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Research article

Extremal values of VDB topological indices over F-benzenoids with equal number of edges

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Abstract: The utilization of molecular structure topological indices is currently a standing operating procedure in the structure-property relations research, especially in QSPR/QSAR study. In the past several year, generous molecular topological indices related to some chemical and physical properties of chemical compounds were put forward. Among these topological indices, the VDB topological indices rely only on the vertex degree of chemical molecular graphs. The VDB topological index of an n-order graph G is defined as

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

where $\{\psi_{ij}\}$ is a set of real numbers, m_{ij} is the quantity of edges linking an i-vertex and another j-vertex. Numerous famous topological indices are special circumstance of this expression. f-benzenoids are a kind of polycyclic aromatic hydrocarbons, present in large amounts in coal tar. Studying the properties of f-benzenoids via topological indices is a worthy task. In this work the extremum TI of f-benzenoids with given number of edges were determined. The main idea is to construct f-benzenoids with maximal number of inlets and simultaneously minimal number of hexagons in Γ_m, where Γ_m is the collection of f-benzenoids with exactly m ($m \ge 19$) edges. As an application of this result, we give a unified approach of VDB topological indices to predict distinct chemical and physical properties such as the boiling point, π-electrom energy, molecular weight and vapour pressure etc. of f-benzenoids with fixed number of edges.

Keywords: VDB topological index; inlet; f-spiral benzenoid; f-linear chain; f-benzenoid

1. Introduction

In mathematics chemistry and biology, a chemical compound can be represented by a molecular graph by converting atoms to vertices and bonds to edges. One of the primary mission of QSAR/QSPR research is to accurately convert molecular graphs into numerical values. Graph theoretic invariants of molecular graphs are called molecular descriptors which can be utilized to simulate the structural information of molecules, in order to make worthwhile physical and chemical properties of these molecules can be acquired by single numerical values. Such kinds of molecular descriptors are also referred to as topological indices.

In the chemical literature, various topological indices relying only on vertex degrees of the molecular graphs can be utilized in QSPR/QSAR investigation on account of them can be obtained directly from the molecular architecture, and can be rapidly calculated for generous molecules (see [1,2]), and we call them VDB (vertex–degree–based) topological indices. To be more precise, for designated non-negative real numbers $\{\psi_{ij}\}$ $(1 \le i \le j \le n-1)$, a *VDB topological index* of a an n-order (molecular) graph G is expressed as

$$TI(G) = \sum_{1\le i\le j\le n-1} m_{ij}\psi_{ij}, \tag{1.1}$$

where m_{ij} is the amount of edges connecting an i-vertex and a j-vertex of G. A great deal of well–known VDB topological indices can be obtained by different ψ_{ij} in expression (1.1). We list some VDB topological indices in Table 1.

Table 1. Some well-known VDB topological indices.

ψ_{ij}	name
$i+j$	First Zagreb index
$\frac{1}{\sqrt{ij}}$	Randić index
$\frac{2\sqrt{ij}}{i+j}$	GA index
$\sqrt{\frac{i+j-2}{ij}}$	ABC index
$\frac{1}{\sqrt{i+j}}$	Sum–connectivity index
$\frac{(ij)^3}{(i+j-2)^3}$	AZI index
$\frac{2}{i+j}$	Harmonic index
$\lvert i-j\rvert$	Albertson index
$\sqrt{i^2+j^2}$	Sombor index
$\frac{ij}{i+j}$	ISI index

The first Zagreb index [3] is the very first VDB topological index, as powerful molecular structure-descriptors [2], Zagreb indices can describe the peculiarities of the degree of branching in molecular carbon-atom skeleton. Thereafter, many VDB topological indices have been put forward to simulate physical, chemical, biological, and other attributes of molecules [4–7]. In 2021, Gutman [8] introduced a new VDB topological index named as the Sombor index which has a linear correlation with the entropy and the enthalpy of vaporization of octanes [9]. Das et al., give sharp bounds for Sombor index of graphs by means of some useful graph parameters and they reveal the relationships between the Sombor index and Zagreb indices of graphs [10]. Recently, Steiner Gutman index was introduced by Mao and Das [11] which incorporate Steiner distance of a connected graph G. Nordhaus-Gaddum-type results for the Steiner Gutman index of graphs were given in [12]. In 2022, Shang study the Sombor index and degree-related properties of simplicial networks [13]. For more details of VDB topological indices, one can see [3, 14–26] and the books [27–29].

Fluoranthene is a eminent conjugated hydrocarbon which abound in coal tar [30]. A *fluoranthene–type benzenoid system* (*f-benzenoid* for short) is formed from two benzenoid units joined by a pentagon [31, 32]. The ordinary structure modality of a f-benzenoid F is shown in Figure 1, where segments X and Y are two benzenoid systems. Each f-benzenoid possesses exactly one pentagon [32]. More and more attention is paid to f-benzenoids after the flash vacuum pyrolysis experiments of these nonalternant polycyclic aromatic hydrocarbons [33].

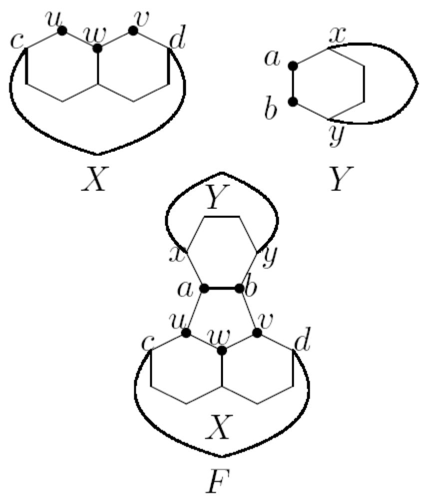

Figure 1. The ordinary structure modality of a f-benzenoid (F) and its construction from two benzenoid systems X and Y.

In the whole article, the terminology and notation are chiefly derived from [34–41]. A vertex of degree k is called a k-vertex, and an edge linking a k-vertex and a j-vertex is designated as a (k, j)-edge. Let n_k be the number of k-vertices and let m_{kj} be the number of (k, j)-edges in the molecular graph G. A benzenoid system without internal vertices is said to be *catacondensed*. Analogously, a f-benzenoid F containing a unique internal vertex is referred to as *catacatacondensed*. We use h-hexagon benzenoid system (or h-hexagon f-benzenoid) to represent a benzenoid system (or f-benzenoid) containing h hexagons.

Let L_h represent the h-hexagon *linear chain* (as shown in Figure 2(a)). An f-benzenoid FL_h ($h \geq 3$) obtaining from pieces $X = L_2$ and $Y = L_{h-2}$ is named as *f-linear chain* (as shown in Figure 2(b)).

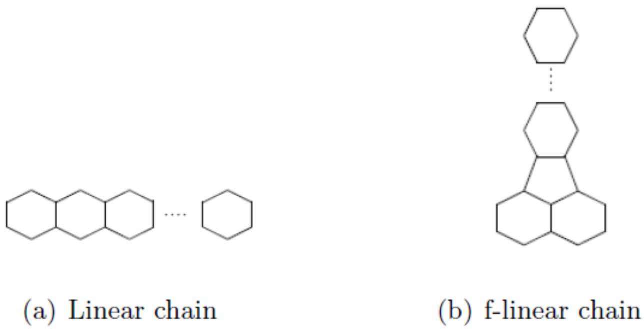

Figure 2. Linear chain and f-linear chain.

A fissure (resp. bay, cove, fjord and lagoon) of a f-benzenoid F is a path of degree sequences $(2, 3, 2)$ (resp. $(2, 3, 3, 2)$, $(2, 3, 3, 3, 2)$, $(2, 3, 3, 3, 3, 2)$ and $(2, 3, 3, 3, 3, 3, 2)$) on the perimeter of F (see Figure 3). Fissures, bays, coves, fjords and lagoons are said to be different kinds of *inlets* and their number are signified by f, B, C, F_j and L, respectively [32, 37]. Inlets determine many electronic and topological properties of f-benzenoids. Then, it can be found that $f+2B+3C+4F_J+5L$ is the number of 3-vertices on the perimeter of F. It is noted that lagoons cannot occur in the theory of benzenoid systems. For convenience, let $r = f + B + C + F_j + L$ to represent the total number of inlets and $b = B+2C+3F_j+4L$ is referred to as the quantity of bay regions, In addition, b is exactly the quantity of $(3, 3)$-edges on the perimeter of F. It is obvious that $b \geq 2$ for any f-benzenoid F.

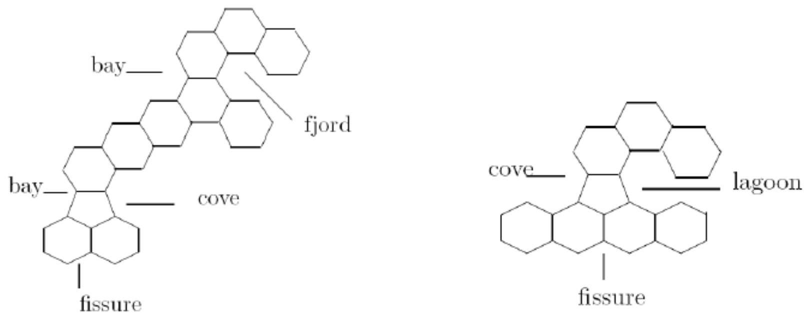

Figure 3. Structural features occurring on the perimeter of f-benzenoids.

It is noted that any f-benzenoid F contains merely either 2-vertex or 3-vertex. The vertices not on the perimeter are said to be *internal*, and we use n_i to represent their number.

Lemma 1.1. [32] *Let F be an n-order, h-hexagon f-benzenoid with m edges and n_i internal vertices. Then*

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

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

Lemma 1.2. [32] *Let F be an n-order and h-hexagon f-benzenoid with r inlets, Then*

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

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

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

From the perspective of mathematics and chemistry, finding the extremal values of some useful TI for significant classes of graphs is very interesting [14, 19, 23, 40–56].

As a matter of convenience, we use Γ_m to represent the collection of f-benzenoids containing exactly m edges. In [45], we derived extremal values for TI among all f-benzenoids with given order. It is noted that structure of f-benzenoids with given order is different from that of f-benzenoids with given number of edges. And we found that the technique for studying TI among all f-benzenoids with given order can not be used directly to investigate TI for all f-benzenoids with fixed number of edges. For this reason, we concentrate on the research of extremal values for TI among all f-benzenoids with given size.

The main idea of this work is to construct f-benzenoids owning maximal r and minimal h at the same time in Γ_m depending on the number m is congruent to $0, 1, 2, 3$ or 4 modulo 5. By making use of this technique, we obtain the extremum of TI over Γ_m and characterize their corresponding graphs on the basis of m is congruent to $0, 1, 2, 3$ or 4 modulo 5. Afterwards the extremums of some well-known TI over Γ_m can be got by use of the previous results.

The structure of this paper is as below. We first determine the maximal r in the set Γ_m in Section 2. By utilizing these results, we find the extremum of several famed TI over Γ_m in Section 3.

2. F–benzenoids with maximal r in Γ_m

We will find the f-benzenoids with maximal r in Γ_m in this section. Figure 4 illustrates three f-benzenoids pertaining to Γ_{42}.

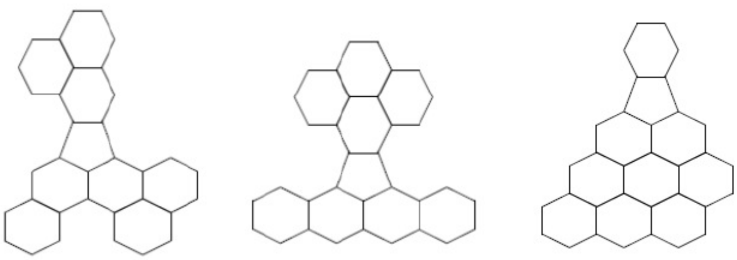

Figure 4. Some f-benzenoids in Γ_{42}.

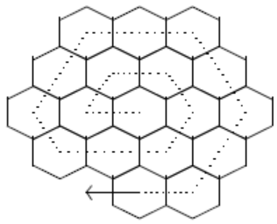

Figure 5. The spiral benzenoid system T_h with maximal number of internal vertices.

At first, we try to obtain the maximum and minimum number of hexagons in any $F \in \Gamma_m$.

The *spiral benzenoid system* [57] T_h is a benzenoid system whose structure is in a "spiral" manner as illustrated in Figure 5. T_h has maximal n_i in all h-hexagon benzenoid systems.

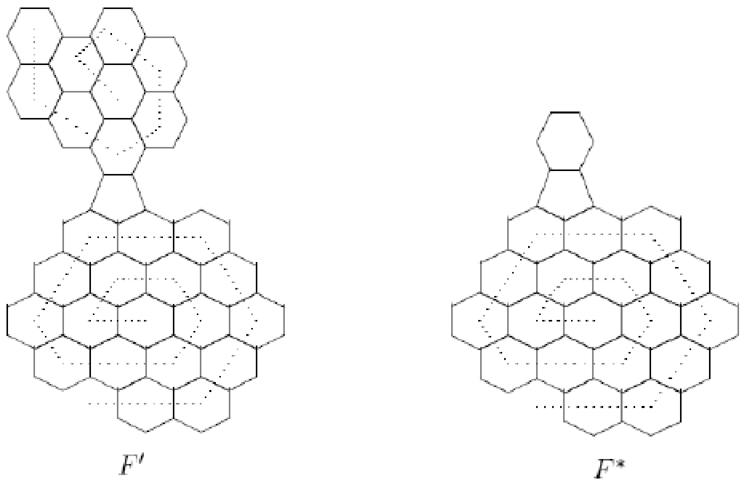

Figure 6. f-benzenoid $F' \in SH_h$ whose two pieces X and Y are both spiral benzenoid systems, and f-spiral benzenoid $F^* \in SH_h$ with two pieces $X = T_{h-1}$ and $Y = T_1$.

As a matter of convenience, let SH_h ($h \geq 3$) represent the collection of f-benzenoids formed by two spiral benzenoids X and Y. Particularly, a *f-spiral benzenoid* is a f-benzenoid $F^* \in SH_h$ in which $X = T_{h-1}$ and $Y = T_1$ (as shown in Figure 6). It is easy to see that that

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

In [40], we proved that for every $F' \in SH_h$ ($h \geq 3$), the inequality

$$n_i(F') \leq n_i(F^*) \tag{2.1}$$

holds, and the following graph operations were introduced.

Operation 1. *For any h-hexagon f-benzenoid F having two segments X and Y, let $h_1 = h(X)$ and $h_2 = h(Y)$. By substituting spiral benzenoid systems T_{h_1} and T_{h_2} for X and Y, severally, another f-benzenoid $F' \in SH_h$ can be obtained (as shown in Figure 7).*

For any h-hexagon f-benzenoid F, when $h = 3$, it is easily checked that

$$n_i(F) = 1 = 2 \times 3 - \lceil \sqrt{12(3-1) - 3} \rceil. \tag{2.2}$$

When $h \geq 4$, let $h_1 = h(X)$ and $h_2 = h(Y)$. Another $F' \in SH_h$ (as shown in Figure 7) in which $X = T_{h_1}$ and $Y = T_{h_2}$ can be acquired by applying Operation 1 to F. It is apparently that $n_i(X) \leq n_i(T_{h_1})$, $n_i(Y) \leq n_i(T_{h_2})$, therefore

$$n_i(F) = n_i(X) + n_i(Y) + 1 \leq n_i(T_{h_1}) + n_i(T_{h_2}) + 1 = n_i(F'). \tag{2.3}$$

So, the following Lemma can be deduced by Eqs (2.1) and (2.3).

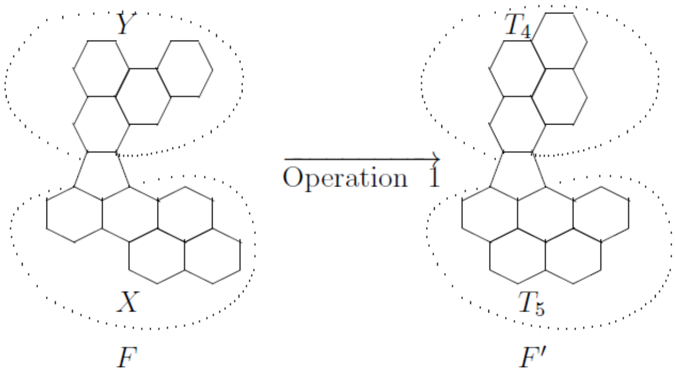

Figure 7. f-benzenoid $F' \in SH_h$ is obtained from F by applying Operation 1 to it.

Lemma 2.1. [41] *Let F be an $h(h \geq 3)$-hexagon f-benzenoid. Then*

$$n_i(F) \leq 2h - \left\lceil \sqrt{12(h-1) - 3} \right\rceil, \tag{2.4}$$

and the equality is established when F is F^*.

For any $F \in \Gamma_m$, $h(F)$ over Γ_m is variable. Sharp bounds for $h(F)$ in Γ_m is given below.

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

$$\left\lceil \frac{1}{5}(m-4) \right\rceil \leq h(F) \leq m - 1 - \left\lceil \frac{1}{3}\left(2m + \sqrt{4m - 31}\right) \right\rceil, \tag{2.5}$$

where $\lceil x \rceil$ is the smallest integer larger or equal to x.

Proof. On one hand, from Lemma 1.1 (ii) we know that $m = 5h(F) + 5 - n_i(F)$. Combining the fact that $n_i(F) \geq 1$ for any $F \in \Gamma_m$, 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 $n_i(F) \leq n_i(F^*)$. 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,

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

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

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

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

Remark 1. *Theorem 2.1 implies that f-spiral benzenoid F^* has the maximal number of hexagons over Γ_m.*

For the sake of obtaining the extremum TI among all f-benzenoids in Γ_m, we need to find the f-benzenoids $F \in \Gamma_m$ possessing maximal r.

Recall that *convex benzenoid systems* (CBS for brevity) are a particular sort of benzenoid systems lack of bay regions [14]. Let $\mathcal{HS}_h$ be the collection of benzenoid systems containing h hexagons.

Lemma 2.2. [42] *Let $H \in \mathcal{HS}_h$. Under the below cases, H is definitely not a CBS:*

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

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

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

Lemma 2.3. [52] *Let $H \in \mathcal{HS}_h$ such that $n_i(H) = 4$. Then H is bound to embody a subbenzenoid system given in Figure 8, there does not exist hexagons which are adjacent to fissures.*

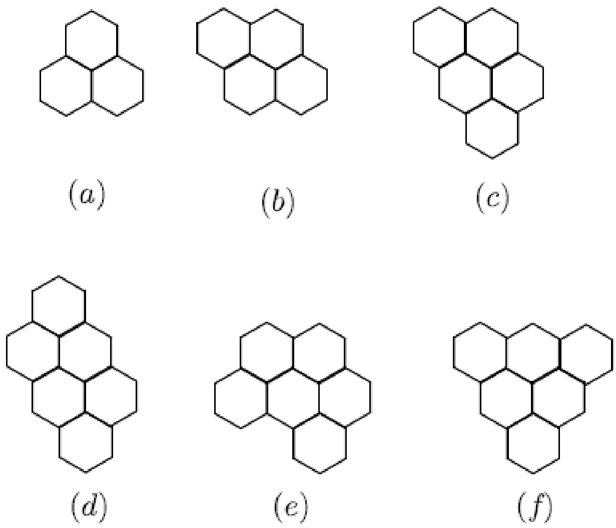

Figure 8. Benzenoid systems with 1, 2, 3 and 4 internal vertices, respectively.

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

Proof. Let S be an h ($h \geq 7$)-hexagon benzenoid system, $n_i(S) = 4$, then by Lemma 2.3 S must contain one of the benzenoid systems of the form given in Figure 7. The proof is carried out in two cases.

Case 1. If these four internal vertices form a path P_4 or a $K_{1,3}$, then S contains one of benzenoid systems (d)–(f) in Figure 7 as its subbenzenoid systems. It is noted that $h \geq 7$, by Lemma 2.2, it must not exist hexagons contiguous to the fissures, so, S has at least one hexagon contiguous to a $(2, 2)$-edge, by means of such hexagons, it is succeeded in converting one of the fissures into a cove, bay or fjord. Hence, $b(S) \geq 1$.

Case 2. If these four internal vertices are not adjacent then S has possibility subbenzenoid systems as follows.
1) There exist one type (a) and one type (c) benzenoid systems in S;
2) There exist two type (b) benzenoid systems in S;
3) There exist two type (a) and one type (b) benzenoid systems in S.
4) There exist four type (a) benzenoid systems in S.
By Lemma 2.2, neither hexagons may be adjacent to the fissures in any of the cases indicated above. Since $h \geq 7$, S has at least one hexagon contiguous to a $(2, 2)$-edge, by means of such hexagons, it is succeeded in making one of the fissures become a cove, bay or fjord. Therefore, $b(S) \geq 1$.

The proof is completed.

Lemma 2.5. [45] *Let F be an h-hexagon f-benzenoid. Then*

1) *If $n_i = 1$, then $r(F) \leq r(FL_h) = 2h - 3$ ($h \geq 3$);*

2) *If $n_i = 2$, then $r(F) \leq r(G_h) = 2h - 4$ ($h \geq 4$);*

3) *If $n_i = 3$, then $r(F) \leq r(R_h) = 2h - 5$ ($h \geq 5$);*

4) *If $n_i = 4$, then $r(F) \leq r(Z_h) = 2h - 6$ ($h \geq 6$).*

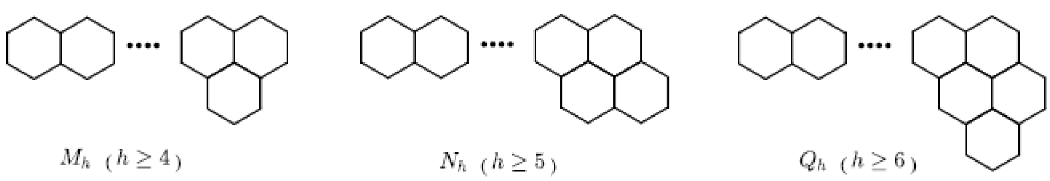

Figure 9. Three types of benzenoid systems.

Next we find the f-benzenoids with maximal r in Γ_m with a fixed n_i. 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.

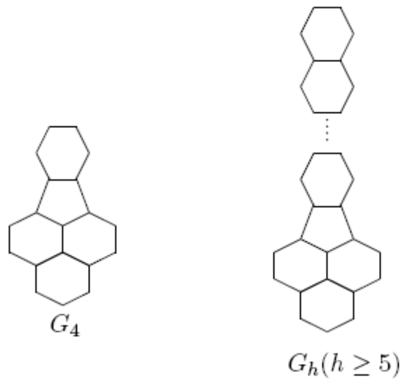

Figure 10. f-benzenoids G_4, and G_h ($h \geq 5$).

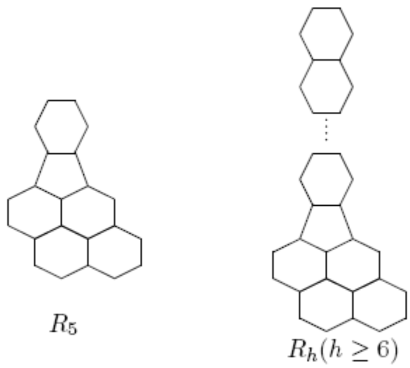

Figure 11. f-benzenoids R_5, and R_h ($h \geq 6$).

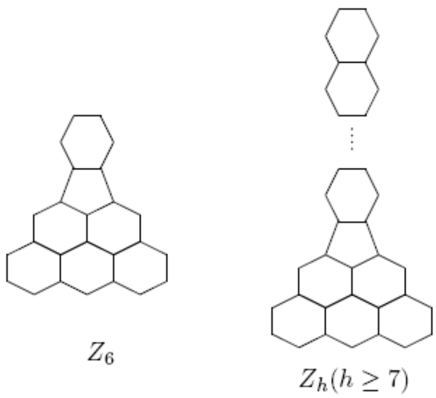

Figure 12. f-benzenoids Z_6, and Z_h ($h \geq 7$).

Lemma 2.6. [41] *Let F be an h-hexagon f-benzenoid. Then*

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

Lemma 2.7. [32] *For any h-hexagon f-benzenoid including n_i internal vertices and b bay regions, the number of* $(2, 2)$*-edge and* $(2, 3)$*-edge are $m_{22} = b + 5, m_{23} = 4h - 2n_i - 2b$, respectively.*

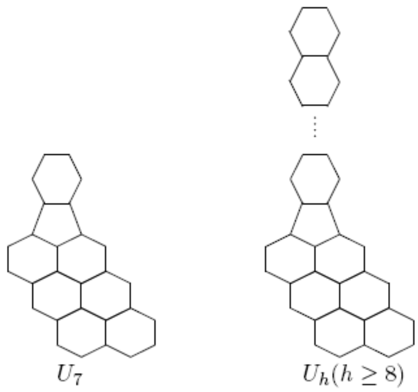

Figure 13. f-benzenoids U_7, and U_h ($h \geq 8$).

From Lemmas 1.2 (ii) and 2.6, we get

$$r = 2h - n_i - b \tag{2.6}$$

Furthermore, by Lemma 1.1 (ii) and Eq (2.6), we deduce

$$r = m - 3h - 5 - b \tag{2.7}$$

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

Proof. Let $h_1 = h(X)$ and $h_2 = h(Y)$, X and Y are two segments of F. If $n_i = 5$, by the structure of f-benzenoid, equality $n_i(X) + n_i(Y) = 4$ holds, so, we have the following five cases.
Case 1. $n_i(X) = 1$, $n_i(Y) = 3$, i.e., there exist one internal vertex and three internal vertices in X and Y, respectively.
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-benzenoid D_1, D_2 or D_3 (see Figure 14). It is clear that $r(F) = r(D_1) = 8 \leq 2h - 7$, $r(F) = r(D_2) = 7 \leq 2h - 7$ or $r(F) = r(D_3) = 8 \leq 2h - 7$.
Subcase 1.1.2. If $h_2 \geq 6$, by Lemma 2.2 and the hypothesis that $n_i(Y) = 3$, Y is not a CBS, so $b(Y) \geq 1$. Furthermore, $b(F) \geq 3$, combining Eq (2.6) we obtain $r = 2h - n_i - b \leq 2h - 8 < 2h - 7$.
Subcase 1.2. If $h_1 \geq 4$, according to Lemma 2.2, X is definitely not a CBS, i.e., $b(X) \geq 1$.
Subcase 1.2.1. If $h_2 = 5$, i.e., $Y = Q_5$. It is clear that $b(F) \geq 4$, then Eq (2.6) deduces $r \leq 2h - 9 < 2h - 7$.
Subcase 1.2.2. If $h_2 \geq 6$, Y is definitely not not a CBS according to Lemma 2.2, so, $b(Y) \geq 1$. It is clear that $b(F) \geq 5$, consequently from Eq (2.6) we obtain $r \leq 2h - 10 < 2h - 7$.
Case 2. $n_i(X) = 3$ and $n_i(Y) = 1$.

Subcase 2.1. If $h_1 = 5$, then $X = Q_5$.
Subcase 2.1.1. If $h_2 = 3$, i.e., $Y = M_3$, then F is the f-benzenoid D_4, D_5, D_6 (see Figure 14), or D_7 (as shown in Figure 15). $r(F) = r(D_4) = 8 \leq 2h-7$, $r(F) = r(D_5) = 7 \leq 2h-7$, $r(F) = r(D_6) = 8 \leq 2h-7$, $r(F) = r(D_7) = 7 \leq 2h-7$.

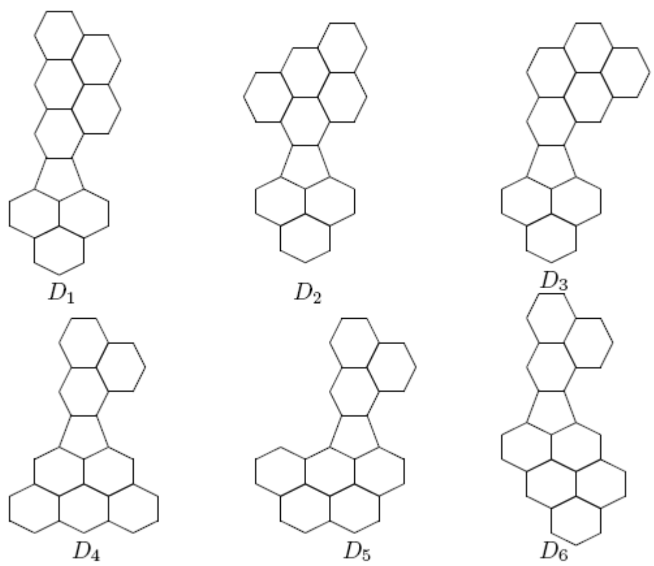

Figure 14. f-benzenoids D_1, D_2, D_3, D_4 and D_5.

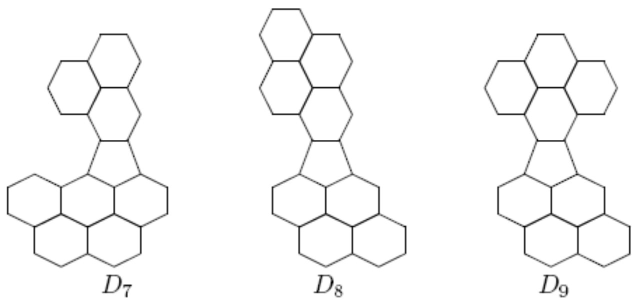

Figure 15. f-benzenoids D_7, D_8 and D_9.

Subcase 2.1.2. If $h_2 \geq 4$, Y is surely not a CBS in light of Lemma 2.2, i.e., $b(X) \geq 1$. Hence, we have $b(F) \geq 4$, it follows from Eq (2.6) that $r \leq 2h-9 < 2h-7$.
Subcase 2.2. If $h_1 \geq 6$, by Lemma 2.2, X is definitely not a CBS, hence $b(X) \geq 1$.
Subcase 2.2.1. If $h_2 = 3$, i.e., $Y = M_3$. We have $b(F) \geq 4$, and Eq (2.6) infers that $r \leq 2h-9 < 2h-7$.
Subcase 2.2.2. f $h_2 \geq 4$, by Lemma 2.2, Y is certainly not a CBS, i.e., $b(X) \geq 1$. Hence we have $b(F) \geq 5$, by Eq (2.6), $r \leq 2h-10 < 2h-7$.
Case 3. $n_i(X) = 2$, $n_i(Y) = 2$, i.e., X and Y both have two internal vertices.
Subcase 3.1. If $h_1 = 4$, we note that $n_i(X) = 2$, so X must be the benzenoid system (b) in Figure 9.

Subcase 3.1.1. If $h_2 = 4$, Y is surely the benzenoid system (b) in Figure 9 according to the hypothesis $n_i(Y) = 2$, therefore, F is D_8 or D_9 (as shown in Figure 15). We get $r(F) = r(D_8) = 8 < 2h - 7$ or $r(F) = r(D_9) = 7 < 2h - 7$.

Subcase 3.1.2. If $h_2 \geq 5$, by Lemma 2.2 and that $n_i(Y) = 2$, Y is not a CBS, so we know that $b(X) \geq 1$. Then $b(F) \geq 4$, by Eq (2.6) and the fact that $n_i = 5$, $r \leq 2h - 9 < 2h - 7$.

Subcase 3.2. If $h_2 = 4$, we note that $n_i(Y) = 2$, so Y must be the benzenoid system (b) in Figure 8.

Subcase 3.2.1. If $h_1 = 4$, X must also be the benzenoid system (b) in Figure 9. Hence, F is D_8 or D_9 (as shown in Figure 15). $r(F) = r(D_8) = 8 \leq 2h - 7$ or $r(F) = r(D_9) = 7 \leq 2h - 7$.

Subcase 3.2.2. If $h_1 \geq 5$, by Lemma 2.2 and $n_i(X) = 2$, X is definitely not a CBS, i.e., $b(X) \geq 1$. Hence, $b(F) \geq 4$, by Eq (2.6) and the fact that $n_i = 5$, we have $r \leq 2h - 9 < 2h - 7$.

Subcase 3.3. If $h_1 \geq 5$, $h_2 \geq 5$, it is noted that $n_i(X) = n_i(Y) = 2$, neither X nor Y are definitely CBS according to Lemma 2.2. So, both $b(X)$ and $b(Y)$ are greater than 1. Hence, $b(F) \geq 5$, on the basis of Eq (2.6) we get $r \leq 2h - 10 < 2h - 7$.

Case 4. $n_i(X) = 4$ and $n_i(Y) = 0$, i.e., X contains four internal vertices, 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 9.

Subcase 4.1.1. If $h_2 = 1$, F is the f-benzenoid D_{10}, D_{11}, D_{12} (see Figure 16), D_{13} (see Figure 17) or U_7 (see Figure 12). $r(F) = r(D_{10}) = 6 \leq 2h - 7$, $r(F) = r(D_{11}) = 6 \leq 2h - 7$, $r(F) = r(D_{12}) = 6 \leq 2h - 7$, $r(F) = r(D_{13}) = 6 \leq 2h - 7$ or $r(F) = r(U_7) = 7 = 2h - 7$.

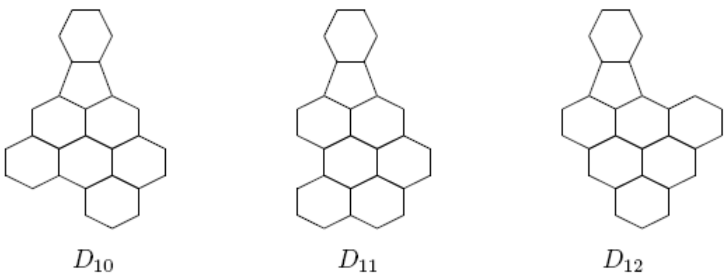

Figure 16. f-benzenoids D_{10}, D_{11} and D_{12}.

Subcase 4.1.2. If $h_2 \geq 2$, we have $b(F) \geq 2$, by Eq (2.6), $r \leq 2h - 7$.

Subcase 4.2. If $h_1 \geq 7$, in the light of Lemma 2.4, X is definitely not a CBS, hence $b(Y) \geq 1$. In this situation $b(F) \geq 3$, we get the inequality $r \leq 2h - 8 < 2h - 7$ according to Eq (2.6).

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

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 $h_1 = 2$, X must be the linear chain L_2. In this event, F is D_{14}, D_{15}, D_{16}, D_{17}, D_{18}, D_{19}, D_{20} or D_{21} (see Figure 17). By further checking, we gain that $r(F) = r(D_{14}) = 7 \leq 2h - 7$, $r(F) = r(D_{15}) = 8 \leq 2h - 7$, $r(F) = r(D_{16}) = 8 \leq 2h - 7$, $r(F) = r(D_{17}) = 7 \leq 2h - 7$, $r(F) = r(D_{18}) = 7 \leq 2h - 7$, $r(F) = r(D_{19}) = 8 \leq 2h - 7$, $r(F) = r(D_{20}) = 6 \leq 2h - 7$ or $r(F) = r(D_{21}) = 6 \leq 2h - 7$.

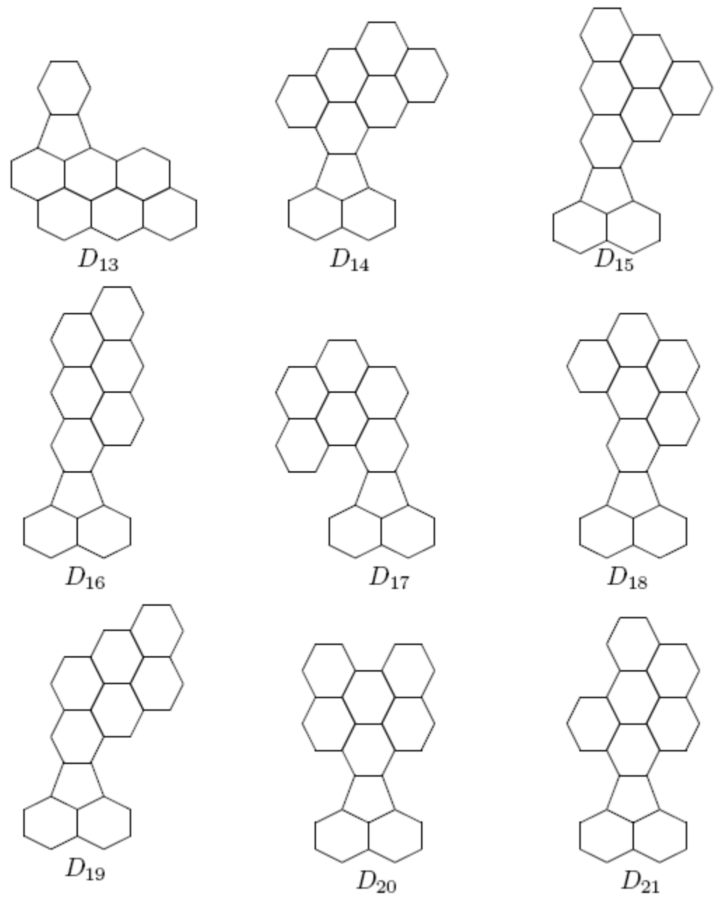

Figure 17. f-benzenoids D_{13}, D_{14}, D_{15}, D_{16}, D_{17}, D_{18}, D_{19}, D_{20} and D_{21}.

Subcase 5.1.2. If $h_1 \geq 3$, bearing in mind that X is a catacondensed benzenoid system and Y is the benzenoid system (d), (e) or (f) in Figure 8, then F must have f-benzenoid D_{14}, D_{15}, D_{16}, D_{17}, D_{18}, D_{19}, D_{20} or D_{21} (see Figure 17) as its subgraph.

Subcase 5.1.2.1. If D_{14} is a subgraph in F, it is obvious that D_{14} has two coves. Since X is a catacondensed benzenoid system and $h_1 \geq 3$, F has at least one hexagon contiguous to a $(2,2)$-edge of X, and such hexagons can convert one fissure into a bay, or convert one cove into a fjord, or convert one fjord into a lagoon. In this instance $b(F) \geq 4$. Consequently, $r \leq 2h - 9 < 2h - 7$ can be got according to Eq (2.6).

Subcase 5.1.2.2. If D_{15}, D_{16} or D_{19} is a subpart f-benzenoid in F, it is obvious each one of D_{15}, D_{16} and D_{19} has a bay and a cove. Since X is a catacondensed benzenoid system and $h_1 \geq 3$, F contains at least one hexagon adjoining a $(2,2)$-edge of X, and such hexagons will make one fissure become a bay, or make one cove become a fjord, or make one fjord become a lagoon. Consequently, $b(F) \geq 4$, by Eq (2.6) it follows that $r \leq 2h - 9 < 2h - 7$.

Subcase 5.1.2.3. If D_{17} is a subpart f-benzenoid in F, it is obvious that D_{17} has a fjord and a bay. Since X is a catacondensed benzenoid system and $h_1 \geq 3$, F has at least one hexagon adjoining a $(2,2)$-edge of X, and such hexagons will convert one fissure into a bay, or convert one cove into a fjord, or convert one fjord into a lagoon. Consequently, $b(F) \geq 4$, by Eq (2.6) it follows that $r \leq 2h - 9 < 2h - 7$.

Subcase 5.1.2.4. If D_{18} is a subpart f-benzenoid in F, it is obvious that D_{18} has a fjord and two bays. Since X is a catacondensed benzenoid system and $h_1 \geq 3$, there exists has at least one hexagon adjoining a $(2, 2)$-edge of X in F, and these hexagons will convert one of the fissures into a bay, or convert one cove into a fjord, or convert one fjord into a lagoon. Consequently, $b(F) \geq 4$, in light of Eq (2.6), $r \leq 2h - 9 < 2h - 7$.
Subcase 5.1.2.5. If D_{20} or D_{21} is a subpart f-benzenoid in F, it is obvious that both D_{20} and D_{21} have a bay and two fjords. Since X is a catacondensed benzenoid system and $h_1 \geq 3$, F contains at least one hexagon adjoining a $(2, 2)$-edge of X, and such hexagons will make one fissure become a bay, or make one cove become a fjord, or make one fjord become a lagoon. Consequently, $b(F) \geq 4$, according to Eq (2.6), $r \leq 2h - 9 < 2h - 7$.
Subcase 5.2. If $h_2 \geq 7$, by Lemma 2.4 and the fact that $n_i(Y) = 4$, Y is certainly not a CBS, i.e., $b(Y) \geq 1$.
Subcase 5.2.1. If $h_1 = 2$, i.e., $X = L_2$. From the structure of f-benzenoid, F is formed from X and Y joined by a pentagon, it is easily seen that there are at least one bay or one cove arisen in the process of construction of F. It is clear that $b(F) \geq 2$, by Eq (2.6) we have $r \leq 2h - 7$.
Subcase 5.2.2. If $h_1 \geq 3$, we know that F is formed by joining from X and Y through a pentagon, in this construction process of F, it is easily seen that there are at least one bay or one cove arisen. Then $b(F) \geq 2$, by Eq (2.6), $r \leq 2h - 7$.

The proof is completed.

We recall that FL_h is the f-linear chain with h hexagons [40]. Extremal f-benzenoids with maximal r in Γ_m were determined in the following theorem.

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 $m \equiv 2(mod5)$, then $r(F) \leq \frac{2m-29}{5} = r(R_{\frac{m-2}{5}})$;*
4) *If $m \equiv 3(mod5)$, then $r(F) \leq \frac{2m-26}{5} = r(G_{\frac{m-3}{5}})$;*
5) *If $m \equiv 4(mod5)$, then $r(F) \leq \frac{2m-23}{5} = r(FL_{\frac{m-4}{5}})$.*

Proof. We know by Eq (2.5) 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 (ii)

$$m = 5h(F) + 5 - n_i(F) = m + 5 - n_i(F),$$

it means that $n_i(F) = 5$. Furthermore, Theorem 2.2 infers 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 (2.7) 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 (ii)

$$m = 5h(F) + 5 - n_i(F) = m + 4 - n_i(F),$$

thus $n_i(F) = 4$. 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 (2.7) and the obvious 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 (ii)

$$m = 5h(F) + 5 - n_i(F) = m + 3 - n_i(F),$$

and so $n_i(F) = 3$. Then $r(F) \leq r(R_{\frac{m-2}{5}})$ by part 3 of Lemma 2.5. So assume now that $h(F) \geq \frac{m-2}{5} + 1$, then by Eq (2.7) 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 $\left\lceil \frac{1}{5}(m-4) \right\rceil = \frac{m-3}{5}$. If $h(F) = \frac{m-3}{5}$, then by Lemma 1.1 (ii)

$$m = 5h(F) + 5 - n_i(F) = m + 2 - n_i(F),$$

thus $n_i(F) = 2$. By Lemma 2.5, $r(F) \leq r(G_{\frac{m-3}{5}})$ and we are done. If $h(F) \geq \frac{m-3}{5} + 1$, then by equality (2.7) 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 $\left\lceil \frac{1}{5}(m-4) \right\rceil = \frac{m-4}{5}$. Since $h \geq \frac{m-4}{5}$ and $b(F) \geq 2$, then by Eq (2.7), we have

$$r(F) = m - 5 - 3h(F) - b(F) \leq m - 5 - \frac{3m-12}{5} - b(F)$$

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

3. Extremal values of TI over Γ_m

In this part, we attempt to find the extremal values of TI over Γ_m.

It is noted that a f-benzenoid F contains only 2-vertex and 3-vertex. Hence, equation (1.1) reduces to

$$TI(F) = m_{22}\psi_{22} + m_{23}\psi_{23} + m_{33}\psi_{33}, \tag{3.1}$$

In the light of Lemmas 1.1 and 1.2,

$$TI(F) = \psi_{22}m + 3(\psi_{33} - \psi_{22})h + (2\psi_{23} - \psi_{22} - \psi_{33})r, \tag{3.2}$$

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

$$\begin{aligned} TI(U) - TI(V) = 3(\psi_{33} - \psi_{22})(h(U) - h(V)) \\ + (2\psi_{23} - \psi_{22} - \psi_{33})(r(U) - r(V)). \end{aligned} \tag{3.3}$$

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

Theorem 3.1. *For any $F \in \Gamma_m$, we have the following results.*

a. *If $s \leq 0$ and $q \geq 0$,*

$$TI(F) \leq \begin{cases} TI(U_{\frac{m}{5}}), & if\ m \equiv 0(mod\ 5) \\ TI(Z_{\frac{m-1}{5}}), & if\ m \equiv 1(mod\ 5) \\ TI(R_{\frac{m-2}{5}}), & if\ m \equiv 2(mod\ 5) \\ TI(G_{\frac{m-3}{5}}), & if\ m \equiv 3(mod\ 5) \\ TI(FL_{\frac{m-4}{5}}), & if\ m \equiv 4(mod\ 5) \end{cases}$$

b. *If $s \geq 0$ and $q \leq 0$,*

$$TI(F) \geq \begin{cases} TI(U_{\frac{m}{5}}), & if\ m \equiv 0(mod\ 5) \\ TI(Z_{\frac{m-1}{5}}), & if\ m \equiv 1(mod\ 5) \\ TI(R_{\frac{m-2}{5}}), & if\ m \equiv 2(mod\ 5) \\ TI(G_{\frac{m-3}{5}}), & if\ m \equiv 3(mod\ 5) \\ TI(FL_{\frac{m-4}{5}}), & if\ m \equiv 4(mod\ 5) \end{cases}$$

Proof. Let $F \in \Gamma_m$. By Eq (2.5)

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

i.e., 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 minimal h over the set Γ_m. Meanwhile, by Theorem 2.3, we have

$$r(F) \leq \begin{cases} r(U_{\frac{m}{5}}), if\ m \equiv 0(mod\ 5) \\ r(Z_{\frac{m-1}{5}}), if\ m \equiv 1(mod\ 5) \\ r(R_{\frac{m-2}{5}}), if\ m \equiv 2(mod\ 5) \\ r(G_{\frac{m-3}{5}}), if\ m \equiv 3(mod\ 5) \\ r(FL_{\frac{m-4}{5}}), if\ m \equiv 4(mod\ 5) \end{cases}$$

i.e., these five f-benzenoids have maximal number of inlets over Γ_m. Hence, for any f-benzenoids $F \in \Gamma_m$ and $V \in \{U_{\frac{m}{5}}, Z_{\frac{m-1}{5}}, R_{\frac{m-2}{5}}, G_{\frac{m-3}{5}}, FL_{\frac{m-4}{5}}\}$, $h(F)-h(V) \geq 0$ and $r(F)-r(V) \leq 0$ hold simultaneously, from Eq (2.7), we have

$$TI(F) - TI(V) = 3s(h(F) - h(V)) + q(r(F) - r(V)).$$

If $s \leq 0$ and $q \geq 0$, then $TI(F) - TI(V) \leq 0$, i.e., V reaches the maximum value of TI over Γ_m. If $s \geq 0$ and $q \leq 0$, then $TI(F) - TI(V) \geq 0$, i.e., V reaches the minimum value of TI over Γ_m. Furthermore, which $V \in \{U_{\frac{m}{5}}, Z_{\frac{m-1}{5}}, R_{\frac{m-2}{5}}, G_{\frac{m-3}{5}}, FL_{\frac{m-4}{5}}\}$ is the extremal graph depending on m is congruent to $0, 1, 2, 3$ or 4 modulo 5.

Example 1. *Values of s and q for several famous TI are listed in Table 2:*

Table 2. Values of s and q for six famous TI.

	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

Therefore, the minimum extreme value of TI for the second Zagreb index, GA index and the AZI index can be determined in the light of Theorems 2.3 and 3.1, and we can obtain the maximum extreme value of TI for the ABC index.

If f-benzenoid $F \in \Gamma_m$, then from the Eqs (2.3) and (2.6) and Lemma 1.1(ii) we have

$$\begin{aligned} TI(F) = {} & (2\psi_{23} - \psi_{33})m + 6(\psi_{33} - \psi_{23})h - (2\psi_{23} - \psi_{22} - \psi_{33})b \\ & - 5(2\psi_{23} - \psi_{22} - \psi_{33}). \end{aligned} \tag{3.4}$$

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

$$\begin{aligned} TI(U) - TI(V) = {} & 6(\psi_{33} - \psi_{23})(h(U) - h(V)) \\ & + (-2\psi_{23} + \psi_{22} + \psi_{33})(b(U) - b(V)). \end{aligned} \tag{3.5}$$

Set $u = 6(\psi_{33} - \psi_{23})$ and keep in mind that $q = 2\psi_{23} - \psi_{22} - \psi_{33}$. Then

$$TI(U) - TI(V) = u(h(U) - h(V)) - q(b(U) - b(V)). \tag{3.6}$$

It is noted that Eq (3.6) can be decided only by h, b and the signs of u and q. For any $F \in \Gamma_m$, We know that

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

and the equality can be achieved precisely when F is the f-spiral benzenoid F^* [41].

In [41], we proved that $n_i(F^*) = 2h - \left\lceil \sqrt{12(h-1) - 3} \right\rceil$. But, $b(F^*) \neq 2$ may occur. It is noticeable if X in F^* is a CBS, F^* is a f-benzenoid satisfying that $b(F^*) = 2$ or 3. For the sake of simplicity, Let $\mathbb{N}$ be the set of positive integers.

The CBS, $W = H(l_1, l_2, l_3, l_4, l_5, l_6)$ (as shown in Figure 18), can be completely determined by the positive integers l_1, l_2, l_3, l_4 [14].

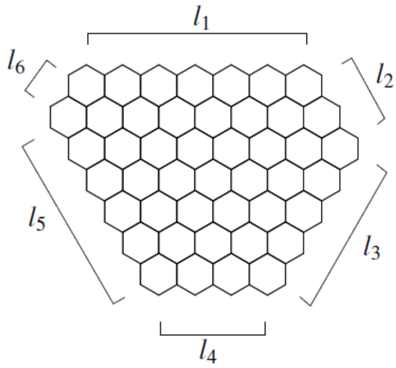

Figure 18. The general form of a CBS. The parameters $l_i \geq 1, i = 1, 2, \cdots, 6$, count the number of hexagons on the respective side of CBS.

The following lemma gave requirements that there exists CBS with maximal n_i [53].

Lemma 3.1. [53] *Let $h \in \mathbb{N}$. The conditions below are isovalent:*

(a) There is a CBS W containing h hexagons and $2h + 1 - \lceil \sqrt{12h-3} \rceil$ number of internal vertices.

(b) There exist $l_1, l_2, l_3, l_4 \in \mathbb{N}$ satisfying the following equation

$$\left.\begin{array}{r} h = l_1 l_3 + l_1 l_4 + l_2 l_3 + l_2 l_4 - l_2 - l_3 \\ -\frac{1}{2} l_1(l_1+1) - \frac{1}{2} l_4(l_4+1) + 1 \\ \lceil \sqrt{12h-3} \rceil = l_1 + 2l_2 + 2l_3 + l_4 - 3 \end{array}\right\} \tag{3.7}$$

If for $h \in \mathbb{N}$, Eq (3.7) has a solution $l_1, l_2, l_3, l_4 \in \mathbb{N}$, then there is a CBS W meeting the conditions that $n_i(W) = n_i(T_h)$.

Now, we concentrate on the research for TI of f-benzenoids. For a $h - 1 \in \mathbb{N}$, supposing that the system below

$$\left.\begin{array}{r} h - 1 = l_1 l_3 + l_1 l_4 + l_2 l_3 + l_2 l_4 - l_2 - l_3 \\ -\frac{1}{2} l_1(l_1+1) - \frac{1}{2} l_4(l_4+1) + 1 \\ \lceil \sqrt{12(h-1)-3} \rceil = l_1 + 2l_2 + 2l_3 + l_4 - 3 \\ \exists\, l_i \in \{l_1, l_2, l_3, l_4, l_5, l_6\},\ l_i = 2 \end{array}\right\} \tag{3.8}$$

has a solution $\{l_1, l_2, l_3, l_4\}$, then a CBS W_{h-1} containing $n_i(W_{h-1}) = 2(h-1) + 1 - \left\lceil \sqrt{12(h-1)-3} \right\rceil$ number of internal vertices exists. Note that $l_i = 2$ in system (3.8), i.e., there exists one fissure on the side of l_i of W_{h-1}, let u, w, v in Figure 1 represent the three vertices of this fissure. Now, we obtain an f-spiral benzenoid F_1^* in which $X = W_{h-1}$ and $Y = L_1$. It is obvious that

$$n_i(F_1^*) = 2h - \left\lceil \sqrt{12(h-1)-3} \right\rceil \tag{3.9}$$

and $b(F_1^*) = 2$. (as shown in Figure 19)

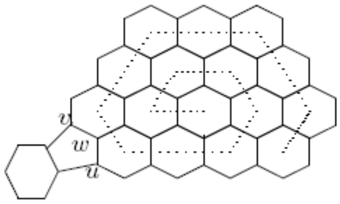

Figure 19. A f-spiral benzenoid F_1^* whose fragment X is a convex spiral benzenoid system W_{h-1}.

Theorem 3.2. *Let $h-1 \in \mathbb{N}$ such that the Eq (3.8) has a solution, and $m = 3h+5+\left\lceil \sqrt{12(h-1)-3} \right\rceil$. Then for any $F \in \Gamma_m$*

1) $TI(F_1^*) \geq TI(F)$, when $u \geq 0$ and $q \geq 0$;

2) $TI(F_1^*) \leq TI(F)$, when $u \leq 0$ and $q \leq 0$.

Proof. From Lemma 1.1 (ii) and Eq (3.9), we have

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

and so

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

It is obvious that $b(F_1^*) = 2$ and $b(F) \geq 2$ for any $F \in \Gamma_m$. Hence by Eq (3.6), we have

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

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

And by Eq (2.5)

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

If $u \geq 0$ and $q \geq 0$ then $TI(F) - TI(F_1^*) \leq 0$, i.e., F_1^* achieves maximal TI in Γ_m. Similarly, if $u \leq 0$ and $q \leq 0$ then $TI(F) - TI(F_1^*) \geq 0$, i.e., F_1^* obtains minimal TI in Γ_m.

Example 2. *The values of u and q for some famous TI are listed in the following Table 3:*

Table 3. Values of u and q for six famous TI.

	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 the minimal values of the Randć index and the the sum–connectivity index in f-spiral benzenoid F_1^* for those h such that Eq (3.8) holds.

Example 3. *Take consideration of the generalized Randć index*

$$R_\alpha(G) = \sum_{1\le i\le j\le n-1} m_{ij}(ij)^\alpha,$$

where $\alpha \in \mathbb{R}$. *Note that*

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

for all $\alpha \in \mathbb{R}$. *Moreover,* $s = 9^\alpha - 4^\alpha \ge 0$ *if and only if* $\alpha \ge 0$ *if and only if* $u = 6(9^\alpha - 6^\alpha) \ge 0$. *Hence, by Theorem 3.1, the minimal value of* $R_\alpha(G)$ *is obtained for all* $\alpha \ge 0$, *and for any* $\alpha \le 0$, *the minimal value of* $R_\alpha(G)$ *can be attained by the f-spiral benzenoid* F_1^* *for those h such that Eq* (3.8) *holds.*

4. Conclusions

This work investigates extremum TI over the collection of f-benzenoids having same number of edges. In practical terms, there are many other types of very useful topological indices for instance graph energy [58–62], Wiener index [63], Randić energy [64], Wiener polarity index [65], incidence energy [66], Harary index [67], entropy measures [68, 69] and HOMO-LUMO index [70]. So, determining these topological indices for f-benzenoids is going to be extraordinary fascinating.

It is noted that the current framework is for studying topological indices of deterministic networks. But random networks would be a very promising direction. In [71, 72], the distance Estrada index of random graphs was discussed, and the author went deeply into (Laplacian) Estrada index for random interdependent graphs. So, studying VDB topological indices of random and random interdependent graphs is another interesting problem.

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Conflict of interest

The authors declare there is no conflict of interest.

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