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ORIGINAL PAPER

Generalizations of Wiener Polarity Index and Terminal Wiener Index

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Abstract In theoretical chemistry, distance-based molecular structure descriptors are used for modeling physical, pharmacologic, biological and other properties of chemical compounds. We introduce a generalized Wiener polarity index $W_k(G)$ as the number of unordered pairs of vertices $\{u, v\}$ of G such that the shortest distance $d(u, v)$ between u and v is k (this is actually the kth coefficient in the Wiener polynomial). For $k = 3$, we get standard Wiener polarity index. Furthermore, we generalize the terminal Wiener index $TW_k(G)$ as the sum of distances between all pairs of vertices of degree k. For $k = 1$, we get standard terminal Wiener index. In this paper we describe a linear time algorithm for computing these indices for trees and partial cubes, and characterize extremal trees maximizing the generalized Wiener polarity index and generalized terminal Wiener index among all trees of given order n.

Keywords Distance in graphs · Wiener polarity index · Terminal Wiener index · Wiener index · Partial cube · Graph algorithm

Mathematics Subject Classification (2000) 05C12, 92E10

1 Introduction

Let $G = (V, E)$ be a connected simple graph with $n = |V|$ vertices and $m = |E|$ edges. For vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of the shortest

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path between u and v in G. The diameter $diam(G)$ is the greatest distance between two vertices of G. Let $d_k(u)$ denotes the number of vertices on distance k from the vertex u. Let $deg(v)$ denotes the degree of the vertex v.

In theoretical chemistry molecular structure descriptors (also called topological indices) are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [11]. There exist several types of such indices, especially those based on vertex and edge distances. Arguably the best known of these indices is the Wiener index W, defined as the sum of distances between all pairs of vertices of the molecular graph [9]

$$W(G) = \sum_{u,v \in V(G)} d(u, v).$$

Besides of use in chemistry, it was independently studied due to its relevance in social science, architecture and graph theory. With considerable success in chemical graph theory, various extensions and generalizations of the Wiener index are recently put forward [3,25].

The Wiener polarity index of a graph G is defined as the number of unordered pairs of vertices $\{u, v\}$ of G such that the shortest distance $d(u, v)$ between u and v is 3,

$$WP(G) = |\{(u, v) \mid d(u, v) = 3,\ u, v \in V\}|.$$

Hosoya [13] found a physico-chemical interpretation of WP. Du et al. [8] described a linear time algorithm for computing the Wiener polarity index of trees, and characterized the trees maximizing the index among all trees of given order. Deng et al. [4–6] and Liu et al. [21] characterized extremal n-vertex trees with given diameter, number of pendent vertices or maximum vertex degree.

For $k \geq 1$, we define the generalized Wiener polarity index as the number of unordered pairs of vertices $\{u, v\}$ of G such that the shortest distance $d(u, v)$ between u and v is k,

$$W_k(G) = \frac{1}{2} \sum_{v \in V(G)} d_k(v) = |\{(u, v) \mid d(u, v) = k,\ u, v \in V\}|.$$

Notice that $W(G) = \sum_{k=1}^{diam(G)} W_k(G)$. If x is a parameter, then the Hosoya polynomial (or Wiener polynomial) of G is defined as [14,23]

$$W(G, x) = \sum_{u,v \in V(G)} x^{d(u,v)} = \sum_{k=1}^{diam(G)} W_k(G) \cdot x^k.$$

Therefore, the generalized Wiener polarity index is basically the kth coefficient in the Hosoya polynomial. For recent survey on the properties of Hosoya polynomial and historical details see [12].

The terminal Wiener index of a graph G is defined by Gutman et al. [10] as the sum of distances between all pairs of pendent vertices of G,

$$TW(G) = \sum_{\substack{u,v \in V(G) \\ deg(u)=deg(v)=1}} d(u, v).$$

Furthermore, the authors described a simple method for computing TW of trees and characterized the trees with minimum and maximum TW. Recently Deng and Zhang [7] studied equiseparability on terminal Wiener index. Independently, Székely et al. [24] introduced the same index (the sum of distances between the leaves of a tree) and studied the correlation between various distance-based topological indices.

For $k \geq 1$, we define the generalized terminal Wiener index as the sum of the distances between all unordered pairs of vertices of degrees k,

$$TW_k(G) = \sum_{\substack{u,v \in V(G) \\ deg(u)=deg(v)=k}} d(u, v).$$

The paper is organized as follows. In Sect. 2 we introduce generalization of the Wiener polarity index $W_k(G)$ and characterize the trees maximizing the generalized Wiener polarity index among all trees of given order, while in Sect. 3 we designed linear algorithm for calculating this index. In Sect. 4 we introduce generalization of the terminal Wiener index and characterize trees maximizing the generalized terminal Wiener index among all trees of given order. In Sect. 5 we present formula for calculation of $TW_k(G)$ for partial cubes and in particular closed formula for TW_3 of coronene series H_k. We close the paper in Sect. 6 by proposing new problems for research.

2 Generalization of Wiener Polarity Index

For $k = 1$, it can be easily seen that $W_1(G) = m$, where m is the number of edges. For $k = 2$, we have

$$W_2(G) = \sum_{v \in V} \binom{deg(v)}{2} = \frac{\sum_{v \in V} deg^2(v)}{2} - m = \frac{M_1(G)}{2} - m,$$

where $M_1(G)$ denotes the first Zagreb index of a graph [22].

For $k = 3$ we have the Wiener polarity index,

$$\begin{aligned} W_3(T) &= \sum_{uv \in E} (deg(v) - 1)(deg(u) - 1) = \sum_{uv \in E} deg(u)deg(v) - \sum_{v \in V} deg^2(v) + m \\ &= M_2(T) - M_1(T) + m, \end{aligned}$$

where $M_2(T)$ denotes the second Zagreb index of a graph [15].

In the following assume that $k \geq 3$. If the diameter of T is less than k, then $W_k(T) = 0$. Therefore, the minimum value of $W_k(T)$ is zero, and it is achieved for all trees with $diam(T) < k$ (for example the star S_n). On the other hand, we will prove that the maximum value of $W_k(T)$ is achieved for a tree with diameter k and with all pendent vertices on distance k.

The group of pendent vertices is defined as the set of all pendent vertices attached to the same unique neighbor. Let A_1 and A_2 be two different groups of pendent vertices with the unique neighbors w_1 and w_2, such that the distance between two arbitrary pendent vertices from these groups is not equal to k. Let p_1 be the number of vertices on distance k from an arbitrary pendent vertex from A_1 and p_2 be the number of vertices on distance k from an arbitrary pendent vertex from A_2. Without loss of generality assume that $p_1 \leq p_2$. If we remove all pendent vertices from A_2 and add them to the group A_1, we get a new tree T' such that

$$W_k(T') - W_k(T) = (|A_1|p_1 + |A_2|p_2) - (|A_1|p_1 + |A_2|p_1) = |A_2|(p_2 - p_1) \geq 0.$$

By repetitive application of this transformation, we will get a new tree with possibly increased generalized Wiener polarity index. The diameter of T' is not greater than the diameter of T and each transformation introduces one new pendent vertex. By choosing two most distant groups of pendent vertices, we will get the extremal tree with diameter equal to k. After that we can apply the transformation finitely many times, until all pendent vertices are on distance k or 2.

Assume that there are p groups of pendent vertices with sizes $a_1, a_2, \ldots, a_p$ and $a_1 + a_2 + \cdots + a_p = q$. Since $diam(T) = k$, we have $n - k + 1 \geq q \geq 2$. The distance between any two pendent vertices not from the same group is equal to k, and therefore

$$W_k(T) = \frac{1}{2}\sum_{i=1}^{p} a_i(q - a_i) = \frac{1}{2}\left(q^2 - \sum_{i=1}^{p} a_i^2\right).$$

The minimum value of $\sum_{i=1}^{p} a_i^2$ under the condition $\sum_{i=1}^{p} a_i = q$ is achieved if and only if all numbers a_i are as close as possible, i. e. $|a_i - a_j| \leq 1$ for all $1 \leq i \leq j \leq p$. This can be easily proved by the transformation $(a_i, a_j) \mapsto (a_i + 1, a_j - 1)$ with $a_j \geq a_i + 2$, since

$$(a_i + 1)^2 + (a_j - 1)^2 - a_i^2 - a_j^2 = 2(a_i - a_j) + 2 < 0.$$

Notice that the tree is uniquely determined by the distances between pendent vertices [27]. A starlike tree is a tree with exactly one vertex of degree ≥ 3. If $p = 2$, we have $W_k(T) = a_1 a_2$ and $a_1 + a_2 = n - k + 1$ and finally

$$W_k(T) = \left\lfloor \frac{n-k+1}{2} \right\rfloor \cdot \left\lceil \frac{n-k+1}{2} \right\rceil$$

Let $p > 2$. For k odd, we can consider two groups of pendent vertices together with the unique path connecting them. The third group of pendent vertices must be on equal distance from both groups and that is impossible. Therefore, the extremal value for odd k is achieved for $p = 2$.

For k even, similarly it can be concluded that there is a unique tree with p groups of pendent vertices (starlike tree with p paths with equal lengths together with groups of pendent vertices attached at the end vertices of these p paths). For $p > 2$, we have

$$n = 1 + p\left(\frac{k}{2} - 1\right) + \sum_{i=1}^{p} a_i = 1 + p\left(\frac{k}{2} - 1\right) + q,$$

and since $p \leq q$, we have $p \leq 2 \cdot \frac{n-1}{k}$. Therefore, using Cauchy–Schwartz inequality it follows

$$\begin{aligned} W_k(T) &= \frac{1}{2}\left(q^2 - \sum_{i=1}^{p} a_i^2\right) \\ &\leq \frac{1}{2}\left(q^2 - \frac{q^2}{p}\right) \\ &= \frac{1}{2}\left(n - 1 - \frac{pk}{2} + p\right)^2 \left(1 - \frac{1}{p}\right). \end{aligned}$$

Let

$$f(p) = \frac{1}{2}\left(n - 1 - \frac{pk}{2} + p\right)^2 \left(1 - \frac{1}{p}\right),$$

for $2 < p < 2 \cdot \frac{n-1}{k} < 2 \cdot \frac{n-1}{k-2}$. The first derivative equals

$$f'(p) = \frac{(2 - 2n - 2p + kp)\left(2 - 2n + 2p - kp - 4p^2 + 2kp^2\right)}{8p^2}.$$

Finally it holds that $f(p)$ is increasing for $2 < p < p^*$ and decreasing for $p^* \leq p < 2 \cdot \frac{n-1}{k}$, where

$$p^* = \frac{k - 2 + \sqrt{(k-2)(16n + k - 18)}}{4(k-2)} = \frac{1}{4} + \frac{1}{4}\sqrt{\frac{16n + k - 18}{k-2}}$$

is the second largest root of $f'(p) = 0$. Therefore, the maximum of the Wiener polarity index for k even should be achieved for $p = 2$ or integers around p^* (see Fig. 1).

3 Linear Algorithm for W_k of Trees

Let T be an arbitrary tree rooted at the vertex 1. We will process the vertices according to the distance from the root vertex or in the recursive depth first search method [2]. For each vertex v, keep the vector $a[v]$ of the length $k + 1$ that stores the number of vertices in the subtree under v on distances $0, 1, 2, \ldots, k$. It follows that $a[v][0] = 1$

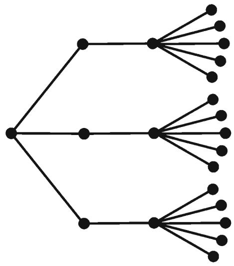

Fig. 1 The extremal tree with maximal generalized Wiener polarity index on $n = 22$ and $k = 6$

and $a[v][1] = deg(v) - 1$ for all vertices different than the root. The matrix a with dimensions $n \times k$ is computed recursively in the first procedure.

In the second procedure we calculate the generalized Wiener polarity index. In DFS tree, for each path of the length k there is a unique vertex v on the smallest distance from the root. Therefore, we need to traverse all vertices v and count the vertices that are on distance k in the subtree under v, such that the unique path connecting these vertices contains v. For the vertices in the subtree under v, we just add $2a[v][k]$. Otherwise, we need to consider all neighbors u of v different than $parent[v]$ and for each $i = 0, 1, \ldots, k-2$ count the number of vertex pairs (x, y) such that:

- x is in the subtree under u and y is not;
- x is on the distance i from u;
- y is on the distance $k - i - 1$ from v and under v.

Finally we counted every vertex pair on distance k twice, as showed in the second procedure. The time and memory complexity is $O(nk)$.

Procedure DFS (*vertex (v)*)

Input: The adjacency list of the tree T with the root vertex $root$.
Output: The array $parent$ and matrix a.

```
a[v][0] = 1;
foreach neighbor u of v do
    if (parent[u] = 0) and (u ≠ root) then
        parent[u] = v;
        DFS(u);
        for i = 0 to k − 1 do
            a[v][i + 1] = a[v][i + 1] + a[u][i];
        end
    end
end
```

4 Generalization of Terminal Wiener Index

For k regular graphs, $TW_k(G) = W(G)$ and $TW_i(G) = 0$ for $i \neq k$. For $k = 1$, we have terminal Wiener index.

Theorem 4.1 ([9]) *Let T be a tree on n vertices. Then,*

$$(n-1)^2 = W(S_n) \leq W(T) \leq W(P_n) = \binom{n+1}{3},$$

with equality if and only if $T \cong S_n$ or $T \cong P_n$.

Theorem 4.2 ([16]) *Let w be a vertex of a nontrivial connected graph G. For non-negative integers p and q, let $G(p,q)$ denote the graph obtained from G by attaching to vertex w pendent paths $P = wv_1v_2\ldots v_p$ and $Q = wu_1u_2\ldots u_q$ of lengths p and q, respectively. If $p \geq q \geq 1$, then*

$$W(G(p,q)) < W(G(p+1, q-1)).$$

For $k = 1$, Gutman et al. [10] characterized the extremal trees within the class of all trees with n vertices that maximize and minimize terminal Wiener index. The path P_n is the unique tree that minimizes TW_1.

Procedure GWP(G)

Input: The adjacency list of the tree T with the root vertex $root$ and the array a.
Output: The generalized Wiener polarity index Wk.

```
Wk = 0;
for v = 1 to n do
    Wk = Wk + 2 · a[v][k];
    foreach neighbor u of v do
        if parent[v] ≠ u then
            for i = 0 to k − 2 do
                Wk = Wk + a[u][i] · (a[v][k − 1 − i] − a[u][k − 2 − i]);
            end
        end
    end
end
return Wk/2;
```

For $k = 2$, the unique tree that maximizes TW_2 is the path P_n. This follows from Theorem 4.1 and the simple fact that in every tree there are at least 2 pendent vertices (there are at most $n-2$ vertices of degree two, and the maximum sum between all such pairs is achieved for path).

Let T^* be the extremal tree that maximizes the generalized terminal Wiener index for $k \geq 3$. It can be easily proved that there are no pendent paths $P = v_1v_2\ldots v_p$ of length greater than 2 or equal to attached at some vertex of T^*. Otherwise, remove pendent edges one by one and subdivide any edge e such that both components of $T^* - e$ contain vertices of degree k—this way we increase TW_k. If such edge does not exist, remove the edge $v_{p-1}v_p$ and add new edge $v_{p-2}v_p$—this way the generalized terminal Wiener index remains the same, or increases if and only if $k = 3$.

Lemma 4.3 *Among trees on n vertices the maximal possible number of vertices of degree $k \geq 2$ is*

$$m(n,k) = \left\lfloor \frac{n-2}{k-1} \right\rfloor.$$

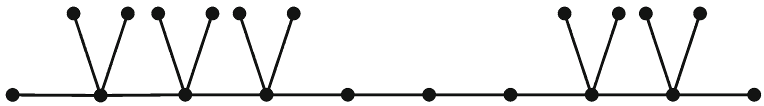

Fig. 2 The extremal tree with maximal generalized terminal Wiener index with $n = 20$ and $k = 4$ ($s = 8$ and $p = 5$)

Proof Consider the induced graph H composed of the vertices of degree k. Let h be the number of vertices in H, and let f be the number of edges in H. Since H is acyclic and possible disconnected, we have $0 \le f \le h - 1$. Furthermore, for the number of edges in tree T holds

$$h \cdot k - (h-1) \le h \cdot k - f \le n - 1.$$

It follows that $h(k-1) \le n-2$, which completes the proof. □

Let $C_{n,k,p}$ be the caterpillar obtained from a path of length $s+2 = n - p \cdot (k-2)$, by attaching $k-2$ pendent vertices to exactly p vertices of a path $P_{s+2} = v_0 v_1 \ldots v_s v_{s+1}$, starting from the vertices v_1 and v_s on the both ends towards center symmetrically (see Fig. 2). The generalized terminal Wiener index can be easily calculated by summing the Wiener index of two paths and the distances between the vertices of two paths:

$$\begin{aligned} TW_k(C_{n,k,p}) &= \sum_{1 \le i, j, \le s} d(v_i, v_j) \\ &= W(P_{\lfloor p/2 \rfloor}) + W(P_{\lceil p/2 \rceil}) + \lfloor p/2 \rfloor \cdot \lceil p/2 \rceil \cdot (s - p + 1) \\ &\quad + \frac{1}{2} \lfloor p/2 \rfloor (\lfloor p/2 \rfloor + 1) \cdot \lceil p/2 \rceil + \frac{1}{2} \lceil p/2 \rceil (\lceil p/2 \rceil + 1) \cdot \lfloor p/2 \rfloor \\ &= \begin{cases} \frac{1}{12} p(3ps - p^2 - 2), & \text{if } p \text{ is even} \\ \frac{1}{12}(p+1)(p-1)(3s - p), & \text{if } p \text{ is odd.} \end{cases} \\ &= \begin{cases} \frac{1}{12} p \left(3np + 5p^2 - 3kp^2 - 2 - 6p\right), & \text{if } p \text{ is even} \\ \frac{1}{12}(p+1)(p-1)(3n + 5p - 3kp - 6), & \text{if } p \text{ is odd.} \end{cases} \end{aligned} \tag{1}$$

We call a caterpillar C 3-bounded if all vertices of C have degree less than or equal to 3.

Theorem 4.4 *Let T be a tree on $n > 4$ vertices. Then*

$$TW_3(T) \le TW_3(C_{n,3,\lfloor n/2 \rfloor - 1}),$$

with equality if and only if $T \cong C_{n,3,\lfloor n/2 \rfloor - 1}$.

Proof Let T^* be a rooted tree with maximal value of generalized terminal Wiener index for $k = 3$. We can also assume that the number of vertices of degree 3 is greater than two.

If T^* is not 3-bounded caterpillar, consider a branching vertex w such that in the subtree under w there are only 3-bounded caterpillars attached at w (it can happen

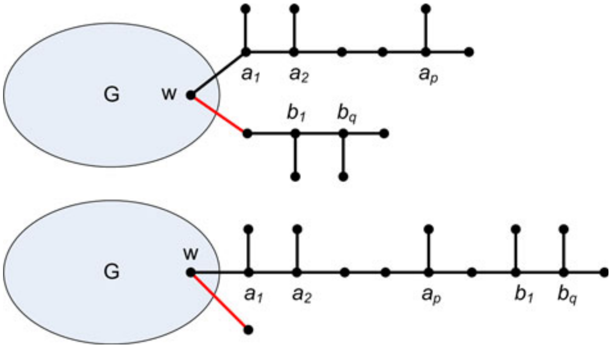

Fig. 3 Transformation that increases generalized terminal Wiener index TW_3

that there are only pendent vertices attached to w). Let C_1 and C_2 be two caterpillars attached at w, such that C_1 has p vertices $v_1, v_2, \ldots, v_p$ of degree 3 and C_2 has q vertices $u_1, u_2, \ldots, u_q$ of degree 3 (see Fig. 3). Without loss of generality, we can assume that the number of vertices of degree 3 in C_1 is greater than or equal to the number of vertices of degree 3, namely $p \geq q$.

Let $a_1, a_2, \ldots, a_p$ be the distances from the vertex w to the vertices $v_1, v_2, \ldots, v_p$ and $b_1, b_2, \ldots, b_q$ be the distance from the vertex w to the vertices $u_1, u_2, \ldots, u_q$. Let $D(w)$ be the sum of distances from the vertex w to the vertices of degree 3 in the subgraph G (see Fig. 3).

The generalized terminal Wiener index of the tree T^* equals

$$TW_3(T^*) = TW_3(G) + (p+q)D(w) + r\left(\sum_{i=1}^{p} a_i + \sum_{j=1}^{q} b_j\right) + \sum_{i<j}(a_j - a_i) + \sum_{i<j}(b_j - b_i) + q \cdot \sum_{i=1}^{p} a_i + p \cdot \sum_{j=1}^{q} b_j,$$

where $r \geq 1$ is the number of vertices of degree 3 in G.

After reattaching the caterpillar C_2 to the end of caterpillar C_1, the degree of vertex w remains the same. The generalized terminal Wiener index of transformed tree T' equals

$$TW_3(T') = TW_3(G) + (p+q)D(w) + r \cdot \sum_{i=1}^{p} a_i + r\left(q \cdot a_p + \sum_{j=1}^{q} b_j\right) + \sum_{i<j}(a_j - a_i) + \sum_{i<j}(b_j - b_i) + q \cdot \left(p \cdot a_p - \sum_{i=1}^{p} a_i\right) + p \cdot \sum_{j=1}^{q} b_j$$

By subtraction, we get

$$TW_3(T') - TW_3(T^*) = rq \cdot a_p + pq \cdot a_p - 2q \cdot \sum_{i=1}^{p} a_i,$$

Since $a_p \geq a_i$ for $i = 1, 2, \ldots, p$, we have

$$\begin{aligned} TW_3(T') - TW_3(T^*) &= q\left(a_p(r+p) - 2\sum_{i=1}^{p} a_i\right) \\ &\geq 2q \cdot \sum_{i=1}^{p}(a_p - a_i) \geq 0, \end{aligned}$$

with equality if and only if $p + r = 2$. Since $p \geq q \geq 1$ and $r \geq 1$, the equality holds iff $p = q = r = 1$.

It follows that using this transformation we can not decrease the generalized terminal Wiener index TW_3. If $deg(w) > 3$, we can remove the pendent edge and subdivide some edge e such that both components of $T^* - e$ contain vertices of degree 3, and further increase the generalized Wiener index. Therefore after these transformations, there is only one 3-bounded caterpillar under w.

Finally, we conclude that the extremal tree is a 3-bounded caterpillar, and it can be easily seen that the maximal value of TW_3 is achieved for caterpillar of the form $C_{n,k,p}$.

For $k = 3$, from (1) we have

$$f(p) = \begin{cases} \frac{1}{12}p\left(3np - 4p^2 - 2 - 6p\right), & \text{if } p \text{ is even} \\ \frac{1}{12}(p+1)(p-1)(3n - 4p - 6), & \text{if } p \text{ is odd.} \end{cases}$$

and

$$f(p) - f(p-2) = \begin{cases} (p-1)(n-2p) - 1, & \text{if } p \text{ is even} \\ (p-1)(n-2p), & \text{if } p \text{ is odd,} \end{cases}$$

which is greater than zero since $n \geq 2p+2$. By direct verification, we get $f(\lfloor \frac{n}{2} \rfloor - 1) > f(\lfloor \frac{n}{2} \rfloor - 2)$ for $n > 4$.

Therefore, it holds

$$TW_3(T) \leq TW_3(C_{n,3,\lfloor n/2 \rfloor - 1}),$$

with equality if and only if $T \cong C_{n,3,\lfloor n/2 \rfloor - 1}$. □

This can be further generalized—for all $k > 3$ the caterpillar that maximizes the function $f(p) = TW_k(C_{n,k,p})$ has maximal generalized terminal Wiener index among trees on n vertices.

5 Calculating TW_k of Partial Cubes

The n-cube Q_n is the graph whose vertex set consists of all binary n-tuples (hence $|V(Q_n)| = 2^n$), two vertices are adjacent if the corresponding tuples differ in precisely one position. The central metric feature of the n cube is the fact that the distance between two vertices is equal to the number of positions in which they differ. A subgraph H of a graph G is called *isometric* if for any vertices u and v of H, $d_H(u, v) = d_G(u, v)$. *Partial cubes* are isometric subgraphs of hypercubes. Important examples of partial cubes are hypercubes, even cycles, (chemical) trees, median graphs, benzenoid systems, phenylenes. The Cartesian product of partial cubes is again a partial cubes.

Let G be a connected graph. Then $e = xy$ and $f = uv$ are in the Djoković–Winkler Θ relation [26] if

$$d(x, u) + d(y, v) \neq d(x, v) + d(y, u).$$

The relation Θ is always reflexive and symmetric, and is transitive on partial cubes. Therefore, Θ partitions the edge set of a partial cube G into equivalence classes $F_1, F_2, \ldots, F_s$, called Θ-classes (or cuts). For any $1 \leq i \leq s$, the graph $G - F_i$ consists of two connected components. The vertex sets of these components will be denoted with $W_{(i,0)}$ and $W_{(i,1)}$, because they can be described as the vertices whose i-th coordinate is 0 and 1, respectively. The sets $W_{(i,\chi)}$, $1 \leq i \leq s$, $\chi \in \{0, 1\}$ are called halfspaces of G, while $W_{(i,0)}$ and $W_{(i,1)}$ are complementary halfspaces [18] and it holds $|W_{(i,0)}| + |W_{(i,1)}| = n$.

Let G be a partial cube with halfspaces $W_{(i,\chi)}$, $1 \leq i \leq s$, $\chi \in \{0, 1\}$. For any $1 \leq i \leq s$ and any $\chi \in \{0, 1\}$, $|W_{(i,\chi)}|^{(k)}$ denotes the number of vertices with degree k in $W_{(i,\chi)}$.

Theorem 5.1 *Let G be a partial cube with halfspaces $W_{(i,\chi)}$, $1 \leq i \leq s$, $\chi \in \{0, 1\}$. Then*

$$TW_k(G) = \sum_{i=1}^{s} |W_{(i,0)}|^{(k)} \cdot |W_{(i,1)}|^{(k)}.$$

Proof G is a partial cube, hence vertices of G can be considered as a binary s-tuple $u = u_1u_2 \ldots u_s$. Moreover, since G is isometric in Q_s, the distance between two vertices is the number of positions in which they differ. Set $\delta(x, y) = 0$ if $x = y$, and $\delta(x, y) = 1$ for $x \neq y$. Then

$$\begin{aligned} TW_k(G) &= \sum_{\substack{u,v \in V(G) \\ deg(u)=deg(v)=k}} d(u, v) \\ &= \sum_{\substack{u,v \in V(G) \\ deg(u)=deg(v)=k}} \sum_{i=1}^{s} \delta(u_i, v_i) \end{aligned}$$

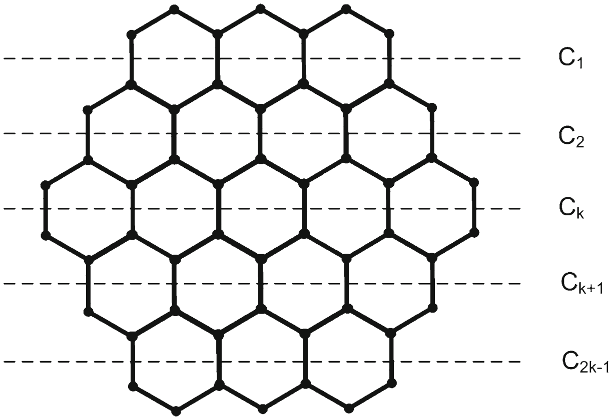

Fig. 4 The Coronene/Circumcoronene H_3

$$= \sum_{i=1}^{s} \left(\sum_{\substack{u,v \in V(G) \\ deg(u)=deg(v)=k}} \delta(u_i, v_i) \right)$$

$$= \sum_{i=1}^{s} |W_{(i,0)}|^{(k)} \cdot |W_{(i,1)}|^{(k)}.$$

This completes the proof. □

An advantage of Theorem 5.1 comparing to computing $TW_k(G)$ by the definition is that we do not need to compute distances, but only to count vertices in the classes. This theorem can be considered as another instance of Klavžar "cut method". For its general description and an overview of its applications in chemical graph theory see survey [19].

As an example, we obtain a closed expression for TW_3 of the coronene/circumcoronene homologous series H_k. In Fig. 4, $2k-1$ horizontal elementary cuts of H_k are presented. There exist two additional groups of $2k-1$ equivalent cuts, obtained by rotating the former group by $\frac{\pi}{3}$ and $-\frac{\pi}{3}$. The number of vertices of H_k equals $n_k = 6k^2$, while there are exactly $6k$ vertices of degree two.

Using symmetry, the contribution of the elementary cut C_i is equal to the contribution of C_{2k-i}, $i = 1, 2, \ldots, k-1$. By induction it follows that for $i = 1, 2, \ldots, k$ the number of vertices above cut C_i equals $i(2k+i)$, while the number of vertices of degree 2 equals $k + 2i$. Therefore by using Theorem 5.1 and described cuts, we have

$$\frac{1}{3} TW_3(H_k) = (3k^2 - 3k)^2 + 2 \sum_{i=1}^{k-1} (2ki + i^2 - k - 2i)(6k^2 - 6k - 2ki - i^2 + k + 2i)$$

$$= \frac{164k^5}{15} - \frac{82k^4}{3} + \frac{58k^3}{3} - \frac{5k^2}{3} - \frac{19k}{15}.$$

Finally, we derive the fifth-order polynomial formula for the generalized terminal Wiener index of H_k

$$TW_3(H_k) = \frac{1}{5}(k-1)k(2k-1)(82k^2 - 82k - 19).$$

Using similar methods as in [1,17,20] one can obtain the closed formulas for other chemical graphs (trees, benzenoid chains, phenylenes,...) and design a linear algorithm for TW_k of benzenoid systems.

6 Concluding Remarks

The Wiener polarity index and the terminal Wiener index are very new molecular-structure descriptors and only a limited number of mathematical and chemical properties were established so far. In this paper we generalized these indices and open new perspectives for the future research.

Another generalization of these indices may be the following

$$W_k^*(G) = |\{(u, v) \mid d(u, v) \leq k,\ u, v \in V\}| = W_1(G) + W_2(G) + \cdots + W_k(G)$$

and

$$TW_k^*(G) = \sum_{\substack{u,v \in V(G) \\ deg(u) \leq k,\ deg(v) \leq k}} d(u, v) \geq TW_1(G) + TW_2(G) + \cdots + TW_k(G).$$

It would be nice to study mathematical and algorithmic properties of these indices and report their chemical relevance. These indices are obtained from the famous Wiener index, which has many applications in chemistry, graph theory and computer science.

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