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Distance Partition Vectors and Distance Based Indices of $(5, 0)$-Nanotubes

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Abstract

In this paper, we calculate the eccentricities and the distance vectors of all vertices of the $(5, 0)$-nanotubes. Building on these computations, we further determine several important distance-based topological indices associated with these nanotubes. Specifically, we investigate the eccentric connectivity index, eccentric adjacency index, first and second eccentric connectivity indices, Wiener index, generalized Wiener index, generalized Wiener polarity index, hyper-Wiener index, and reciprocal complementary Wiener index. These

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indices are instrumental in characterizing the structural and connectivity attributes of nanotubes, offering significant insights into their topological properties. The arguments from this paper could be readily adapted to obtain similar results for (6,0)-nanotubes.

1 Introduction

A fullerene is a molecule made entirely of carbon atoms organized into a closed, hollow structure [15]. These structures can take various shapes, including spheres, ellipsoids, or cylindrical tubes. Mathematically, fullerene graphs are 3-connected, cubic planar graphs composed exclusively of pentagonal and hexagonal faces [4]. According to Euler's formula, every fullerene must contain exactly twelve pentagonal faces, regardless of its overall size or shape. The first discovered fullerene molecule, C_{60}, consists of 60 carbon atoms arranged in a structure resembling Richard Buckminster Fuller's geodesic dome [13]. This resemblance inspired its name, buckminsterfullerene. The discovery of C_{60} marked a pivotal moment, laying the foundation for fullerene chemistry and the advent of nanotechnology. Grünbaum and Motzkin [9] demonstrated that fullerene graphs with n vertices exist for all even $n \geq 24$ and for $n = 20$. While the number of pentagonal faces in a fullerene graph is minimal compared to the hexagonal faces, their arrangement is cruical in determining the graph's overall shape. When the pentagonal faces are evenly distributed, the fullerene graph achieves icosahedral symmetry, with the dodecahedron being the smallest example. Fullerene graphs can also form tubular structures, a specialized class known as nanotubes.

Nanotubical graphs are essential for modeling and understanding carbon nanotubes, an allotrope of carbon characterized by their hollow cylindrical structure, with walls that are only one atom thick. The carbon atoms are arranged in a hexagonal lattice, and the tubes typically have a diameter of 1-3 nanometers. Carbon nanotubes were first discovered in 1991 (open-ended) [12] and later in 1996 (close-ended) [17]. While carbon nanotubes are often associated with fullerenes, they don't have to be capped with fullerene structures at their ends. Open-ended carbon nanotubes, which lack these fullerene caps, are also common and have their own unique properties and applications. Renowned for their exceptional mechanical strength and electrical properties, carbon nanotubes are at the forefront of nanotechnology and materials science. The mathematical framework provided by nanotubical graphs facilitates the analysis of their topological and geometrical properties, offering deeper insights into their unique characteristics and applications.

In this paper, we will focus on close-ended nanotubes, which are a type of fullerene graphs with distinct structural characteristics. These graphs are cylindrical, with both ends capped by subgraphs, which are primarily pentagonal (five-sided faces) and possibly a few hexagons. These pentagons allow the structure to curve and close, forming the ends of the tube. The cylindrical section of a nanotube is derived from a planar hexagonal grid, where points along two parallel lines are identified and connected. The method used to roll this hexagonal grid into a cylindrical form is described by a pair of integers (p_1, p_2), which determine the rolling pattern and overall structure of the nanotube [18]. Numbers p_1 and p_2 are the components of the translation vector between atoms on the hexagonal grid that will overlap when the tube is formed.

Although many mathematical properties of fullerenes have already been established [2–6, 8, 18], numerous others remain unexplored. In this paper, we calculate the eccentricities and the distance vectors of all vertices of the $(5, 0)$-nanotubes. Building on these computations, we further determine several important distance-based topological indices associated with these nanotubes. Topological indices, in general, assist in comparing different nanotube structures, helping to determine how small changes in topology affect performance in nanotechnology applications. The indices we analyzed help describe various aspects of molecular graphs, such as connectivity, branching, and transport properties, and therefore play an important role in characterizing the structural and connectivity properties of the nanotubes. For example, the eccentric connectivity index shows how well-connected distant parts of the nanotube are, which is relevant for electrical conductivity, mechanical stability, and molecular interactions. The eccentric adjacency index measures how eccentricities vary along adjacent atoms and it is useful for understanding transport phenomena, such as heat or charge distribution, while the first and second eccentric connectivity indices are useful in predicting reactivity, stability, and electronic properties. Other indices that we calculate are much more familiar. The paper is organized as follows. Section 2, Preliminaries, presents the fundamental definitions and results required for this paper. In Section 3, we analyze the distance partition vectors of a $(5,0)$-nanotube as a function of its length and the type of vertex, distinguishing between two vertex types: incoming and outgoing. In Section 4, we evaluate or establish bounds for various distance-based topological indices of the given structures, including the eccentric connectivity index, eccentric adjacency index, first and second Zagreb eccentricity indices, Wiener index, generalized Wiener index, generalized Wiener polarity index, hyper-Wiener index, and reciprocal complementary Wiener index.

2 Preliminaries

This paper follows the standard notation and terminology of graph theory as outlined in [7]. For $u, v \in V(G)$, the distance $d_G(u, v)$ between vertices u and v is defined as the number of edges in a shortest path connecting them in G. Vertices at distance j from vertex v in G are referred to as the j-neighbors of v and the number of such vertices is denoted by $n_j(v)$.

Let C_{10k}, $k \geq 2$ be a $(5,0)$-nanotube. There are many ways to represent a nanotube geometrically. We can use a Schlegel diagram or display the nanotube unrolled. In both representations, we define the initial layer L_0 as the set of vertices incident to the pentagon p which is the center of a cap and set $F_0 = \{p\}$. For each $i = 1, \ldots, k$ the set of faces F_i contains all the faces incident with vertices form L_{i-1} that are not already in F_{i-1}. Similarly, L_i contains all the vertices incident to a face from F_i that are not contained in L_{i-1}. Thus, the nanotube C_{10k} is composed of $k+1$ layers. The first and last layers, L_0 and L_k, each contain 5 vertices, while every intermediate layer has 10 vertices. In the unrolled form of C_{10k}, the layers are arranged from left to right, with the vertices of layer L_0 positioned as the leftmost vertices and the vertices of layer L_k as the rightmost vertices, see Figure 1.

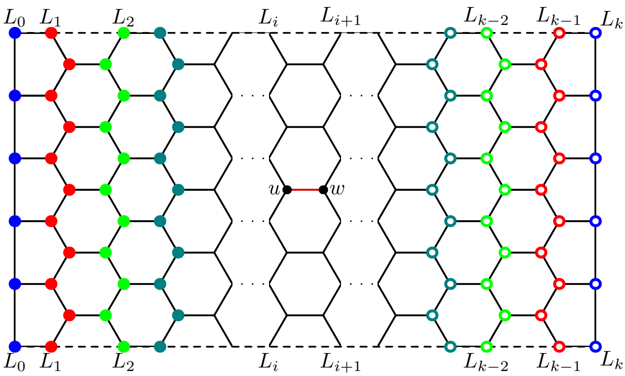


Figure 1. The layers of a $(5, 0)$-nanotube. The filled blue vertices belong to layer L_0, while the hollow blue vertices are in layer L_k. Similarly, the filled red vertices are in L_1 whereas the hollow red vertices belong to layer L_{k-1}, etc. The vertex $u \in L_i$ is an outgoing vertex, while the vertex $w \in L_{i+1}$ is an incoming vertex.

Let $e = uw$ be an edge in C_{10k}, where $u \in L_i$ and $w \in L_{i+1}$. We refer to the vertex u as an outgoing vertex for L_i, and the vertex w as an incoming vertex for L_{i+1}, see Figure 1. Note that all vertices in the initial layer are outgoing, while those in the final layer are incoming. Additionally, each intermediate layer is composed of 5 outgoing and 5 incoming vertices, which alternate along the layer. For $0 \leq i < k$ $(0 < i \leq k)$ denote by L_i^{out} (L_i^{in}) the set of 5 outgoing (ingoing) vertices of L_i.

Definition 1. Let G be a nonempty finite connected graph and v a vertex of G. The distance partition $\pi_d(v)$ relative to v is a collection of disjoint sets:

- $D_0 = \{v\}$,
- $D_j = \{u : d(v, u) = j\}$, $j = 1, 2, 3, \ldots, \text{ecc}(v)$,

where $\text{ecc}(v)$ is the eccentricity of v, i.e. $\text{ecc}(v) = \max_{u \in V(G)} d(v, u)$.

Definition 2. Let G be a nonempty finite connected graph and v a vertex of G. The distance partition vector $\text{DV}(v) \in \mathbb{N}^{\text{diam}(G)}$ of a vertex v is defined as

$$\text{DV}(v) = (n_0(v), n_1(v), \ldots, n_{\text{diam}(G)}(v)),$$

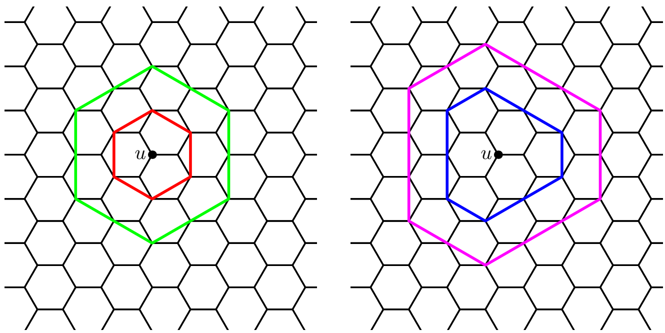
where $n_j(v) = |D_j|$ for $j = 0, 1, \ldots, \text{ecc}(v)$, and $n_j(v) = 0$ for $\text{ecc}(v) < j \leq$

diam(G).

For simplicity, in the next sections, we will omit zero components of DV(v), leaving only the first ecc(v) nonzero components. Note that $n_0(v) = 1$ for each $v \in V(G)$.

3 Distance partition vectors of (5, 0)-nanotube

As noted in [5], on the infinite regular hexagonal grid the number of j-neighbors is $3j$ for any vertex v. Furthermore, from a geometric standpoint, when $j > 1$, the convex hull of these vertices, considered as points in the plane, forms a hexagon H_j, with all such vertices evenly distributed along its sides, see Figure 2. (For $j = 1$, the convex hull is a triangle.)



(*a*) (*b*)

Figure 2. (a) The hexagons H_2 (red) and H_4 (green) with respect to the vertex u. (b) The hexagons H_3 (blue) and H_5 (pink) with respect to the vertex u.

The following result from [5] holds.

Proposition 1. *For $j > 1$, let H_j denote the hexagon formed by the j-neighbors of a vertex v in an infinite hexagonal grid. When j is even, each side of H_j contains exactly $j/2 + 1$ vertices. For odd j, three nonadjacent sides contain precisely $\lceil j/2 \rceil$ vertices, while the remaining three sides contain $\lceil j/2 \rceil + 1$ vertices.*

Remark. From Figure 2 we can see that for each $j > 1$, there are two vertical sides of H_j. Let j be odd. If v is an outgoing (incoming) vertex, then the left (right) vertical side contains $\lceil j/2 \rceil + 1$ its j-neighbors, while the right (left) vertical side contains $\lceil j/2 \rceil$ j-neighbors.

By rolling the hexagonal grid by the vector $5\vec{i} + 0\vec{j}$, and placing the pentagonal caps at both ends of the cylinder, we obtain C_{10k}. In this configuration, for a vertex $v \in V(C_{10k})$, its j-neighbors may either stay on the sides of the hexagons H_j or shift to different positions, depending on the location of v and the distance j. Andova et al. [5] studied the distances of vertices in an infinite open (p_1, p_2)-nanotube G. For each $j \in \mathbb{N}$, they determined the number of j-neighbors of a vertex $v \in V(G)$.

Theorem 2. *Let v be an arbitrary vertex in an infinite open (p_1, p_2)-nanotube and let $q \in \mathbb{N}$, $q \leq p_1 - p_2$. Then*

$$n_j(v) = \begin{cases} 3j, & 1 \leq j < p_1 + p_2; \\ 3j - (p_2 + 1), & j = p_1 + p_2; \\ 3j - 2(p_2 + 2q), & j = p_1 + p_2 + q; \\ 2(p_1 + p_2), & j \geq 2p_1. \end{cases}$$

From Theorem 2 we obtain the numbers $n_j(v)$ of vertices at distance j from v in an infinite open $(5, 0)$-nanotube:

$$n_j(v) = \begin{cases} 3j, & 1 \leq j < 5; \\ 3j - 1, & j = 5; \\ 15 - q, & j = 5 + q,\ 1 \leq q \leq 4; \\ 10, & j \geq 10. \end{cases} \tag{1}$$

Since C_{10k} is finite, its distance vectors differ from those of an infinite open $(5, 0)$-nanotube. However, the following observations show that the distance vectors can be very different only if $v \in L_0 \cup L_k$.

Observation 1. *Let $x \in L_i$ and $y \in L_j$, where $0 \leq i \leq j \leq k$. Then there is a shortest path between x and y using only the vertices of $L_i, L_{i+1}, \ldots, L_j$.*

For $i = j = 1$ and $i = j = k - 1$, there may exist shortest paths between x and y that use vertices from L_0 and L_k, respectively. In all other cases every shortest path between x and y uses only the vertices of $L_i, L_{i+1}, \ldots, L_j$.

Observation 2. *Let $x \in L_i$ and $y \in L_j$, where $1 \le i < j \le k$ or $i = 0$ and $j > 2$. Then there is a shortest path between x and y that passes through at most two vertices in each layer $L_i, L_{i+1}, \ldots, L_{j-1}$.*

According to Observation 2, there exists a shortest path between x and y that uses the smallest possible number of vertices of $L_i, L_{i+1}, \ldots, L_{j-1}$ and the remaining vertices of the path are from L_j.

Observations 1 and 2 are significant when determining eccentricities of vertices and calculating the distance vectors.

The smallest $(5, 0)$-nanotube is the dodecahedron C_{20} created only by the two caps. Since it is a vertex-transitive graph, all of its vertices belong to a single orbit under the automorphism group of C_{20}. From the structure and the symmetry of C_{10k}, $k \ge 3$ it follows that there are k orbits of the automorphism group $\mathrm{Aut}(C_{10k})$, each having 10 vertices. We denote them by $O_0 = L_0^{\mathrm{out}} \cup L_k^{\mathrm{in}}$, $O_1 = L_1^{\mathrm{in}} \cup L_{k-1}^{\mathrm{out}}$, $O_2 = L_1^{\mathrm{out}} \cup L_{k-1}^{\mathrm{in}}$, $\ldots$, $O_{k-1} = L_{\lfloor k/2 \rfloor}^{\mathrm{out}} \cup L_{\lceil k/2 \rceil}^{\mathrm{in}}$. Note that for $s \ge 0$, it holds $O_{2s} = L_s^{\mathrm{out}} \cup L_{k-s}^{\mathrm{in}}$ and $O_{2s+1} = L_{s+1}^{\mathrm{in}} \cup L_{k-s-1}^{\mathrm{out}}$. Furthermore, when k is even, all 10 vertices of the orbit O_{k-1} belong to $L_{k/2}$. Therefore, to determine distance vectors of all vertices from C_{10k}, it is sufficient to calculate the distance partition vector of only one vertex from each orbit.

Before we calculate distance partition vectors of vertices of C_{10k}, $k \ge 6$, let us mention a result from [3] concerning the diameter of C_{10k}:

Lemma 1. *We have*

$$\mathrm{diam}(C_{10k}) = \begin{cases} 2k+1, & k = 2; \\ 2k, & k = 3, 4; \\ 2k-1, & k \ge 5. \end{cases} \tag{2}$$

Now we calculate eccentricities of vertices in C_{10k}, $k \ge 2$. Because of the symmetry of C_{10k} for $v \in L_i^{\mathrm{in}}$ and $u \in L_{k-i}^{\mathrm{out}}$ we have $\mathrm{ecc}(v) = \mathrm{ecc}(u)$. So it suffices to consider eccentricities of vertices of L_i^{in} for $1 \le i \le \lfloor k/2 \rfloor$ and L_i^{out} for $0 \le i \le \lfloor (k-1)/2 \rfloor$.

Lemma 2. *For eccentricities of vertices of C_{10k} we have*

i) If $k = 2$, then $\mathrm{ecc}(v) = 5$ for all $v \in V(C_{10k})$.

ii) If $k = 3$, then $\mathrm{ecc}(v) = 6$ for all $v \in V(C_{10k})$.

iii) If $k \geq 4$ and $v \in L_i^{\mathrm{in}} \cup L_{k-i}^{\mathrm{out}}$ for $1 \leq i \leq \lfloor k/2 \rfloor$, then

$$\mathrm{ecc}(v) = 2(k-i) + \delta,$$

where $\delta = 2$ if $(k,i) = (4,2)$, $\delta = 1$ for $(k,i) \in \{(4,1),(5,2),(6,3)\}$, and $\delta = 0$ otherwise.

iv) If $k \geq 4$ and $v \in L_i^{\mathrm{out}} \cup L_{k-i}^{\mathrm{in}}$ for $0 \leq i \leq \lfloor (k-1)/2 \rfloor$, then

$$\mathrm{ecc}(v) = 2(k-i) - 1 + \delta,$$

where $\delta = 2$ if $(k,i) \in \{(4,1),(5,2)\}$, $\delta = 1$ if $(k,i) \in \{(4,0),(5,1),(6,2),(7,3)\}$, and $\delta = 0$ otherwise.

Proof. Denote

$$V_1 = \bigcup_{i=1}^{\lfloor k/2 \rfloor} L_i^{\mathrm{in}} \bigcup \bigcup_{i=0}^{\lfloor (k-1)/2 \rfloor} L_i^{\mathrm{out}} \quad \text{and} \quad V_2 = \bigcup_{i=\lfloor k/2 \rfloor + 1}^{k} L_i^{\mathrm{in}} \bigcup \bigcup_{i=\lfloor k/2 \rfloor}^{k-1} L_i^{\mathrm{out}}.$$

It suffices to consider the vertices $v \in V_1$. Then, the vertices at the biggest distance from v must be in V_2 (see Figure 1), somewhere close to L_k. We consider all the possible cases and start with incoming vertices.

Case 1: $v \in L_{k-1}^{\mathrm{in}}$. This is possible only if $k = 2$ since $v \in V_1$. Then all vertices of L_k^{in} are at distance at most 4 from v, but there is a vertex of L_{k-1}^{out} which is at distance 5 from v (use Observations 1 and 2 for a shortest path). So $\mathrm{ecc}(v) = 5$.

Case 2: $v \in L_{k-2}^{\mathrm{in}}$. This is possible only if $k \in \{3,4\}$. Then all vertices of L_k^{in} are at distance at most 5 from v, but there is a vertex of L_{k-1}^{in} which is at distance 6 from v. So $\mathrm{ecc}(v) = 6$.

Case 3: $v \in L_{k-3}^{\mathrm{in}}$. This is possible only if $k \in \{4,5,6\}$. Then all vertices of L_k^{in} are at distance at most 7 from v, and one of them is at distance exactly 7 from v, so as one vertex of L_{k-1}^{out}. So $\mathrm{ecc}(v) = 7$.

Case 4: $v \in L^{\rm in}_{k-i}$ for $i \geq 4$. Then all vertices of $L^{\rm in}_k$ are at distance exactly $2(k-i)$ from v.

Now we consider the cases $v \in L^{\rm out}_i$. Here the case $v \in L^{\rm out}_{k-1}$ is impossible since that would mean $k = 1$.

Case 5: $v \in L^{\rm out}_{k-2}$. If $k = 2$ then $v \in L^{\rm out}_0$ and there is a unique vertex of $L^{\rm in}_2$ at distance 5 from v, all other vertices are closer. So $\text{ecc}(v) = 5$. Now suppose that $v \notin L^{\rm out}_0$. This is possible only if $k = 3$. Then all vertices of $L^{\rm in}_k$ are at distance at most 5 from v, but there is a vertex of $L^{\rm out}_{k-1}$ at distance 6 from v. So $\text{ecc}(v) = 6$.

Case 6: $v \in L^{\rm out}_{k-3}$. If $k = 3$ then $v \in L^{\rm out}_0$. Then all vertices of $L^{\rm in}_k$ and L_{k-1} are at distance at most 6 from v (for the latter one should use paths having first edges in L_0) and two vertices of $L^{\rm in}_k$ are at distance exactly 6 from v. So $\text{ecc}(v) = 6$. Now suppose that $v \notin L^{\rm out}_0$. This is possible only if $k \in \{4, 5\}$. Then all vertices of $L^{\rm in}_k$ are at distance at most 6 from v, but there is a vertex of $L^{\rm in}_{k-1}$ at distance 7 from v. So $\text{ecc}(v) = 7$.

Case 7: $v \in L^{\rm out}_{k-4}$. This is possible only if $k \in \{4, 5, 6, 7\}$. Then all vertices of $L^{\rm in}_k$ are at distance at most 8 from v, one being at distance exactly 8 from v. Also one vertex of $L^{\rm out}_{k-1}$ has distance 8 from v if $k \geq 4$. So $\text{ecc}(v) = 8$.

Case 8: $v \in L^{\rm out}_{k-i}$ for $i \geq 5$. Then all vertices of $L^{\rm in}_k$ are at distance exactly $2(k-i) - 1$ from v.

Observe that if $k = 2$, then $\text{ecc}(v) = 5$ (Cases 1 and 5), while if $k = 3$, then $\text{ecc}(v) = 6$ (Cases 2, 5 and 6). ■

Observe that Lemma 1 is a consequence of Lemma 2, and the diameter is achieved by the vertices of $L^{\rm out}_0$. In the next table, we show eccentricities of the vertices of V_1 when $4 \leq k \leq 7$. If $k \in \{2, 3\}$, then all the vertices have the same eccentricity, and if $k \geq 8$, then there is no irregularity.

	$L^{\rm out}_0$	$L^{\rm in}_1$	$L^{\rm out}_1$	$L^{\rm in}_2$	$L^{\rm out}_2$	$L^{\rm in}_3$	$L^{\rm out}_3$
$k = 4$	8	7	7	6			
$k = 5$	9	8	8	7	7		
$k = 6$	11	10	9	8	8	7	
$k = 7$	13	12	11	10	9	8	8

Table 1. Eccentricities of vertices of V_1 for $4 \leq k \leq 7$.

For $k \geq 2$ and each $i = 0, 1, \ldots, k$, the layer L_i divides the nanotube C_{10k} into two distinct parts (one of them being empty if $i = 0$ or $i = k$). The left-hand side part consists of layers L_j for $j = 0, 1, \ldots, i-1$, while the right-hand side part consists of layers L_j for $j = i+1, \ldots, k$. By $L(v)$ and $R(v)$ we denote the distance partition vector for the left-hand side part and the right-hand side part, respectively, and by $D(v)$ we denote the distance partition vector within the layer L_i.

By Observations 1 and 2, the following statement holds.

Proposition 3. *Let $k \geq 2$ and let v be a vertex from C_{10k} such that $v \in L_i$, $0 \leq i \leq k$. Then*

$$D(v) = \begin{cases} (1,2,2), & \text{if } i \in \{0,k\}; \\ (1,2,2,2,2,1), & \text{otherwise,} \end{cases} \tag{3}$$

and

$$\mathrm{DV}(v) = L(v) + D(v) + R(v). \qquad \blacksquare$$

By symmetry, if $u \in L_i^{\mathrm{in}}$ then for $v \in L_{k-i}^{\mathrm{out}}$ we have $R(u) = L(v)$, and if $u \in L_i^{\mathrm{out}}$ then for $v \in L_{k-i}^{\mathrm{in}}$ we have $R(u) = L(v)$. Hence, it suffices to calculate $L(v)$. These vectors are presented in the following table.

$L(v)$	$v \in L_i^{\mathrm{in}}$	$v \in L_i^{\mathrm{out}}$
$i=1$	(0,1,2,2)	(0,0,2,2,1)
$i=2,\ k=2$	(0,1,4,6,3,1)	
$i=2,\ k\geq 3$	(0,1,2,4,4,3,1)	(0,0,2,3,5,4,1)
$i=3,\ k=3$	(0,1,4,6,6,6,2)	
$i=3,\ k\geq 4$	(0,1,2,4,5,7,5,1)	(0,0,2,3,5,6,7,2)
$i=4,\ k=4$	(0,1,4,6,6,6,6,5,1)	
$i=4,\ k\geq 5$	(0,1,2,4,5,7,7,7,2)	(0,0,2,3,5,6,7,6,6)
$i=5,\ k=5$	(0,1,4,6,6,6,6,5,6,5)	
$i=5,\ k\geq 6$	(0,1,2,4,5,7,7,7,6,6)	(0,0,2,3,5,6,7,6,6,5,5)
$i=k,\ k\geq 6$	$(0,1,4,6,6,6,6,5,6,5^{\#(2k-9)})$	
$6\leq i\leq k-1$, $k\geq 7$	$(0,1,2,4,5,7,7,7,6,6,5^{\#2(i-5)})$	$(0,0,2,3,5,6,7,6,6,5^{\#2(i-4)})$

Table 2. Distance partition vectors for the left-hand side in C_{10k}. The notation $5^{\#k}$ represents a sequence of k elements, all equal to 5.

Now using Proposition 3 we get the following theorem from Table 2.

Theorem 4. *Let $k \geq 10$. Moreover, let $x =$ 'in' or $x =$ 'out' if k is even. Then the distance partition vectors of all vertices of C_{10k} are listed in Table 3.* ∎

We remark that the rows for $i = 5$ are redundant since the following two (those in which $i > 5$) are valid also for $i = 5$. We have them emphasize the change at $i = 5$.

Observe that for $i > 5$, the distance vectors for $v \in L_i^{\text{in}}$ and $v \in L_i^{\text{out}}$ differ only by the parity of exponents at 10 and by the exponent at 5. Therefore, we can unify the description of these distance vectors using the orbits O_t, where $t \geq 9$, since the orbit O_9 consists of all vertices from $L_5^{\text{in}} \cup L_{k-5}^{\text{out}}$. However, distance vectors for vertices in orbits O_0, O_1, …,O_8 are slightly different (see the first 9 lines of Table 3).

	Distance vector DV(v)
$i = 0$ and $v \in L_i^{\text{out}}$	$(1,3,6,6,6,6,6,5,6,5^{\#(2k-9)})$
$i = 1$ and $v \in L_i^{\text{in}}$	$(1,3,6,7,7,7,7,6,6,5^{\#(2k-10)})$
$i = 1$ and $v \in L_i^{\text{out}}$	$(1,3,6,8,8,8,7,7,6,6,5^{\#(2k-12)})$
$i = 2$ and $v \in L_i^{\text{in}}$	$(1,3,6,9,11,10,8,6,6,5^{\#(2k-12)})$
$i = 2$ and $v \in L_i^{\text{out}}$	$(1,3,6,9,12,12,8,7,6,6,5^{\#(2k-14)})$
$i = 3$ and $v \in L_i^{\text{in}}$	$(1,3,6,9,12,14,12,7,6,5^{\#(2k-14)})$
$i = 3$ and $v \in L_i^{\text{out}}$	$(1,3,6,9,12,14,14,9,6,6,5^{\#(2k-16)})$
$i = 4$ and $v \in L_i^{\text{in}}$	$(1,3,6,9,12,14,14,13,8,5^{\#(2k-16)})$
$i = 4$ and $v \in L_i^{\text{out}}$	$(1,3,6,9,12,14,14,13,12,6,5^{\#(2k-18)})$
$i = 5$ and $v \in L_i^{\text{in}}$	$(1,3,6,9,12,14,14,13,12,11,5^{\#(2k-19)})$
$i = 5$ and $v \in L_i^{\text{out}}$	$(1,3,6,9,12,14,14,13,12,11,10,5^{\#(2k-21)})$
$i > 5$ and $v \in L_i^{\text{in}}$	$(1,3,6,9,12,14,14,13,12,11,10^{\#(2i-10)},5^{\#(2k-4i+1)})$
$i > 5$ and $v \in L_i^{\text{out}}$	$(1,3,6,9,12,14,14,13,12,11,10^{\#(2i-9)},5^{\#(2k-4i-1)})$
$i = \lfloor k/2 \rfloor$, k is odd, and $v \in L_i^{\text{in}}$	$(1,3,6,9,12,14,14,13,12,11,10^{\#(k-11)},5,5,5)$
$i = \lfloor k/2 \rfloor$, k is odd, and $v \in L_i^{\text{out}}$	$(1,3,6,9,12,14,14,13,12,11,10^{\#(k-10)},5)$
$i = k/2$, k is even, and $v \in L_i^{x}$	$(1,3,6,9,12,14,14,13,12,11,10^{\#(k-10)},5)$
$t \geq 9$ and $v \in O_t$	$(1,3,6,9,12,14,14,13,12,11,10^{\#(t-9)},5^{\#(2k-2t-1)})$

Table 3. Distance partition vectors for vertices of C_{10k}, for $k \geq 10$. Unless otherwise stated, $i < \lfloor k/2 \rfloor$. The notation $a^{\#p}$ represent a sequence of p elements, all equal to a.

4 Distance based indices of $(5, 0)$-nanotubes

In this section, we determine exact values or establish bounds for a wide range of chemical indices for C_{10k}. We start with indices based on eccentricities.

Eccentric connectivity index [16] of G is

$$\xi_c(G) = \sum_{v \in V(G)} \deg_G(v) \cdot \mathrm{ecc}_G(v),$$

where $\deg_G(v)$ is the degree of v in G.

Eccentric adjacency index [1] of G is

$$\xi^{\mathrm{ad}}(G) = \sum_{v \in V(G)} \frac{\mathrm{SG}(v)}{\mathrm{ecc}_G(v)},$$

where $\mathrm{SG}(v)$ is the sum of degrees of neighbours of v.

The eccentricity version of the Zagreb indices was first introduced by Vukičević and Graovac [19]. *First Zagreb eccentricity index* is defined by

$$\xi_1(G) = \sum_{v \in V(G)} \mathrm{ecc}_G^2(v),$$

and *second Zagreb eccentricity index* is

$$\xi_2(G) = \sum_{uv \in E(G)} \big(\mathrm{ecc}_G(u) \cdot \mathrm{ecc}_G(v)\big).$$

By Lemma 2, the eccentricities are regular if $k \geq 8$. Namely, if $v \in O_i$, $0 \leq i \leq k-1$, then $\mathrm{ecc}(v) = 2k - 1 - i$. Therefore, in the next statement, we assume that $k \geq 8$. For smaller k, the indices could be easily calculated by a computer.

Theorem 5. *Let* $k \geq 8$. *Then*
(a) $\xi_c(C_{10k}) = 45k^2 - 15k$;
(b) $90\ln(2) \leq \xi^{\mathrm{ad}}(C_{10k}) \leq 90\big(\ln(2k-1) - \ln(k-1)\big)$;
(c) $\xi_1(C_{10k}) = \dfrac{5}{3}k(14k^2 - 9k + 1)$;
(d) $\xi_2(C_{10k}) = 35k^3 - \frac{45}{2}k^2 - 5k + \delta$,

where $\delta = \frac{15}{2}$ *if* k *is odd and* $\delta = 10$ *if* k *is even.*

Proof. (a) Since each orbit of C_{10k} has 10 vertices, by Lemma 2 we have

$$\begin{aligned}\xi_c(C_{10k}) &= \sum_{v\in V(C_{10k})} \deg(v)\cdot \mathrm{ecc}(v) = 10\sum_{t=k}^{2k-1} 3t \\ &= 30\Big(\sum_{t=1}^{2k-1} t - \sum_{t=1}^{k-1} t\Big) = 30\Big(\frac{4k^2-2k}{2} - \frac{k^2-k}{2}\Big) = 45k^2 - 15k.\end{aligned}$$

(b) We have

$$\xi^{\mathrm{ad}}(C_{10k}) = \sum_{v\in V(C_{10k})} \frac{9}{\mathrm{ecc}(v)} = 10\sum_{t=k}^{2k-1}\frac{9}{t} = 90\sum_{t=k}^{2k-1} t^{-1}.$$

Calculating the area below $f(x) = x^{-1}$ and using the fact that $f(x) = x^{-1}$ is positive and decreasing for all $x > 0$, we infer

$$\int_k^{2k} x^{-1}dx \le \sum_{t=k}^{2k-1} t^{-1} \le \int_{k-1}^{2k-1} x^{-1}dx,$$

and so

$$90\big(\ln(2k) - \ln(k)\big) \le \xi^{\mathrm{ad}}(C_{10k}) \le 90\big(\ln(2k-1) - \ln(k-1)\big).$$

Since $\ln(2k) = \ln(2) + \ln(k)$, we obtain the result.

(c) We have

$$\begin{aligned}\xi_1(C_{10k}) &= \sum_{v\in V(C_{10k})} \mathrm{ecc}^2(v) \\ &= 10\sum_{t=k}^{2k-1} t^2 = 10\left(\sum_{t=1}^{2k-1} t^2 - \sum_{t=1}^{k-1} t^2\right) \\ &= 10\left[\frac{(2k-1)2k(4k-1)}{6} - \frac{(k-1)k(2k-1)}{6}\right] \\ &= \frac{5}{3}k(14k^2 - 9k + 1).\end{aligned}$$

(d) To calculate $\xi_2(C_{10k})$, note that there are 5 edges with both endvertices in L_0^{out} and 5 edges with both endvertices in L_k^{in}. Furthermore, there are 5 edges with one endvertex in L_t^{out} and the other in L_{t+1}^{in}, where $0 \le t \le k-1$, and 10 edges with one endvertex in L_t^{in} and the other in L_t^{out}, where $1 \le t \le k-1$. Considering the orbits, there are 10 edges with both endvertices in the last orbit O_{k-1} if k is even, but there are only 5 edges with both endvertices in the last orbit O_{k-1} if k is odd. Therefore, it is natural to consider two cases according to the parity of k.

Case 1. *k is odd.* In the calculation below, in the first expression we consider the edges between O_{k-1} and O_{k-2}, O_{k-3} and O_{k-4}, ..., O_2 and O_1. In each case, there are 20 edges between these orbits. In the second expression we consider edges between O_{k-2} and O_{k-3}, O_{k-4} and O_{k-5}, ..., O_1 and O_0. In each case, there are 10 edges between these orbits. Then we consider the 5 edges with both endvertices in O_{k-1} and finally the 10 edges with both endvertices in O_0. We have

$$\begin{aligned}
\xi_2(C_{10k}) &= 20 \sum_{j=1}^{\frac{k-1}{2}} 2(k-j)[2(k-j)-1] + 10 \sum_{j=0}^{\frac{k-3}{2}} [2(k-j)-1]2(k-j-1) \\
&\quad + 5k^2 + 10(2k-1)^2 \\
&= 120 \sum_{j=1}^{\frac{k-3}{2}} (k-j)^2 - 100 \sum_{j=1}^{\frac{k-3}{2}} (k-j) + 35k(3k-2) \\
&= 120 \left[\sum_{t=1}^{k-1} t^2 - \sum_{t=1}^{\frac{k+1}{2}} t^2 \right] - 100 \left[\sum_{t=1}^{k-1} t - \sum_{t=1}^{\frac{k+1}{2}} t \right] + 35k(3k-2) \\
&= 35k^3 - \tfrac{45}{2}k^2 - 5k + \tfrac{15}{2}.
\end{aligned}$$

Case 2. *k is even.* Here, in the first expression we consider the edges between O_{k-2} and O_{k-3}, O_{k-4} and O_{k-5}, ..., O_2 and O_1, while in the second expression we consider the edges between O_{k-1} and O_{k-2}, O_{k-3} and O_{k-4}, ..., O_1 and O_0. Then we consider 10 edges with both endvertices in O_{k-1} and 10 edges with both endvertices in O_0. We get

$$\begin{aligned}\xi_2(C_{10k}) &= 20\sum_{j=1}^{\frac{k-2}{2}} 2(k-j)[2(k-j)-1] + 10\sum_{j=0}^{\frac{k-2}{2}}[2(k-j)-1]2(k-j-1) \\ &\quad + 10k^2 + 10(2k-1)^2 \\ &= 120\sum_{j=1}^{\frac{k-2}{2}}(k-j)^2 - 100\sum_{j=1}^{\frac{k-2}{2}}(k-j) + 10(9k^2-9k+1) \\ &= 120\left[\sum_{t=1}^{k-1} t^2 - \sum_{t=1}^{k/2} t^2\right] - 100\left[\sum_{t=1}^{k-1} t - \sum_{t=1}^{k/2} t\right] + 10(9k^2-9k+1) \\ &= 35k^3 - \tfrac{45}{2}k^2 - 5k + 10. \qquad \blacksquare\end{aligned}$$

Observe that by Theorem 5 we have $\lim_{k\to\infty} \xi^{\mathrm{ad}}(C_{10k}) = 90\ln(2)$.

Now we calculate indices using the distance sequences.

Generalized Wiener polarity index [10], $W_j(G)$, is the number of unordered pairs of vertices $u, v \in V(G)$ such that $d_G(u,v) = j$. When $j = 3$, we get the *polarity index* [20].

Observe that $W_j(G) = 0$ if $j > \mathrm{diam}(G)$, and for $k \geq 5$, the diameter of C_{10k} is $2k-1$, by Lemma 1.

Theorem 6. *Let $k \geq 10$. Then, the values of $W_j(C_{10k})$ for $k \geq 10$ and $j = 1, \ldots, 2k-1$ are given in Table 4.*

j	$W_j(C_{10k})$	j	$W_j(C_{10k})$	j	$W_j(C_{10k})$
1	$15k$	4	$60k-80$	7	$65k-220$
2	$30k$	5	$70k-135$	8	$60k-230$
3	$45k-30$	6	$70k-180$	9	$55k-250$
≥ 10	$50k-25j$				

Table 4. Generalized Wiener polarity index of C_{10k} for $k \geq 10$ and $j = 1, \ldots, 2k-1$.

Proof. The graph C_{10k} has k orbits, each with 10 vertices. Further, every pair of vertices, say u and v, with distance $d(u,v)$ is counted twice in Table 3; once in the row corresponding to u and once in the row corresponding to v. So using the distance sequences from Table 3 we have

$W_1(C_{10k}) = \frac{10}{2} \cdot 3k = 15k$, $W_2(C_{10k}) = \frac{10}{2} \cdot 6k = 30k$, $W_3(C_{10k}) = \frac{10}{2}(9k - 1 - 2 - 3) = 45k - 30$ and $W_4(C_{10k}) = \frac{10}{2}(12k - 1 - 4 - 5 - 6) = 60k - 80$. In a similar way we obtain values of $W_j(C_{10k})$ for $j = 5, \ldots, 9$ as given in Table 4. Now we calculate $W_j(C_{10k})$ when $j \geq 10$. We distinguish two cases.

Case 1: $10 \leq j \leq k - 1$. In Table 3, we have 5's in the first rows and 10's in the last rows on j-th position (ignoring the very last row, of course). When $j = k - i$, then in i rows we have 10's and in the remaining $k - i$ rows we have 5's. So

$$W_j(C_{10k}) = \frac{10}{2} \cdot 10(k - j) + \frac{10}{2} \cdot 5j = 50k - 25j.$$

Case 2: $k \leq j \leq 2k - 1$. Observe that the longest sequence of 10's appears in the row that is above the last one in Table 3. So if there is a non-zero number on i-th position, where $i \geq k$, then this number is 5. If $j = k + i$, then there are i orbits with 0 on j-th position, and $k - i$ orbits with 5 on j-th position. So

$$W_j(C_{10k}) = \frac{10}{2} \cdot 5\big(k - (j - k)\big) = 50k - 25j. \qquad \blacksquare$$

Using generalized Wiener polarity indices we can calculate other chemical indices. The most famous chemical index is the Wiener index.

Wiener index, $W(G)$, is the sum of distances in G [20]. That is

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

The *hyper-Wiener index* is defined [14] as

$$\mathrm{WW}(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (d(u, v) + d^2(u, v)).$$

Finally, the *reciprocal complementary Wiener index* [11] is

$$\mathrm{RCW}(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{\mathrm{diam}(G) + 1 - d(u, v)}$$

Denote $R_k = \sum_{j=1}^{9} \frac{W_j(C_{10k})}{2k-j}$. By Theorem 6, we obtain

$$R_k = \frac{15k}{2k-1} + \frac{30k}{2k-2} + \frac{45k-30}{2k-3} + \frac{60k-80}{2k-4} + \frac{70k-135}{2k-5} + \frac{70k-180}{2k-6} + \frac{65-220k}{2k-7} + \frac{60k-230}{2k-8} + \frac{55k-250}{2k-9}.$$

Theorem 7. *Let* $k \geq 10$. *Then*
(a) $W(C_{10k}) = \frac{5}{3}(20k^3 + 235k - 402)$;
(b) $\mathrm{WW}(C_{10k}) = \frac{25}{6}(4k^4 + 4k^3 - k^2 + 407k - 864)$;
(c) $\mathrm{RCW}(G) = R_k + 50k - 250$.

Proof. (a) Since C_{10k} has diameter $2k-1$, we can use the generalized Wiener polarity index to calculate the Wiener index. By using Theorem 6, we obtain

$$\begin{aligned} W(C_{10k}) &= \sum_{j=1}^{2k-1} j \cdot W_j(C_{10k}) = \sum_{j=1}^{9} j \cdot W_j(C_{10k}) + \sum_{j=10}^{2k-1} j(50k - 25j) \\ &= 2650k - 7795 + \frac{25}{3}(4k^3 - 271k + 855) \\ &= \frac{5}{3}(20k^3 + 235k - 402). \end{aligned}$$

(b) Denote $\Delta = \sum_{\{u,v\} \subseteq V(C_{10k})} d^2(u,v)$. We use a formula $\sum_{j=1}^{a} j^3 = \frac{a^2}{4}(a+1)^2$ to obtain

$$\begin{aligned} \Delta &= \sum_{j=1}^{2k-1} j^2 \cdot W_j(C_{10k}) = \sum_{j=1}^{9} j^2 \cdot W_j(C_{10k}) + \sum_{j=10}^{2k-1} j^2(50k - 25j) \\ &= 17250k - 57155 + \frac{25}{3}(4k^4 - k^2 - 1710k + 6075) \\ &= \frac{5}{3}(20k^4 - 5k^2 + 1800k - 3918). \end{aligned}$$

Since $\mathrm{WW}(C_{10k}) = \frac{1}{2}\left(W(C_{10k}) + \Delta\right)$, by using ($a$) we obtain the result.
(c) We write a formula for $\mathrm{RCW}(G)$ by usind generalized Wiener polarity

index and obtain

$$\begin{aligned}\mathrm{RCW}(C_{10k}) &= \sum_{j=1}^{2k-1} \frac{W_j(C_{10k})}{2k-j} = R_k + \sum_{j=10}^{2k-1} \frac{50k-25j}{2k-j} \\ &= R_k + 25(2k-10).\end{aligned}$$ ■

Generalized Wiener index, $W^\alpha(G)$, is defined as

$$W^\alpha(G) = \sum_{\{u,v\}\subseteq V(G)} d^\alpha(u,v),$$

where α is any real number. If $\alpha = 1$, we get the Wiener index, and if $\alpha = 0$, then $W^0(G) = \binom{|V(G)|}{2}$. If $\alpha = -1$, then $W^{-1}(G) = H(G)$, where $H(G)$ is the Harary index of G. For chemical purpuses, both $W^{\frac{1}{2}}$, and the general case W^α are examined.

Obviously, $W^\alpha(C_{10k}) = \sum_{j=1}^{2k-1} j^\alpha W_j(C_{10k})$. When α is a positive integer, a compact formula for $W^\alpha(C_{10k})$ can be derived like the cases $\alpha = 1$ and $\alpha = 2$; see the proof of Theorem 7. For other values of α, one can obtain bounds for $W^\alpha(C_{10k})$.

Observe that

$$\sum_{j=10}^{2k-1} j^\alpha W_j(C_{10k}) = \sum_{j=10}^{2k-1} j^\alpha(50k-25j) = 50k\sum_{j=10}^{2k-1} j^\alpha - 25\sum_{j=10}^{2k-1} j^{\alpha+1}.$$

For any real number $\beta \neq 0$, the function $f(x) = x^\beta$ is monotonic on its domain. If f is increasing, then for integers a and b with $1 < a < b$, we have

$$\int_{a-1}^{b} f(x)dx < \sum_{i=a}^{b} f(i) < \int_{a}^{b+1} f(x)dx. \tag{4}$$

If f decreases, the inequalities in (4) are reversed. Using the notation $\int_a^b f(x)\,dx = [F(x)]_a^b$, we derive the following result from inequalities in (4).

Theorem 8. *Let* $\alpha \in \mathbb{R} \setminus \{0,1\}$. *Denote* $W_9^\alpha = \sum_{j=1}^{9} j^\alpha \cdot W_j(C_{10k})$. *We* *have*

$$W_9^\alpha + L < W^\alpha(C_{10k}) < W_9^\alpha + P,$$

where

(a) $L = \frac{50k}{\alpha+1}\Big[x^{\alpha+1}\Big]_{10}^{2k} - \frac{25}{\alpha+2}\Big[x^{\alpha+2}\Big]_{9}^{2k-1}$ *and* $P = \frac{50k}{\alpha+1}\Big[x^{\alpha+1}\Big]_{9}^{2k-1} - \frac{25}{\alpha+2}\Big[x^{\alpha+2}\Big]_{10}^{2k}$ *if* $\alpha < 0$ *and* $\alpha \notin \{-1,-2\}$*;*

(b) $L = \frac{50k}{\alpha+1}\Big[x^{\alpha+1}\Big]_{9}^{2k-1} - \frac{25}{\alpha+2}\Big[x^{\alpha+2}\Big]_{9}^{2k-1}$ *and* $P = \frac{50k}{\alpha+1}\Big[x^{\alpha+1}\Big]_{10}^{2k} - \frac{25}{\alpha+2}\Big[x^{\alpha+2}\Big]_{10}^{2k}$ *if* $0 < \alpha < 1$*;*

(c) $L = \frac{50k}{\alpha+1}\Big[x^{\alpha+1}\Big]_{9}^{2k-1} - \frac{25}{\alpha+2}\Big[x^{\alpha+2}\Big]_{10}^{2k}$ *and* $P = \frac{50k}{\alpha+1}\Big[x^{\alpha+1}\Big]_{10}^{2k} - \frac{25}{\alpha+2}\Big[x^{\alpha+2}\Big]_{9}^{2k-1}$ *if* $1 < \alpha$*;*

(d) $L = 50k\Big[\ln(x)\Big]_{10}^{2k} - 50k + 250$ *and* $P = 50k\Big[\ln(x)\Big]_{9}^{2k-1} - 50k + 250$ *if* $\alpha = -1$*;*

(e) $L = -50k\Big[x^{-1}\Big]_{10}^{2k} - 25\Big[\ln(x)\Big]_{9}^{2k-1}$ *and* $P = -50k\Big[x^{-1}\Big]_{9}^{2k-1} - 25\Big[\ln(x)\Big]_{10}^{2k}$ *if* $\alpha = -2$.

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