic hexagonal systems in $\mathcal{HS}_{18}$

By Theorem 2.2, given a positive integer h, we can construct a minimal element of $\mathcal{HS}_h$ from a solution of the system of equations (6). What happens if there is no solution?

Corollary 2.4 *Let h be a positive integer such that the system of equations (6) has no solution. Then the spiral T_h is a minimal element of $\mathcal{HS}_h$.*

Proof. First of all we note that the number of bay regions in a spiral hexagonal system is 0 or 1. Since $p(T_h) = 2u$ then by Theorem 2.2 and our hypothesis, $b(T_h) = 1$. On the other hand, if $S \in \mathcal{HS}_h$, then by equation (3)

$$\chi(S) - \chi(T_h) = \left(\frac{1}{2} - \alpha\right)(n(S) - (2h + 1 + u)) + \alpha(b(S) - 1) \qquad (7)$$

If $b(S) = 0$ then $n(S) - (2h + 1 + u) \geq 1$ and so

$$\chi(S) - \chi(T_h) \geq \left(\frac{1}{2} - \alpha\right) - \alpha = \frac{1}{2} - 2\alpha > 0$$

If $b(S) \geq 1$ then by (2) and (7), $\chi(S) - \chi(T_h) \geq 0$. Hence, T_h is a minimal element of $\mathcal{HS}_h$. ■

From our results above, given $h \in \mathbb{N}$, the problem of finding a minimal element of $\mathcal{HS}_h$ is completely determined by the existence of solutions in $\mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$ of the system of equations (6). Note that equation

$$2q + 3r + 2s + t - 1 = u \qquad (8)$$

gives a bound for each of the values of q, r, s and t. More precisely, if $(q, r, s, t) \in \mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$ is a solution of (8), then

$$\begin{array}{ll} 1 \leq q \leq \left\{\frac{u+1}{2}\right\} & , \quad 0 \leq r \leq \left\{\frac{u+1}{3}\right\} \\ 1 \leq s \leq \left\{\frac{u+1}{2}\right\} & , \quad 0 \leq t \leq \{u+1\} \end{array}$$

Therefore we can check among all (finite) possible values of (q, r, s, t) $\left(\left\{\frac{u+1}{2}\right\}^2 \cdot \left(\left\{\frac{u+1}{3}\right\} + 1\right) \cdot (\{u+1\} + 1)\right.$ possibilities) which of them is a solution of equation (8), and then among these, which are solutions of equation

$$rq + \frac{1}{2}(r-1)r + (s+t)(q+r) - \frac{1}{2}t(t+1) = h$$

However, this process can be extremely long for large h. We will show in our next result a more effective algorithm.

Theorem 2.5 *Let $(q, r, s, t) \in \mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$ be a solution of the system of equations (6). Then*

$$t = \frac{u-3}{6} \pm \frac{1}{12}z$$

$$r = \frac{t-3+u}{6} \pm y$$

and

$$(q,s) = \left(\frac{-3r+4t+1+u \pm x}{4}, \frac{-3r-3t+1+u \mp x}{4}\right)$$

where $(x,y,z) \in \mathbb{N} \times \mathbb{N} \times \mathbb{N}$ *is a solution of the equation*

$$21x^2 + 3y^2 + z^2 = 28\left(u^2 + 3 - 12h\right) \tag{9}$$

Proof. Assume that $(q,r,s,t) \in \mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$ is a solution of (6). Then by simple algebraic manipulations,

$$(q,s) = \left(\frac{-3r+t+1+u \pm \sqrt{A(r,t)}}{4}, \frac{-3r-3t+1+u \mp \sqrt{A(r,t)}}{4}\right)$$

where

$$A(r,t) = -7r^2 + 2tr - 6r + 2ur - 7t^2 - 6t + 2ut + 1 + 2u + u^2 - 16h$$

Since q, r, s, t, u and h are integers, $A(r,t) = x^2$ for some integer x, which we may assume non-negative. Then solving for r in this equation we obtain

$$r = \frac{t-3+u \pm \sqrt{B(t)}}{7}$$

where

$$B(t) = -48t^2 - 48t + 16ut + 16 + 8u + 8u^2 - 112h - 7x^2$$

As above, $B(t) = y^2$ for some non-negative integer y. It follows then

$$t = \frac{u-3}{6} \pm \frac{1}{12}\sqrt{C}$$

where

$$C = 84 + 28u^2 - 336h - 3y^2 - 21x^2$$

Finally, $C = z^2$ for $z \in \mathbb{N}$. Consequently,

$$h = \frac{1}{4} + \frac{1}{12}u^2 - \frac{1}{112}y^2 - \frac{1}{16}x^2 - \frac{1}{336}z^2$$

or equivalently

$$21x^2 + 3y^2 + z^2 = 28\left(u^2 + 3 - 12h\right)$$

Note that since $u = \left\{\sqrt{12h-3}\right\}$ then $(u-1)^2 < 12h - 3 \leq u^2$ and so the right member of (9) is non-negative. ■

If $(q,r,s,t) \in \mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$ is a solution of (6) then Theorem 2.5 gives tight bounds for t. In fact, let $p = \sqrt{28(u^2+3-12h)}$. Since $0 \leq z \leq p$ then

$$t = \frac{u-3}{6} + \frac{1}{12}z \Longrightarrow \frac{u-3}{6} \leq t \leq \frac{u-3}{6} + \frac{1}{12}p$$

and

$$t = \frac{u-3}{6} - \frac{1}{12}z \Longrightarrow \frac{u-3}{6} - \frac{1}{12}p \leq t \leq \frac{u-3}{6}$$

Based on this observation we can give a more effective algorithm as follows:

Algorithm 2.6 *Let $h \in \mathbb{N}$ and $u = \left\{\sqrt{12h-3}\right\}$. Set $p = \sqrt{28(u^2+3-12h)}$,*

$$Z_1(t) = 2(u-3) - 12t, \qquad Z_2(t) = -Z_1(t)$$

$$R_1(t,y) = \frac{t-3+u}{6} + y, \quad R_2(t,y) = \frac{t-3+u}{6} - y$$

and

$$f(x,y,z) = 21x^2 + 3y^2 + z^2 - p^2$$

1. *For each integer $t_0 \in \left[\frac{u-3}{6} - \frac{1}{12}p, \frac{u-3}{6}\right]$ compute $Z_1(t_0)$.*
2. *Find the non-negative solutions of*

$$f(x,y,Z_1(t_0)) = 0$$

3. *For each solution $(x_0, y_0, Z_1(t_0))$ in step 2, compute $R_1(t_0,y_0)$ and $R_2(t_0,y_0)$.*
4. *If $R_i(t_0,y_0) \in \mathbb{N}$ ($i = 1$ or 2), solve the following system of equations for (q,r,s,t) :*

$$\left.\begin{array}{c} rq + \frac{1}{2}(r-1)r + (s+t)(q+r) - \frac{1}{2}t(t+1) = h \\ 2q + 3r + 2s + t - 1 = u \\ r = R_i(t_0,y_0) \\ t = t_0 \end{array}\right\}$$

5. *Repeat steps 1 through 4 for each $t_0 \in \left[\frac{u-3}{6}, \frac{u-3}{6} + \frac{1}{12}p\right]$ substituting $Z_1(t_0)$ by $Z_2(t_0)$*
6. *Choose solutions $(q,r,s,t) \in \mathbb{N}^* \times \mathbb{N} \times \mathbb{N}^* \times \mathbb{N}$ given in step 4.*

Then by Theorem 2.5, every solution of (6) will be obtained in step 6.

We note that each of the steps in the algorithm can be easily computed using a math software system. We used MAPLE 7 in our next examples.

Example 2.7 *Let $h = 350$. Then $u = \left\{\sqrt{12 \cdot 350 - 3}\right\} = 65$ and so for each integer $t_0 \in \left[\frac{u-3}{6} - \frac{1}{12}p, \frac{u-3}{6}\right] = \left[8, \frac{31}{3}\right]$ we compute $Z_1(t_0)$ and for each $t_0 \in \left[\frac{u-3}{6}, \frac{u-3}{6} + \frac{1}{12}p\right] = \left[\frac{31}{3}, \frac{38}{3}\right]$ we compute $Z_2(t_0)$. The following Table contains the information given by the algorithm.*

	Step 1	*Step 2*	*Step 3*	*Step 4*
t_0	$Z_1(t_0)$	$(x_0, y_0, Z_1(t_0))$	$R_1(t_0, y_0)$ $R_2(t_0, y_0)$	(q, r, s, t)
8	28	$(0, 0, 28)$	10	$(11, 10, 3, 8)$
			10	$(11, 10, 3, 8)$
9	16	$(1, 3, 16)$	12	*
			58/7	*
		$(4, 8, 16)$	79/7	*
			9	$(13, 9, 2, 9), (11, 9, 4, 9)$
		$(5, 1, 16)$	72/7	*
			10	*
10	4	$(6, 2, 4)$	74/7	*
			10	$(10, 10, 3, 10)$
		$(5, 9, 4)$	81/7	*
			9	*
		$(0, 16, 4)$	88/7	*
			8	$(13, 8, 3, 10)$
		$(4, 12, 4)$	12	$(9, 12, 1, 10)$
			60/7	*

t_0	$Z_2(t_0)$	$(x_0, y_0, Z_2(t_0))$	$R_1(t_0, y_0)$ $R_2(t_0, y_0)$	(q, r, s, t)
11	8	*	*	*
12	20	$(1, 11, 20)$	85/7	*
			9	*
		$(2, 10, 20)$	12	*
			64/7	*
		$(4, 4, 20)$	78/7	*
			10	$(11, 10, 1, 12)$

The solutions for the system of equations (6) when $h = 350$ and $u = 65$ are given in the last column of the Table. In particular, for each of these

solutions (q,r,s,t), *the hexagonal system* $S = S(q,r,s,t)$ *is minimal in* $\mathcal{HS}_{350}$.

Example 2.8 *Let* $h = 2712805$. *In this case,* $u = 5706$ *and so we compute* $Z_1(t_0)$ *for* $t_0 \in [921, 950]$ *and* $Z_2(t_0)$ *for* $t_0 \in [951, 980]$. *For each of these values of* t_0, *it can be checked that the equations*

$$f(x, y, Z_1(t_0)) = 0 \text{ and } f(x, y, Z_2(t_0)) = 0$$

have no solutions. Therefore, the system of equations (6) has no solution. It follows from Corollary 2.4, that the spiral $T_{2712805}^{\cdot}$ *is a minimal element of* $\mathcal{HS}_{2712805}$.

3 Hexagonal systems with maximal connectivity index

The hexagonal systems E_h depicted in Figure 5 have maximal connectivity index in the class $\mathcal{CHS}_h$ of catacondensed hexagonal systems ([15, Corollary 7]). We will show in this section that they are also maximal in $\mathcal{HS}_h$.

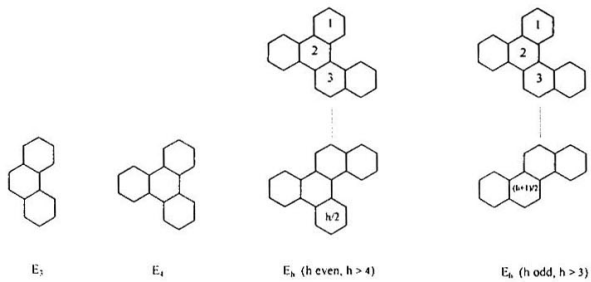


Figure 5: Maximal hexagonal systems in $\mathcal{HS}_h$

For each $h \in \mathbb{N}$ ([15, Examples 4 and 5]), $n(E_h) = 4h + 2$ and

$$b(E_h) = \begin{cases} \frac{3h-6}{2} & \text{if } h \text{ is even} \\ \frac{3h-7}{2} & \text{if } h \text{ is odd} \end{cases}$$

Given $S \in \mathcal{HS}_h$, since $n(S) = 4h + 2 - n_i(S)$ it follows from equation (3)

$$\chi(E_h) - \chi(S) = \begin{cases} \left(\frac{1}{2} - \alpha\right) n_i(S) + \alpha\left(\frac{3h-6}{2} - b(S)\right) & \text{if } h \text{ is even} \\ \left(\frac{1}{2} - \alpha\right) n_i(S) + \alpha\left(\frac{3h-7}{2} - b(S)\right) & \text{if } h \text{ is odd} \end{cases}$$

Bearing in mind the relation $b(S) = m_{22}(S) - 6$, to show that $\chi(S) \leq \chi(E_h)$ is equivalent to show that

$$m_{22}(S) \leq \left(\frac{1}{2\alpha} - 1\right) n_i(S) + \frac{3h + x}{2} \tag{10}$$

where $x = \begin{cases} 6 \text{ if } h \text{ is even} \\ 5 \text{ if } h \text{ is odd} \end{cases}$.

Theorem 3.1 *Let $S \in \mathcal{HS}_h$. Then inequality (10) holds. In particular, E_h has maximal connectivity index in $\mathcal{HS}_h$.*

Proof. We use induction on $n_i(S)$. If $n_i(S) = 0$ then S is a catacondensed hexagonal system and the result follows from ([15, Theorem 6]). Assume as inductive hypothesis, that (10) holds when $n_i(S) \leq k$, $k \geq 0$. Let $S_0 \in \mathcal{HS}_h$ such that $n_i(S_0) = k + 1$. We can choose an internal vertex v of S_0 such that not all of its adjacent vertices are internal. We consider the following cases: (a) v is a vertex of S_0 with three adjacent external vertices a, b and c (see Figure 6).

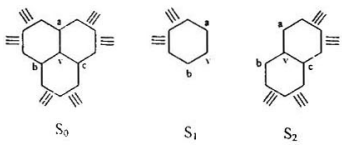


Figure 6: The hexagonal system S_0 splitted into sub-hexagonal systems S_1 and S_2

Then we can split S_0 into sub-hexagonal systems S_1 and S_2 such that

$$\begin{aligned} h &= h_1 + h_2 \\ n_i(S_0) &= n_i(S_1) + n_i(S_2) + 1 \\ m_{22}(S_0) &\leq m_{22}(S_1) + m_{22}(S_2) \end{aligned}$$

where h_1 and h_2 denote the number of hexagons of S_1 and S_2, respectively. Moreover, if h is even then h_1 and h_2 have the same parity. Therefore if h_1 and h_2 are even, then by our inductive hypothesis

$$\begin{aligned} m_{22}(S_0) &\leq m_{22}(S_1) + m_{22}(S_2) \\ &\leq \left(\frac{1}{2\alpha} - 1\right)(n_i(S_1) + n_i(S_2)) + \frac{3(h_1 + h_2) + 6}{2} \\ &= \left(\frac{1}{2\alpha} - 1\right)(n_i(S_0) - 1) + \frac{3h + 6}{2} \\ &\leq \left(\frac{1}{2\alpha} - 1\right) n_i(S_0) + \frac{3h + 6}{2} \end{aligned}$$

Similarly, if h_1 and h_2 are odd. On the other hand, if h is odd then h_1 and h_2 have opposite parity. Consequently, if h_1 is even and h_2 is odd then

$$\begin{aligned} m_{22}(S_0) &\leq m_{22}(S_1) + m_{22}(S_2) \\ &\leq \left(\frac{1}{2\alpha} - 1\right)(n_i(S_1) + n_i(S_2)) + \frac{3h_1 + 6}{2} + \frac{3h_2 + 5}{2} \\ &= \left(\frac{1}{2\alpha} - 1\right)(n_i(S_0) - 1) + \frac{3h}{2} + \frac{11}{2} \\ &\leq \left(\frac{1}{2\alpha} - 1\right) n_i(S_0) + \frac{3h + 5}{2} \end{aligned}$$

If h_1 is odd and h_2 is even is similar.

(b) v is a vertex of S_0 with two adjacent external vertices a and c (see Figure 7).

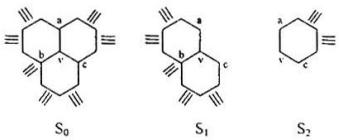


Figure 7: The hexagonal system S_0 splitted into sub-hexagonal systems S_1 and S_2

Then we split S_0 into sub-hexagonal systems S_1 and S_2 and an analogous argument as in case (a) shows that inequality (10) holds for $m_{22}(S_0)$.

(c) Assume that S_0 does not have internal vertices of the types considered in cases (a) or (b). Then there exists an internal vertex v of S_0 with adjacent external vertex a as shown in Figure 8

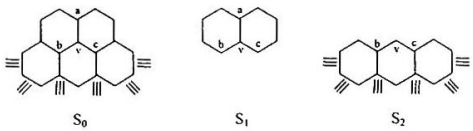


Figure 8: The hexagonal system S_0 splitted into sub-hexagonal systems S_1 and S_2

In this case.

$$\begin{aligned} h &= 2 + h_2 \\ n_i(S_0) &= 1 + n_i(S_2) \\ m_{22}(S_0) &\leq 6 + m_{22}(S_2) \end{aligned}$$

If h is even then h_2 is even and so

$$\begin{aligned} m_{22}(S_0) &\leq 6 + m_{22}(S_2) \\ &\leq 6 + \left(\frac{1}{2\alpha} - 1\right) n_i(S_2) + \frac{3h_2 + 6}{2} \\ &= 6 + \left(\frac{1}{2\alpha} - 1\right)(n_i(S_0) - 1) + \frac{3(h-2) + 6}{2} \\ &= \left(\frac{1}{2\alpha} - 1\right)(n_i(S_0) - 1) + \frac{3h + 12}{2} \\ &\leq \left(\frac{1}{2\alpha} - 1\right) n_i(S_0) + \frac{3h + 6}{2} \end{aligned}$$

Similarly if h is odd. This ends the proof. ■

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