A Survey on Terminal Wiener Index

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Abstract

The *terminal Wiener index* $TW = TW(G)$ of a graph G is equal to the sum of distances between all pairs of pendent vertices of G. This distance–based molecular structure descriptor was put forward quite recently [I. Gutman, B. Furtula, M. Petrović, *J. Math. Chem.* **46** (2009) 522–531]. In this survey we outline the hitherto established properties of TW. In particular, we describe a simple method for computing TW of trees, characterize the trees with minimum and maximum TW, and provide a formula for calculating TW of thorn graphs.

1. Introduction

Let G be a connected graph with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $\mathbf{E}(G) = \{e_1, e_2, \ldots, e_m\}$. The *distance* between the vertices v_i and v_j, $v_i, v_j \in \mathbf{V}(G)$, is equal to the length (= number of edges) of the shortest path starting at v_i and ending at v_j (or vice versa) [1], and will be denoted by $d(v_i, v_j|G)$.

The oldest molecular structure descriptor (topological index) is the one put forward in 1947 by Harold Wiener [2], nowadays referred to as the *Wiener index* and denoted by W. It is defined as the sum of distances between all pairs of vertices of a (molecular) graph:

$$W = W(G) = \sum_{\{u,v\} \subseteq \mathbf{V}(G)} d(u, v|G) = \sum_{1 \le i < j \le n} d(v_i, v_j|G) \ . \tag{1}$$

Details on the chemical applications and mathematical properties of the Wiener index can be found in the reviews [3–5].

The square matrix of order n whose (i,j)-entry is $d(v_i, v_j|G)$ is called the *distance matrix* of G. Also this matrix has been much studied by mathematical chemists, for details see [6, 7]. From the distance matrix not only the Wiener index, but also numerous other structure descriptors can be derived [8, 9].

In a number of recently published articles, the so-called *terminal distance matrix* [10, 11] or *reduced distance matrix* [12] of trees was considered.

If an n-vertex graph G has k pendent vertices (= vertices of degree one), labeled by $v_1, v_2, \ldots, v_k$, then its terminal distance matrix is the square matrix of order k whose (i,j)-entry is $d(v_i, v_j|G)$. In what follows, we denote this matrix by $\mathbf{TD} = \mathbf{TD}(G)$.

Practically all researches on $\mathbf{TD}$ (and, eventually, on the terminal Wiener index) were concerned with trees (= connected acyclic graphs). The reason for this is evident: It is easy to envisage that in the case of non-tree graphs G, in the matrix $\mathbf{TD}(G)$ the information on the structure of G may be almost completely missing.

In particular, if the graph G has no pendent vertices, then G has no terminal distance matrix (i. e., the dimension of $\mathbf{TD}$ is zero). If G has a single pendent vertex, then $\mathbf{TD}(G)$ has dimension one and its unique matrix element is zero. If G has two just two pendent vertices, both adjacent to the same vertex, then irrespective of the actual structure of this graph, $\mathbf{TD}(G)$ is of the form

$$\begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix} .$$

In the case of trees the situation is less pessimistic. Namely, any n-vertex tree has k pendent vertices, and $2 \leq k \leq n-1$. The unique n-vertex trees with $k=2$ and $k=n-1$ are, respectively, the *path* (P_n) and the *star* (S_n). It is important to know that the terminal distance matrix of a tree T determines the entire distance matrix of T, and thus completely determines the tree T itself [13].

Terminal distance matrices of trees were used for modeling amino acid sequences of proteins and the genetic code [10, 11, 14], and were proposed to serve as a source of novel molecular–structure descriptors [10, 11].

Motivated by the previous researches on the terminal distance matrix and on its chemical applications, the present authors have conceived the *terminal Wiener index* $TW(G)$ of a graph G as *the sum of the distances between all pairs of its pendent vertices* [15].

Without loss of generality, we may assume that the graph G has n vertices of which k vertices, labeled by $v_1, v_2, \ldots, v_k$, are pendent. Let thus $\mathbf{V}_1(G) = \{v_1, v_2, \ldots, v_k\}$ be the set of pendent vertices of G. In harmony with the previously introduced notation, $\mathbf{V}_1(G) \subseteq \mathbf{V}(G)$. Then, in analogy with Eq. (1), we define

$$TW = TW(G) = \sum_{\{u,v\} \subseteq \mathbf{V}_1(G)} d(u,v|G) = \sum_{1 \leq i < j \leq k} d(v_i, v_j|G) \ . \tag{2}$$

In order to illustrate the above definition, we show how the terminal Wiener index is computed for the tree T_1 depicted in Fig. 1. Here we directly apply Eq. (2).

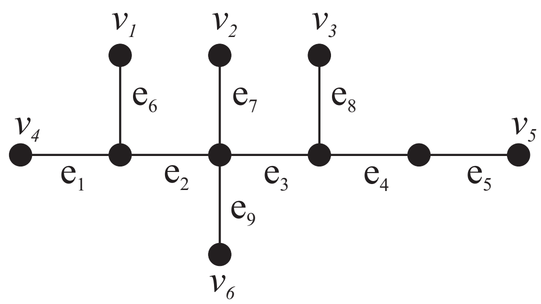

Fig. 1. A tree T_1 whose terminal Wiener index is equal to 51.

The tree T_1 has six pendent vertices - $v_1, v_2, \ldots, v_6$. Therefore the summation on the right–hand side of (2) contains $\binom{6}{2} = 15$ terms, and we have:

$$\begin{aligned}
TW(T_1) &= d(v_1,v_2|T_1) + d(v_1,v_3|T_1) + d(v_1,v_4|T_1) + d(v_1,v_5|T_1) + d(v_1,v_6|T_1) \\
&+ d(v_2,v_3|T_1) + d(v_2,v_4|T_1) + d(v_2,v_5|T_1) + d(v_2,v_6|T_1) + d(v_3,v_4|T_1) \\
&+ d(v_3,v_5|T_1) + d(v_3,v_6|T_1) + d(v_4,v_5|T_1) + d(v_4,v_6|T_1) + d(v_5,v_6|T_1) \\
&= 3+4+2+5+3+3+3+4+2+4+3+3+5+3+4 = 51 \ .
\end{aligned}$$

2. Elementary properties of the terminal Wiener index

Directly from its definition, Eq. (2), the following properties of TW are immediate:

1. If the graph G has no pendent vertices ($k = 0$, $\mathbf{V}_1(G) = \emptyset$), then $TW(G) = 0$.

2. If the graph G has a single pendent vertex ($k = 1$, $\mathbf{V}_1(G) = \{v_1\}$), then $TW(G) = 0$.

3. If the graph G has exactly two pendent vertices ($k = 2$, $\mathbf{V}_1(G) = \{v_1, v_2\}$), then $TW(G) = d(v_1, v_2|G)$.

4. In particular, if the two vertices from point 3 are adjacent to the same vertex of G, then $TW(G) = 2$.

5. As a special case of point 3, $TW(P_n) = n - 1$.

6. The star S_n has $n - 1$ pendent vertices, all adjacent to the same vertex. Therefore,

$$TW(S_n) = \binom{n-1}{2} \times 2 = (n-1)(n-2) \ .$$

The above listed properties of TW confirm the conclusions that it is purposeful to restrict the considerations to trees.

3. A modified Wiener's "first theorem"

In this section we are concerned with trees. Recall that any tree T with n vertices has $n - 1$ edges, and has at least two pendent vertices.

The first question that should be asked in connection with the terminal Wiener index is how it could be efficiently computed. For this a result that is fully analogous to Wiener's "first theorem" for the ordinary Wiener index [2, 16] was reported in [15].

In his seminal article [2] Wiener communicated the formula

$$W(T) = \sum_{e \in \mathbf{E}(T)} n_1(e) \cdot n_2(e) \tag{3}$$

which holds for any tree T. This result may be viewed as the first theorem ever for the Wiener index. In formula (3) e stands for an edge, whereas $n_1(e)$ and $n_2(e)$ are the number of vertices lying on the two sides of e; the summation in (3) goes over all edges of the respective tree T. If T has n vertices, then $n_1(e) + n_2(e) = n$ for all edges e.

In the paper [7] no proof of formula (3) was put forward. However, the proof of (3) is easy [16]: Instead of summing the distances (= the number of edges in the shortest paths) between all pairs of vertices in the tree T, we may count how many times a particular edge e lies on the (unique) shortest path between two vertices, and then add these counts over all edges of the underlying tree. The number of shortest paths that go through the edge e is equal to $n_1(e) \cdot n_2(e)$.

Using the same idea we obtain [15]:

Theorem 1. Let T be an n-vertex tree with k pendent vertices, and let e be its edge. Denote by $p_1(e)$ and $p_2(e)$ the number of pendent vertices of T, lying on the two sides of e. Then

$$TW(T) = \sum_{e \in \mathbf{E}(T)} p_1(e) \cdot p_2(e) \tag{4}$$

with the summation embracing all the $n-1$ edges of T.

Proof. Instead of summing the distances between all pairs of pendent vertices in the tree T, we count how many times a particular edge e lies on the shortest path between two pendent vertices, and then add these counts over all edges of the underlying tree. Such shortest paths will start at $p_1(e)$ pendent vertices (those lying on one side of e) and end at $p_2(e)$ pendent vertices (those lying on the other side of e). Thus their number is $p_1(e) \cdot p_2(e)$, which leads to Eq. (4). ■

It should be noted that for all edges of the tree T,

$$p_1(e) + p_2(e) = k \qquad \text{and} \qquad p_1(e), p_2(e) \geq 1 \; .$$

Consequently,

$$k - 1 \leq p_1(e) \cdot p_2(e) \leq \left\lfloor \frac{k}{2} \right\rfloor \left\lceil \frac{k}{2} \right\rceil \; .$$

If e is a pendent edge, then $p_1(e) \cdot p_2(e) = k - 1$.

For the tree T_1 (see Fig. 1) we immediately get:

$$\begin{array}{ll}
p_1(e_1) = 1 \; ; \; p_2(e_1) = 5 & \qquad p_1(e_2) = 2 \; ; \; p_2(e_2) = 4 \\[6pt]
p_1(e_3) = 4 \; ; \; p_2(e_3) = 2 & \qquad p_1(e_4) = 5 \; ; \; p_2(e_4) = 1 \\[6pt]
p_1(e_5) = 5 \; ; \; p_2(e_5) = 1 & \qquad p_1(e_6) = 1 \; ; \; p_2(e_6) = 5 \\[6pt]
p_1(e_7) = 1 \; ; \; p_2(e_7) = 5 & \qquad p_1(e_8) = 1 \; ; \; p_2(e_8) = 5 \\[6pt]
p_1(e_9) = 1 \; ; \; p_2(e_9) = 5 &
\end{array}$$

and therefore formula (4) yields:

$$\begin{aligned} TW(T_1) &= (1\times 5)+(2\times 4)+(4\times 2)+(5\times 1)+(1\times 5) \\ &+ (1\times 5)+(1\times 5)+(1\times 5)+(1\times 5) = 51 \ . \end{aligned}$$

This example shows that the calculation of TW by means of formula (4) is somewhat easier than by using the definition (2). However, the true value of formula (4) is in enabling one to deduce a number of general properties of the terminal Wiener index of trees.

4. Variable terminal Wiener index

A generalization of the Wiener–index concept, based on Eq. (3), was proposed in 2004 by Vukičević, Žerovnik, and one of the present authors [17]. Thus, the *variable Wiener index* was defined as

$$W_\lambda(T) = \sum_{e\in \mathbf{E}(T)} [n_1(e)\cdot n_2(e)]^\lambda \tag{5}$$

where λ is a real number. In full analogy to this, bearing in mind Eq. (4), Deng and Zhang put forward the *variable terminal Wiener index*, defined as [18]

$$TW_\lambda(T) = \sum_{e\in \mathbf{E}(T)} [p_1(e)\cdot p_2(e)]^\lambda \ . \tag{6}$$

Until now, there is no report on any chemical application of TW_λ, and its only established mathematical property is the one mentioned in the subsequent section.

Needless to say, for $\lambda = 1$ the variable Wiener and variable terminal Wiener indices reduce to the ordinary Wiener and terminal Wiener indices, respectively.

5. Terminal–equiseparable trees

In this section it will be assumed that the quantities $n_1(e)$ and $n_2(e)$, as well as $p_1(e)$ and $p_2(e)$, encountered in Section 3, are chosen so that $n_1(e) \geq n_2(e)$ and $p_1(e) \geq p_2(e)$.

Let T' and T'' be two n-vertex trees, with edge sets $\mathbf{E}(T') = \{e'_1, e'_2, \ldots, e'_{n-1}\}$ and $\mathbf{E}(T'') = \{e''_1, e''_2, \ldots, e''_{n-1}\}$. If it is possible to label the edges of T' and T'' so that $n_1(e'_i) = n_1(e''_i)$ holds for all $i = 1, 2, \ldots, n-1$, then the trees T' and T'' are said to be *equiseparable*

[19]. Then, of course, also $n_2(e'_i) = n_2(e''_i)$ holds for all $i = 1, 2, \ldots, n-1$. Equiseparability of trees has numerous intriguing mathematical and chemical consequences, for details see [20–24]. For our considerations it suffices to note that for any value of the parameter λ, cf. Eq. (5), equiseparable trees have equal variable Wiener indices. In particular, such trees have also equal Wiener indices.

Equiseparability is a very frequent phenomenon among trees. Namely, it was shown that [23],

$$\lim_{n\to\infty} \frac{\#EST(n)}{\#T(n)} = 1 \tag{7}$$

where $\#EST(n)$ is the number of n-vertex trees having an equiseparable mate, and $\#T(n)$ is the total number of n-vertex trees. Eq. (7) means that almost all trees have an equiseparable mate.

Deng and Zhang [18] extended the concept of equiseparability to terminal vertices. They defined *terminal–equiseparability* as follows. If for two n-vertex trees T' and T'', the equality $p_1(e'_i) = p_1(e''_i)$ holds for all $i = 1, 2, \ldots, n-1$, then T' and T'' are *terminal–equiseparable*.

The same authors [18] described methods for constructing pairs of terminal–equiseparable trees. This turned out to be easy, and fully analogous to what earlier was proposed for equiseparable trees [20]. We state here two simple results of this kind:

Theorem 2. All n-vertex trees with exactly 3 pendent vertices are mutually terminal–equiseparable.

Proof. Since $k = 3$, on one side of each edge there is one, and on the other side two pendent vertices. Therefore, for any edge e of any tree with $k = 3$, it is $p_1(e) = 2$ and $p_2(e) = 1$. ■

Theorem 3. If the trees T' and T'' are terminal–equiseparable, then for all values of the parameter λ, $TW_\lambda(T') = TW_\lambda(T'')$. In particular, $TW(T') = TW(T'')$.

Proof. Take into account Eq. (6). ■

Without proof we state the much less easy:

Theorem 4. [18]

$$\lim_{n\to\infty} \frac{\#TEST(n)}{\#T(n)} = 1$$

where $\#TEST(n)$ is the number of n-vertex trees having a terminal–equiseparable mate, and $\#T(n)$ is the total number of n-vertex trees. Therefore, almost all trees have a terminal–equiseparable mate.

6. Tree with minimal terminal Wiener index

For the considerations that follow one should recall that the summation on the right–hand side of Eq. (4) goes over $n-1$ (non-zero) terms.

Because 1 is the minimal possible value for the product $p_1(e) \cdot p_2(e)$, it immediately follows that $n-1$ is the minimal possible value that the terminal Wiener index may assume for n-vertex trees. Because any tree different from P_n possesses at least one edge e for which $p_1(e) \cdot p_2(e) \geq 2$, we conclude that $TW(T) > n-1$ holds for all n-vertex trees $T \ncong P_n$. By this, as a straightforward consequence of Eq. (4) we obtained:

Theorem 5. [15] For any n-vertex tree, $TW(T) \geq n-1$. Equality $TW(T) = n-1$ holds if and only if $T \cong P_n$. ■

Thus the path is the tree with minimal terminal Wiener index. The finding of the tree(s) with maximal TW is less easy and will be achieved in the subsequent two sections.

7. Trees with fixed number of pendent vertices having minimal and maximal terminal Wiener index

In this section we restrict our consideration to n-vertex trees having a fixed number k of pendent vertices. Such trees have also k pendent edges, and, consequently, k summands on the right–hand side of Eq. (4) are equal to $k-1$. Formula (4) can thus be rewritten as

$$TW(T) = k(k-1) + \sum_{e'} p_1(e') \cdot p_2(e') \tag{8}$$

where e' are the non-pendent edges of T . Note that there exist $n-1-k$ such edges.

The only n-vertex tree with $k = 2$ is the path P_n. Therefore, in what follows, we assume that $3 \leq k \leq n-1$.

In view of the fact that $p_1(e')+p_2(e') = k$, the minimal value of the product $p_1(e') \cdot p_2(e')$ is $k-1$. Therefore, if for all non-pendent edges e' the product $p_1(e') \cdot p_2(e')$ is equal to $k-1$, then the respective tree will have minimal possible TW-value. Such trees do exist.

A tree is said to be *starlike of degree* k if exactly one of its vertices has degree greater than two, and this degree is equal to k, $k \geq 3$. In Fig. 2 are depicted all 12-vertex starlike trees of degree 4.

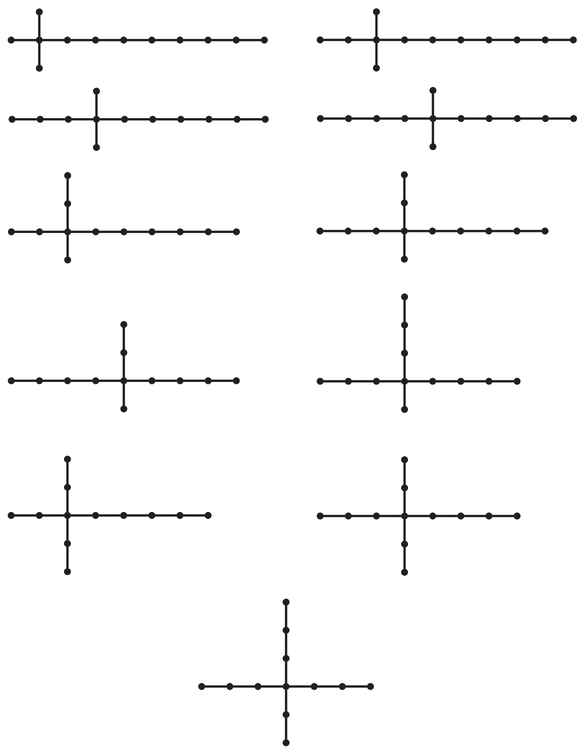

Fig. 2. The 12-vertex starlike trees of degree 4. Among 12-vertex trees with 4 pendent vertices these all have minimal terminal Wiener index, equal to 33.

Theorem 6. [15] Among n-vertex trees with a fixed number k of pendent vertices, $k \geq 3$, the starlike trees of degree k have minimal terminal Wiener index. All n-vertex starlike trees of degree k have $TW = (n-1)(k-1)$.

Proof. It is easy to see that among trees, only the starlike trees have the property that either $p_1(e) = 1$ or $p_2(e) = 1$ holds for any edge e. ■

From Theorem 6 we see that $TW = 33$ holds for all the eleven trees depicted in Fig. 2.

From this example one concludes that there are numerous non-isomorphic trees having the same TW-value. In other words, the isomer–discriminating power of the terminal Wiener index is very low. In particular, all trees with 3 pendent vertices are starlike, and thus all such trees with same number n of vertices have same TW-values, equal to $2(n-1)$. (The same conclusion would follow also from Theorems 2 and 3.)

We now begin the search for trees with k pendent vertices and maximal TW. For reason just explained, we are not interested in the case $k = 3$.

In Section 3 it has been explained that the maximal possible value of the product $p_1(e') \cdot p_2(e')$ is $\lfloor k/2 \rfloor \cdot \lceil k/2 \rceil$. Then from Eq. (8) we conclude that the maximal possible value of TW is $k(k-1) + (n-1-k)\lfloor k/2 \rfloor \lceil k/2 \rceil$, provided that there exist n-vertex trees with k pendent vertices, for which all non-pendent edges e' have the property

$$p_1(e') \cdot p_2(e') = \left\lfloor \frac{k}{2} \right\rfloor \left\lceil \frac{k}{2} \right\rceil \, . \tag{9}$$

Indeed, such trees do exist (see below). We thus arrive at:

Theorem 7. [15] Among n-vertex trees with a fixed number k of pendent vertices, $k \geq 4$, the trees whose all non-terminal edges e' satisfy condition (9) have maximal terminal Wiener index. All such trees have

$$TW = k(k-1) + (n-1-k) \left\lfloor \frac{k}{2} \right\rfloor \left\lceil \frac{k}{2} \right\rceil \, . \tag{10}$$

Proof. We have already seen that the right–hand side of Eq. (10) is the maximal possible value that TW may assume. What remains is to demonstrate that there are trees satisfying Eq. (10). The construction of such trees proceeds as follows:

(a) If k is even, $4 \leq k < n-1$, then the required tree is obtained from the path P_{n-k} by attaching to each of its terminal vertices $k/2$ new pendent vertices. This tree is unique.

(b) If k is odd, $5 \leq k < n-1$, then the required tree is obtained from the path P_{n-k} by attaching to each of its terminal vertices $(k-1)/2$ new pendent vertices, and by attaching one more pendent vertex to some vertex of P_{n-k}. There exist $\lceil (n-k)/2 \rceil$ distinct trees of this kind.

(c) If $k = n-1$, then the respective tree is the star, having no non-pendent edges at all.

It can easily be verified that the above described trees have n vertices, k pendent vertices and that their non-pendent edges satisfy condition (9). It is also straightforward to see that these are the only trees with such properties. ■

The trees with 12 vertices and various number of pendent vertices, having maximal terminal Wiener index are shown in Fig. 3.

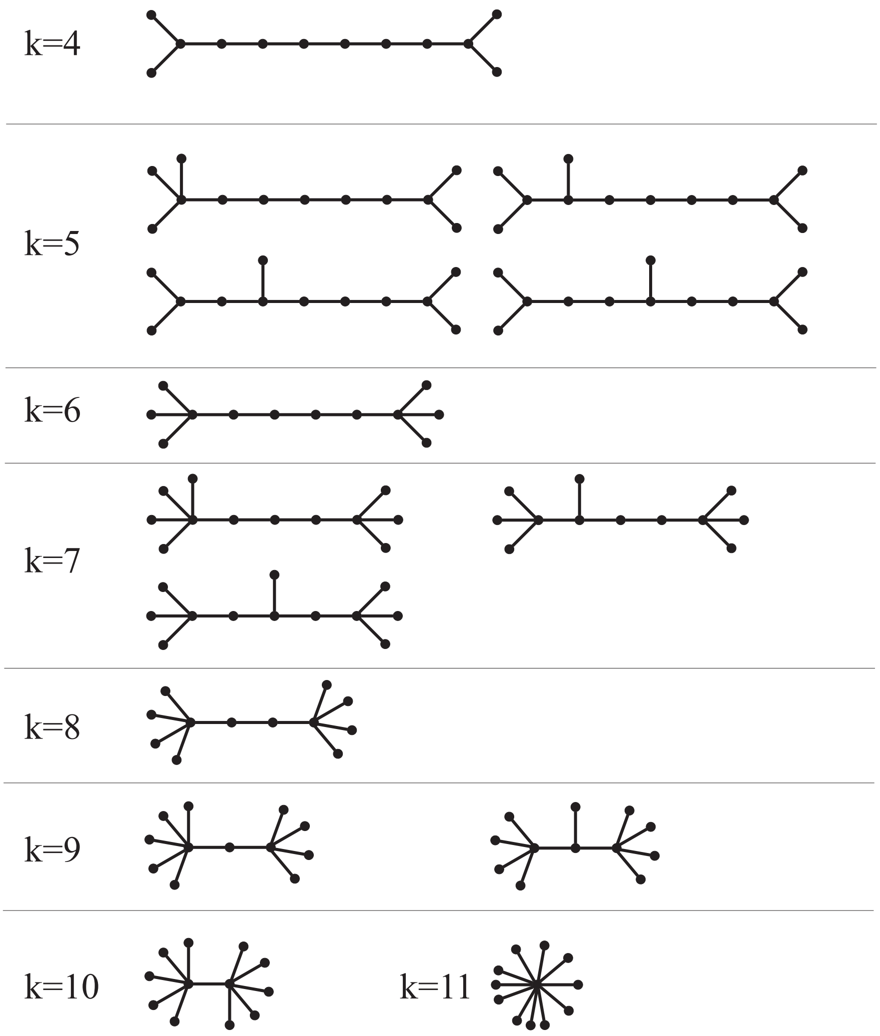

Fig. 3. Trees with $n = 12$ vertices and k pendent vertices, having maximal terminal Wiener index. For even values of k such trees are unique. For odd values of k there exist $\lceil (n-k)/2 \rceil$ distinct trees of this kind; in particular, 4, 3, 2, and 1 for $k = 5$, $k = 7$, $k = 9$, and $k = 11$, respectively.

8. Trees with maximal terminal Wiener index

In the preceding section we determined the n-vertex trees with a fixed number k of pendent vertices, for which TW is maximal.

In Fig. 4 are depicted all n-vertex trees with maximal terminal Wiener index, for $9 \leq n \leq 16$. These may give an idea which value of k needs to be chosen in order to get a maximum TW-value.

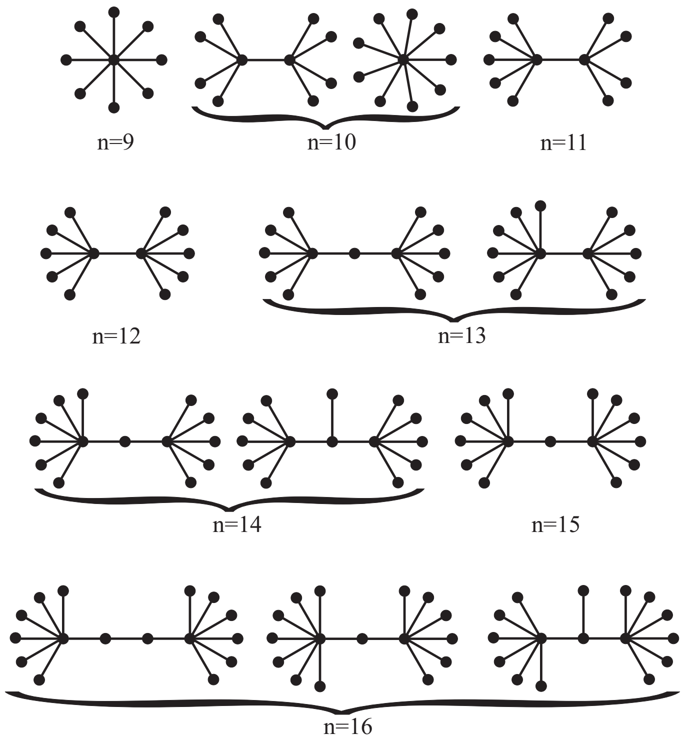

Fig. 4. The n-vertex trees with maximal terminal Wiener index, for $n = 9, 10, \ldots, 16$.

In order to find the n-vertex tree(s) for which TW is maximal we only have to determine the value of k for which the right–hand side of Eq. (10) is maximal. The solution of this not quite easy mathematical problem was found in [15]. We state it without proof.

Theorem 8. [15] Within the class of all trees with n vertices the following holds.

(a) If $3 \leq n \leq 9$, then the star S_n has maximal terminal Wiener index, equal to $(n-1)(n-2)$.

(b) If $n = 3s$, $s = 4, 5, 6, \ldots$, then the tree with $k = 2s + 2$ pendent vertices (specified in the proof of Theorem 4) has maximal terminal Wiener index, equal to $s^3 + 3\,s^2 + s - 1$.

This tree is unique.

(c) If $n = 3s+1$, $s = 3,4,5,\ldots$, then the trees with $k = 2s+2$ and $k = 2s+3$ pendent vertices (specified in the proof of Theorem 4) have maximal terminal Wiener indices, all equal to $s^3 + 4\,s^2 + 3s$. There are $\lceil s/2 \rceil$ distinct trees of this kind.

(d) If $n = 3s+2$, $s = 3,4,5,\ldots$, then the trees with $k = 2s+3$ pendent vertices (specified in the proof of Theorem 4) have maximal terminal Wiener indices, all equal to $s^3+5\,s^2+6s+2$. There are $\lceil (s-1)/2 \rceil$ distinct trees of this kind.

9. Terminal Wiener index of thorn graphs

Let G a connected n-vertex graph with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$, and let $\mathbf{a} = (a_1, a_2, \ldots, a_n)$ be an n-tuple of non-negative integers. The *thorn graph* $G(\mathbf{a})$ is the graph obtained by attaching a_i pendent vertices to the vertex v_i of G for $i = 1,2,\ldots,n$. The a_i pendent vertices attached to the vertex v_i will be called the thorns of v_i .

Theorem 9. [25] If $a_i > 0$ for all $i = 1,2,\ldots,n$, then

$$TW(G(\mathbf{a})) = 2\sum_{i=1}^{n} \binom{a_i}{2} + \sum_{1 \le i < j \le n} a_i\,a_j\,[d(v_i,v_j|G) + 2] \ . \tag{11}$$

Proof. We obtain formula (11) by applying Eq. (2). Consider first the thorns attached to a given vertex v_i . Each of these are at distance 2, and therefore their contribution to $TW(G(\mathbf{a}))$ is $\binom{a_i}{2} \times 2$. This leads to the first term on the right–hand side of (11).

Consider a thorn attached to vertex v_i and a thorn attached to vertex v_j , $i \neq j$. Their distance is by two greater than the distance between v_i and v_j . Since there are $a_i \times a_j$ pairs of thorns of this kind, their contribution to $TW(G(\mathbf{a}))$ is equal to $a_i\,a_j\,[d(v_i,v_j|G) + 2]$. This leads to the second terms on the right–hand side of (11). ■

Corollary 9.1. Formula (11) remains valid also if some a_i's are equal to zero, provided that the corresponding vertices of the graph G are not pendent.

Corollary 9.2. If $a_1 = a_2 = \cdots = a_n = a > 0$, then

$$TW(G(\mathbf{a})) = a^2\,W(G) + an(an-1) \ . \tag{12}$$

Proof. Start with Eq. (11) and apply the definition (1) of the Wiener index of the graph G. This yields

$$TW(G(\mathbf{a})) = na(a-1) + a^2\ [W(G) - n(n-1)]$$

which is then easily transformed into Eq. (12). ■

Theorem 10. [25] Let G be a connected n-vertex graph, and let $v_1, v_2, \ldots, v_k$ be its pendent vertices. Choose the n-tuple $\mathbf{a}$ so that

$$a_i = \begin{cases} a & \text{for } i = 1, 2, \ldots, k \\ 0 & \text{for } i = k+1, \ldots, n \end{cases}$$

and let $a > 0$. Then

$$TW(G(\mathbf{a})) = a^2\, TW(G) + ak(ak-1)\ . \tag{13}$$

Proof. Start with Eq. (11) and apply the definition (2) of the terminal Wiener index of the graph G. This yields

$$TW(G(\mathbf{a})) = ka(a-1) + a^2\ [TW(G) - k(k-1)]$$

which is then easily transformed into Eq. (13). ■

Note that if in the above theorem $a = 0$, then $TW(G(\mathbf{a})) \equiv TW(G)$.

By means of Theorem 10 it is possible to recursively compute the terminal Wiener indices of certain dendrimers. An example of a dendrimer series to which formula (13) is applicable is shown in Fig. 5.

Let D_0, D_1, D_2, ... be a series of dendrimer graphs. Let for $h = 1, 2, \ldots,$ the dendrimer graph D_h be obtained so that a pendent vertices are attached to each pendent vertex of D_{h-1}. For an illustration see Fig. 5.

Let k_h be the number of pendent vertices of D_h. Then from Theorem 10 we get the recurrence relations:

$$\begin{aligned} TW(D_{h+1}) &= a^2\, TW(D_h) + a\, k_h(a\, k_h - 1) \\ k_{h+1} &= a\, k_h\ . \end{aligned}$$

In the examples depicted in Fig. 5, $a = 2$. It is easy to check that $TW(D_0) = 12$ and

$k_0 = 3$. Then

$$\begin{aligned}
TW(D_1) &= a^2\, TW(D_0) + a\, k_0(a\, k_0 - 1) = 2^2 \cdot 12 + 2 \cdot 3 \cdot (2 \cdot 3 - 1) = 78 \\
k_1 &= a\, k_0 = 2 \cdot 3 = 6 \\
TW(D_2) &= a^2\, TW(D_1) + a\, k_1(a\, k_1 - 1) = 2^2 \cdot 78 + 2 \cdot 6 \cdot (2 \cdot 6 - 1) = 444 \\
k_2 &= a\, k_1 = 2 \cdot 6 = 12 \\
TW(D_3) &= a^2\, TW(D_2) + a\, k_2(a\, k_2 - 1) = 2^2 \cdot 444 + 2 \cdot 12 \cdot (2 \cdot 12 - 1) = 2328 \\
k_3 &= a\, k_2 = 2 \cdot 12 = 24 \\
TW(D_4) &= a^2\, TW(D_3) + a\, k_3(a\, k_3 - 1) = 2^2 \cdot 2328 + 2 \cdot 24 \cdot (2 \cdot 24 - 1) = 11568 \\
k_4 &= a\, k_3 = 2 \cdot 24 = 48
\end{aligned}$$

etc.

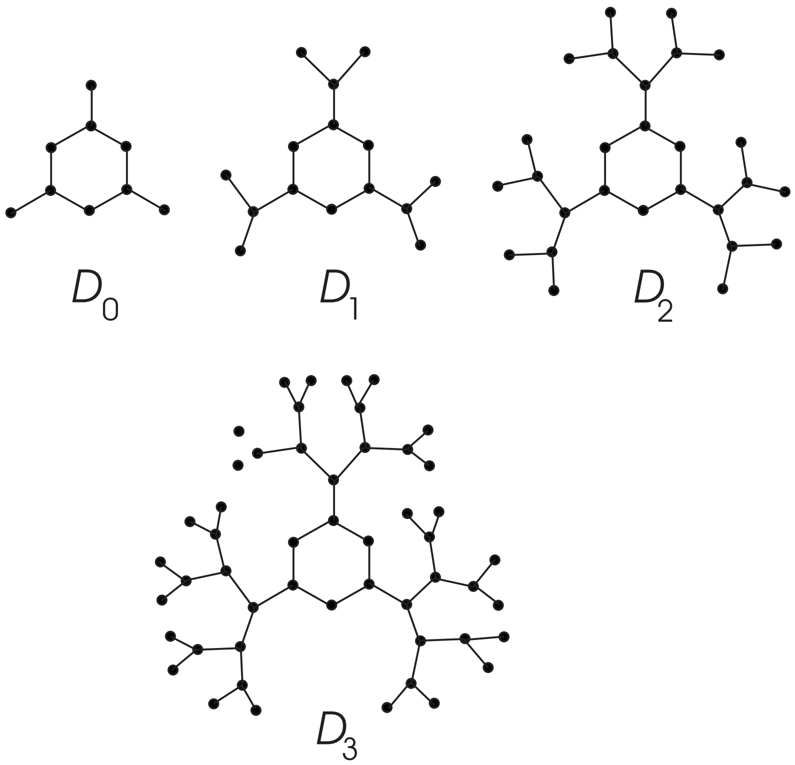

Fig. 5. The first four members of a series of dendrimer graphs. Their terminal Wiener indices are calculated recursively as $TW(D_0) = 12$, $TW(D_1) = 78$, $TW(D_2) = 444$, $TW(D_3) = 2328$, $\ldots$; for details see text.

10. Concluding remarks

As already mentioned, the terminal Wiener index is a very new molecular–structure descriptor. Only a limited number of its mathematical properties were established so far; practically all of these are outlined in the present survey.

Until now no attempt was reported to find some chemical application of TW or, at least, to investigate how TW is correlated with the usually employed physico–chemical properties of alkanes (octane isomers, in particular). The readers of this survey are invited and encouraged to help filling this gap.

The variable terminal Wiener index, Eq. (6), was introduced *ad hoc* [18], and practically nothing is known about it. What first would have to be done is to find a convincing argument (either chemical or mathematical) why such a quantity should be considered at all. Otherwise, the idea should better be abandoned.

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