Extremal values of vertex–degree–based topological indices over fluoranthene-type benzenoid systems with equal number of edges

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Abstract

Let G be a graph with n vertices. A vertex–degree–based topological index is defined from a set of real numbers $\{\psi_{ij}\}$ as $$TI(G)=\sum_{1\leq i\leq j\leq n-1}m_{ij}\psi_{ij},$$ where m_{ij} is the number of edges of G connecting a vertex of degree i with a vertex of degree j. Many of the well–known topological indices are particular cases of this expression, including all Randi\'{c}-type connectivity indices. In this work we determine extremal values for TI over the set of fluoranthene–type benzenoid systems with a fixed number of edges. The main idea consists in constructing fluoranthene–type benzenoid systems with maximal number of inlets in Γ_{m} which have simultaneously minimal number of hexagons, where Γ_{m} is the set of fluoranthene–type benzenoid systems with exactly $m(m\geq19)$ edges.

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Abstract

Let G be a graph with n vertices. A vertex–degree–based topological index is defined from a set of real numbers $\{\psi_{ij}\}$ as

$$TI(G) = \sum_{1 \le i \le j \le n-1} m_{ij}\psi_{ij},$$

where m_{ij} is the number of edges of G connecting a vertex of degree i with a vertex of degree j. Many of the well–known topological indices are particular cases of this expression, including all Randić-type connectivity indices. In this work we determine extremal values for TI over the set of fluoranthene–type benzenoid systems with a fixed number of edges. The main idea consists in constructing fluoranthene–type benzenoid systems with maximal number of inlets in Γ_m which have simultaneously minimal number of hexagons, where Γ_m is the set of fluoranthene–type benzenoid systems with exactly $m(m \ge 19)$ edges.

Keywords: vertex–degree–based topological index, connectivity index, inlet, fluoranthene–type benzenoid system.

1 Introduction

In the chemical literature, a great variety of topological indices (molecular structure descriptors) have been and are currently considered in applications to QSPR/QSAR studies(see [14, 59]). Many of them depend only on the degrees of the vertices of the underlying molecular graph (i.e., graphs which represent chemicals) and are now called vertex–degree–based topological indices. More precisely, given nonnegative real numbers $\{\psi_{ij}\}$ $(1 \le i \le j \le n-1)$, a *vertex–degree–based topological index* (*VDB topological index* for short) of a (molecular) graph G with n vertices is expressed as

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

where m_{ij} is the number of edges of G connecting a vertex of degree i with a vertex of degree j. Many of the well–known VDB topological indices are particular cases of this expression, for example, if for every $1 \le i \le j \le n-1$ the numbers are $\psi_{ij} = \frac{1}{\sqrt{ij}}$, then we obtain the Randić index; if $\psi_{ij} = ij$ then the second Zagreb index is obtained [28], in the atom–bond connectivity index $\psi_{ij} = \sqrt{\frac{i+j-2}{ij}}$ [15], in the geometric–arithmetic index $\psi_{ij} = \frac{2\sqrt{ij}}{i+j}$ [60], in the sum–connectivity index $\psi_{ij} = \frac{1}{\sqrt{i+j}}$ [65], in the augmented Zagreb index $\psi_{ij} = \frac{(ij)^3}{(i+j-2)^3}$ [16] and in the harmonic index $\psi_{ij} = \frac{2}{i+j}$ [64], just to mention a few. Details of these and other VDB topological indices can be found in the books [26, 27, 44] and [7, 8, 13, 17, 21, 22, 37, 38].

In [39], we derived extremal values for TI over the set of fluoranthene–type benzenoid systems with given order. Our interest in this work is to study the extremal values of a TI of the form (1) over fluoranthene–type benzenoid systems with a fixed number of edges. For the definition of hexagonal systems and details of this theory we refer to [25].

Fluoranthene is a well–known tetracyclic conjugated hydrocarbon, present in large amounts in coal tar [6]. It consists of a benzene and a naphthalene unit, joined through a five–membered ring. Other polycyclic conjugated hydrocarbon, consisting of two benzenoid units joined through a five-membered ring are referred as *fluoranthene–type benzenoid system* (*f-benzenoid* for short) [20, 24]. A few examples of f-benzenoids are presented in Figure 1.

In what follows we will represent the f-benzenoid by means of their molecular graphs [24]. This, in particular, means that the carbon atoms are represented by vertices, and the carbon–carbon bonds by edges. The molecular graphs of f-benzenoid are then defined in the following manner. Let X be a benzenoid system [24]. Let u and v be two vertices of X whose degree is two, and which both are adjacent to a vertex w of degree 3. Let Y be another benzenoid system. Let a and b be two adjacent vertices of Y whose degree is two. The f-benzenoid F is obtained by joining (with a new

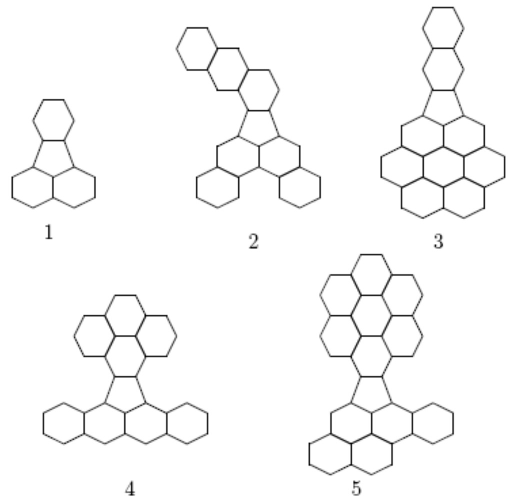


Figure 1: Examples of fluoranthene-type benzenoid systems. 1 and 2 are cata–catacondensed, 3 is peri–catacondensed, 4 is cata–pericondensed, and 5 is peri–pericondensed.

edge) the vertices u and a , and by joining (with a new edge) the vertices v and b (see Figure 2).

What first needs to be noticed is that the vertices a, b, v, w, u of F form a five-membered cycle. Each f-benzenoid possesses (by definition) exactly one five-membered cycle.

The f-benzenoids considered by us must pertain to plane graphs composed of regular hexagonals and a regular pentagon, all having the same edge lengths. Non–adjacent hexagon and hexagon–pentagon pairs must neither touch nor overlap (we exclude the helicenic and other geometrically non–plane species from the class of f-benzenoids). For more about f–benzenoid,

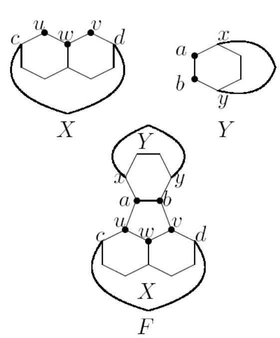
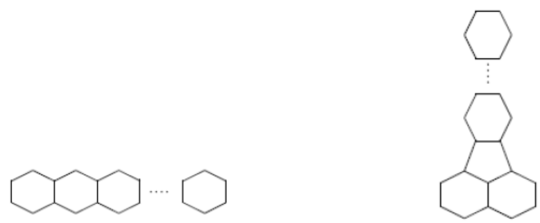


Figure 2: The general form of an f-benzenoid (F) and its construction from two benzenoid systems X and Y



(a) Linear chain (b) f-linear chain

Figure 3: Linear chain and f-linear chain.

one can see [24].

Throughout this paper, the notation and terminology are mainly taken from [9, 10, 19, 34, 35, 41, 42]. A benzenoid system is said to be *catacondensed* if it has no internal vertices; otherwise it is pericondensed [25]. In view of this, we propose the following classification of f–benzenoid. If the f–benzenoid F has just a single internal vertex, then it is said to be *cata–catacondensed*. This happens when both fragments X and Y (as shown in Figure 2) are catacondensed benzenoid systems.

Let L_h denote the *linear chain* with h hexagons(as shown in Figure 3(a)). A cata–catacondensed f–benzenoid is called an *f–linear chain* when fragment X is L_2 and Y is L_{h-2}, and which is denoted as FL_h, $h \geq 3$ (as shown in Figure 3(b)).

The following definitions were introduced in [24, 25]. If one goes along the perimeter of an f–benzenoid F, then a fissure (resp. a bay, cove, fjord, or lagoon) corresponds to a sequence of three (resp. four, five, six, or seven) consecutive vertices on the perimeter, of which the first and the last are vertices of degree 2 and the rest are vertices of degree 3. (For examples see Figure 4). The number of fissures, bays, coves, fjords and lagoons are denoted, respectively, by f, B, C, F_j and L.

Fissures, bays, coves, fjords and lagoons are called various types of *inlets*. The total number of inlets on the perimeter of F, $f+B+C+F_j+L$, will be denoted by r. There is another parameter $b = B + 2C + 3F_j + 4L$, called the *number of bay regions*, will be useful later. It is easy to see that $b \geq 2$ for all f–benzenoids, and b is just the number of $(3,3)$-type edges on the perimeter. Evidently, $f + 2B + 3C + 4F_j + 5L$ is the number of vertices of degree 3 on the perimeter.

First of all, all vertices in an f-benzenoid have degrees equal to 2 or 3, so, in further text, a i-vertex denotes a vertex of degree i, and a (i,j)-edge stands for an edge connecting a i-vertex with a j-vertex. The number of

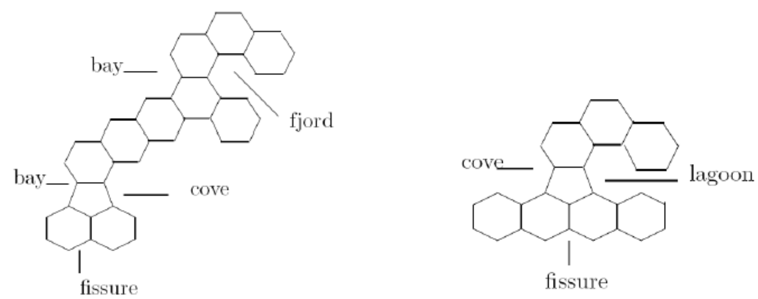


Figure 4: Structural features occurring on the boundary of f–benzenoids.

i-vertices and (i, j)-edges in the graph considered will be denoted by n_i and m_{ij}, respectively.

If F is an f–benzenoid with n vertices, m edges and h hexagons, then F possesses $h + 1$ cycles (h hexagons and a pentagon), so, $m = n + h$, and $n_2 + n_3 = n$, $2n_2 + 3n_3 = 2m$, it can be shown that $n_2 = n - 2h$, $n_3 = 2h$.

Some vertices of F lie on its perimeter. These will be referred to as *external vertices*, and their numbers are denoted by n_{ex}.

The vertices that are not external are said to be *internal*, and their numbers are denoted by n_i. Claearly, $n_{ex} + n_i = n$.

An f–benzenoid with h hexagons and n_i internal vertices represents a benzenoid hydrocarbon of the formula $C_{4h+5-n_i}H_{2h+5-n_i}$.

Lemma 1.1 [24] *Let F be an f–benzenoid with n vertices, m edges h hexagons and n_i internal vertices, Then*

(a) *the number of internal edges $m_i = h + n_i$;*

(b) $n = 4h + 5 - n_i$;

(c) $m = 5h + 5 - n_i$.

Lemma 1.2 [24] *Let F be an f–benzenoid with n vertices, h hexagons and r inlets, Then*

(a) $m_{22} = n - 2h - r$;

(b) $m_{23} = 2r$;

(c) $m_{33} = 3h - r$.

From a mathematical and chemical point of view, it is of great interest to find the extremal values of some useful VDB topological indices

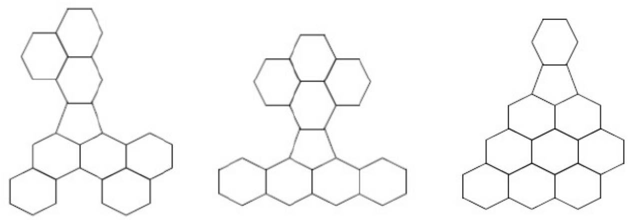


Figure 5: Some f–benzenoids in Γ_{42}

such as connectivity index, general connectivity index, second Zagreb index, atom–bond connectivity index, sum–connectivity index, geometric–arithmetic index, augmented Zagreb index, harmonic index for significant classes of graphs. Many results concerning this topic can be found in [2, 7, 17, 23, 30, 32, 38, 39, 40, 41, 42, 43, 48, 49, 52, 53, 54, 57, 61, 62].

In this paper, we will determine the extremal values of a VDB topological index TI over the f–benzenoids with equal number of edges m, and we will characterize the corresponding f–benzenoids depending if the number of edges m is congruent to 0, 1, 2, 3 or 4 modulo 5. Then we will apply these results to find the extremal values of some well-known VDB topological indices over f–benzenoids with fixed number of edges m.

2 Maximal number of inlets in Γ_m

Let Γ_m denote the set of f–benzenoids with exactly m edges. We will find in this section the f–benzenoids with maximal number of inlets in Γ_m and then, we will apply this result in the study of extremal values of VDB topological indices. Figure 5 shows several f–benzenoids belonging to Γ_{42}.

Note that the number of hexagons in f–benzenoids belonging to Γ_m is variable. So, we try to find the lower and upper bounds for the number of hexagons in any $F \in \Gamma_m$. Firstly, we recall the concept of the spiral benzenoid system [29].

The *spiral benzenoid system* T_h is an hexagonal system with maximal number of internal vertices which are constructed by the "spiral" method illustrated in Figure 6.

By analogy with an extremal benzenoid system, an *extremal f–benzenoid* is defined by possessing the maximum number of internal vertices for a given number of hexagons: $n_i = (n_i)_{max}$ [42].

For convenience, we let $SH_h (h \geq 3)$ denote the set of all f–benzenoids whose two fragments X and Y are both spiral benzenoids. Especially, an f–benzenoid system $F^* \in SH_h$ with two fragments $X = T_{h-1}$ and $Y = T_1$ is

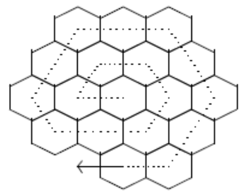


Figure 6: The spiral benzenoid system T_h with maximal number of internal vertices. Hexagons have to be added one-by-one, going along the indicated spiral line.

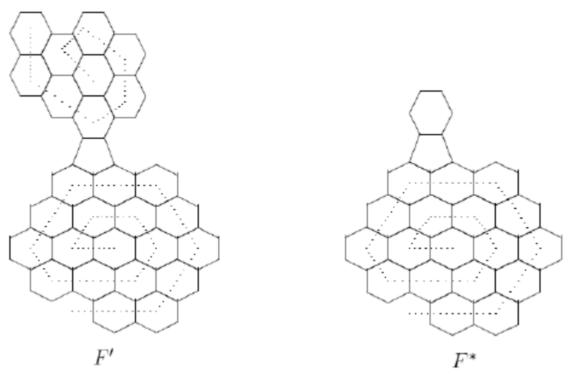


Figure 7: f–benzenoid $F' \in SH_h$ whose two fragments X and Y are both spiral benzenoid systems, and f–spiral benzenoid $F^* \in SH_h$ with two fragments $X = T_{h-1}$ and $Y = T_1$.

called an *f-spiral benzenoid* (as shown in Figure 7). It is obvious that

$$n_i(F^*) = 2h - \lceil \sqrt{12(h-1)-3}\, \rceil.$$

Lemma 2.1 [42] *For any f–benzenoid F with $h \geq 3$ hexagons, we have*

$$n_i(F) \leq n_i(F^*) = 2h - \left\lceil \sqrt{12(h-1)-3} \right\rceil. \tag{2}$$

The following theorem gives the upper and lower bounds for the number of hexagons in f–benzenoids $F \in \Gamma_m$.

Theorem 2.1 *For any f–benzenoid $F \in \Gamma_m$,*

$$\left\lceil \frac{1}{5}(m-4) \right\rceil \leq h(F) \leq m - 1 - \left\lceil \frac{1}{3}\left(2m + \sqrt{4m-31}\right) \right\rceil, \tag{3}$$

where $h(F)$ denotes the number of hexagons in F. $\lceil x \rceil$ is the smallest integer not smaller than x.

Proof. On one hand, from Lemma 1.1 (c) we know that $m = 5h(F) + 5 - n_i(F)$. Combining the fact that for any f–benzenoid F, $n_i(F) \geq 1$, we get

$$h(F) \geq \left\lceil \frac{1}{5}(m-4) \right\rceil .$$

On the other hand, by Lemma 2.1 we know that

$$n_i(F) \leq n_i(F^*) = 2h - \left\lceil \sqrt{12(h-1)-3} \right\rceil .$$

Consequently, from $m = 5h(F) + 5 - n_i(F)$ we have

$$m - 3h(F) - 5 \geq \left\lceil \sqrt{12(h(F)-1)-3} \right\rceil \geq \sqrt{12(h(F)-1)-3}.$$

Hence,

$$(3h(F) + (3-m))^2 \geq 4m - 31.$$

By observing the fact that $3h(F) + (3-m) < 0$, we deduce

$$3h(F) + (3-m) \leq -\sqrt{4m-31},$$

i.e.,

$$h(F) \leq m - 1 - \left\lceil \frac{1}{3}\left(2m + \sqrt{4m-31}\right) \right\rceil .$$

This completes the proof. ∎

Remark 1 *From Theorem 2.1 we know that the f–spiral benzenoid F^* has the maximal number of hexagons over Γ_m.*

One crucial problem in the study of extremal values of topological indices is to find among all f–benzenoid in Γ_m, the f–benzenoids which have maximal number of inlets. We will show that in SH_h, the f–benzenoid F with maximal number of inlets has minimal number of hexagons $h(F) = \lceil \frac{1}{5}(m-4) \rceil$.

In order to prove this result we need some preliminaries lemmas. Recall that the *convex benzenoid systems* is a special class of benzenoid systems in which there are no bay regions [7]. We denote by $\mathcal{HS}_h$ the set of benzenoid systems with h hexagons.

Lemma 2.2 [2] *Let $H \in \mathcal{HS}_h$. In each of the following conditions H is not a convex benzenoid system:*

(a) *If $h \geq 4$ and $n_i = 1$;*

(b) *If $h \geq 5$ and $n_i = 2$;*

(c) *If $h \geq 6$ and $n_i = 3$.*

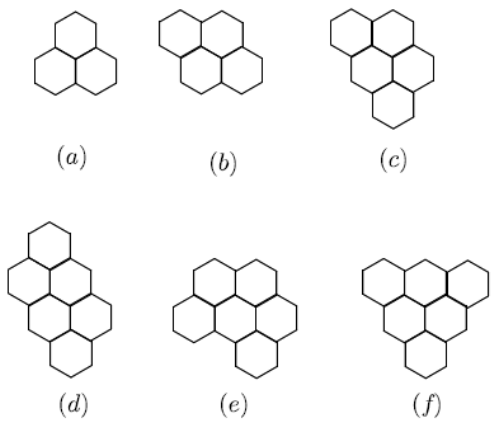


Figure 8: Benzenoid systems with 1, 2, 3 and 4 internal vertices, respectively

Lemma 2.3 [54] *Let $H \in \mathcal{HS}_h$ such that $n_i(H) = 4$. Then H must contain a subbenzenoid system of the form given in Figure 8, where no hexagons are adjacent to the fissures.*

Lemma 2.4 *Let $H \in \mathcal{HS}_h$. If $h \geq 7$ and $n_i(H) = 4$, then H is not a convex benzenoid system.*

Proof. If $h = 6$ then H is one of the benzenoid systems (d), (e) and (f) in Figure 8. It is clear that both (d) and (f) are convex benzenoid systems, but (e) is not. If $h \geq 7$, by Lemma 2.3, H has a subbenzenoid system as in Figure 8, where no hexagons are adjacent to the fissures. Since $h \geq 7$ there must exist hexagons adjacent to a $(2,2)$-edge, and these hexagons will transform one of the fissures into a bay, cove or fjord. Consequently, $b(H) \geq 1$.

Lemma 2.5 [38] *Let F be a f–benzenoid with h hexagons. Then*

$$r(F) \leq \begin{cases} r(FL_h) = 2h - 3 \ (h \geq 3), & if \ n_i = 1 \\ r(G_h) = 2h - 4 \ (h \geq 4), & if \ n_i = 2 \\ r(R_h) = 2h - 5 \ (h \geq 5), & if \ n_i = 3 \\ r(Z_h) = 2h - 6 \ (h \geq 6), & if \ n_i = 4 \end{cases}$$

Next we find the f–benzenoids with maximal number of inlets in Γ_m with a fixed number of internal vertices. Recall that M_h, N_h and Q_h (see Figure 9) are benzenoid systems, and G_h (see Figure 10), R_h (see Figure 11), Z_h (see Figure 12) are f–benzenoids.

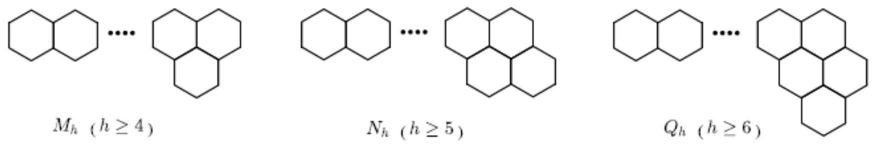


Figure 9: Three types of benzenoid systems

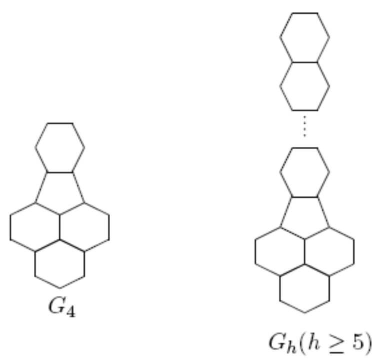


Figure 10: f-benzenoids G_4, and $G_h(h \geq 5)$

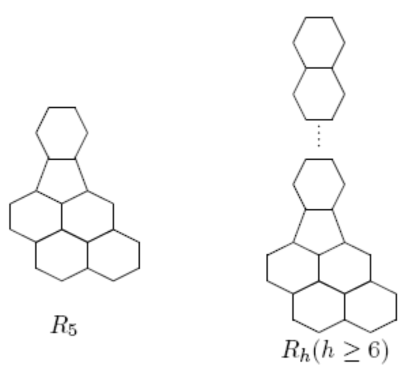
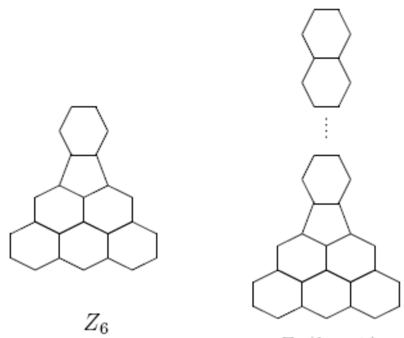
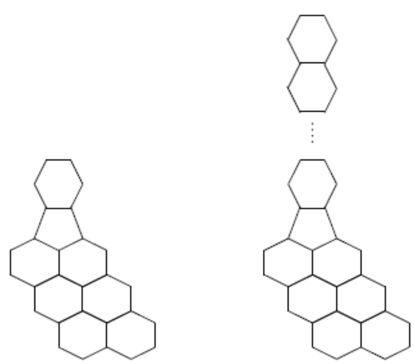


Figure 11: f-benzenoids R_5, and $R_h(h \geq 6)$



Z_6 $Z_h(h \geq 7)$

Figure 12: f-benzenoids Z_6, and $Z_h(h \geq 7)$



U_7 $U_h(h \geq 8)$

Figure 13: f-benzenoids U_7, and $U_h(h \geq 8)$

Lemma 2.6 [42] *For any f–benzenoid F with h hexagons,*

$$r(F) \leq r(FL_h) = 2h - 3.$$

Lemma 2.7 [24] *If a f–benzenoid has h hexagons, n_i internal vertices, and b bay regions, then the counts of edges of type $(2,2)$ and $(2,3)$ are $m_{22} = b+5, m_{23} = 4h - 2n_i - 2b$.*

Combining Lemma 1.2 (b) and Lemma 2.6, we get

$$r = 2h - n_i - b \tag{4}$$

Furthermore, by Lemma 1.1 (c) and equation (4), we deduce

$$r = m - 3h - 5 - b \tag{5}$$

Theorem 2.2 *Let F be a f–benzenoid with h hexagons. If $n_i = 5$, then $r(F) \leq r(U_h) = 2h - 7$ $(h \geq 7)$.*

Proof. Let X and Y be two fragments in F, h_1 and h_2 denote the number of hexagons in X and Y, respectively. If $n_i = 5$, the proof proceeds in five cases.

Case 1 $n_i(X) = 1$, and $n_i(Y) = 3$, i.e., X has an internal vertex, but Y has three internal vertices.

Subcase 1.1 If $h_1 = 3$, then $X = M_3$.

Subcase 1.1.1 If $h_2 = 5$, i.e., $Y = Q_5$, then F is the f–benzenoids D_1, D_2 or D_3 (see Figure 14). It is easy to see that $r(F) = r(D_1) = 8$, $r(F) = r(D_2) = 7$ or $r(F) = r(D_3) = 8$.

Subcase 1.1.2 If $h_2 \geq 6$, then by Lemma 2.2, Y is not a convex benzenoid system, i.e., $b(Y) \geq 1$. In this case $b(F) \geq 3$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 8 < 2h - 7$.

Subcase 1.2 If $h_1 \geq 4$, then by Lemma 2.2, X is not a convex benzenoid system, i.e., $b(X) \geq 1$.

Subcase 1.2.1 If $h_2 = 5$, i.e., $Y = Q_5$. It is easy to see that $b(F) \geq 4$, consequently from equation (4) we deduce $r = 2h - n_i - b \leq 2h - 9 < 2h - 7$.

Subcase 1.2.2 If $h_2 \geq 6$, then by Lemma 2.2, Y is not a convex benzenoid system, i.e., $b(Y) \geq 1$. It is easy to see that $b(F) \geq 5$, consequently from equation (4) we deduce $r = 2h - n_i - b \leq 2h - 10 < 2h - 7$.

Case 2 $n_i(X) = 3$ and $n_i(Y) = 1$, i.e., X has three internal vertices, but Y has one internal vertex.

Subcase 2.1 If $h_1 = 5$, then $X = Q_5$.

Subcase 2.1.1 If $h_2 = 3$, ie., $Y = M_3$, then F is the f–benzenoids D_4, D_5, D_6 (see Figure 14), or D_7 (as shown in Figure 15). $r(F) = r(D_4) = 8$, $r(F) = r(D_5) = 7$, $r(F) = r(D_6) = 8$, $r(F) = r(D_7) = 7$.

Subcase 2.1.2 If $h_2 \geq 4$, by Lemma 2.2, Y is not a convex benzenoid system, i.e., $b(X) \geq 1$. In this case we have $b(F) \geq 4$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 9 < 2h - 7$.

Subcase 2.2 If $h_1 \geq 6$, by Lemma 2.2, X is not a convex benzenoid system, i.e., $b(X) \geq 1$.

Subcase 2.2.1 If $h_2 = 3$, ie., $Y = M_3$. In this case we have $b(F) \geq 4$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 9 < 2h - 7$.

Subcase 2.2.2 f $h_2 \geq 4$, by Lemma 2.2, Y is not a convex benzenoid system, i.e., $b(X) \geq 1$. In this case we have $b(F) \geq 5$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 10 < 2h - 7$.

Case 3 $n_i(X) = 2$ and $n_i(Y) = 2$, i.e., X and Y both have two internal vertices.

Subcase 3.1 If $h_1 = 4$, then $X = N_4$.

Subcase 3.1.1 If $h_2 = 4$, F is the f–benzenoids D_8 or D_9 (as shown in Figure 15). $r(F) = r(D_8) = 8$ or $r(F) = r(D_9) = 7$.

Subcase 3.1.2 If $h_2 \geq 5$, by Lemma 2.2, Y is not a convex benzenoid system, i.e., $b(X) \geq 1$. Then $b(F) \geq 4$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 9 < 2h - 7$.

Subcase 3.2 If $h_2 = 4$, i.e., $Y = N_4$.

Subcase 3.2.1 If $h_1 = 4$, i.e., $X = N_4$. F is the f–benzenoid D_8 or D_9(as shown in Figure 15). $r(F) = r(D_8) = 8$ or $r(F) = r(D_9) = 7$.

Subcase 3.2.2 If $h_1 \geq 5$, by Lemma 2.2, X is not a convex benzenoid system, i.e., $b(X) \geq 1$. In this case, $b(F) \geq 4$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 9 < 2h - 7$.

Subcase 3.3 If $h_1 \geq 5$, $h_2 \geq 5$, by Lemma 2.2, neither X nor Y are convex benzenoid systems, i.e., $b(X) \geq 1$ and $b(Y) \geq 1$. In this case $b(F) \geq 5$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 10 < 2h - 7$.

Case 4 $n_i(X) = 4$ and $n_i(Y) = 0$, i.e., X has four internal vertex, Y is a catacondensed benzenoid system.

Subcase 4.1 If $h_1 = 6$, then X is the benzenoid system (d), (e) or (f) in Figure 8.

Subcase 4.1.1 If $h_2 = 1$, F is the f–benzenoids D_{10}, D_{11}, D_{12} (see Figure 16), D_{13} (see Figure 17) or U_7 (see Figure 13). $r(F) = r(D_{10}) = 6$, $r(F) = r(D_{11}) = 6$, $r(F) = r(D_{12}) = 6$, $r(F) = r(D_{13}) = 6$ or $r(F) = r(U_7) = 7$.

Subcase 4.1.2 If $h_2 \geq 2$, then $b(F) \geq 2$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 7$.

Subcase 4.2 If $h_1 \geq 7$, by Lemma 2.4, X is not a convex benzenoid system, i.e., $b(Y) \geq 1$. In this case $b(F) \geq 3$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 8 < 2h - 7$.

Case 5 $n_i(X) = 0$ and $n_i(Y) = 4$, i.e., X is a catacondensed benzenoid system, Y has four internal vertex.

Subcase 5.1 If $h_2 = 6$, then Y is the benzenoid system (d), (e) or (f) in Figure 8.

Subcase 5.1.1 If $h_1 = 2$, F is the f–benzenoids D_{14}, D_{15}, D_{16}, D_{17}, D_{18}, D_{19}, D_{20} or D_{21} (see Figure 17). $r(F) = r(D_{14}) = 7$, $r(F) = r(D_{15}) = 8$, $r(F) = r(D_{16}) = 8$, $r(F) = r(D_{17}) = 7$, $r(F) = r(D_{18}) = 7$, $r(F) = r(D_{19}) = 8$, $r(F) = r(D_{20}) = 6$ or $r(F) = r(D_{21}) = 6$.

Subcase 5.1.2 If $h_1 \geq 3$, then $b(F) \geq 4$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 9 < 2h - 7$.

Subcase 5.2 If $h_2 \geq 7$, by Lemma 2.4, Y is not a convex benzenoid system, i.e., $b(Y) \geq 1$.

Subcase 5.2.1 If $h_1 = 2$, i.e., $X = L_2$. In this case $b(F) \geq 4$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 9 < 2h - 7$.

Subcase 5.2.2 If $h_1 \geq 3$, then $b(F) \geq 5$, by equation (4) it follows that $r = 2h - n_i - b \leq 2h - 10 < 2h - 7$.

This completes the proof. ∎

Now we can find the f–benzenoids with maximal number of inlets in Γ_m, the set of f–benzenoids with m edges. We recall that FL_h is the f–linear chain with h hexagons.

Theorem 2.3 *Let $F \in \Gamma_m$. Then*

1. *If $m \equiv 0(mod5)$, then $r(F) \leq \frac{2m-35}{5} = r(U_{\frac{m}{5}})$;*
2. *If $m \equiv 1(mod5)$, then $r(F) \leq \frac{2m-32}{5} = r(Z_{\frac{m-1}{5}})$;*
3. *If $m \equiv 2(mod4)$, then $r(F) \leq \frac{2m-29}{5} = r(R_{\frac{m-2}{5}})$;*
4. *If $m \equiv 3(mod5)$, then $r(F) \leq \frac{2m-26}{5} = r(G_{\frac{m-3}{5}})$;*

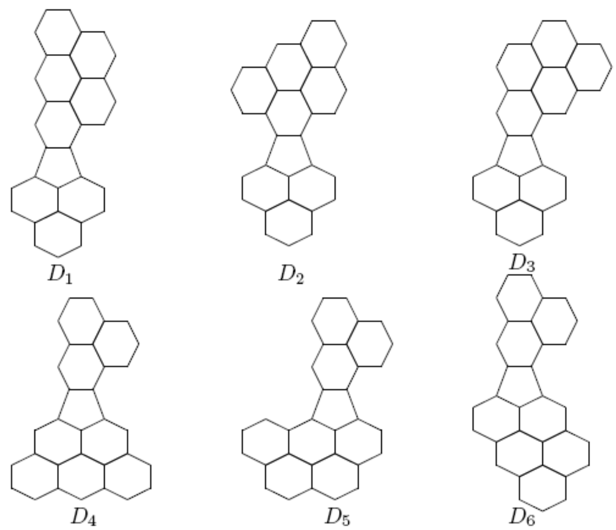


Figure 14: f-benzenoids D_1, D_2, D_3, D_4 and D_5

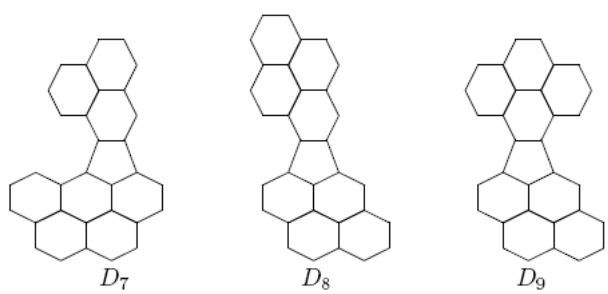


Figure 15: f-benzenoids D_7, D_8 and D_9

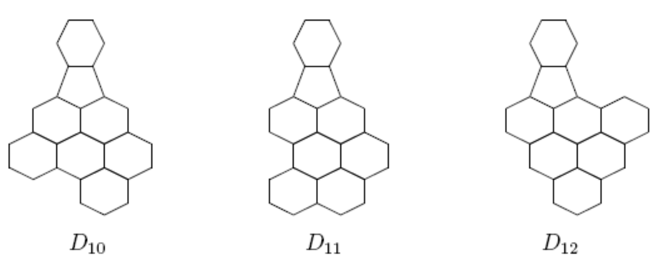


Figure 16: f-benzenoids D_{10}, D_{11} and D_{12}

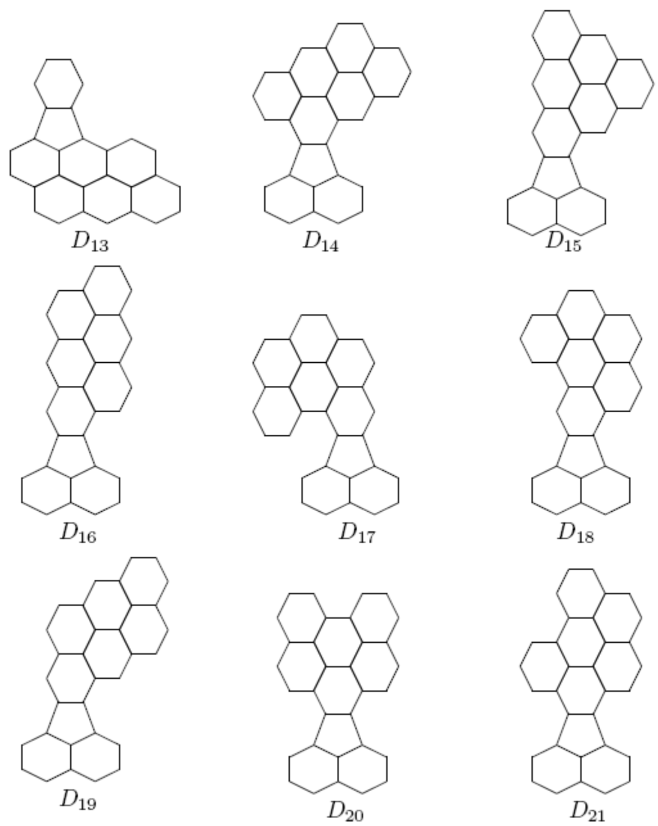


Figure 17: f-benzenoids D_{13}, D_{14}, D_{15}, D_{16}, D_{17}, D_{18}, D_{19}, D_{20} and D_{21}

5. *If* $m \equiv 4(mod5)$, *then* $r(F) \leq \frac{2m-23}{5} = r(FL_{\frac{m-4}{5}})$.

Proof. We know by equation (3) that

$$\left\lceil \frac{1}{5}(m-4) \right\rceil \leq h(F) \leq m-1-\left\lceil \frac{1}{3}\left(2m+\sqrt{4m-31}\right) \right\rceil.$$

1. If $m \equiv 0(mod5)$, then $\left\lceil \frac{1}{5}(m-4) \right\rceil = \frac{m}{5}$. If $h = \frac{m}{5}$, then by Lemma 1.1 (c)

$$m = 5h(F) + 5 - n_i(F) = 5(\frac{m}{5}) + 5 - n_i(F) = m + 5 - n_i(F),$$

and so $n_i(F) = 5$. Now we can apply Theorem 2.2, to conclude that $r(F) \leq r(U_{\frac{m}{5}})$ and we are done. So assume now that $h(F) \geq \frac{m}{5} + 1$, then by equality (5) and the fact that $b(F) \geq 2$

$$r(F) = m - 5 - 3h(F) - b(F) \leq m - 5 - 3(\frac{m}{5} + 1) - b(F)$$

$$\leq \frac{2m}{5} - 10 = \frac{2m-50}{5} \leq \frac{2m-35}{5} = r(U_{\frac{m}{5}}).$$

2. If $m \equiv 1(mod5)$, then $\left\lceil \frac{1}{5}(m-4) \right\rceil = \frac{m-1}{5}$. If $h(F) = \frac{m-1}{5}$, then by Lemma 1.1 (c)

$$m = 5h(F) + 5 - n_i(F) = 5(\frac{m-1}{5}) + 5 - n_i(F) = m + 4 - n_i(F),$$

and so $n_i(F) = 4$. Then $r(F) \leq r(Z_{\frac{m-1}{5}})$ by part 4 of Lemma 2.5. Otherwise $h(F) \geq \frac{m-1}{5} + 1$, then by equality (5) and the fact that $b(F) \geq 2$

$$r(F) = m - 5 - 3h(F) - b(F) \leq m - 5 - 3(\frac{m-1}{5} + 1) - b(F)$$

$$\leq \frac{2m+3}{5} - 10 = \frac{2m-47}{5} \leq \frac{2m-32}{5} = r(Z_{\frac{m-1}{5}}).$$

3. If $m \equiv 2(mod5)$, then $\left\lceil \frac{1}{5}(m-4) \right\rceil = \frac{m-2}{5}$. If $h(F) = \frac{m-2}{5}$, then by Lemma 1.1 (c)

$$m = 5h(F) + 5 - n_i(F) = 5(\frac{m-2}{5}) + 5 - n_i(F) = m + 3 - n_i(F),$$

and so $n_i(F) = 3$. It follows from Lemma 2.5 part 3 that $r(F) \leq r(R_{\frac{m-2}{5}})$. So assume now that $h(F) \geq \frac{m-2}{5} + 1$, then by equation (5) and the fact that $b(F) \geq 2$

$$r(F) = m - 5 - 3h(F) - b(F) \leq m - 5 - 3(\frac{m-2}{5} + 1) - b(F)$$

$$\leq \frac{2m+6}{5} - 10 = \frac{2m-44}{5} \leq \frac{2m-29}{5} = r(R_{\frac{m-2}{5}}).$$

4. If $m \equiv 3(mod5)$, then $\lceil \frac{1}{5}(m-4) \rceil = \frac{m-3}{5}$. If $h(F) = \frac{m-3}{5}$, then by Lemma 1.1 (c)

$$m = 5h(F) + 5 - n_i(F) = 5(\frac{m-3}{5}) + 5 - n_i(F) = m + 2 - n_i(F),$$

and so $n_i(F) = 2$. By Lemma 2.5 part 2, to conclude that $r(F) \leq r(G_{\frac{m-3}{5}})$ and we are done. So assume now that $h(F) \geq \frac{m-3}{5} + 1$, then by equality (5) and the fact that $b(F) \geq 2$

$$r(F) = m - 5 - 3h(F) - b(F) \leq m - 5 - 3(\frac{m-3}{5} + 1) - b(F)$$
$$\leq \frac{2m+9}{5} - 10 = \frac{2m-41}{5} \leq \frac{2m-26}{5} = r(G_{\frac{m-3}{5}}).$$

5. If $m \equiv 4(mod5)$, then $\lceil \frac{1}{5}(m-4) \rceil = \frac{m-4}{5}$. Since $h \geq \frac{m-4}{5}$, then by equation (5) and the fact that $b(F) \geq 2$

$$r(F) = m - 5 - 3h(F) - b(F) \leq m - 5 - \frac{3m-12}{5} - b(F)$$
$$\leq \frac{2m+12}{5} - 7 = \frac{2m-23}{5} = r(FL_{\frac{m-4}{5}}).$$

This completes the proof. ∎

3 Extremal values of VDB topological indices over Γ_m

In this section, we will try to find the extremal values of VDB topological indices over Γ_m.

Let TI be a VDB topological index induced by the real nonnegative numbers $\{\psi_{ij}\}$ $(1 \leq i \leq j \leq n-1)$. In the particular case that F is an f–benzenoid, only vertices of degree 2 and 3 appear and so equation (1) reduces to

$$TI(F) = m_{22}\psi_{22} + m_{23}\psi_{23} + m_{33}\psi_{33}, \tag{6}$$

By Lemmas 1.1 and 1.2, we get

$$TI(F) = \psi_{22}m + 3(\psi_{33} - \psi_{22})h + (2\psi_{23} - \psi_{22} - \psi_{33})r, \tag{7}$$

If $U, V \in \Gamma_m$ then clearly

$$\begin{aligned} TI(U) - TI(V) = 3(\psi_{33} - \psi_{22})(h(U) - h(V)) \\ + (2\psi_{23} - \psi_{22} - \psi_{33})(r(U) - r(V)). \end{aligned} \tag{8}$$

For convenience, we set $s = \psi_{33} - \psi_{22}$, $q = 2\psi_{23} - \psi_{22} - \psi_{33}$.

Theorem 3.1 *Let TI be a VDB topological index of the form (7) induced by the nonnegative real numbers $\{\psi_{22}, \psi_{23}, \psi_{33}\}$. Assume that $s \leq 0$ and $q \geq 0$ (resp. $s \geq 0$ and $q \leq 0$). Then the maximal(resp. minimal) TI–value over Γ_m is attained in:*

1. $U_{\frac{m}{5}}$ *if* $m \equiv 0(mod5)$*;*
2. $Z_{\frac{m-1}{5}}$ *if* $m \equiv 1(mod5)$*;*
3. $R_{\frac{m-2}{5}}$ *if* $m \equiv 2(mod4)$*;*
4. $G_{\frac{m-3}{5}}$ *if* $m \equiv 3(mod5)$*;*
5. $FL_{\frac{m-4}{5}}$ *if* $m \equiv 4(mod5)$*.*

Proof. Let $F \in \Gamma_m$. Note that by equation (3)

$$h(F) \geq \left\lceil \frac{1}{5}(m-4) \right\rceil = \begin{cases} h(U_{\frac{m}{5}}), & if\ m \equiv 0(mod5) \\ h(Z_{\frac{m-1}{5}}), & if\ m \equiv 1(mod5) \\ h(R_{\frac{m-2}{5}}), & if\ m \equiv 2(mod5) \\ h(G_{\frac{m-3}{5}}), & if\ m \equiv 3(mod5) \\ h(FL_{\frac{m-4}{5}}), & if\ m \equiv 4(mod5) \end{cases}$$

Hence by Theorem 2.3 the f–benzenoids $U_{\frac{m}{5}}$, $Z_{\frac{m-1}{5}}$, $R_{\frac{m-2}{5}}$, $G_{\frac{m-3}{5}}$ and $FL_{\frac{m-4}{5}}$ have simultaneously maximal number of inlets and minimal number of hexagons over the set Γ_m of f–benzenoids with m edges. Hence the result follows from equation (8) and the signs of q and s.
This completes the proof. ∎

Example 1 *The following Table 1 contains the values of s and q for several well–known topological indices:*

Table 1: Values of s and q for six well–known topological indices

	ij	$\frac{1}{\sqrt{ij}}$	$\frac{2\sqrt{ij}}{i+j}$	$\frac{1}{\sqrt{i+j}}$	$\frac{(ij)^3}{(i+j-2)^3}$	$\sqrt{\frac{i+j-2}{ij}}$
q	-1	-0.0168	-0.0404	-0.0138	-3.390	0.040
s	5	-0.1667	0	-0.091	3.390	-0.040

Hence, by Theorems 2.3 and 3.1 we can deduce in the case of the second Zagreb index, geometric–arithmetic index and the augmented Zagreb index we can determine the minimal value of TI, and for the atom–bond–connectivity index we can determine the maximal value of TI.

If F is an f–benzenoid with m edges, then from the equations (4), (7) and Lemma 1.1(c) we deduce

$$\begin{aligned} TI(F) = {} & (2\psi_{23} - \psi_{33})m + 6(\psi_{33} - \psi_{23})h - (2\psi_{23} - \psi_{22} - \psi_{33})b \\ & - 5(2\psi_{23} - \psi_{22} - \psi_{33}). \end{aligned} \tag{9}$$

Consequently, for f–benzenoids $U, V \in \Gamma_m$

$$\begin{aligned} TI(U) - TI(V) = {} & 6(\psi_{33} - \psi_{23})(h(U) - h(V)) \\ & + (-2\psi_{23} + \psi_{22} + \psi_{33})(b(U) - b(V)). \end{aligned} \tag{10}$$

Set $u = 6(\psi_{33} - \psi_{23})$ and keep the notation for q introduced earlier. Then

$$TI(U) - TI(V) = u(h(U) - h(V)) - q(b(U) - b(V)). \tag{11}$$

As we can see this expression only depends on the number of hexagons and the number of bay regions. We know from equation (3) that the maximal value possible of hexagons in a f–benzenoid with m edges is

$$m - 1 - \left\lceil \frac{1}{3}\left(2m + \sqrt{4m - 31}\right) \right\rceil,$$

and this occurs precisely in the f–spiral hexagon system F^*.

By the structure of the f–spiral benzenoid system F^*, we know that $n_i(F^*) = 2h - \left\lceil \sqrt{12(h-1)} - 3 \right\rceil$. But, $b(F^*)$ may not always equal to 2. It is obvious that if fragment X of F^* satisfies that $b(X) = 0$, i.e., X is a convex benzenoid system, we can get a f–benzenoid F^* such that $b(F^*) = 2$ or 3.

But, we know that the fragment X constructed by the "spiral" method are not necessarily convex (and may have a single bay, i.e., $B = 1$). So, it is naturally for us to find a method to transform a spiral benzenoid system into a convex benzenoid system with equal number of internal vertices.

The structure of a convex benzenoid system W can be specified as $W = H(a_1, a_2, a_3, a_4, a_5, a_6)$ for positive integers $a_1, a_2, a_3, a_4, a_5, a_6$. Their general form is depicted in Figure 18. It has been demonstrated [7] that W is completely determined by the parameters a_1, a_2, a_3, a_4, since it must be

$$a_5 = a_1 + a_2 - a_4, \qquad a_6 = a_3 + a_4 - a_1.$$

Fortunately, the authors in [57] precisely determined necessary and sufficient conditions for the existence of convex benzenoid systems with maximal number of internal vertices.

Lemma 3.1 [57] *Let h be a positive integer. The following conditions are equivalent:*

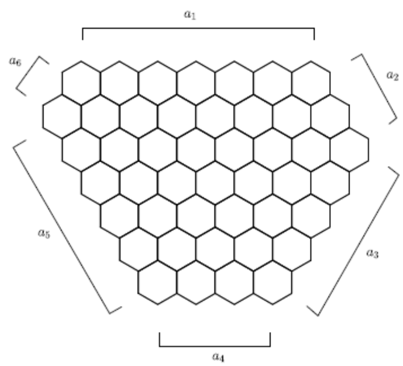


Figure 18: The general form of a convex benzenoid system (CHS). The parameters $a_i \geq 1, i = 1, 2, \cdots, 6$, count the hexagons on the respective side of CHS.

(a) *There exists a convex benzenoid system W with h hexagons satisfying*

$$n_i(W) = 2h + 1 - \lceil \sqrt{12h - 3}\ \rceil;$$

(b) *There exist a set of positive integers a_1, a_2, a_3, a_4 which are solutions of the system of equation*

$$\left.\begin{array}{c} h = a_1a_3 + a_1a_4 + a_2a_3 + a_2a_4 - a_2 - a_3 \\ -\frac{1}{2}a_1(a_1+1) - \frac{1}{2}a_4(a_4+1) + 1 \\ \lceil \sqrt{12h-3}\ \rceil = a_1 + 2a_2 + 2a_3 + a_4 - 3 \end{array}\right\} \tag{12}$$

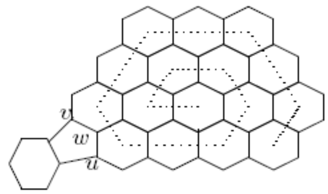
If the system of equation (12) has a solution for a positive integer h, then there exists a convex benzenoid system W such that $n_i(W) = n_i(T_h)$. But, Rada et al. [57] show that not for every positive integer h there is a solution for the system of equation (12). As a byproduct, they show that given a positive integer h, the existence of convex benzenoid systems with maximal number of internal vertices imply the existence of a solution to the following Diophantine equation

$$21x^2 + 3y^2 + z^2 = 28(\lceil \sqrt{12h-3}\ \rceil^2 - (12h - 3)).$$

This gives a method to find values of h for which there are no convex benzenoid systems which satisfy $n_i(W) = n_i(T_h)$.

We now return to the study of TI of f–benzenoids. If the following system

$$\left.\begin{array}{c} h - 1 = a_1a_3 + a_1a_4 + a_2a_3 + a_2a_4 - a_2 - a_3 \\ -\frac{1}{2}a_1(a_1+1) - \frac{1}{2}a_4(a_4+1) + 1 \\ \lceil \sqrt{12(h-1)-3}\ \rceil = a_1 + 2a_2 + 2a_3 + a_4 - 3 \\ \exists\ a_i \in \{a_1, a_2, a_3, a_4, a_5, a_6\},\ a_i = 2 \end{array}\right\} \tag{13}$$



F_1^*

Figure 19: An f–spiral benzenoid F_1^* whose fragment X is a convex spiral benzenoid system W_{h-1}

has a solution $\{a_1, a_2, a_3, a_4\}$ for a positive integer $h-1$, then there exists a convex spiral benzenoid system W_{h-1} such that

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

Note that element a_i in the set $\{a_1, a_2, a_3, a_4, a_5, a_6\}$ equal to 2, we let W_{h-1} be the X fragment, and it is obvious that W_{h-1} possess only one fissure on the side of a_i. Let the three vertices of this fissure be u, w, v in Figure 2, and let Y be a single hexagon, then we get an f–spiral benzenoid F_1^* with h hexagons such that $n_i(F_1^*) = 2h - \left\lceil \sqrt{12(h-1)-3} \right\rceil$ and $b(F_1^*) = 2$. (as shown in Figure 19)

Theorem 3.2 *Let $h-1$ be a positive integer such that the system of equation* (13) *has a solution, and $m = 3h + 5 + \left\lceil \sqrt{12(h-1)-3} \right\rceil$. Then*

1. *If $u \geq 0$ and $q \geq 0$, then TI reaches its maximal value in F_1^* over Γ_m;*
2. *If $u \leq 0$ and $q \leq 0$, then TI reaches its minimal value in F_1^* over Γ_m.*

Proof. Since $n_i(F_1^*) = 2h - \left\lceil \sqrt{12(h-1)-3} \right\rceil$. Then

$$n(F_1^*) = 4h + 5 - (2h - \left\lceil \sqrt{12(h-1)-3} \right\rceil) = 2h + 5 + \left\lceil \sqrt{12(h-1)-3} \right\rceil$$

and so F_1^* has m edges. Also we know by hypothesis that $b(F_1^*) = 2$. On the other hand, $m = 3h + 5 + \left\lceil \sqrt{12(h-1)-3} \right\rceil$ implies that

$$h = m - 1 - \left\lceil \frac{1}{3}\left(2m + \sqrt{4m-31}\right) \right\rceil .$$

Hence by equations (3) and (11) it follows that for any f–benzenoid $F \in \Gamma_m$

$$TI(F) - TI(F_1^*) = u(h(F) - h(F_1^*)) - q(b(F) - b(F_1^*))$$

$$= u\left[h(F) - \left(m - 1 - \left\lceil \frac{1}{3}\left(2m + \sqrt{4m-31}\right)\right\rceil\right)\right] - q[b(F) - 2]$$

It is easy to see that $b(F) \geq 2$. It is clear now that if $u \geq 0$ and $q \geq 0$ then $TI(F) - TI(F_1^*) \leq 0$ which implies that F_1^* reaches its maximal value over Γ_m. Similarly, if $u \leq 0$ and $q \leq 0$ then $TI(F) - TI(F_1^*) \geq 0$ which implies that F_1^* reaches its minimal value over Γ_m.
This completes the proof. ∎

Example 2 *The following Table 2 contains the values of* u *and* q *for several well–known topological indices:*

Table 2: Values of u and q for six well–known topological indices

	ij	$\frac{1}{\sqrt{ij}}$	$\frac{2\sqrt{ij}}{i+j}$	$\frac{1}{\sqrt{i+j}}$	$\frac{(ij)^3}{(i+j-2)^3}$	$\sqrt{\frac{i+j-2}{ij}}$
q	-1	-0.0168	-0.0404	-0.0138	-3.390	0.040
u	18	-0.449	0.121	-0.233	20.344	-0.242

Hence, by Theorem 3.1 we can deduce in the case of the Randć index and the the sum–connectivity index we can determine the minimal value of TI *in f–spiral benzenoid* F_1^* *for those* h *such that equation* (13) *holds.*

Example 3 *Consider the generalized Randć index determined by the numbers* $\psi_{ij} = (ij)^\alpha$, *where* $\alpha \in \mathbb{R}$. *Note that*

$$q = 2(6^\alpha) - 4^\alpha - 9^\alpha = -4^\alpha((\frac{3}{2})^\alpha - 1)^2 \leq 0$$

for all $\alpha \in \mathbb{R}$. *Moreover,* $s = 9^\alpha - 4^\alpha \geq 0$ *if and only if* $\alpha \geq 0$ *if and only if* $u = 6(9^\alpha - 6^\alpha) \geq 0$. *Hence for all* $\alpha \geq 0$ *the minimal value of the generalized Randić index is determined by Theorem 3.1 and for all* $\alpha \leq 0$, *the minimal value is attained by the f–spiral benzenoid* F_1^* *for those* h *such that equation* (13) *holds.*

4 Conclusions

In this work we determine extremal values for VDB topological indices over the set Γ_m of f–benzenoids with a equal number of edges. As future work, it would be also interesting to consider the values of other topological indices of f–benzenoids, such as Wiener index [33] and Wiener polarity index [51], the Harary index [1], graph energy [31, 36, 46, 47, 63], Randić energy [11], incidence energy [3], matching energy [50], energy of matrix [18], HOMO-LUMO index [45], entropy measures [4, 5], molecular identification numbers [12].

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