MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **78** (2017) 469-486

ISSN 0340 - 6253

Extremal Values of the Number of Inlets and Number of Bay Regions over Pericondensed Hexagonal Systems

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(Received October 26, 2016)

Abstract

In this paper we find extremal values of the number of inlets and the number of bay regions over $\mathcal{PHS}_h$, the set of pericondensed hexagonal systems with h hexagons. As an application, we determine extremal values of vertex-degree-based topological indices over $\mathcal{PHS}_h$.

1 Introduction

In this paper we study a special class of hexagonal systems, the so-called pericondensed hexagonal systems. These are hexagonal systems with at least one internal vertex. For the definition of hexagonal systems and details of their theory we refer to the book [11]. 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.

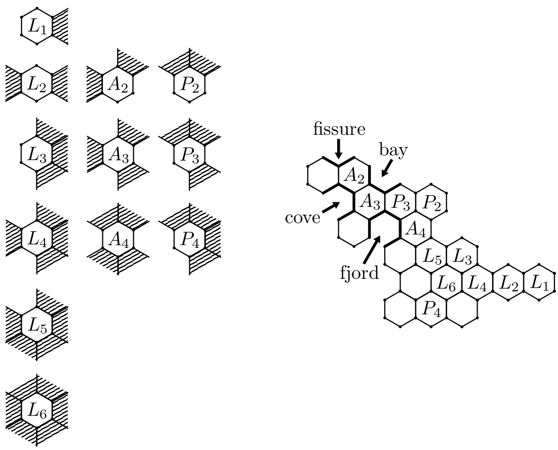


Figure 1. The twelve types of hexagons that can occur in hexagonal systems and the structural features on the perimeter of a hexagonal system.

When going along the perimeter of a hexagonal system H, certain features may be encountered [11], called fissure, bay, cove and fjord, which correspond respectively to vertex degree sequences $(2,3,2)$, $(2,3,3,2)$, $(2,3,3,3,2)$ and $(2,3,3,3,3,2)$ (see Figure 1). The number of fissures, bays, coves and fjords are denoted respectively by $f(H), B(H), C(H)$ and $F(H)$. The parameter

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

is called the number of inlets of H [18].

Another quantity much studied in the theory of hexagonal systems is the number of bay regions $b = b(H)$ defined as

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

When H is a hexagonal system with h hexagons, these two quantities are connected via the relation [2]

$$r = 2(h-1) - (b + n_i), \tag{1}$$

where n_i is the number of internal vertices H has.

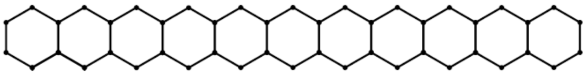
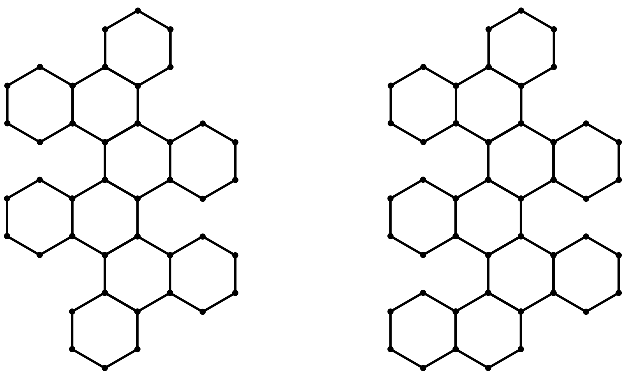


Figure 2. Linear hexagonal chain L_h.

Recall that H is a catacondensed hexagonal system if $n_i(H) = 0$ and it is a pericondensed hexagonal system if $n_i(H) \geq 1$. We will denote by $\mathcal{HS}_h$ the set of hexagonal systems, $\mathcal{CHS}_h$ the set of catacondensed hexagonal systems and $\mathcal{PHS}_h$ the set of pericondensed hexagonal systems with h hexagons. In [2] it was shown that the linear hexagonal chain L_h (see Figure 2) attains the maximal value of r among all hexagonal systems in $\mathcal{HS}_h$ and consequently in $\mathcal{CHS}_h$, since L_h is a catacondensed hexagonal system. In [19] it was shown that the minimal value of r over $\mathcal{CHS}_h$ is attained in the hexagonal system E_h (see Figure 3), and recently the authors in [4] found that the minimal value of r over $\mathcal{HS}_h$ is attained in B_h (see Figure 4). Hence the extremal value problem of r over $\mathcal{CHS}_h$ and $\mathcal{HS}_h$ is settled.



E_h (h even) $\qquad$ E_h (h odd)

Figure 3. Hexagonal systems with maximal value of b over $\mathcal{HS}_h$.

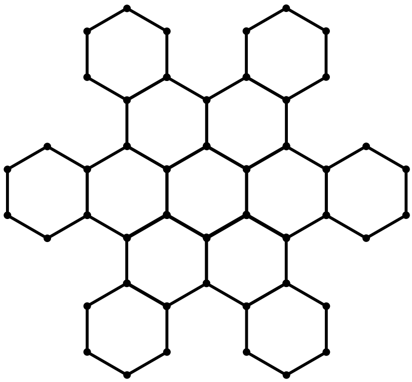


Figure 4. Hexagonal system B_h with minimal number of inlets over $\mathcal{HS}_h$.

Regarding the number of bay regions b over $\mathcal{CHS}_h$, since $n_i(H) = 0$ for all $H \in \mathcal{CHS}_h$, it follows from (1) that

$$r(H) = 2(h-1) - b(H),$$

and so

$$b(H) \leq b(E_h) = \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil, \tag{2}$$

for all $H \in \mathcal{CHS}_h$. The minimal value of b over $\mathcal{CHS}_h$ is clearly attained in L_h, since $b(L_h) = 0$. In $\mathcal{HS}_h$ the minimal is attained in convex hexagonal systems, i.e. hexagonal systems W for which $b(W) = 0$ (see [2]), and the maximal in E_h as you can see in [3].

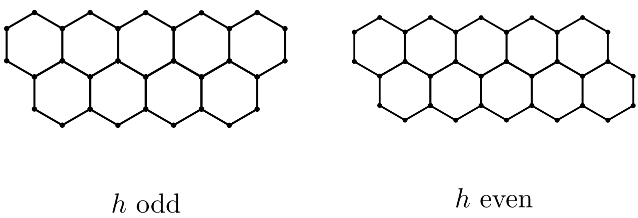


Figure 5. Convex pericondensed hexagonal systems.

So naturally arises the question: is it possible to find sharp upper and lower bounds for r and b over $\mathcal{PHS}_h$? It turns out that the minimal value of r is attained again in B_h, since B_h is a pericondensed hexagonal system. Also, it is easy to construct convex pericondensed hexagonal systems (see Figure 5) and so these have minimal b over $\mathcal{PHS}_h$. Moreover, we show in Theorem 2.1 of this paper that M_h (see Figure 6) attains the maximal value of r among all hexagonal systems in $\mathcal{PHS}_h$.

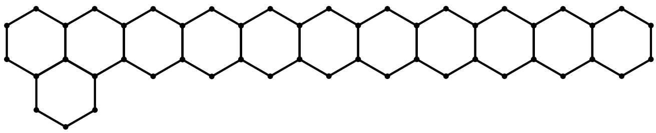
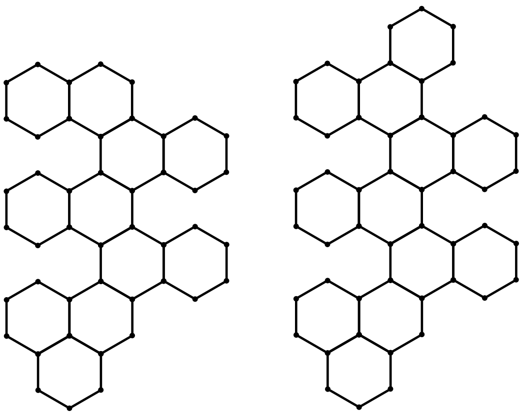


Figure 6. Hexagonal systems M_h with maximal number of inlets over $\mathcal{PHS}_h$.

Perhaps the most interesting question is:

Problem 1.1 *Which pericondensed hexagonal systems attain the maximal value of b.*

In our main result we give a sharp upper bound for the value of b over $\mathcal{PHS}_h$. More precisely, we show in Theorem 2.3 that $b(H) \leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil$ for all $H \in \mathcal{PHS}_h$ $(h \geq 4)$. Moreover, the pericondensed hexagonal system F_h (see Figure 7) attains the maximal value of b.



F_h (h odd) F_h (h even)

Figure 7. Hexagonal system with maximal value of b over $\mathcal{PHS}_h$.

As an application of the results mentioned above, we determine extremal values of vertex-degree-based topological indices over $\mathcal{PHS}_h$. Recall that a vertex-degree-based topological index TI of G is defined as

$$TI(G) = \sum_{1 \le i \le j \le n-1} m_{ij}\varphi_{ij} \tag{3}$$

where $\{\varphi_{ij}\}$ is a set of non-negative real numbers and $1 \le i \le j \le n-1$, and m_{ij} is the number of i-j-edges, i.e. edges between vertices of degree i and degree j ([9], [12], [13], [15], [21]). Many of the well-known topological indices are particular cases of this expression; for instance, when $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ we obtain the Randić index ([24]), one of the most widely used in applications to physical and chemical properties ([6], [16], [17], [25]). Due to the success of the Randić index many other topological indices appeared in the mathematical-chemistry literature, which are particular cases of the formula given in (3): in the second Zagreb index $\varphi_{ij} = ij$ [10], in the atom-bond-connectivity index $\varphi_{ij} = \sqrt{\frac{i+j-2}{ij}}$ [7], in the geometric-arithmetic index $\varphi_{ij} = \frac{2\sqrt{ij}}{i+j}$ [26], in the sum-connectivity index $\varphi_{ij} = \frac{1}{\sqrt{i+j}}$ [29], in the augmented Zagreb index $\varphi_{ij} = \frac{(ij)^3}{(i+j-2)^3}$ [8] and in the harmonic index $\varphi_{ij} = \frac{2}{i+j}$ [28], just to mention a few.

Results on the extremal values of TI over $\mathcal{HS}_h$ and $\mathcal{CHS}_h$ have appeared recently in the literature ([1], [2], [3], [5], [20], [22], [23]). In this paper we address the extremal value problem over $\mathcal{PHS}_h$. More specifically, under certain conditions on the set of numbers $\{\varphi_{ij}\}$ (which most of the well-known topological indices satisfy), we find extremal values of TI over $\mathcal{PHS}_h$ (Theorems 3.1 and 3.2).

2 Extremal values of the number of inlets and number of bay regions

We first determine the extremal values of r over $\mathcal{PHS}_h$. It was shown in [4] that the hexagonal system B_h (see Figure 4) has $\left\lceil \sqrt{3(h-1)} \right\rceil$ inlets and this is the minimal number of inlets among all hexagonal systems in $\mathcal{HS}_h$. Since B_h is a pericondensed hexagonal system, then B_h attains the minimal number of inlets in $\mathcal{PHS}_h$.

Theorem 2.1 *Let $h \ge 4$. Then for all $P \in \mathcal{PHS}_h$*

$$\left\lceil \sqrt{3(h-1)} \right\rceil = r(B_h) \le r(P) \le r(M_h) = 2(h-2).$$

Proof. We only have to prove the upper bound. Let $P \in \mathcal{PHS}_h$ and assume that

$n_i(P) \geq 2$. Then $b(P) + n_i(P) \geq 2$ and so by (1)

$$\begin{aligned} r(P) &= 2(h-1) - (b(P) + n_i(P)) \\ &\leq 2(h-1) - 2 = 2(h-2) \end{aligned}$$

If $n_i(P) = 1$ then $b(P) \geq 1$ by [1, Lemma 2.3]. Hence $b(P) + n_i(P) \geq 2$ and again $r(P) \leq 2(h-2)$. Finally, it is easy to show that $r(M_h) = 2(h-2)$ (see Figure 6). ■

Now we look at the bounds for b over $\mathcal{PHS}_h$. For every positive integer h we can easily construct convex pericondensed hexagonal systems as we can see in Figure 5. These have obviously minimal number of bay regions in $\mathcal{PHS}_h$. So now we are interested in finding the maximal number of bay regions among all hexagonal systems in $\mathcal{PHS}_h$. We know that the maximal value of b over $\mathcal{HS}_h$ is attained in the catacondensed hexagonal system E_h (see Figure 3). This result appeared in [Cru-13, Theorem 3.4] and its proof is based on a (long and complicated) result by Wu and Deng [27, Theorem 10] about the general connectiviy index R_α of hexagonal systems. We now give a simpler proof that depends directly on the structure of the hexagonal system, and a small variation of this result will give us the maximal value of b over $\mathcal{PHS}_h$.

Recall that every hexagonal system with $h \geq 2$ hexagons is obtained from a hexagonal system with $h-1$ hexagons by adding a hexagon of type L_1 (one-contact addition), or P_2 (two-contact addition), or L_3 (three-contact addition), or P_4 (four-contact addition) or L_5 (five-contact-addition) (see [11]). In particular, every hexagonal system has one of the mentioned hexagons: L_1, P_2, L_3, P_4 and L_5. The proof of our next result is based on this observation.

Another well-known relation [11] we will use frequently from now on is

$$m_{22}(H) = b(H) + 6. \tag{4}$$

Theorem 2.2 *Let $H \in \mathcal{HS}_h$ with $h \geq 2$. Then*

$$b(H) \leq \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil .$$

Proof. The proof is by induction on h. It is easy to check the result for $h = 2, 3, 4$. Let $h \geq 5$ and assume that the result is true for any hexagonal system with less than h hexagons. Let H be a hexagonal system with h hexagons. We consider several cases:

1. H contains a L_3, P_4 or L_5 hexagon, or a P_2 hexagon of the form depicted in Figure 8. In this case we will show that there exists a (sub)hexagonal system H_1 with $h-1$ hexagons such that $b(H) \leq b(H_1)+1$. If this is so then by induction we easily obtain

$$b(H) \leq b(H_1) + 1 \leq \left\lceil \frac{3}{2}(h-1) - \frac{7}{2} \right\rceil + 1 \leq \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil .$$

Note that in each case, splitting H into the dark shadowed (sub)hexagonal system H_1 of $h-1$ hexagons and the corresponding hexagon L_3, P_4, L_5 or P_2, we obtain at least five new 2-2-edges. Hence

$$m_{22}(H) \leq m_{22}(H_1) + 6 - 5 = m_{22}(H_1) + 1,$$

and from relation (4) we deduce

$$b(H) \leq b(H_1) + 1.$$

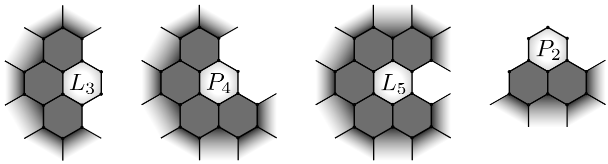


Figure 8. Hexagonal systems used in the proof of Theorem 2.2, case 1.

2. H contains a P_2 hexagon of the form depicted in Figure 9. In this case we will show that there exist (sub)hexagonal systems H_1 and H_2 of H, with $h_1 \geq 2$ and $h_2 \geq 2$ hexagons respectively, such that $h = h_1 + h_2$ and $b(H) \leq b(H_1) + b(H_2) + 3$. Then by induction

$$b(H) \leq b(H_1) + b(H_2) + 3 \leq \left\lceil \frac{3}{2}h_1 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + 3 \leq \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil .$$

Splitting H into the two hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system, we obtain at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

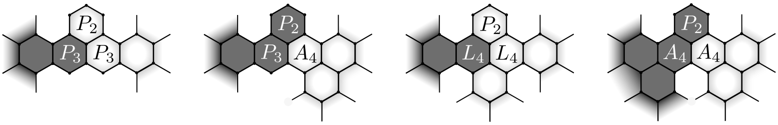


Figure 9. Hexagonal systems used in the proof of Theorem 2.2, case 2.

3. H contains a L_1 hexagon and the hexagon adjacent to it is not A_3. In this case we show that there exist two (sub)hexagonal systems H_1 and H_2 of H, with $h_1 \geq 2$ and $h_2 \geq 2$ hexagons respectively, such that $h = h_1 + h_2$ and $b(H) \leq b(H_1) + b(H_2) + 3$ and the result follows as in part 2 of this theorem.

   Let X be the hexagon adjacent to the L_1 hexagon in H. Then X must be L_2, A_2, P_3 or L_4 (see Figure 10). In each case, we split H into the two hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system, obtaining at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

   or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

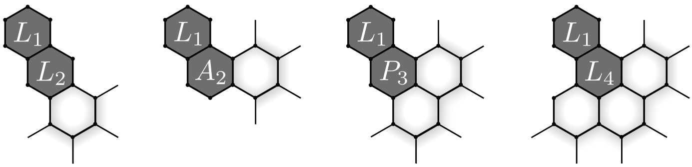


Figure 10. Hexagonal systems used in the proof of Theorem 2.2, case 3.

4. H contains a A_3 hexagon and X is one of the hexagons next to it which is not A_3 nor L_1. Then we will show that there exist (sub)systems H_1 and H_2 of H, with $h_1 \geq 2$ and $h_2 \geq 2$ hexagons respectively, such that $h = h_1 + h_2$ and $b(H) \leq b(H_1) + b(H_2) + 3$ The result would follow as in part 2 of this theorem.

   Clearly X must be a L_2, L_4, A_2 or P_3 hexagon (see Figure 11). In each case, we split system H into the two (sub)hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system, obtaining at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

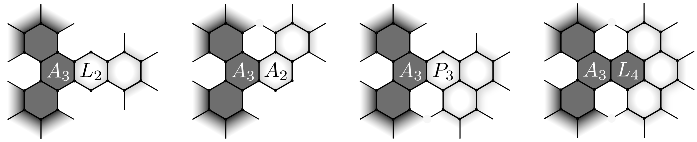


Figure 11. Hexagonal systems used in the proof of Theorem 2.2, case 4.

5. Finally, all hexagons in H are L_1 or A_3. Then H is a catacondensed hexagonal system and the result follows by (2). ■

Now we can find the maximal value of b over the set $\mathcal{PHS}_h$.

Theorem 2.3 *Let $H \in \mathcal{PHS}_h$ with $h \geq 4$. Then*

$$b(H) \leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil.$$

Proof. The proof is by induction on h. It is easy to check the result for $h = 4, 5, 6$. Let $h \geq 7$ and assume that the result is true for any pericondensed hexagonal system with less than h hexagons. Let H be a pericondensed hexagonal system with h hexagons. First assume that $n_i(H) \geq 5$.

1. H contains a L_3, P_4 or L_5 hexagon, or a P_2 hexagon of the form depicted in Figure 8. Then by part 1 of the proof of Theorem 2.2, there exists a (sub)hexagonal system H_1 with $h-1$ hexagons such that $b(H) \leq b(H_1) + 1$. Moreover, since $n_i(H) \geq 5$, $H_1 \in \mathcal{PHS}_{h-1}$. Hence by induction we deduce

$$b(H) \leq b(H_1) + 1 \leq \left\lceil \frac{3}{2}(h-1) - \frac{11}{2} \right\rceil + 1 \leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil.$$

2. H satisfies any of the cases 2, 3 or 4 in the proof of Theorem 2.2. Then there exist two (sub)hexagonal systems H_1 and H_2 of H, with $h_1 \geq 2$ and $h_2 \geq 2$ hexagons respectively, such that $h = h_1 + h_2$ and $b(H) \leq b(H_1) + b(H_2) + 3$. Since $n_i(H) \geq 5$,

one of the two hexagonal systems is pericondensed, say H_1. Then by induction we deduce

$$\begin{aligned} b(H) &\leq b(H_1) + b(H_2) + 3 \leq \left\lceil \frac{3}{2}h_1 - \frac{11}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + 3 \\ &\leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil . \end{aligned}$$

The only possibility left is case 5 in Theorem 2.2, but this cannot occur since $H \in \mathcal{PHS}_h$. So we only have to consider when $1 \leq n_i(H) \leq 4$.

If $n_i(H) = 4$ then the proof works the same as in the case $n_i(H) \geq 5$ except when there is a L_5 hexagon. Note that in the splitting of H in that case, none of the (sub)hexagonal systems is pericondensed. However, if $n_i(H) = 4$ then we can split H (see Figure 12) into the two (sub)hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system with at least four hexagons. In this case, we obtain at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

Since H_1 is pericondensed (with exactly one internal vertex), the results follow as in part 2 of this theorem. Note that if H_1 has exactly three hexagons, then one of these hexagons is a P_2 hexagon and the results follows as in part 1 of this theorem.

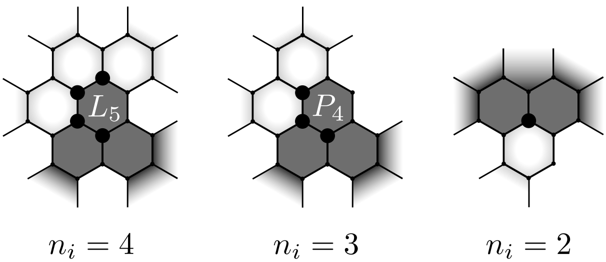


Figure 12. Pericondensed hexagonal systems with $n_i \in \{2, 3, 4\}$.

If $n_i(H) = 3$ then H does not contain a L_5 hexagon. Again, the proof works as in the case $n_i(H) \geq 5$ except when H contains a P_4 hexagon. However, since $n_i(H) = 3$ we can split H into the two (sub)hexagonal systems H_1 and H_2 (see Figure 12), where H_1 is the dark shadowed (sub)hexagonal system with at least four hexagons. In this case, we obtain at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

Since H_1 is pericondensed (with exactly one internal vertex), the results follow as in part 2 of this theorem. Note that if H_1 has exactly three hexagons, then one of these hexagons is a P_2 hexagon and the results follows as in part 1 of this theorem.

If $n_i(H) = 2$, H is of the form depicted in Figure 12. Note that one internal vertex is highlighted and the other one belongs to the dark shadowed (sub)hexagonal system. We split system H into the two (sub)hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system. If H_2 has two or more hexagons, we obtain at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

Since H_1 is pericondensed, the results follow as in part 2 of this theorem.

On the other hand, if H_2 consists of only one hexagon then the system H has the form (a) or the form (b) depicted in Figure 13. Note that in case (b) one internal vertex is highlighted and the other one belongs to the dark shadowed (sub)hexagonal system. In each case, we split system H into the two (sub)hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system.

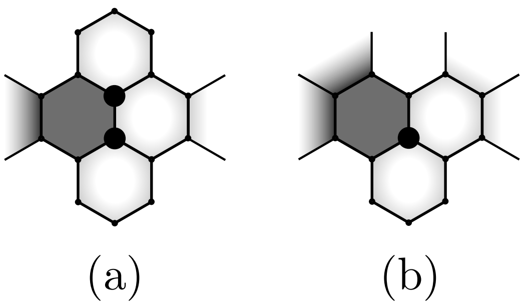


Figure 13. Pericondensed hexagonal systems with $n_i = 2$ when H_2 consists of only one hexagon.

In case (a) we obtain at least five new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 5,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 1.$$

Since neither H_1 nor H_2 are pericondensed, by Theorem 2.2 we deduce

$$\begin{aligned} b(H) &\leq b(H_1) + b(H_2) + 1 \leq \left\lceil \frac{3}{2}h_1 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + 1 \\ &\leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil . \end{aligned}$$

In case (b) we obtain at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

Since H_1 is pericondensed, the results follow as in part 2 of this theorem.

Finally, if $n_i(H) = 1$, we split H into three (sub) hexagonal system H_1, H_2 and H_3 of H as depicted in Figure 14, where $h = h_1 + h_2 + h_3$. If $h_2 = h_3 = 1$ then

$$m_{22}(H) \leq m_{22}(H_1) + 6 + 6 - 4 - 4 - 3 = m_{22}(H_1) + 1,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + 1.$$

From Theorem 2.2

$$\begin{aligned} b\,(H) &\leq b\,(H_1) + 1 \leq \left\lceil \frac{3}{2}(h-2) - \frac{7}{2} \right\rceil + 1 \\ &\leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil . \end{aligned}$$

If $h_2 > 1$ and $h_3 = 1$ then

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) + 6 - 4 - 3 - 3 = m_{22}(H_1) + m_{22}(H_2) - 4,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 2.$$

From Theorem 2.2 and the fact that $h = h_1 + h_2 + 1$ we obtain

$$\begin{aligned} b\,(H) &\leq b\,(H_1) + b\,(H_2) + 2 \\ &\leq \left\lceil \frac{3}{2}h_1 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + 2 \\ &\leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil . \end{aligned}$$

Now, if $h_2 > 1$ and $h_3 > 1$ we obtain at least nine new 2-2-edges. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) + m_{22}(H_3) - 9,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + b\,(H_3) + 3.$$

It follows from Theorem 2.2 and the fact that $h = h_1 + h_2 + h_3$ that

$$\begin{aligned} b\,(H) &\leq b\,(H_1) + b\,(H_2) + b\,(H_3) + 3 \\ &\leq \left\lceil \frac{3}{2}h_1 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_3 - \frac{7}{2} \right\rceil + 3 \\ &\leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil . \end{aligned}$$

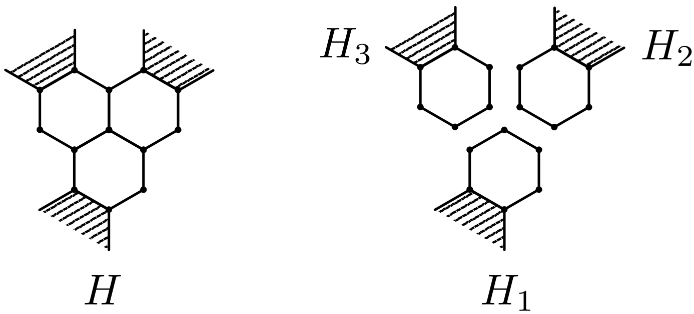


Figure 14. Split of pericondensed (sub)hexagonal system H with $n_i = 1$.

■

The hexagonal system F_h depicted in Figure 7 have maximal value of b over the set of pericondensed hexagonal systems with h hexagons.

3 Extremal values of TI over $\mathcal{PHS}_h$

We first note that a hexagonal system only has vertices of degree 2 and 3, so the expression for TI given in (3) simplifies as

$$TI\,(H) = m_{22}\varphi_{22} + m_{23}\varphi_{23} + m_{33}\varphi_{33}. \tag{5}$$

From the well known relations [18] in a hexagonal system H with n vertices and h hexagons

$$\begin{aligned} m_{22} &= n - 2h - r + 2 \\ m_{23} &= 2r \\ m_{33} &= 3h - r - 3, \end{aligned}$$

the fact that

$$n = 4h + 2 - n_i$$

and from (5), we deduce that for any two hexagonal systems $S, U \in \mathcal{HS}_h$

$$TI\,(S) - TI\,(U) = q\,[r\,(S) - r\,(U)] + \varphi_{22}\,[n_i\,(U) - n_i\,(S)]\,, \tag{6}$$

where

$$q = 2\varphi_{23} - \varphi_{22} - \varphi_{33}.$$

By (1) we can also express the variation of TI in terms of the number of bay regions

$$TI\,(S) - TI\,(U) = q\,[b\,(U) - b\,(S)] + (q + \varphi_{22})\,[n_i\,(U) - n_i\,(S)]\,. \tag{7}$$

Most of the topological indices studied in the literature satisfy the condition

$$-\varphi_{22} \le q < 0, \tag{8}$$

as we can see in Table 1.

	ij	$\frac{1}{\sqrt{ij}}$	$\frac{2\sqrt{ij}}{i+j}$	$\frac{2}{i+j}$	$\frac{1}{\sqrt{i+j}}$	$\frac{(ij)^3}{(i+j-2)^3}$	$\sqrt{\frac{i+j-2}{ij}}$
q	-1	-.0168	-.0404	-.0333	-.0138	-3.3906	.0404
φ_{22}	4	.5	1	.5	.5	8	0.70

Table 1. Values of q and φ_{22} for well-known VDB topological indices.

We next find the minimal value of TI over $\mathcal{PHS}_h$ under the condition (8). Recall that the spiral hexagonal system S_h has maximal number of internal vertices

$$n_i\,(S_h) = 2h + 1 - \left\lceil \sqrt{12h - 3} \right\rceil$$

among all hexagonal systems in $\mathcal{HS}_h$ [14]. In [22] we characterize the values of h for which there exists a convex hexagonal system W with maximal number of internal vertices, i.e.

$$n_i\,(W) = 2h + 1 - \left\lceil \sqrt{12h - 3} \right\rceil. \tag{9}$$

Note that $W \in \mathcal{PHS}_h$. Hence we deduce from [22, Theorems 1.1 and 3.1]:

Theorem 3.1 *Let TI be a vertex-degree-based topological index of the form (3).*

1. *If there exists a convex hexagonal system W with h hexagons satisfying (9) and $-\varphi_{22} \leq q < 0$ then W has minimal TI-value among all hexagonal systems in $\mathcal{PHS}_h$.*

2. *If there is no convex hexagonal system with h hexagons satisfying (9) and $\frac{-\varphi_{22}}{2} \leq q < 0$, then the spiral S_h has minimal TI-value over $\mathcal{PHS}_h$.*

The maximal TI-value in $\mathcal{PHS}_h$ is attained in the pericondensed hexagonal system F_h (see Figure 7), as we can see in our next result.

Theorem 3.2 *Let TI be a vertex-degree-based topological index of the form (3). If $-\varphi_{22} \leq q < 0$ then F_h has maximal TI-value over $\mathcal{PHS}_h$.*

Proof. Let $P \in \mathcal{PHS}_h$. Then $n_i(P) \geq 1$. It follows from (7) and Theorem 2.3 that

$$\begin{aligned} TI(F_h) - TI(P) &= q\left[b(P) - b(F_h)\right] + (q+\varphi_{22})\left[n_i(P) - n_i(F_h)\right] \\ &= q\left[b(P) - \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil\right] + (q+\varphi_{22})\left[n_i(P) - 1\right] \geq 0. \end{aligned}$$

Consequently, $TI(F_h) \geq TI(P)$ for all $P \in \mathcal{PHS}_h$. ∎

Remark 3.3 *The condition $\frac{-\varphi_{22}}{2} \leq q < 0$ holds for most of the well-known topological indices, as we can see in Table 1. Consequently, for all these indices the extremal values of TI over $\mathcal{PHS}_h$ are determined for all h, by Theorems 3.1 and 3.2.*

In the case of the Atom-Bond-Connectivity index $q > 0$.

Theorem 3.4 *Let TI be a vertex-degree-based topological index of the form (3). If $q > 0$ then M_h has maximal TI-value among all hexagonal systems in $\mathcal{PHS}_h$.*

Proof. Let $P \in \mathcal{PHS}_h$. Then $n_i(P) \geq 1$. By (6) and Theorem 2.1

$$\begin{aligned} TI(M_h) - TI(P) &= q\left[r(M_h) - r(P)\right] + \varphi_{22}\left[n_i(P) - n_i(M_h)\right] \\ &= q\left[2(h-2) - r(P)\right] + \varphi_{22}\left[n_i(P) - 1\right] \geq 0. \end{aligned}$$

Hence $TI(M_h) \geq TI(P)$ for all $P \in \mathcal{PHS}_h$. ∎

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