

## On extremal trees with respect to the F-index

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### Abstract

In a study on the structure–dependency of the total  $\pi$ -electron energy from 1972, Trinajstić and one of the present authors have shown that it depends on the sums  $\sum_{v \in V} d(v)^2$  and  $\sum_{v \in V} d(v)^3$ , where  $d(v)$  is the degree of a vertex  $v$  of the underlying molecular graph  $G$ . The first sum was later named *first Zagreb index* and over the years became one of the most investigated graph–based molecular structure descriptors. On the other hand, the second sum, except in very few works on the general first Zagreb index and the zeroth–order general Randić index, has been almost completely neglected. Recently, this second sum was named *forgotten index*, in short the *F-index*, and shown to have an exceptional applicative potential. In this paper we examine the trees extremal with respect to the *F-index*.

**Keywords:** F-index; general first Zagreb index; molecular trees; topological indices; trees.

### 1. Introduction

The first and the second Zagreb indices, introduced by Gutman & Trinajstić (1972) are among the oldest graph–based molecular structure descriptors, so-called topological indices (Balaban *et al.* (1983); Devillers & Balaban (1990); Gutman (2013)). For a graph  $G$  with a vertex set  $V(G)$  and an edge set  $E(G)$ , these are defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} d(u)d(v), \quad (1)$$

where the degree of a vertex  $v \in V(G)$ , denoted by  $d(v)$ , is the number of the first neighbors of  $v$ .

Over the years these indices have been thoroughly examined and used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. More about their physico–chemical applications and mathematical properties can be found in Nikolić *et al.* (2003), Gutman (2013), Furtula *et al.* (2013), Gutman & Das (2004), Das & Gutman (2004), Zhou (2004), Gutman *et al.* (2015), Liu & You (2010) respectively, as well as in the references cited therein. The sum of squares of vertex degrees was also independently studied in quite a few mathematical

papers (Das (2003; 2004); Bell (1992); Caen (1998); Cioabă (2006); Peled *et al.* (1999)).

In an early work on the structure–dependency of the total  $\pi$ -electron energy by Gutman & Trinajstić (1972) beside the first Zagreb index, it was indicated that another term on which this energy depends is of the form

$$F(G) = \sum_{v \in V(G)} d(v)^3. \quad (2)$$

For unexplainable reasons, the above sum, except (implicitly) in a few works about the general first Zagreb index (Li & Zhao (2004); Li & Zheng (2005)) and the zeroth–order general Randić index (Hu *et al.* (2005)) has been completely neglected. Very recently, Furtula and one of the present authors succeeded to demonstrate that  $F(G)$  has a very promising applicative potential (Furtula & Gutman (2015)). They proposed that  $F(G)$  be named the *forgotten topological index*, or shortly the *F-index*.

Before the publication of the paper Furtula & Gutman (2015), the F-index was not examined as such. On the other hand, in some earlier studies on degree–based graph invariants, it appears as a special case.

The *general first Zagreb index* of a graph  $G$  is defined as

$$M_1^\alpha(G) = \sum_{v \in V(G)} d(v)^\alpha = \sum_{uv \in E(G)} [d(u)^{\alpha-1} + d(v)^{\alpha-1}],$$

for  $\alpha \in \mathbb{R}, \alpha \neq 0$ . (3)

and its first occurrence in the literature seems to be the work by Li & Zhao (2004). Observe that  $M_1^3(G) = F(G)$ . In Li & Zhao (2004) the trees with the first three smallest and largest general first Zagreb index were characterized. In Li & Zhao (2004) and Li & Zheng (2005) among other things, it was shown that for  $\alpha > 1$ , the star  $S_n$  is the tree on  $n$  vertices with maximal  $M_1^\alpha$  whereas the path  $P_n$  is the tree on  $n$  vertices with minimal  $M_1^\alpha$ -value. Needless to say that these results directly apply to the F-index ( $\alpha = 3$ ). More results and information about the general first Zagreb index can be found in Gutman (2014), Hu *et al.* (2005), Liu & Liu (2010), Li & Zhao (2004), Li & Zheng (2005), Su *et al.* (2012), Zhang & Zhang (2006).

The *Randić (or connectivity)* index was introduced by Randić (1975) and is defined as

$$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}. \quad (4)$$

Later, Kier & Hall (1997) have introduced the so-called *zeroth-order Randić index*

$${}^0R = {}^0R(G) = \sum_{v \in V(G)} d(v)^{-\frac{1}{2}}, \quad (5)$$

which was generalized by Li & Zheng (2005). It was named the *zeroth-order general Randić index* and was defined as

$${}^0R_\alpha = {}^0R_\alpha(G) = \sum_{v \in V(G)} d(v)^\alpha \quad (6)$$

for any real number  $\alpha$ . Evidently,  ${}^0R_3(G) = F(G)$ .

Hu *et al.* (2005) characterized graphs of maximal degree at most 4 (molecular graphs), with given number of vertices and edges, and with extremal (maximum or minimum) zeroth-order general Randić index. This, again, in the special case  $\alpha = 3$  renders results for the F-index.

Here, we extend the work on trees with extremal values of F-index, by considering trees with bounded maximal degree. Since the paths are the trees with minimal F-index also in this case, we consider here the characterization of trees with bounded maximal degree that have maximal F-value.

In the sequel we introduce notation that will be used in the rest of the paper. For  $u, v, x, y \in V(G)$  such that

$uv \in E(G), xy \notin E(G)$ , we denote by  $G - uv$  the graph that is obtained by deleting the edge  $uv$  from  $G$  and by  $G + xy$  the graph that is obtained by adding the edge  $xy$  to  $G$ . By  $\Delta = \Delta(G)$  we denote the maximal degree of  $G$ . A sequence  $D = [d_1, d_2, \dots, d_n]$  is *graphical* if there is a graph whose vertex degrees are  $d_i, i = 1, \dots, n$ . If in addition  $d_1 \geq d_2 \geq \dots \geq d_n$ , then  $D$  is a *degree sequence*. Furthermore, the notation  $D(G) = [x_1^{n_1}, x_2^{n_2}, \dots, x_t^{n_t}]$  means that the degree sequence is comprised of  $n_i$  vertices of degree  $x_i$ , where  $i = 1, 2, \dots, t$ .

A tree is said to be *rooted* if one of its vertices has been designated as the *root*. In a rooted tree, the *parent* of a vertex is the vertex adjacent to it on the path to the root; every vertex except the root has a unique parent. A vertex is a parent of a subtree, if this subtree is attached to the vertex. A *child* of a vertex  $v$  is a vertex of which  $v$  is the parent.

## 2. Results

First, we characterize trees with maximal degree at most  $\Delta$  that have maximal F-index.

### 2.1. Trees with bounded maximal degree

**Theorem 2.1.** *Let  $T$  be a tree with maximal F-index among the trees with  $n$  vertices and maximal degree at most  $\Delta$ . Then the following holds:*

- (i) *If  $(n - 2) \bmod (\Delta - 1) = 0$ , then  $T$  contains  $\frac{n-2}{\Delta-1}$  vertices of degree  $\Delta$  and  $\frac{n(\Delta-2)+2}{\Delta-1}$  vertices of degree 1.*
- (ii) *Otherwise,  $T$  contains  $\frac{n-1-x}{\Delta-1}$  vertices of degree  $\Delta$ ,  $\frac{(n-1)(\Delta-2)+x}{\Delta-1}$  vertices of degree 1 and one vertex of degree  $x$ , where  $x$  is uniquely determined by  $2 \leq x \leq \Delta - 1$  and  $(n - 1 - x) \bmod (\Delta - 1) = 0$ .*

**Proof.** We may assume that  $T$  is a rooted tree, whose root is a vertex with degree  $\Delta$ . First, we show that  $T$  is comprised of vertices of degrees  $\Delta$  and 1, and in some cases of one additional vertex  $u$ , with  $2 \leq d(u) \leq \Delta - 1$ . Assume that this is not true and that  $T$  has more than one such vertex. Denote by  $V_d$  the set of all vertices of  $T$  whose degrees are different from  $\Delta$  and 1. Denote by  $n_i$  the number of vertices of tree  $T$  of degree  $i, \forall i = 1, 2, \dots, \Delta$ . We assume that for the degrees of the vertices of  $V_d$  the order  $d(u) \geq \dots \geq d(v)$  holds. Let  $w$  be a child vertex of  $v$ .

Delete the edge  $vw$  and add the edge  $uw$  to  $T$ , obtaining a tree  $T'$ . After this transformation, the degree of  $u$  increases by one, while the degree of  $v$  decreases by one, and the degree set  $V_d$  changed into  $V'_d$ . It holds that

$$F(T') - F(T) = (d(u) + 1)^3 - d(u)^3 + (d(w) - 1)^3 - d(w)^3 > 0. \quad (7)$$

It holds that  $|V'_d| \leq |V_d|$ , with strict inequality if  $d(u) = \Delta - 1$  or  $d(v) = 2$ . If  $|V'_d| \geq 2$  we choose from  $V'_d$  a vertex with maximal degree and a vertex with minimal degree, and we repeat the above operation, obtaining a tree with larger F-index. We proceed on iteratively with the same type of transformation until the transformed  $V_d$  has cardinality 1 or 0, and thus obtain a contradiction to the assumption that  $T$  has more than one vertex with degree different from 1 and  $\Delta$ . It follows that  $T$  has a degree sequence  $[\Delta^{n_\Delta}, 1^{n_1}]$  or  $[\Delta^{n_\Delta}, x^1, 1^{n_1}]$ ,  $2 \leq x \leq \Delta - 1$ .

Observe that any transformation on  $T$  will result in a tree with  $|V_d| > 1$  or will disconnect  $T$ . Thus, we conclude that  $T$  must have one of the two above presented degree sequences.

Next, with respect to the cardinality of  $|V_d|$ , we determine the parameters  $n_\Delta$ ,  $n_1$ , and  $x$ .

Case 1.  $|V_d| = 0$ . In this case the degree sequence of  $T$  is  $[\Delta^{n_\Delta}, 1^{n_1}]$  where the equations

$$\begin{aligned} \sum_{i=1}^{\Delta} n_i &= n_\Delta + n_1 = n \text{ and} \\ \sum_{i=1}^{\Delta} i n_i &= \Delta n_\Delta + n_1 = 2(n - 1) \end{aligned} \quad (8)$$

hold. The above equations have the integer solution

$$n_\Delta = \frac{n - 2}{\Delta - 1}, \quad n_1 = \frac{n(\Delta - 2) + 2}{\Delta - 1}, \quad (9)$$

for  $(n - 2) \bmod (\Delta - 1) = 0$ .

Case 2.  $|V_d| = 1$ . Here the degree sequence of  $T$  is  $[\Delta^{n_\Delta}, x^1, 1^{n_1}]$ , with

$$\begin{aligned} \sum_{i=1}^{\Delta} n_i &= n_\Delta + n_1 + 1 = n \text{ and} \\ \sum_{i=1}^{\Delta} i n_i &= \Delta n_\Delta + n_1 + x = 2(n - 1). \end{aligned} \quad (10)$$

The above equations give the integer solution

$$n_\Delta = \frac{n - 1 - x}{\Delta - 1}, \quad n_1 = \frac{(n - 1)(\Delta - 2) + x}{\Delta - 1}, \quad (11)$$

for  $(n - 1 - x) \bmod (\Delta - 1) = 0$ .

□

As straightforward consequence of Theorem 2.1, we obtain the maximal value of the F-index for trees with maximal degree  $\Delta$ .

Corollary 2.1. *Let  $T$  be a tree with maximal F-index among the trees with  $n$  vertices and maximal degree at most  $\Delta$ . Then,*

(i) if  $(n - 2) \bmod (\Delta - 1) = 0$ ,

$$F(T) = \Delta(\Delta + 1)(n - 2) + 2(n - 1);$$

(ii) otherwise,

$$F(T) = (\Delta^2 + \Delta + 2)(n - 1) - (\Delta^2 + \Delta + 1)x + x^3,$$

where  $x$  is uniquely determined by  $2 \leq x \leq \Delta - 1$  and  $n - 1 - x \bmod (\Delta - 1) = 0$ .

Proof. If  $(n - 2) \bmod (\Delta - 1) = 0$ , by Theorem 2.1,  $T$  has degree sequence  $[\Delta^{n_\Delta}, 1^{n_1}]$ , where  $n_\Delta = (n - 2) / (\Delta - 1)$  and  $n_1 = (n(\Delta - 2) + 2) / (\Delta - 1)$ . Thus,

$$\begin{aligned} F(T) &= \Delta^3 \frac{n - 2}{\Delta - 1} + \frac{n(\Delta - 2) + 2}{\Delta - 1} \\ &= \Delta(\Delta + 1)(n - 2) + 2(n - 1). \end{aligned} \quad (12)$$

Otherwise,  $T$  has degree sequence  $[\Delta^{n_\Delta}, x^1, 1^{n_1}]$ , where  $n_\Delta = (n - 1 - x) / (\Delta - 1)$ ,  $n_1 = ((n - 1)(\Delta - 2) + x) / (\Delta - 1)$ . Then,

$$\begin{aligned} F(T) &= \Delta^3 \frac{n - (x + 1)}{\Delta - 1} + \frac{(n - 1)(\Delta - 2) + x}{\Delta - 1} + x^3 \\ &= \frac{(\Delta^3 + \Delta - 2)n + (1 - \Delta^3)x - (\Delta^3 + \Delta - 2)}{\Delta - 1} + x^3 \\ &= (\Delta^2 + \Delta + 2)(n - 1) - (\Delta^2 + \Delta + 1)x + x^3. \end{aligned} \quad (13)$$

□

## 2.2. Molecular trees

For the special case of molecular trees, i.e.,  $\Delta \leq 4$ , we obtain the following result. Recall that such trees provide the graph representation of the so-called saturated hydrocarbons or alkanes (Gutman & Polansky (1986); Balaban *et al.* (1983)) and are of major importance in theoretical chemistry.

Theorem 2.2. *Let  $T$  be a molecular tree with maximal F-index among the trees with  $n$  vertices. Then the following holds:*

- If  $(n - 2) \bmod 3 = 0$ , then  $T$  contains  $\frac{n-2}{3}$  vertices of degree 4 and  $\frac{2n+2}{3}$  vertices of degree 1. Its F-index is

$$F(T) = 22n - 42.$$

- Otherwise,  $T$  contains  $\frac{n-1-x}{3}$  vertices of degree 4,  $\frac{2(n-1)+x}{3}$  vertices of degree 1 and one vertex of degree  $x$ , where  $x$  is uniquely determined by  $2 \leq x \leq 3$  and  $(n-1-x) \bmod 3 = 0$ . Its F-index is

$$F(T) = 22(n-1) - 21x + x^3.$$

Proof. For  $n = 2, 3, 4, 5$  the star  $S_n$  maximizes the F-index (Li & Zhao (2004)). For  $n = 6$  and  $\Delta \leq 4$ , the possible degree sequences of  $T$  are  $(4, 2, 1, 1, 1, 1)$ ,  $(3, 3, 1, 1, 1, 1)$ ,  $(3, 2, 2, 1, 1, 1)$  and  $(2, 2, 2, 2, 1, 1)$ . The first of these degree sequences corresponds to the largest F-index,  $F(T)$ .

Thus, the corresponding degree sequences of  $T$  for  $n = 2, 3, 4, 5, 6$  satisfy the theorem.

In the rest of the proof we assume that  $n \geq 7$ . First, we show that  $T$  has maximal degree  $\Delta = 4$ . A tree with maximal degree  $\Delta$  we denote by  $T_\Delta$ . By Corollary 2.1(i),  $F(T_2) = 8n - 14$ . Further, we distinguish between two case.

Case 1.  $(n-2) \bmod 2 = 0$ .

By Corollary 2.1(i), we have that  $F(T_3) = 14n - 26$ . Since  $(n-2) \bmod 2 = 0$ , it follows that  $(n-2) \bmod 3 \neq 0$ , and by Corollary 2.1(ii),  $F(T_4) = 22(n-1) - 21x + x^3$ , where  $x = 2$  or  $x = 3$ . For  $n \geq 7$ ,  $F(T_4) > F(T_3) > F(T_2)$  is satisfied.

Case 2.  $(n-2) \bmod 2 \neq 0$ .

By Corollary 2.1(ii),  $F(T_3) = 14(n-1) - 13x + x^3$ , where  $x = 2$  or  $x = 3$ .

Subcase 2.1.  $(n-2) \bmod 3 = 0$ .

By Corollary 2.1(i),  $F(T_4) = 22n - 42$ . For  $n \geq 7$  and  $x = 2, 3$ , it holds that  $F(T_4) > F(T_3) > F(T_2)$ .

Subcase 2.2.  $(n-2) \bmod 3 \neq 0$ .

By Corollary 2.1(ii),  $F(T_4) = 22(n-1) - 21x + x^3$ . Again, a straightforward calculation yields that  $F(T_4) > F(T_3) > F(T_2)$ .

So, we have shown that for  $n \geq 3, 4, 5$  the tree with maximal F-index has maximal degree  $n-1$ , and for  $n \geq 5$  it has maximal degree  $\Delta = 4$ . Setting  $\Delta = 4$  in Theorem 2.1 and Corollary 2.1, we complete the proof.  $\square$

We would like to note that the results of Theorem 2.2 coincide with the results of Theorem 2.2 in Hu *et al.* (2005), pertaining to the zeroth-order general Randić index of a graph, when  $\alpha = 3$  and  $m = n - 1$ .

### 2.3. Observations and computational results

Degree sequences of trees with bounded maximal degree and maximal  $F(T)$  are fully characterized by Theorem 2.1. We would like to note that, alternatively, one can obtain a complete characterization by solving the integer linear programming problem presented in Lemma 2.1. We denote the number of vertices of tree  $T$  of degree  $i$  by  $n_i$ ,  $\forall i = 1, 2, \dots, \Delta$  and the number of edges, connecting a vertex of degree  $i$  with a vertex of degree  $j$ , by  $m_{ij}$ .

Lemma 2.1. *Let  $T$  be a tree with maximal F-index among all trees with  $n$  vertices and maximal degree  $\Delta$ . Then, the trees with maximal F-index are completely described by solving the maximization problem*

$$\begin{aligned} & \text{maximize } F = \sum_{i=1}^{\Delta} i^3 n_i \\ & \text{subject to } \sum_{i=1}^{\Delta} n_i = n, \\ & \sum_{i=1}^{\Delta} i n_i = 2(n-1), \\ & \sum_{i=2}^{\Delta-1} n_i \leq 1, \\ & \sum_{j=1, j \neq i}^{\Delta} m_{ij} + 2m_{ii} = i n_i \quad 1 \leq i \leq \Delta, \\ & 0 \leq n_i \leq n-1, \quad 1 \leq i \leq \Delta, \\ & 0 \leq m_{ij} \leq n-2, \quad 1 \leq i, j \leq \Delta. \end{aligned}$$

For experimental proposes we have solve the above linear programming problem for trees with  $\Delta = 4$  (molecular trees) and trees with  $\Delta = 5$ . Needless to say the obtained characterization coincide with that from Theorem 2.1. All trees with maximal F-index of order up to 20 and maximal degree 4 and 5 are given in Figures 1. and 2., respectively.

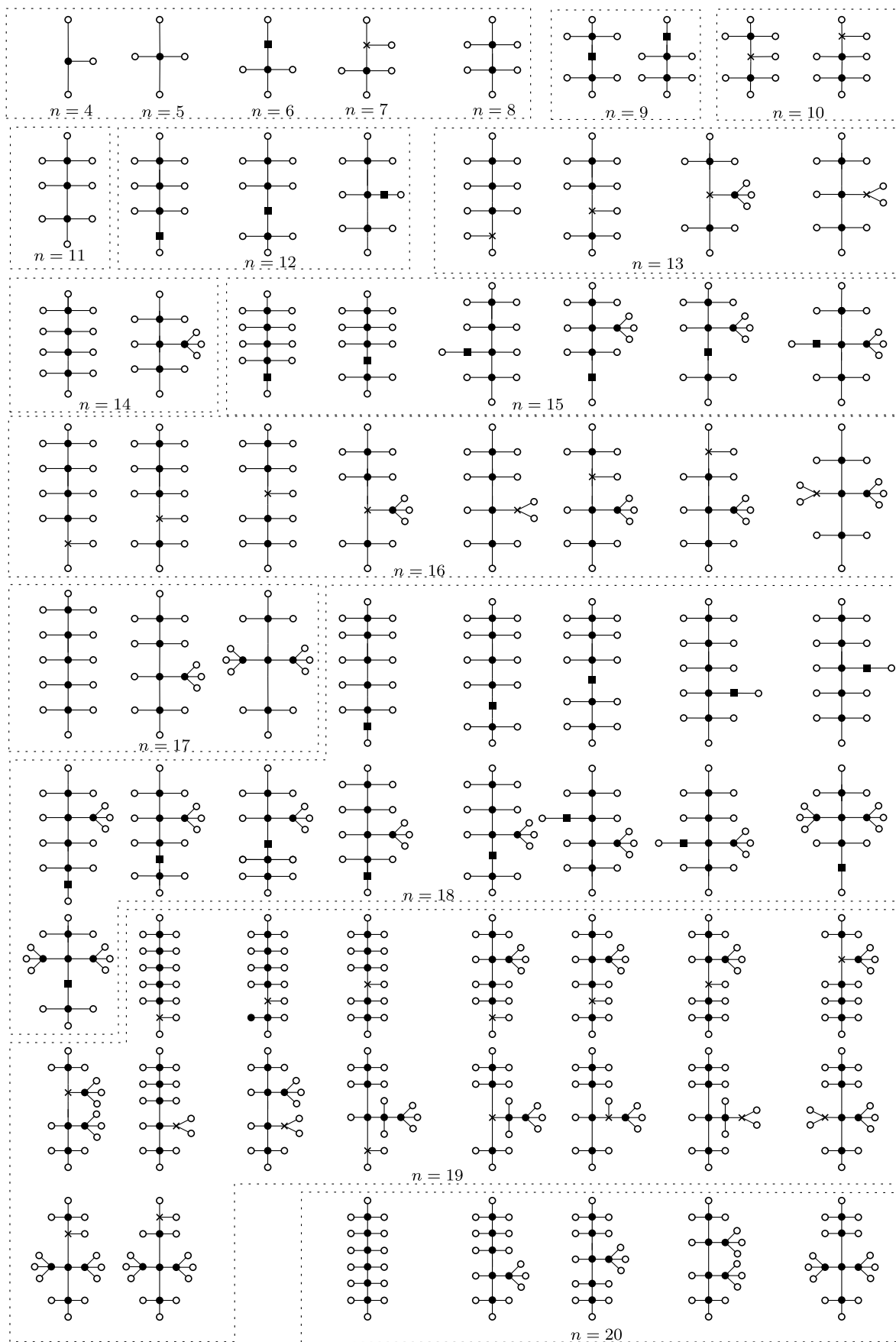


Fig. 1. Extremal chemical trees of orders  $n = 4, \dots, 20$  with respect to the F-index.

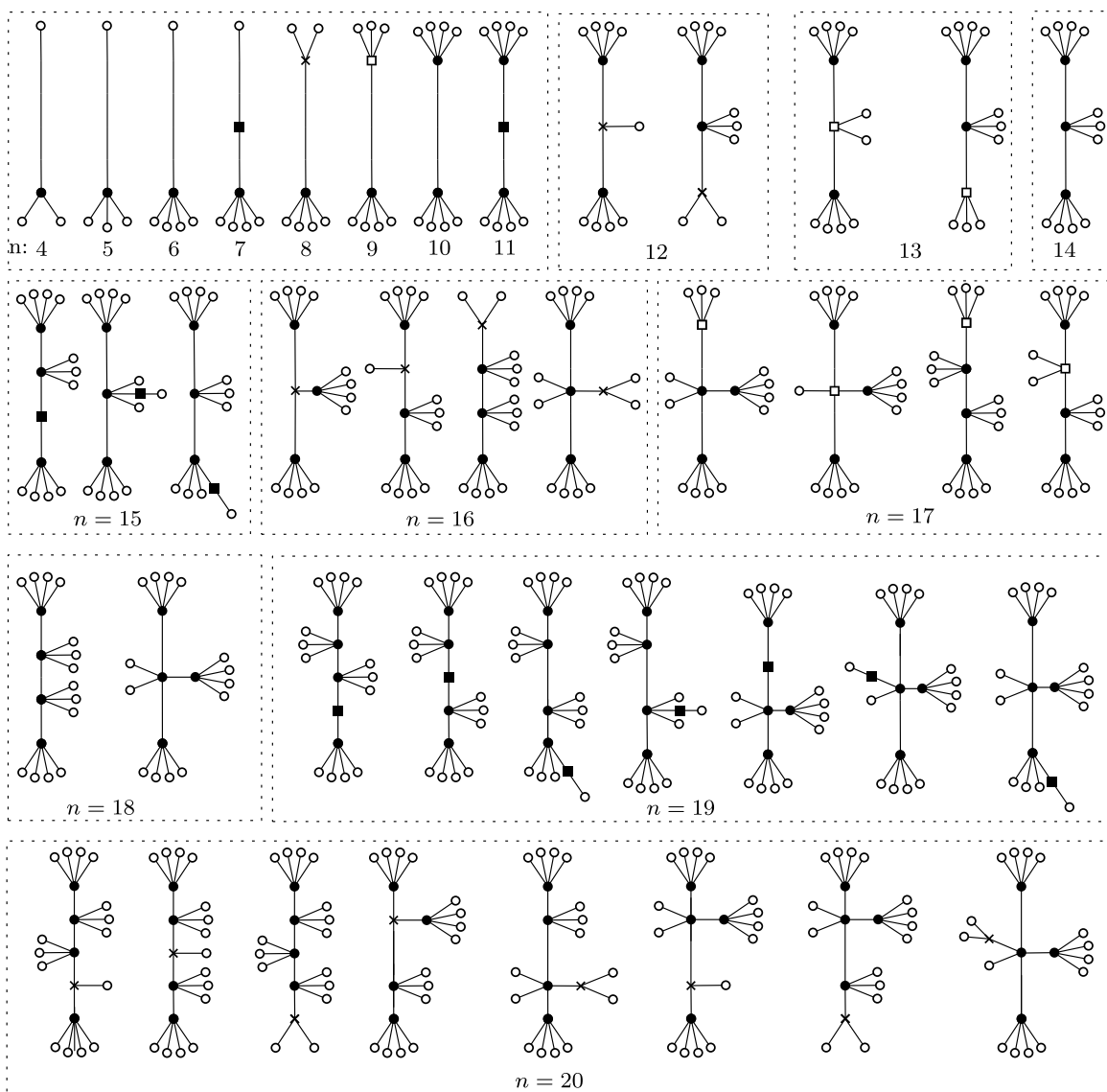


Fig. 2. Extremal trees of orders  $n = 4, 5, \dots, 20$ ,  $\Delta = 5$  with respect to the F-index.

### 3. Conclusion

The *F-index* is a graph-based molecular structure descriptor that has an exceptional applicative potential. In this paper we have characterized the extremal trees with  $n$  vertices and arbitrarily large maximal degree  $\Delta$  with respect to the *F-index*. Additionally, we have presented some computational results. The computations were focused on molecular trees and on trees with maximal degree  $\Delta = 5$  of order up to 20.

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## حول الأشجار الحرجة بالنسبة إلى المعامل التبولوجي - $F$

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### ملخص

في الدراسة البحثية المنشورة في عام 1972 عن اعتمادية التكوين الجزئي على الطاقة الكلية للإلكترون -  $\pi$  فإن الباحث Trinajstić مع المؤلف الثالث للبحث الحالي قد برهننا أن الطاقة الكلية للإلكترون تعتمد على مجموع مربعات درجات رؤوس الرسم الجزئي الكامنة للإلكترون. وفيما بعد أطلق على مجموع مربعات درجات رؤوس رسم ما مسمى المعامل التبولوجي «معامل زغرب الأول للرسم». وخلال السنوات فيما بعد 1972 أصبح معامل زغرب الأول أحد أهم واصفات التكوين الجزئي المعتمد على الرسم أو الشكل الجزئي. وعلى الجانب الآخر فإن مجموع مكعبات درجات رؤوس الرسم (فيما عدا أبحاث نادرة جدا بخصوص معامل زغرب الأول العام ومعامل راندك العام ذي الرتبة الصفرية) غالباً ما قد تم إهمالها تماماً. حديثاً فإن مجموع مكعبات درجات رؤوس الرسم أطلق عليها المعامل المنسي أو للاختصار معامل -  $F$  كما تبين أن لديه إمكانات تطبيقية استثنائية. في هذا البحث فإننا ندرس ونحدد الأشجار الحرجة ذات القيم العظمى بالنسبة إلى المعامل -  $F$ .