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BRANCHINGS IN TREES AND THE CALCULATION OF THE WIENER INDEX OF A TREE

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Abstract

The Wiener index is a topological index introduced as structural descriptor for molecular graphs of alkanes (trees). It is defined as the sum of distances between all pairs of vertices in a tree. Branchings and linear segments are natural characteristics of the structure of trees (every vertex of degree 3 or greater defines a branching point; a path between neighboring branching points forms a segment). A novel formula for the calculation of the Wiener index of a tree based on distances between branching points is derived.

1. Introduction

The Wiener index is a well-known distance-based topological index introduced originally as structural descriptor for acyclic organic molecules [1]. In most cases the chemical applications of the Wiener index deal with molecular graphs of alkanes, that are trees. For a tree T, this topological index is defined as the sum of distances between all unordered pairs of its vertices [2]:

$$W(T) = \sum_{\{u,v\} \subseteq V(T)} d(u,v), \qquad (1)$$

where $d(u,v)$ is the number of edges in a shortest path connecting the vertices u and v.

Many important relationships have been established between the structure of alkanes and their physico-chemical properties (see books [3–5] and reviews [6–13]). Recent progress in chemical synthesis also inspires great interest in new classes of extremely

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branched acyclic molecules [14]. Mathematical properties of the Wiener index and methods for the calculation W for various classes of abstract and molecular graphs have been described in mathematical and chemical literature (see selected articles [15–37]).

In this paper we consider structural characteristics that reflect branchings in trees. Several known formulas will be modified using these characteristics. A novel formula for the calculation of the Wiener index is presented.

2. Branchings in trees

Branchings and linear segments are natural characteristics of the structure of trees. A vertex v is said to be a *branching point* of a tree T if $\deg(v) \geq 3$. The paths are the only trees without a branching point. Denote by $B(T)$ the set of all branching points of T. The set of all pendent vertices of T together with $B(T)$ will be denoted by $BP(T)$. If T has p vertices then $0 \leq |B(T)| \leq (p-2)/2$ and $2 \leq |BP(T)| \leq p$.

Branching points decompose a tree into segments. A *segment* of T is a path–subtree S whose terminal vertices belong to $BP(T)$, i. e., every internal vertex v of S has $\deg_T(v) = 2$. In other words, only terminal vertices of a segment may be branching or pendent vertices in the respective tree. For example, all gomeomorphically reducible trees have the same number of segments. The length of a segment S is equal to the number of edges in S and it is denoted by ℓ_S. The following parts of S will be also considered: $S^0 = S \setminus \{u, v\}$ and $S^* = S \setminus \{u\}$, where u and v are the terminal vertices of S. By construction, $\ell_{S^0} = \ell_S - 2$ and $\ell_{S^*} = \ell_S - 1$.

The *distance of a vertex* v, $d_T(v)$, is the sum of distances between v and all other vertices of T, i.e. $d_T(v) = \sum_{u \in V(T)} d_T(v, u)$. Then the Wiener index can be written in the following manner

$$W(T) = \frac{1}{2} \sum_{v \in V(T)} d_T(v). \tag{2}$$

As an illustration of methods based on branching points, we recall two formulas for the calculation of the Wiener index. Every vertex v with their neighbors define a *star* with center at v. These formulas demonstrate that it is sufficient to examine stars for branching points and remaining parts of a tree.

The first method was elaborated by Canfield et al. [15]. It is a recursive approach for calculation of the Wiener index of a general tree. Let $T_1, T_2, \ldots, T_m$ be trees with disjoint

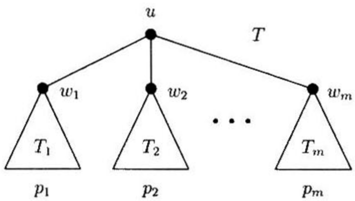

Figure 1. Branching point u of a tree T.

vertex sets and orders $p_1, p_2, \ldots, p_m$, $m \geq 2$, and $w_i \in V(T_i)$ for $i = 1, 2, \ldots, m$. In the general case, any tree T on more than two vertices can be represented as shown in Fig. 1.

Proposition 1 [15]. *Let T be a tree on $p \geq 3$ vertices. Then*

$$W(T) = \sum_{i=1}^{m} \left[W(T_i) + (p - p_i)\, d_{T_i}(w_i) - p_i^2 \right] + p(p-1).$$

Doyle and Graver derived a non-recursive formula for the Wiener index [16, 17]. Their formula does not contain distances between vertices in a tree.

Proposition 2 [16]. *Let T be a tree on p vertices. Then*

$$W(T) = \binom{p+1}{3} - \sum_{u \in B(T)} \sum_{1 \leq i < j < k \leq m} p_i\, p_j\, p_k\,.$$

The first term on the right–hand side of this equation is just the Wiener index of the p-vertex path.

3. Branching points, segments and calculations

In this section we generalize several known formulas for the Wiener index using tree's segments. Since all segments may be regarded as elementary pieces of a tree, we also formulate results in terms of W for segments.

The next useful equalities follows from the definition of a segment. Let T be a p-vertex tree. Then

$$\sum_{S \in T} W(S) = \sum_{S \in T} W(S^*) + \frac{1}{2} \left(\sum_{S \in T} \ell_S^2 + p - 1 \right),$$

$$\sum_{S\in T} W(S^*) = \frac{1}{6}\left(\sum_{S\in T} \ell_S^3 - p + 1\right),$$

$$\sum_{S\in T} \ell_S = p - 1.$$

1. First we consider a formula discovered by Wiener [1]. It is based on the observation that $W(T)$ is equal to the number of edges in the paths between all pairs of vertices of the tree T. Let $e = (x, y)$ be an edge of T. Then let $n_1(e)$ be the number of vertices of T lying closer to x than to y and let $n_2(e)$ be the number of vertices of T lying closer to y than to x. The quantities $n_1(e)$ and $n_2(e)$ can be formally defined for an edge $e = (x, y)$ as $n_1(e) = |\{v \mid v \in V(T),\, d_T(v, x) < d_T(v, y)\}|$ and $n_2(e) = |\{v \mid v \in V(T),\, d_T(v, y) < d_T(v, x)\}|$.

Proposition 3 [1]. *Let T be a tree on p vertices. Then*

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

Formula (3) can be easily generalized in terms of segments. If all internal vertices and all edges of a segment S are deleted from a tree, we have two nontrivial connected components. Denote by $n_1(S)$ and $n_2(S)$ the number of vertices of these components, $n_1(S) + n_2(S) = p(T) - \ell_S + 1$.

Proposition 4. *Let T be a tree on p vertices. Then*

$$W(T) = \sum_S n_1(S)\, n_2(S)\, \ell_S + \frac{1}{6} \sum_S \ell_S(\ell_S - 1)(3p - 2\ell_S + 1) \tag{4}$$

where the summations go over all segments of T.

Proof. Let $S = (v_0, v_1, ..., v_{\ell_S})$ be an arbitrary segment of T. For every edge e of S, we express quantities $n_1(e)$ and $n_2(e)$ through $n_1(S)$ and $n_2(S)$. Let $e_i = (v_i, v_{i+1})$. Since $n_1(e_i) = n_1(S) + i$, we have $n_2(e_i) = n_2(S) + \ell_S - i - 1$ for $i = 0, 1, ..., \ell_S - 1$. Therefore, all edges of S make the following contribution to the sum of eq. (3):

$$\sum_{i=0}^{\ell_S - 1} (n_1(S) + i)(n_2(S) + \ell_S - i - 1) = n_1(S)\, n_2(S)\, \ell_S + \frac{1}{6}\ell_S(\ell_S - 1)(3p - 2\ell_S + 1).$$

The proof is completed by summing this equation over all segments of T. □

If every segment of T is an edge (i. e., $\ell_S = 1$ for any S), then eq. (3) coincides with its modification (4). Since $n_1(S)$ and $n_2(S)$ are just the numbers of vertices lying on the two sides of S, it is sufficient to count the vertices from only one side of each segment.

Corollary 1. *Let T be a tree on p vertices. Then*

$$W(T) = \sum_S n_1(S)\, n_2(S)\, \ell_S + (p+1) \sum_S W(S) - (p+3) \sum_S W(S^*)$$

where the summations go over all segments of T.

2. It is known a formula that shows how irregularity of the distances of adjacent vertices influences W.

Proposition 5 [18]. *Let T be a tree on p vertices. Then*

$$W(T) = \frac{1}{4}\left[p^2(p-1) - \sum_{(u,v)\in E(T)} [d_T(v) - d_T(u)]^2\right]. \qquad (5)$$

Every edge of a tree makes a non-negative contribution to the sum of eq. (5). For vertices of any pendent edge, $[d_T(v) - d_T(u)]^2 = (n-2)^2$ and this value is maximal among all edges. The minimal value of $[d_T(v) - d_T(u)]^2$, equal to zero, will be achieved on a bicentral tree. For computational purposes it is convenient to use the equality $d(v) - d(u) = n_2(e) - n_1(e)$ [20].

Proposition 6. *Let T be a tree on p vertices. Then*

$$W(T) = \frac{1}{12}\left[(3p^2+1)(p-1) - 3\sum_S \frac{1}{\ell_S} [d_T(u) - d_T(v)]^2 - \sum_S \ell_S^3\right] \qquad (6)$$

where the summations go over all segments of T.

Proof. Denote by T_v and T_u the trees obtained by deleting a segment S with terminal vertices v and u from a tree T. If $n_1(S) = |V(T_v)|$ and $n_2(S) = |V(T_u)|$, then

$$\begin{aligned} d(v) - d(u) &= \sum_{x\in V(T_v)} [d(v,x) - d(u,x)] + \sum_{y\in V(T_u)} [d(v,y) - d(u,y)] \\ &= \sum_{x\in V(T_u)} \ell_S - \sum_{y\in V(T_v)} \ell_S = \ell_S[n_2(S) - n_1(S)]. \end{aligned}$$

Since $4n_1(S)n_2(S) = [n_1(S)+n_2(S)]^2 - [n_1(S)-n_2(S)]^2$ and $n_1(S)+n_2(S) = p - \ell_S + 1$, we have $4n_1(S)n_2(S) = (p-\ell_S+1)^2 - [d(v)-d(u)]^2/\ell_S^2$. Substituting the latter equation back into (3), we obtain eq. (6). □

Corollary 2. *Let T be a tree on p vertices. Then*

$$W(T) = \frac{1}{4}\left[p^2(p-1) - \sum_S \frac{1}{\ell_S}[d(v) - d(u)]^2 - 2\sum_S W(S^*)\right]$$

where the summations go over all segments of T.

3. The right–hand side of eq. (2) may be regarded as a half–sum of vertex distances with unit weights. The next formula demonstrates how to compute the Wiener index if the weights are the vertex degrees.

Proposition 7 [19]. *Let T be a tree on p vertices. Then*

$$W(T) = \frac{1}{4}\left[p(p-1) + \sum_{v \in V(T)} \deg(v)\, d_T(v)\right]. \tag{7}$$

Recall that the degree of a vertex v is the number of edges in a star with center at v. A *generalized star* associated with a vertex v consists of this vertex and all segments beginning at v. The number of edges in a generalized star is denoted by q_v. The set of such stars covers every edge of a tree twice, i. e., $\sum_v q_v = 2(p(T) - 1)$.

In order to determine the Wiener index, we can consider only generalized stars corresponding to the vertices of $BP(T)$.

Proposition 8. *Let T be a tree on p vertices. Then*

$$W(T) = \frac{1}{12}\left[(3p+1)(p-1) + 3\sum_{v \in BP(T)} q_v\, d_T(v) - \sum_S \ell_S^3\right] \tag{8}$$

where the second summation goes over all segments of T.

Proof. By Proposition 7,

$$W(T) = \frac{1}{4}\left(p(p-1) + \sum_{v \in BP(T)} \deg(v) d_T(v) + 2\sum_{S \in T}\sum_{v \in V(S^0)} d_T(v)\right). \tag{9}$$

We now calculate the last sum of eq. (9).

Lemma 1. *Let S be a segment with terminal vertices x and y in a tree T. Then*

$$\sum_{v \in V(S^0)} d_T(v) = \frac{1}{2}(\ell_S - 1)[d_T(x) + d_T(y)] - \frac{1}{6}\ell_S(\ell_S^2 - 1).$$

Proof. Denote by T_x and T_y the trees obtained by deleting the segment S with terminal vertices x and y from a tree T. Let $n_1(S) = |V(T_x)|$, $n_2(S) = |V(T_y)|$ and $S^0 = (v_1, v_2, ..., v_{\ell_S - 1})$. Then for $i = 1, 2, ..., \ell_S - 1$

$$\begin{aligned} d_T(v_i) &= \sum_{u \in V(T_x)} d(v_i, u) + \sum_{u \in V(T_y)} d(v_i, u) + \sum_{j=1}^{\ell_S - 1} d(v_i, v_j) \\ &= \sum_{u \in V(T_x)} [d(v_i, x) + d(x, u)] + \sum_{u \in V(T_y)} [d(v_i, y) + d(y, u)] + d_{S^0}(v_i) \\ &= \sum_{u \in V(T_x)} d(x, u) + \sum_{u \in V(T_y)} d(y, u) + i\, n_1(S) + (\ell_S - i) n_2(S) + d_{S^0}(v_i). \qquad (10) \end{aligned}$$

The sum of the first and the second terms of eq. (10) we express through the distances of terminal vertices of the segment. Then

$$\begin{aligned} d_T(x) &= \sum_{u \in V(T_x)} d(x, u) + \sum_{u \in V(T_y)} [d(x, y) + d(y, u)] + d_{S^*}(x) \\ &= \sum_{u \in V(T_x)} d(x, u) + \sum_{u \in V(T_y)} d(y, u) + \ell_S n_2(S) + d_{S^*}(x). \qquad (11) \end{aligned}$$

For the second terminal vertex of the segment,

$$d_T(y) = \sum_{u \in V(T_x)} d(x, u) + \sum_{u \in V(T_y)} d(y, u) + \ell_S n_1(S) + d_{S^*}(y). \qquad (12)$$

Summing expressions (11) and (12), we have

$$\sum_{u \in V(T_x)} d(x, u) + \sum_{u \in V(T_y)} d(y, u) = \frac{1}{2}[d_T(x) + d_T(y) - \ell_S(p - \ell_S + 1) - \ell_S(\ell_S - 1)]. \qquad (13)$$

Substituting eq. (13) into (10) and then summing eq. (10) over all $i = 1, 2, ..., \ell_S - 1$, we obtain

$$\begin{aligned} \sum_{i=1}^{\ell_S - 1} d_T(v_i) &= \frac{1}{2}(\ell_S - 1)[d_T(x) + d_T(y)] + 2W(S^*) - \frac{1}{2}\ell_S(\ell_S - 1)^2 \\ &+ n_1(S) \sum_{i=1}^{\ell_S - 1} i + n_2(S) \sum_{i=1}^{\ell_S - 1} (\ell_S - i) - \frac{1}{2}(\ell_S - 1)(p - \ell_S + 1). \qquad (14) \end{aligned}$$

It can be noted that the expression in the second line of (14) is equal to zero. □

Applying Lemma 1 to the last sum of eq. (9), we have

$$W(T) = \frac{1}{4}\Bigg(p(p-1) + \sum_{S \in T} (\ell_S - 1)[d_T(x) + d_T(y)] + \sum_{v \in BP(T)} \deg(v) d_T(v) -$$

$$- \frac{1}{3}\sum_{S\in T}\ell_S(\ell_S^2-1)\Big)$$

$$= \frac{1}{4}\Bigg(p(p-1) + \sum_{v\in BP(T)}(\ell_{i_1}+\ell_{i_2}+\ldots+\ell_{i_k}-k)d_T(v)$$

$$+ \sum_{v\in BP(T)}\deg(v)d_T(v) - \frac{1}{3}\sum_{S\in T}\ell_S(\ell_S^2-1)\Bigg)$$

where $k = deg(v)$ and $\ell_{i_1}, \ell_{i_2}, \ldots, \ell_{i_k}$ are lengths of segments beginning at v. □

Corollary 3. *Let T be a tree on p vertices. Then*

$$W(T) = \frac{1}{4}\left[p(p-1) + \sum_{v\in BP(T)} q_v\, d(v) - \sum_S W(S^*)\right]$$

where the second summation goes over all segments of T.

4. New formula for the calculation of the Wiener index

Consider two distinct generalized stars of T with branching points u, v and the numbers of vertices q_u and q_v. These stars and the path between v and u form a *double (generalized) star* of the respective tree. Let $q_{uv} = q_u - \ell$, where ℓ is the length of the unique segment coming from the vertex u and belonging to the path between u and v. The distance of an arbitrary vertex v in a tree T may be expressed through the distances from v to all branching points of T.

Lemma 2. *Let T be a tree on p vertices and v be the j-th vertex of an arbitrary segment S_m, $1 \le j \le \ell_{S_m}+1$. Then*

$$d_T(v) = \sum_{u\in B(T)} d(v,u)\, q_{uv} + \frac{1}{2}\left(\sum_S \ell_S^2 + p - 1\right) - (j-1)(\ell_{S_m}+1-j)$$

where the second summation goes over all segments of T.

Proof. Let T_0 be a tree and $u \in V(T_0)$. Consider a sequence of trees $T_0, T_1, \ldots, T_k$ such that T_i is obtained from T_{i-1} by joining the vertex u with the terminal vertex of a new path H_i of order $\ell_i + 1$, $i = 1, 2, \ldots, k$. It is clear that an arbitrary tree T can be constructed by these operations, beginning from one-vertex tree T_0. Every path H_i forms a segment in T. For an arbitrary vertex $v \in V(T_0)$, we calculate its distance in T_k.

Let $v \in BP(T_0)$. Then

$$\begin{aligned}
d_{T_1}(v) &= d_{T_0}(v) + \sum_{x \in V(H_1)} d_{T_1}(v,x) = d_{T_0}(v) + \sum_{x \in V(H_1)} [d_{T_0}(v,u) + d_{H_1}(u,x)] \\
&= d_{T_0}(v) + \ell_1 d_{T_0}(v,u) + \frac{1}{2}\ell_1(\ell_1+1), \\
d_{T_2}(v) &= d_{T_1}(v) + \ell_2 d_{T_1}(v,u) + \frac{1}{2}\ell_2(\ell_2+1), \\
&\dots \\
d_{T_k}(v) &= d_{T_{k-1}}(v) + \ell_k d_{T_{k-1}}(v,u) + \frac{1}{2}\ell_k(\ell_k+1).
\end{aligned}$$

Since $d_{T_i}(v,u) = d_{T_{i-1}}(v,u)$ for all $i = 1, 2, ..., k$,

$$d_{T_k}(v) = d_{T_0}(v) + (\ell_1 + \ell_2 + ... + \ell_k) d_{T_k}(v,u) + \frac{1}{2}\sum_{i=1}^{k} \ell_i(\ell_i+1).$$

Suppose that $T_0 = v$ and $T = T_k$ for some k. Since $d_{T_0}(v) = 0$ and $\ell_1 + \ell_2 + ... + \ell_k = q_{uv}$, the lemma is proved for vertices of $BP(T)$.

Let v be the internal j-th vertex of some segment S_m. The proof is similar to the above reasoning except of two steps. Namely, two parts of S_m with lengths $j-1$ and $\ell_{S_m} - j + 1$ are considered as paths H_1 and H_2. These paths are attached to the vertex $v = T_0$ and form a single segment in T. In this case

$$\begin{aligned}
d_{T_1}(v) &= \frac{1}{2}j(j-1), \\
d_{T_2}(v) &= d_{T_1}(v) + \frac{1}{2}(\ell_{S_m} - j + 1)(\ell_{S_m} - j + 2) \\
&= \frac{1}{2}\ell_{S_m}(\ell_{S_m} + 1) - (j-1)(\ell_{S_m} - j + 1). \quad \square
\end{aligned}$$

For a double star, define $Q_{uv} = [q_v - \deg(v) + 2]\, q_{uv} + [q_u - \deg(u) + 2]\, q_{vu}$. It is clear that $Q_{uv} = Q_{vu}$. If u is a pendent vertex and v is a branching point in a tree then $q_{uv} = 0$ and $Q_{uv} = (q_u + 1) q_{vu}$. If the vertices u and v are both pendent then $q_{vu} = q_{uv} = 0$ and, therefore, $Q_{uv} = 0$. The next result shows how to compute the Wiener index of T through weighted distances between vertices of $BP(T)$.

Proposition 9. *Let T be a tree on p vertices. Then*

$$W(T) = \frac{1}{12}\left[(3p+1)(p-1) + 3 \sum_{\{u,v\} \subseteq BP(T)} d(u,v)\, Q_{uv} + \sum_S \ell_S^2 (3p - \ell_S)\right]$$

where the second summation goes over all segments of T.

Proof. Define the quantity q_{uv} for an internal vertex of a segment. Let $v \in S^0$ and $u \in BP(T)$. If u is a non-terminal vertex of S, then q_{uv} is defined as in the case of branching points. If u is a terminal vertex of S, we assume $q_{uv} = 0$.

Lemma 2 and eq. (2) immediately imply the following equality

$$W(T) = \frac{1}{4}\left(2 \sum_{v \in V(T)} \sum_{u \in BP(T)} d(v,u) q_{uv} + p\left(\sum_{S \in T} \ell_S^2 + p - 1\right) - 2 \sum_{S \in T} W(S^*)\right). \quad (15)$$

Because $q_{uv} = 0$ for a pendent vertex u, the set $B(T)$ can be replaced by $BP(T)$.

Consider the double sum of eq. (15) separately for the vertices of degree 2 and the other vertices of a tree. Then we can write

$$\begin{aligned} &\sum_{v \in V(T)} \sum_{u \in BP(T)} d(v,u) q_{uv} = \\ &= \sum_{v \in BP(T)} \sum_{u \in BP(T)} d(v,u) q_{uv} + \sum_{v \in V(T) \setminus BP(T)} \sum_{u \in BP(T)} d(v,u) q_{uv} \\ &= \sum_{\{v,u\} \subseteq BP(T)} d(v,u)(q_{uv} + q_{vu}) + \sum_{S \in T} \sum_{v \in V(S^0)} \sum_{u \in BP(T)} d(v,u) q_{uv}. \end{aligned} \quad (16)$$

In order to determine the last term of (16), consider a segment S with terminal vertices x and y. Let T_x and T_y be the trees obtained by deleting the segment S from T. It is clear that for every internal vertex v of the segment $q_{uv} = q_{ux}$ if $u \in BP(T_x)$ and $q_{uv} = q_{uy}$ if $u \in BP(T_y)$. For convenience, assume $q_{vv} = 0$ for an arbitrary vertex v of T. Then

$$\begin{aligned} &\sum_{v \in V(S^0)} \sum_{u \in BP(T)} d(v,u) q_{uv} = \\ &= \sum_{v \in V(S^0)} \left(\sum_{u \in BP(T_x)} [d(v,x) + d(x,u)] q_{ux} + \sum_{u \in BP(T_y)} [d(v,y) + d(y,u)] q_{uy} \right) \\ &= \sum_{v \in V(S^0)} \left(d(v,x) \sum_{u \in BP(T_x)} q_{ux} + d(v,y) \sum_{u \in BP(T_y)} q_{uy} + \sum_{u \in BP(T_x)} d(x,u) q_{ux} \right. \\ &\left. + \sum_{u \in BP(T_y)} d(y,u) q_{uy} \right). \end{aligned} \quad (17)$$

For the first and the second terms of eq. (17), we have

$$\begin{aligned} &\sum_{v \in V(S^0)} \left(d(v,x) \sum_{u \in BP(T_x)} q_{ux} + d(v,y) \sum_{u \in BP(T_y)} q_{uy} \right) = \\ &\qquad = [1 + 2 + \ldots + (\ell_S - 1)] \left(\sum_{u \in BP(T_x)} q_{ux} + \sum_{u \in BP(T_y)} q_{uy} \right) \\ &\qquad = \frac{1}{2} \ell_S (\ell_S - 1)(p - \ell_S - 1). \end{aligned} \quad (18)$$

Denote the sum of the third and the fourth terms of eq. (17) by F. Replacing the sets $B(T_x)$ and $B(T_y)$ by $BP(T)$, we can write

$$F = \sum_{u\in BP(T_x)} d(x,u)q_{ux} + \sum_{u\in BP(T_y)} [d(x,u) - \ell_S]q_{uy} = \sum_{u\in BP(T)} d(x,u)q_{ux} - \ell_S \sum_{u\in BP(T_y)} q_{uy}$$

$$= \sum_{u\in BP(T_x)} [d(y,u) - \ell_S]q_{ux} + \sum_{u\in BP(T_y)} d(y,u)q_{uy} = \sum_{u\in BP(T)} d(y,u)q_{uy} - \ell_S \sum_{u\in BP(T_x)} q_{ux}.$$

Therefore,

$$F = \frac{1}{2}\left(\sum_{u\in BP(T)} d(x,u)q_{ux} + \sum_{u\in BP(T)} d(y,u)q_{uy} - \ell_S(p - \ell_S - 1)\right). \tag{19}$$

Substituting (18) and (19) back into (17), we obtain

$$\sum_{v\in V(S^0)} \sum_{u\in BP(T)} d(v,u)q_{uv} = \frac{1}{2}(\ell_S - 1)\left(\sum_{u\in BP(T)} d(x,u)q_{ux} + \sum_{u\in BP(T)} d(y,u)q_{uy}\right).$$

Then the triple sum of (16) can be rewritten as follows

$$\frac{1}{2}\sum_{S\in T}(\ell_S - 1)\left(\sum_{u\in BP(T)} d(x,u)q_{ux} + \sum_{u\in BP(T)} d(y,u)q_{uy}\right) =$$

$$= \frac{1}{2}\sum_{v\in BP(T)}\left([q_v - deg(v)] \sum_{u\in BP(T)} d(v,u)q_{uv}\right)$$

$$= \frac{1}{2}\sum_{\{v,u\}\subseteq BP(T)} d(u,v)[(q_v - deg(v))q_{uv} + (q_u - deg(u))q_{vu}]. \tag{20}$$

The proof of proposition follows from eqs. (15), (16) and (20). □

Corollary 4. *Let T be a tree on p vertices. Then*

$$W(T) = \frac{1}{4}\left[\sum_{\{u,v\}\subseteq BP(T)} d(u,v)\,Q_{uv} + 2p\sum_S W(S) - 2(p+1)\sum_S W(S^*)\right] \tag{21}$$

where the second and the third summations go over all segments of T.

5. Example of calculation of the Wiener index

As an illustration consider the dendrimer–like tree T shown in Fig. 2. This tree has 52 segments of length 10 and, therefore, $p = \sum_S l_S + 1 = 521$ vertices. All vertices of the set $BP(T)$ are marked by big circles. In order to calculate the first term of eq. (21), we consider two types of pairs of vertices.

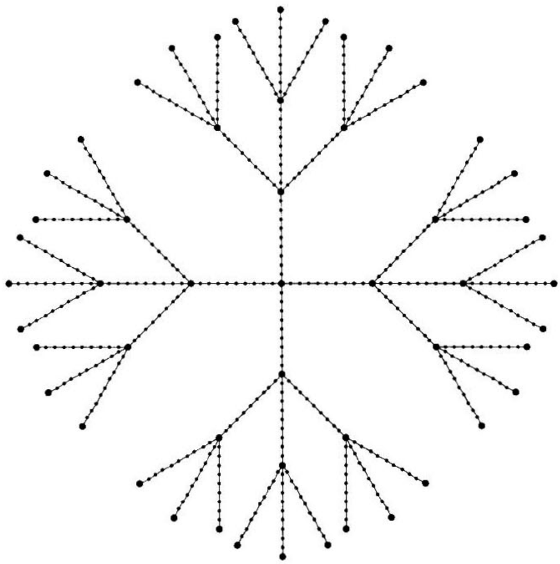

Figure 2. Dendrimer–like tree T.

Let $u, v \in BP(T)$ and $\deg(u) = 1$, $\deg(v) = 4$. Let u be fixed and v goes over all branching points of T. Then there is one vertex v such that $d(u,v) = 10$ and $d(u,v) = 20$, three vertices v with $d(u,v) = 30$ and $d(u,v) = 40$, and nine vertices v for which $d(u,v) = 50$. For every such pair, $Q_{uv} = (10+1)(4 \cdot 10 - 10) = 330$. Since the tree T has 36 symmetrical pendent vertices, we have

$$36 \sum_{v \in B(T)} d(u,v)\, Q_{uv} = 36 \cdot 330 \cdot (1 \cdot 10 + 1 \cdot 20 + 3 \cdot 30 + 3 \cdot 40 + 9 \cdot 50) = 8{,}197{,}200.$$

Let $u, v \in BP(T)$ and $\deg(u) = \deg(v) = 4$. For every pair of such vertices, $Q_{uv} = 2\,(4 \cdot 10 - 4 + 2)(4 \cdot 10 - 10) = 2280$. It is not hard to count that the tree T contains 16 pairs of vertices at distance 10, 30 pairs of vertices at distance 20, 36 pairs of vertices at distance 30, and 54 pairs of vertices at distance 40. Therefore,

$$\sum_{\{u,v\} \subseteq B(T)} d(u,v)\, Q_{uv} = 2280 \cdot (16 \cdot 10 + 30 \cdot 20 + 36 \cdot 30 + 54 \cdot 40) = 9{,}120{,}000.$$

Because $l_S = 10$ for every segment S of T, $W(S) = 220$ and $W(S^*) = 165$. This implies

$$2p\sum_S W(S) - 2(p+1)\sum_S W(S^*) = 2 \cdot 52 \cdot (521 \cdot 220 - 522 \cdot 165) = 2{,}962{,}960.$$

Finally, we have

$$W(T) = \frac{1}{4}(8{,}197{,}200 + 9{,}120{,}000 + 2{,}962{,}960) = 5{,}070{,}040.$$

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