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Extremal Values of Vertex–Degree Topological Indices Over Hexagonal Systems

Roberto Cruz, Hernán Giraldo, Juan Rada

Instituto de Matemáticas, Universidad de Antioquia
Medellín, Colombia

rcruz@matematicas.udea.edu.co, heragis@matematicas.udea.edu.co, jrada@matematicas.udea.edu.co

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Abstract

We find an upper bound for the number of bay regions over the set of hexagonal systems with h hexagons. We also determine extremal values of vertex-degree based topological indices over the set of all hexagonal systems with a fixed number of hexagons.

1 Introduction

A great variety of vertex-degree-based topological indices (molecular structure descriptors) have been considered in the mathematico-chemical literature [9]. Given nonnegative real numbers $\Psi(i,j)$ for every $1 \leq i \leq j \leq n-1$, they are of the form

$$TI = TI(G) = \sum_{1 \leq i \leq j \leq n-1} m_{ij}\, \Psi(i,j) \tag{1}$$

where G is a graph with n vertices and m_{ij} is the number of edges of G connecting a vertex of degree i with a vertex of degree j. Many important topological indices are of this type, for instance, the second Zagreb index is obtained by setting $\Psi(i,j) = ij$ [5], in the connectivity index $\Psi(i,j) = \frac{1}{\sqrt{ij}}$ [14], in the atom-bond connectivity index $\Psi(i,j) = \sqrt{\frac{i+j-2}{ij}}$ [3], in the geometric-arithmetic index $\Psi(i,j) = \frac{2\sqrt{ij}}{i+j}$ [15], in the sum-connectivity index $\Psi(i,j) = \frac{1}{\sqrt{i+j}}$ [18], in the augmented Zagreb index $\Psi(i,j) = \frac{(ij)^3}{(i+j-2)^3}$ [4] and in the harmonic index $\Psi(i,j) = \frac{2}{i+j}$ [17], just to mention a few.

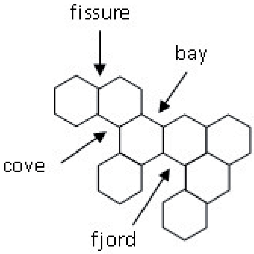

Figure 1. Different types of inlets in a hexagonal system

Our interest in this paper is to study the maximal and minimal values of a topological index TI of the form (1) over the class of all hexagonal systems with a fixed number of hexagons. The motivation comes from the papers [6, 10, 13, 16], where extremal values of different topological indices of the form (1) are considered over the set of hexagonal systems with a fixed number of hexagons.

For the definition of hexagonal systems and details of this theory we refer to [7]. When going along the perimeter of a hexagonal system, then a fissure, bay, cove, and fjord are, respectively, paths with degree sequences

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

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

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

was introduced in [11] and is called the number of inlets of S. Another useful parameter associated to a hexagonal system is the so-called number of bay regions of S, denoted by $b = b(S)$, and defined as

$$b(S) = B(S) + 2C(S) + 3F(S)$$

which counts the number of edges on the perimeter, connecting two vertices of degree 3. If $b\,(S) = 0$ then we say that S is a convex hexagonal system [2].

We will denote by $n_i\,(S)$ the number of internal vertices of the hexagonal system S. Recall that S is a catacondensed hexagonal system if $n_i\,(S) = 0$.

Since any hexagonal system S has only vertices of degree 2 and 3, the general expression for TI given in (1) simplifies as

$$TI(S) = m_{22}\,\Psi(2,2) + m_{23}\,\Psi(2,3) + m_{33}\,\Psi(3,3) \tag{2}$$

From the well known relations [11] in a hexagonal system S with n vertices and h hexagons

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

we deduce from (2) that

$$\begin{aligned} TI\,(S) &= \Psi\,(2,2)\,n+\left[3\Psi\,(3,3)-2\Psi\,(2,2)\right]h \\ &+ \left[2\Psi(2,3)-\Psi(2,2)-\Psi(3,3)\right]r \\ &+ \left[2\Psi(2,2)-3\Psi(3,3)\right]. \end{aligned} \tag{3}$$

From the fact that $n = 4h + 2 - n_i$, it follows from relation (3) that if S and U are hexagonal systems with h hexagons then

$$TI\,(S)-TI\,(U)=q\,[r\,(S)-r\,(U)]+\Psi\,(2,2)\,[n_i\,(U)-n_i\,(S)] \tag{4}$$

where $q = 2\Psi\,(2,3) - \Psi\,(2,2) - \Psi(3,3)$.

Surprisingly, most of the topological indices studied in the literature satisfy the condition

$$-\Psi\,(2,2) \le q < 0$$

as we can see in the Table of Example 3.6. It turns out that under this condition, we completely solve in this paper the problem of finding the maximal and minimal value of a topological index of the form (1), over the set $\mathcal{HS}_h$ of all hexagonal systems with h hexagons. In Theorem 3.1 part (4) we show that the minimal value is attained in the hexagonal system W with maximal number of inlets, a hexagonal system which was introduced in [2]. In order to find the maximal value, we previously show in Theorem 3.4 a sharp upper bound of the number of bay regions over $\mathcal{HS}_h$, based on a result of Wu and Deng [16]. As a consequence, in Theorem 3.5 we show that the maximal value is attained in E (see Figure 4), a catacondensed hexagonal system introduced in [12]. Another application of Theorem 3.4 is given in Theorem 3.7, where we solve a problem proposed by Wu and Deng [16].

We also find the maximal TI-value when $q > 0$ and the minimal TI-value when $q < -\Psi\,(2,2)$ in Theorem 3.1.

Finally, in Section 2 we solve the extremal TI-value problem but in the class of convex hexagonal systems with a fixed number of hexagonos.

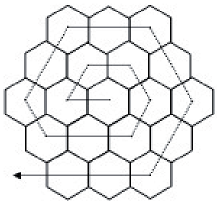

Figure 2. Spiral hexagonal system

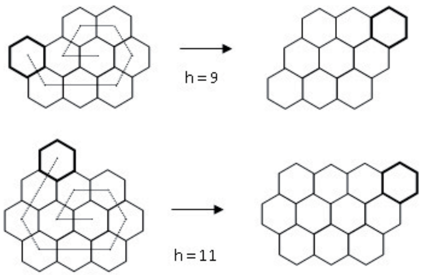

Figure 3. Convex hexagonal system with maximal number of internal vertices

2 Convex hexagonal systems with extremal TI-value

Recall that Harary and Harborth [8] constructed the "spiral" hexagonal systems (see Figure 2), hexagonal systems with maximal number of internal vertices.

In other words, if S is a hexagonal systems with h hexagons and F is a spiral hexagonal system with h hexagons then

$$n_i(S) \leq n_i(F) = 2h + 1 - \left\lceil \sqrt{12h - 3} \right\rceil \tag{5}$$

where $\lceil x \rceil$ denotes the least integer greater or equal to x. Depending on h, the number of bay regions in a spiral hexagonal system can be 0 or 1. However, it was shown in [2] that for every h there exists a convex hexagonal system W (i.e. a hexagonal system such that $b(W) = 0$) with h hexagons and maximal number of internal vertices

$$n_i(W) = 2h + 1 - \left\lceil \sqrt{12h - 3} \right\rceil . \tag{6}$$

These were constructed by modifying the spiral hexagonal systems S such that $b(S) = 1$ (see Figure 3). We can rely on this result to determine the extremal values of a TI of the form (1) over the set $\mathcal{CHS}_h$ of all convex hexagonal systems with h hexagons.

Theorem 2.1 *Let TI be a vertex-degree topological index of the form (2) and set $p = 2\Psi(2,3) - \Psi(3,3)$. Let W be a convex hexagonal system with h hexagons such that (6) holds and let C be a catacondensed hexagonal system with h hexagons. Then:*

1. *If $p = 0$ then TI is constant over $\mathcal{CHS}_h$;*
2. *If $p > 0$ then W (resp. C) has minimal (resp. maximal) TI-value over $\mathcal{CHS}_h$;*
3. *If $p < 0$ then W (resp. C) has maximal (resp. minimal) TI-value over $\mathcal{CHS}_h$.*

Proof. From [2] we know that

$$r(S) = 2h(S) - n_i(S) - 2$$

for every convex hexagonal system S. Hence by (4), for every $S, U \in \mathcal{CHS}_h$

$$\begin{aligned} TI(S) - TI(U) &= q\left[r(S) - r(U)\right] + \Psi(2,2)\left[n_i(U) - n_i(S)\right] \\ &= \left[n_i(U) - n_i(S)\right]\left[q + \Psi(2,2)\right] = \left[n_i(U) - n_i(S)\right] p \ . \end{aligned}$$

1. Clearly, if $p = 0$ then TI is constant over $\mathcal{CHS}_h$. 2. Assume that $p > 0$. Let $W \in \mathcal{CHS}_h$ such that (6) holds and let C be a catacondensed hexagonal system (i.e., $n_i(C) = 0$). Then for every $S \in \mathcal{CHS}_h$

$$TI(S) - TI(W) = \left[n_i(W) - n_i(S)\right] p \geq 0$$

and

$$TI(S) - TI(C) = -n_i(S)\, p \leq 0$$

which shows that W has minimal TI-value and C has maximal TI-value over $\mathcal{CHS}_h$. 3. The proof is similar to part 2. ■

3 Hexagonal systems with extremal TI-value

We next consider the problem of extremal TI-values over the set $\mathcal{HS}_h$ of all hexagonal systems with h hexagons.

Theorem 3.1 *Let TI be a vertex-degree topological index of the form (2) and set $q = 2\Psi(2,3) - \Psi(2,2) - \Psi(3,3)$. Then*

1. *If $q = 0$ then the catacondensed hexagonal systems (resp. spiral hexagonal systems) have maximal (resp. minimal) TI-value over $\mathcal{HS}_h$;*

2. *If $q > 0$ then the linear hexagonal chain has maximal TI-value over $\mathcal{HS}_h$;*

3. *If $q \leq -\Psi(2,2)$ then the linear hexagonal chain has minimal TI-value over $\mathcal{HS}_h$;*

4. *If $-\Psi(2,2) \leq q < 0$ then the convex hexagonal system W has minimal TI-value over $\mathcal{HS}_h$.*

Proof. Let S be a hexagonal system with h hexagons.

1. Assume that $q = 0$ and denote by F the spiral hexagonal system with h hexagons. Then by (4) and (5)

$$TI(F) - TI(S) = \Psi(2,2)\,[n_i(S) - n_i(F)] \leq 0 \;.$$

Consequently F has minimal TI-value. If V is a catacondensed hexagonal system then $n_i(V) = 0$ which implies

$$TI(V) - TI(S) = \Psi(2,2)\,[n_i(S)] \geq 0$$

and so V has maximal TI-value.

2. Suppose that $q > 0$ and let L be the linear hexagonal system with h hexagons. It was shown in [2] that $r(S) \leq r(L) = 2(h-1)$. Since $n_i(L) = 0$ and $n_i(S) \geq 0$ it follows from (4) that

$$TI(L) - TI(S) = q\,[r(L) - r(S)] + \Psi(2,2)\,[n_i(S)] \geq 0 \;.$$

Thus L has maximal TI-value.

3. Suppose that $q \leq -\Psi(2,2)$. Recall that in [2] we have

$$r(S) + n_i(S) = 2(h-1) - b(S)\,. \tag{7}$$

Since $r(L) - r(S) \geq 0$ and $b(S) \geq 0$ then

$$\begin{aligned} TI(L) - TI(S) &= q\,[r(L) - r(S)] + \Psi(2,2)\,[n_i(S)] \\ &\leq -\Psi(2,2)\,[r(L) - r(S)] + \Psi(2,2)\,[n_i(S)] \\ &= \Psi(2,2)\,[(r(S) + n_i(S)) - 2(h-1)] \\ &= \Psi(2,2)\,[-b(S)] \leq 0 \;. \end{aligned}$$

Thus L has minimal TI value.

4. Assume that $-\Psi(2,2) \leq q < 0$. Since $n_i(S) - n_i(W) \leq 0$ it follows from (7), (4) and the fact that $b(W) = 0$ that

$$\begin{aligned} TI(W) - TI(S) &= q[r(W) - r(S)] + \Psi(2,2)[n_i(S) - n_i(W)] \\ &\leq q[r(W) - r(S)] + (-q)[n_i(S) - n_i(W)] \\ &= q[r(W) + n_i(W) - (r(S) + n_i(S))] \\ &= q\,b(S) \leq 0\ . \end{aligned}$$

Consequently W has minimal TI-value. ■

Example 3.2 *Consider the case where $\Psi(i,j) = k > 0$ for every $2 \leq i \leq j \leq 3$. Then*

$$\begin{aligned} TI(S) &= m_{22}\Psi(2,2) + m_{23}\Psi(2,3) + m_{33}\Psi(3,3) \\ &= k \cdot (m_{22} + m_{23} + m_{33}) = k \cdot m(S) \end{aligned}$$

where $m(S)$ is the number of edges the hexagonal system $S \in \mathcal{HS}_h$ has. We apply Theorem 3.1 (part 1 since $q = 0$) to conclude that the catacondensed hexagonal systems have maximal TI-value, and the minimal TI-value is attained in the spiral hexagonal systems. This is consistent with Harary–Harborth's paper "Extremal Animals" [8], where they show that

$$3h + \left\lceil \sqrt{12h - 3} \right\rceil \leq m(S) \leq 5h + 1\ .$$

The upper bound occurs in the catacondensed hexagonal systems and the lower bound in the spiral hexagonal systems.

What can we say about the maximal TI-value for $q < 0$? In order to give an answer to this question recall that the general connectivity indices were introduced by Bollobás and Erdös [1] as the vertex-degree topological index where $\Psi(i,j) = [ij]^\alpha$, for every $\alpha \in \mathbb{R}$. It is denoted by R_α. In other words, for a graph G

$$R_\alpha(G) = \sum_{uv} [d(u)\, d(v)]^\alpha$$

where uv runs over the set of all edges of G.

Let E be the catacondensed hexagonal system with h hexagons [12] (see Figure 4).

It was shown in [12] that $r(E) = \left\lceil \frac{h}{2} + 1 \right\rceil$ and since $n_i(E) = 0$ it follows from (7) that

$$b(E) = 2(h-1) - \left\lceil \frac{h}{2} + 1 \right\rceil = \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil \tag{8}$$

In a recent paper the following result was proved:

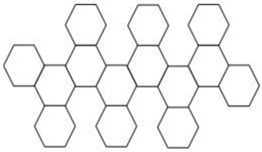

Figure 4. Catacondensed hexagonal system with minimal number of inlets

Theorem 3.3 *[16, Theorem 10] Let $S \in \mathcal{HS}_h$. Then $R_\alpha(E) \geq R_\alpha(S)$ for every $\alpha < \frac{ln2}{ln3-ln2}$.*

Based on this result we can find an upper bound for the number of bay regions over the set $\mathcal{HS}_h$.

Theorem 3.4 *For every $S \in \mathcal{HS}_h$*

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

Proof. From (4)

$$R_\alpha(E) - R_\alpha(S) = q\left[r(E) - r(S)\right] + \Psi(2,2)\left[n_i(S)\right] \tag{9}$$

where

$$\begin{aligned} q &= 2\Psi(2,3) - \Psi(2,2) - \Psi(3,3) \\ &= 2\cdot 6^\alpha - 4^\alpha - 9^\alpha \end{aligned}$$

and

$$\Psi(2,2) = 4^\alpha .$$

Hence from (9) and Theorem 3.3 we deduce

$$\begin{aligned} 0 &\leq \frac{R_\alpha(E) - R_\alpha(S)}{4^\alpha} \\ &= \frac{2\cdot 6^\alpha - 4^\alpha - 9^\alpha}{4^\alpha}\left[r(E) - r(S)\right] + n_i(S) \\ &= \left[2\cdot\left(\frac{3}{2}\right)^\alpha - 1 + \left(\frac{3}{2}\right)^{2\alpha}\right]\left[r(E) - r(S)\right] + n_i(S) \\ &= -\left[\left(\frac{3}{2}\right)^\alpha - 1\right]^2\left[r(E) - r(S)\right] + n_i(S) \end{aligned}$$

for every $\alpha < \frac{ln2}{ln3-ln2}$. Equivalently,

$$\left[\left(\frac{3}{2}\right)^{\alpha} - 1\right]^{2} [r(E) - r(S)] \leq n_i(S) \tag{10}$$

for every $\alpha < \frac{ln2}{ln3-ln2}$. Consequently, letting $\alpha \to -\infty$ on both sides of (10) it follows that

$$r(E) - r(S) \leq n_i(S) \tag{11}$$

Hence from (11), (7) and (8)

$$\begin{aligned} b(S) &= 2(h-1) - r(S) - n_i(S) \\ &\leq 2(h-1) - r(E) = 2(h-1) - \left\lceil \frac{h}{2} + 1 \right\rceil \\ &= b(E). \end{aligned}$$

■

One application of Theorem 3.4 to the study of topological indices is the following:

Theorem 3.5 *Let TI be a vertex-degree topological index of the form (2) and set $q = 2\Psi(2,3) - \Psi(2,2) - \Psi(3,3)$. If*

$$-\Psi(2,2) \leq q < 0$$

then E has maximal TI-value over $\mathcal{HS}_h$.

Proof. Let $S \in \mathcal{HS}_h$. By (4) and (7)

$$\begin{aligned} TI(E) - TI(S) &= q[r(E) - r(S)] + \Psi(2,2)[n_i(S)] \\ &= q[b(S) - b(E) + n_i(S)] + \Psi(2,2)[n_i(S)] \\ &= q[b(S) - b(E)] + [q + \Psi(2,2)][n_i(S)]. \end{aligned} \tag{12}$$

By Theorem 3.4 we know that $b(S) - b(E) \leq 0$ and since $q < 0$ then

$$q[b(S) - b(E)] \geq 0.$$

On the other hand, $n_i(S) \geq 0$ and by hypothesis $q + \Psi(2,2) > 0$, hence

$$[q + \Psi(2,2)][n_i(S)] \geq 0$$

and the result follows from (12). ■

Let us examine now the list of the most important vertex-degree-based topological indices.

Example 3.6 *We consider a topological index of the form*

$$TI = TI(S) = m_{22}\Psi(2,2) + m_{23}\Psi(2,3) + m_{33}\Psi(3,3)$$

Recall that

$$q = 2\Psi(2,3) - \Psi(2,2) - \Psi(3,3).$$

The following table contains information that allows us to determine the extreme values of TI from the theorems described above (Theorems 3.1 and 3.5).

	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*
$\Psi(2,2)$	*4*	*.5*	*1*	*.5*	*.5*	*8*	*0.70*
Minimal	**W**	**W**	**W**	**W**	**W**	**W**	*
Maximal	**E**	**E**	**E**	**E**	**E**	**E**	**L**

As we can see, the second Zagreb index, the connectivity index, the geometric-arithmetic index, the sum-connectivity index, the harmonic index and the augmented Zagreb index satisfy $-\Psi(2,2) \leq q < 0$. Consequently, by Theorem 3.1 (part 4) the minimal value of these topological indices is the convex hexagonal system W and by Theorem 3.5, the maximal value is the catacondensed hexagonal system E. By Theorem 3.1 part 2, the maximal value of the atom-bond connectivity index is attained in L since $q > 0$ in this case.

Finally, we present an answer to a problem proposed in [16, Problem 1] related to the general connectivity index R_α:

Theorem 3.7 *Let R_α be the general connectivity index. Then*

1. *If $\alpha \geq \frac{ln(2)}{ln(3)-ln(2)}$ then the linear hexagonal chain L has minimal R_α-value over $\mathcal{HS}_h$;*
2. *If $\alpha \leq \frac{ln(2)}{ln(3)-ln(2)}$ then the convex hexagonal system W has minimal R_α-value and the catacondensed hexagonal system E has maximal R_α-value over $\mathcal{HS}_h$.*

Proof. As we noted in the proof of Theorem 3.4, $q = -4^\alpha\left[\left(\frac{3}{2}\right)^\alpha - 1\right]^2$ and so $q < 0$ for every $\alpha \in \mathbb{R}$, $\alpha \neq 0$. On the other hand,

$$q + \Psi(2,2) = 2 \cdot 6^\alpha - 9^\alpha.$$

It can be easily checked that

$$q + \Psi(2,2) \leq 0 \Leftrightarrow \alpha \geq \frac{\ln(2)}{\ln(3) - \ln(2)}.$$

Hence, if $\alpha \geq \frac{\ln(2)}{\ln(3)-\ln(2)}$ then $q \leq -\Psi(2,2)$, which implies by Theorem 3.1 (part 3) that the linear hexagonal chain L has minimal R_α-value. If $\alpha \leq \frac{\ln(2)}{\ln(3)-\ln(2)}$ then

$$-\Psi(2,2) \leq q < 0$$

and so by Theorem 3.1 (part 4), the convex hexagonal system W has minimal TI-value over $\mathcal{HS}_h$ and by Theorem 3.5, E has maximal TI-value over $\mathcal{HS}_h$. ■

In conclusion, the extremal value problem of a topological index of the form (1) over the set $\mathcal{HS}_h$ is completely solved when $-\Psi(2,2) \leq q \leq 0$. We know the maximal value when $q > 0$ and the minimal value when $q < -\Psi(2,2)$. However, we do not have an answer for the following problem.

Problem 3.8 *The following questions remain open:*

1. *Find the minimal TI-value over $\mathcal{HS}_h$ when $q > 0$;*

2. *Find the maximal TI-value over $\mathcal{HS}_h$ when $q < -\Psi(2,2)$.*

Bearing in mind (4) and (7), Problem 3.8 is equivalent to find the maximal and minimial value of the function

$$S \rightsquigarrow b(S) + \frac{q + \Psi(2,2)}{q} n_i(S)$$

where S runs over the set $\mathcal{HS}_h$. Note that whether $q > 0$ or $q < -\Psi(2,2)$, we have $\frac{q+\Psi(2,2)}{q} > 0$. The difficulty here is that the maximal value of the function $b(S)$ occurs when $n_i(S)$ is minimal, and viceversa.

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