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On the distance matrix of an infinite class of fullerene graphs

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Abstract. Let G be a graph. The distance $d(u,v)$ between two vertices u and v of G is the minimum length of the paths connecting them. The aim of this paper is computing the distance matrix of infinite familiy of fullerene graph A_{10n}.

Keywords. distance, distance matrix, fullerene.

1 Introduction

A fullerene is a cubic three connected graph with pentagons and hexagons, see [1,5]. All graphs in this paper are simple and connected. The vertex and edge sets of graph G are denoted by $V(G)$ and $E(G)$, respectively. If $x,y \in V(G)$ be two arbitrary vertices of G, then the distance $d(x,y)$ between x and y is defined as the length of the minimum path connecting them. The matrix $[d_{ij}]$ consisting of all distances between vertices of a graph G is known as the distance matrix. The Wiener index is a useful number associated with the structure of a molecule is defined as:

$$W(G) = \frac{1}{2} \sum_{x,y \in V(G)} d(x,y),$$

see [2–4, 6]. Here, we compute the distance matrix of the fullerene graph A_{10n} depicted in Figure 1.

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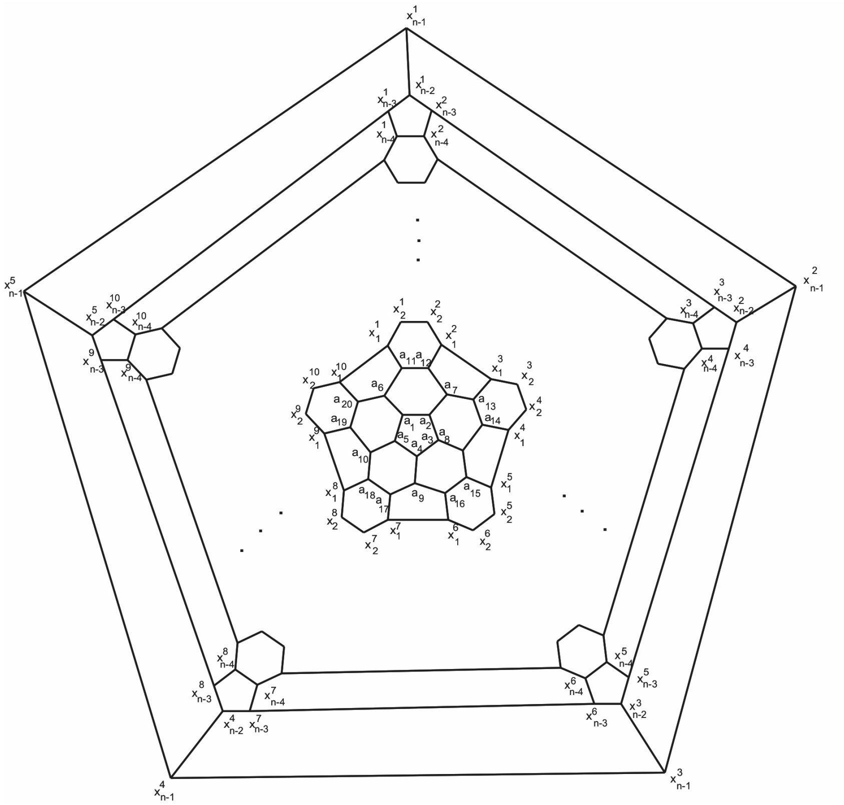

Figure 1. The fullerene graph A_{10n}.

2 Main Results

A zig−zag nanotube with m rows and n columns of hexagons is denoted by $NT(m,n)$, as shown in Figure 2. By combining a nanotube $NT(10,n)$ with two copies of cap B (Figure 3) as shown in Figure 4, the resulted graph is a fullerene, which has $10n$ vertices and exactly $5n-10$ hexagonal faces denoted by A_{10n}, see Figure 1. For computing the distance matrix of A_{10n}, first we compute the distance between two arbitary vertices of nanotube $NT(10,n)$. To do this, we can divide the set of vertices of $NT(10,n)$ to $n-4$ subsets as shown in Figure 1. The vertices of the i-th layer $(1 \leq i \leq n-4)$ are labled by $x_i^1, \cdots, x_i^{10}$.

Here, we determine the distance matrix of zig−zag nanotube $NT(m,n)$, where $m = 10$. Let $1 \leq i, r \leq n$ and $1 \leq j \leq 10$. One can see that the path $x_i^j \rightarrow x_{i+1}^j \rightarrow \cdots \rightarrow x_r^j$ is the shortest path between x_i^j and x_r^j. This yields that $d(x_i^j, x_r^j) = |r-i|$. Also we can see that if $1 \leq i \leq n-3$, then

$$d(x_i^j, x_r^{j+1}) = |r-i| + 1, \tag{1}$$

where $i \neq r$. It is clear if we suppose that j is odd, then $d(x_i^j, x_i^{j+1}) = 3$ if i is odd, and $d(x_i^j, x_i^{j+1}) = 1$, otherwise. Now suppose that j is even. Then, $d(x_i^j, x_i^{j+1}) = 1$ if i is odd, and $d(x_i^j, x_i^{j+1}) = 3$, otherwise. Note that, it is enough to compute the distance between vertices of each $x_r^j (j \neq 1, j \leq 6)$ with the vertices of x_i^1 .

First, we report the distance between some vertices x_r^j and x_r^1 in Tables 1 and 2.

Table 1. Distances between vertices x_r^j and x_r^1.

j	r	$d(x_r^j, x_r^1)$	The shortest path
3	even, $2 \leq r \leq n-4$	4	$x_r^3 \to x_{r-1}^3 \to x_{r-1}^2 \to x_r^2 \to x_r^1$
3	odd, $1 \leq r \leq n-5$	4	$x_r^3 \to x_r^2 \to x_{r+1}^2 \to x_{r+1}^1 \to x_r^1$
4	even, $2 \leq r \leq n-4$	5	$x_r^4 \to x_r^3 \to x_{r-1}^3 \to x_{r-1}^2 \to x_r^2 \to x_r^1$
4	odd, $3 \leq r \leq n-5$	7	$x_r^4 \to x_{r-1}^4 \to x_{r-1}^3 \to x_{r-2}^3 \to x_{r-2}^2 \to x_{r-1}^2 \to x_{r-1}^1 \to x_r^1$
5	even, $2 \leq r \leq n-6$	8	$x_r^5 \to x_{r+1}^5 \to x_{r+1}^4 \to x_{r+2}^4 \to x_{r+2}^3 \to x_{r+1}^3 \to x_{r+1}^2 \to x_r^2 \to x_r^1$
5	odd, $3 \leq r \leq n-5$	8	$x_r^5 \to x_r^4 \to x_{r+1}^4 \to x_{r+1}^3 \to x_r^3 \to x_r^2 \to x_{r+1}^2 \to x_{r+1}^1 \to x_r^1$
6	even, $2 \leq r \leq n-6$	9	$x_r^6 \to x_r^5 \to x_{r-1}^5 \to x_{r-1}^4 \to x_r^4 \to x_r^3 \to x_{r-1}^3 \to x_{r-1}^2 \to x_r^2 \to x_r^1$
6	odd, $3 \leq r \leq n-5$	9	$x_r^6 \to x_r^7 \to x_{r+1}^7 \to x_{r+1}^8 \to x_r^8 \to x_r^9 \to x_{r+1}^9 \to x_{r+1}^{10} \to x_r^{10} \to x_r^1$

Table 2. Distances between vertices x_r^j and x_r^1.

Vertices	$d(x,y)$	Vertices	$d(x,y)$
(x_{n-3}^1, x_{n-3}^2)	2	(x_{n-3}^1, x_{n-3}^5)	6
(x_{n-3}^1, x_{n-3}^3)	3	(x_1^1, x_1^5)	9
(x_{n-2}^1, x_{n-2}^2)	3	(x_{n-2}^1, x_{n-2}^3)	4
(x_1^1, x_1^4)	6	(x_{n-4}^1, x_{n-4}^6)	8
(x_{n-1}^1, x_{n-1}^2)	1	(x_{n-3}^1, x_{n-3}^6)	6
(x_{n-3}^1, x_{n-3}^4)	5	(x_{n-1}^1, x_{n-1}^3)	2
(x_{n-2}^1, x_{n-2}^2)	3	(x_1^1, x_1^6)	8
(x_{n-4}^1, x_{n-4}^5)	7		

• Let $j = 3$. We find the distance between the vertices x_r^3 and x_i^1. First, suppose that r is even. We have two following cases:

Case 1. Let $r < i$, $2 \leq r \leq n-6$ and $1 \leq i \leq n-3$. The path $x_r^3 \to x_{r+1}^3 \to x_{r+1}^2 \to x_i^1$ is the shortest path between vertices x_r^3 and x_i^1. So by using Eq.(1) and next argument, we conclude that if $r+1 = i$, then $d(x_r^3, x_i^1) = 5$ and otherwise

$$d(x_r^j, x_i^1) = 3 + |(r+1) - i|.$$

Let $2 \leq r \leq n-4$. If $i = n-2$, by regarding to the last path we have $d(x_r^3, x_{n-2}^1) = 2 + |r + 1 - i|$.

If $i = n-1$, the path $x_r^3 \to x_{n-2}^2 \to x_{n-1}^1$ is the shortest path and so $d(x_r^3, x_{n-1}^1) = 1 + |i - r|$.

Case 2. Let $r > i$, $2 \le r \le n-4$ and $1 \le i \le n-5$. The path $x_r^3 \to x_{r-1}^3 \to x_{r-1}^2 \to x_i^1$ is the shortest path between vertices x_r^3 and x_i^1. So, if $r - 1 = i$, then $d(x_r^3, x_i^1) = 5$ and otherwise

$$d(x_r^3, x_i^1) = 3 + |(r-1) - i|.$$

Now, suppose that r is odd. Again two following cases hold:

Case 1. Let $r < i$, $1 \le r \le n-5$ and $1 \le i \le n-3$. The path $x_r^3 \to x_r^2 \to x_i^1$ is the shortest path between vertices x_r^3 and x_i^1. So

$$d(x_r^3, x_i^1) = 2 + |r - i|.$$

Let $1 \le r \le n-3$. Similarly, if $i = n-2$, then $d(x_r^3, x_{n-2}^1) = 1 + |r - i|$. If $i = n-1$, by regarding the path $x_r^3 \to x_{n-1}^2 \to x_{n-1}^1$ we have $d(x_r^3, x_{n-1}^1) = 1 + |r - i|$.

Case 2. Let $r > i$ and $1 \le r, i \le n-3$. Similar to the last case we have

$$d(x_r^3, x_i^1) = 2 + |r - i|.$$

• Let $j = 4$. Here, we find the distance between the vertices x_r^4 and x_i^1. First, suppose that r is even. We have two following cases:

Case 1. Let $r < i$, $2 \le r \le n-6$ and $1 \le i \le n-3$. The path $x_r^4 \to x_r^3 \to x_{r+1}^3 \to x_{r+1}^2 \to x_i^1$ is the shortest path between vertices x_r^4 and x_i^1. So, we conclude that if $r + 1 = i$, then $d(x_r^3, x_i^1) = 6$ and otherwise

$$d(x_r^4, x_i^1) = 4 + |(r+1) - i|.$$

Let $2 \le r \le n-4$. Similarly, if $i = n-2$, then $d(x_r^4, x_{n-2}^1) = 3 + |r + 1 - i|$ and if $i = n-1$, by considering the path $x_r^4 \to x_{n-1}^2 \to x_{n-1}^1$ then $d(x_r^4, x_{n-1}^1) = 1 + |i - r|$.

Case 2. Let $r > i$, $2 \le r \le n-4$ and $1 \le i \le n-5$. The path $x_r^4 \to x_r^3 \to x_{r-1}^3 \to x_{r-1}^2 \to x_i^1$ is the shortest path between vertices x_r^4 and x_i^1. So, if $r - 1 = i$, then $d(x_r^4, x_i^1) = 6$ and otherwise

$$d(x_r^4, x_i^1) = 4 + |(r-1) - i|.$$

If $r = n-2$ and $1 \le i \le n-4$, the path $x_r^2 \to x_{r-1}^3 \to x_{r-1}^2 \to x_{r-2}^2 \to x_{r-2}^1 \to x_i^1$ is the shortest path between vertices x_{n-2}^2 and x_i^1. So we have

$$d(x_{n-2}^2, x_i^1) = 4 + |r - 2 - i|.$$

If $r = n-1$, $1 \le i \le n-3$, the path $x_r^2 \to x_r^1 \to x_{r-1}^1 \to x_{r-2}^1 \to x_i^1$ is the shortest path between vertices x_{n-1}^2 and x_i^1. So we have

$$d(x_{n-1}^2, x_i^1) = 3 + |r - 2 - i|.$$

Now, suppose that r is odd. We have two following cases:

Case 1. Let $r < i$, $1 \leq r \leq n-7$ and $1 \leq i \leq n-3$. The path $x_r^4 \to x_{r+1}^4 \to x_{r+1}^3 \to x_{r+2}^3 \to x_{r+2}^2 \to x_i^1$ is the shortest path between vertices x_r^4 and x_i^1. So, we conclude that if $r+2 = i$, then $d(x_r^4, x_i^1) = 7$ and otherwise

$$d(x_r^4, x_i^1) = 5 + |(r+2) - i|.$$

Let $1 \leq r \leq n-5$. If $i = n-2$, then $d(x_r^4, x_{n-2}^1) = 4 + |r+2-i|$ and if $i = n-1$, then $d(x_r^4, x_{n-1}^1) = 1 + |i-r|$.

Case 2. Let $r > i$, $3 \leq r \leq n-5$ and $1 \leq i \leq n-6$. The path $x_r^4 \to x_{r-1}^4 \to x_{r-1}^3 \to x_{r-2}^3 \to x_{r-2}^2 \to x_i^1$ is the shortest path between vertices x_r^4 and x_i^1. So, we conclude that if $r-2 = i$, then $d(x_r^4, x_i^1) = 7$ and otherwise

$$d(x_r^4, x_i^1) = 5 + |(r-2) - i|.$$

Similar to the last case if $r = n-3$ and $1 \leq i \leq n-6$ then for $r-2 = i$, $d(x_r^4, x_i^1) = 7$ and otherwise

$$d(x_r^4, x_i^1) = 5 + |(r-2) - i|.$$

• Let $j = 5$. We find the distance between the vertices x_r^5 and x_i^1. First, suppose that r is even. We have two following cases:

Case 1. Let $r < i$, $2 \leq r \leq n-8$ and $1 \leq i \leq n-3$. The path $x_r^5 \to x_{r+1}^5 \to x_{r+1}^4 \to x_{r+2}^4 \to x_{r+2}^3 \to x_{r+3}^3 \to x_{r+3}^2 \to x_i^1$ is the shortest path between vertices x_r^5 and x_i^1. So, we conclude that if $r+3 = i$, then $d(x_r^5, x_i^1) = 9$ and otherwise

$$d(x_r^5, x_i^1) = 7 + |(r+3) - i|.$$

If $i = n-2$ and $2 \leq r \leq n-6$, then $d(x_r^5, x_{n-2}^1) = 6 + |r+3-i|$ and if $i = n-1$ and $2 \leq r \leq n-6$, then $d(x_r^5, x_{n-1}^1) = 2 + |r-i|$.

Case 2. Let $r > i$ and $4 \leq r \leq n-6$ and $1 \leq i \leq n-7$. The path $x_r^5 \to x_{r-1}^5 \to x_{r-1}^4 \to x_{r-2}^4 \to x_{r-2}^3 \to x_{r-3}^3 \to x_{r-3}^2 \to x_i^1$ is the shortest path between vertices x_r^5 and x_i^1. So, we conclude that if $r-3 = i$, then $d(x_r^5, x_i^1) = 9$ and otherwise

$$d(x_r^5, x_i^1) = 7 + |(r-3) - i|.$$

If $r = n-4$ and $1 \leq i \leq n-6$, then similar to the last case if $r-3 = i$, then $d(x_r^5, x_i^1) = 9$ and otherwise we have

$$d(x_r^5, x_i^1) = 7 + |(r-3) - i|.$$

Now, suppose that r is odd. We have two following cases:

Case 1. Let $r < i$, $1 \le r \le n-7$ and $1 \le i \le n-3$. The path $x_r^5 \to x_r^4 \to x_{r+1}^4 \to x_{r+1}^3 \to x_{r+2}^3 \to x_{r+2}^2 \to x_i^1$ is the shortest path between vertices x_r^5 and x_i^1. So, we conclude that if $r+2 = i$, then $d(x_r^5, x_i^1) = 8$ and otherwise

$$d(x_r^5, x_i^1) = 6 + |(r+2) - i|.$$

Let $1 \le r \le n-5$. If $i = n-2$, then $d(x_r^5, x_{n-2}^1) = 5 + |r+2-i|$ and if $i = n-1$, then $d(x_r^5, x_{n-1}^1) = 2 + |r-i|$.

Case 2. Let $r > i$, $3 \le r \le n-5$ and $1 \le i \le n-6$. The path $x_r^5 \to x_r^4 \to x_{r-1}^4 \to x_{r-1}^3 \to x_{r-2}^3 \to x_{r-2}^2 \to x_i^1$ is the shortest path between vertices x_r^5 and x_i^1. So, we conclude that if $r-2 = i$, then $d(x_r^5, x_i^1) = 8$ and otherwise

$$d(x_r^5, x_i^1) = 6 + |(r-2) - i|.$$

If $r = n-3$ and $1 \le i \le n-6$, then similar to the last case if $r-2 = i$, then $d(x_r^5, x_i^1) = 8$ and otherwise

$$d(x_r^5, x_i^1) = 6 + |(r-2) - i|.$$

• Let $j = 6$. We find the distance between the vertices x_r^6 and x_i^1. First, suppose that r is even. We have two following cases:

Case 1. Let $r < i$, $2 \le r \le n-4$ and $1 \le i \le n-3$. The path $x_r^6 \to x_r^5 \to x_{r+1}^5 \to x_{r+1}^4 \to x_{r+2}^4 \to x_{r+2}^3 \to x_{r+3}^3 \to x_{r+3}^2 \to x_i^1$ is the shortest path between vertices x_r^6 and x_i^1. So, we conclude that if $r+3 = i$, then $d(x_r^6, x_i^1) = 10$ and otherwise

$$d(x_r^6, x_i^1) = 8 + |(r+3) - i|.$$

Let $2 \le r \le n-6$. If $i = n-2$, by regarding the path $x_r^6 \to x_{n-1}^3 \to x_{n-1}^2 \to x_{n-1}^1 \to x_{n-2}^1$ we have $d(x_r^6, x_{n-2}^1) = 3 + |i+1-r|$ and if $i = n-1$, then $d(x_r^6, x_{n-1}^1) = 2 + |i-r|$.

Case 2. Let $r > i$, $4 \le r \le n-6$ and $1 \le i \le n-7$. The path $x_r^6 \to x_r^5 \to x_{r-1}^5 \to x_{r-1}^4 \to x_{r-2}^4 \to x_{r-2}^3 \to x_{r-3}^3 \to x_{r-3}^2 \to x_i^1$ is the shortest path between vertices x_r^6 and x_i^1. So, we conclude that if $r-3 = i$, then $d(x_r^6, x_i^1) = 10$ and otherwise

$$d(x_r^6, x_i^1) = 8 + |(r-3) - i|.$$

Similarly, if $r = n-4$, $1 \le i \le n-6$, for $r-3 = i$, $d(x_r^6, x_i^1) = 10$ and otherwise

$$d(x_r^6, x_i^1) = 8 + |(r-3) - i|.$$

if $r = n-2$ and $1 \le i \le n-3$, by considering the path $x_{n-2}^3 \to x_{n-1}^3 \to x_{n-1}^2 \to x_{n-1}^1 \to x_i^1$ we have

$$d(x_{n-2}^3, x_i^1) = 3 + |(r+1) - i|.$$

Now, suppose that r is odd. Two following cases hold:

Case 1. Let $r < i$, $3 \leq r \leq n-7$ and $3 \leq i \leq n-3$. Suppose $r+4 > i$, the path $x_r^6 \to x_r^7 \to x_{r+1}^7 \to x_{r+1}^8 \to x_{r+2}^8 \to x_{r+2}^9 \to x_{r+3}^9 \to x_{r+3}^{10} \to x_{r+2}^{10} \to x_{r+2}^1 \to x_i^1$ is the shortest path between vertices x_r^6 and x_i^1. This yields that

$$d(x_r^6, x_i^1) = 9 + |(r+2) - i|.$$

If $r+4 = i$, then $d(x_r^6, x_i^1) = 9$. Suppose $r+4 < i$, the path $x_r^6 \to x_r^7 \to x_{r+1}^7 \to x_{r+1}^8 \to x_{r+2}^8 \to x_{r+2}^9 \to x_{r+3}^9 \to x_{r+3}^{10} \to x_{r+4}^{10} \to x_{r+4}^1 \to x_i^1$ is the shortest path between vertices x_r^6 and x_i^1. This means that

$$d(x_r^6, x_i^1) = 9 + |(r+4) - i|.$$

Let $r = 1$, $i > 5$ and $i \neq n-1$. So

$$d(x_1^6, x_i^1) = 9 + |(r+4) - i|.$$

Let $1 \leq r \leq n-7$. If $i = n-2$, by regarding the path $x_r^6 \to x_{r+1}^6 \to x_{r+1}^5 \to x_{r+2}^5 \to x_{r+2}^4 \to x_{r+3}^4 \to x_{r+3}^3 \to x_{r+4}^3 \to x_{r+4}^2 \to x_i^1$ we have $d(x_r^6, x_{n-2}^1) = 8 + |r+4-i|$ and if $i = n-1$, then $d(x_r^6, x_{n-1}^1) = 2 + |i-r|$.

Case 2. Let $r > i$, $3 \leq r \leq n-5$ and $1 \leq i \leq n-6$. Suppose $r-3 \geq i$, the path $x_r^6 \to x_r^7 \to x_{r-1}^7 \to x_{r-1}^8 \to x_{r-2}^8 \to x_{r-2}^9 \to x_{r-3}^9 \to x_{r-3}^{10} \to x_{r-4}^{10} \to x_{r-4}^1 \to x_i^1$ is the shortest path between vertices x_r^6 and x_i^1. So we have

$$d(x_r^6, x_i^1) = 9 + |(r-4) - i|.$$

if $i = r-2$, then $d(x_r^6, x_i^1) = 9$ and if $i = r-1$, then $d(x_r^6, x_i^1) = 10$. Similarly, if $r = n-3$, $1 \leq i \leq n-6$ and $r-3 \geq i$, then $d(x_r^6, x_i^1) = 9 + |(r-4) - i|$. If $i = r-2$, then $d(x_r^6, x_i^1) = 9$ and if $i = r-1$, then $d(x_r^6, x_i^1) = 10$. If $r = n-1$ and $1 \leq i \leq n-2$, then $d(x_{n-1}^3, x_i^1) = r+2-i$. The other cases are reported in the Table 3.

Table 3. Vertices and distances between them.

Vertices	$d(x,y)$	Vertices	$d(x,y)$	Vertices	$d(x,y)$
(x^3_{n-3}, x^1_{n-2})	2	(x^5_{n-4}, x^1_{n-2})	6	(x^6_{n-4}, x^1_{n-5})	9
(x^3_{n-3}, x^1_{n-1})	3	(x^5_{n-4}, x^1_{n-1})	5	(x^6_2, x^1_1)	9
(x^1_{n-4}, x^1_{n-3})	4	(x^5_{n-4}, x^1_{n-5})	8	(x^6_1, x^1_1)	8
(x^4_{n-4}, x^1_{n-3})	5	(x^5_2, x^1_1)	8	(x^6_1, x^1_2)	9
(x^2_{n-2}, x^1_{n-1})	2	(x^5_{n-5}, x^1_{n-4})	7	(x^6_1, x^1_3)	9
(x^2_{n-2}, x^1_{n-3})	4	(x^5_{n-5}, x^1_{n-3})	7	(x^6_1, x^1_4)	11
(x^2_{n-1}, x^1_{n-2})	2	(x^5_{n-3}, x^1_{n-2})	5	(x^6_1, x^1_5)	9
(x^4_{n-5}, x^1_{n-4})	6	(x^5_{n-3}, x^1_{n-1})	4	(x^6_{n-3}, x^1_{n-2})	5
(x^4_{n-5}, x^1_{n-3})	6	(x^5_{n-3}, x^1_{n-5})	7	(x^6_{n-5}, x^1_{n-2})	7
(x^4_{n-3}, x^1_{n-2})	4	(x^5_{n-3}, x^1_{n-4})	6	(x^6_{n-5}, x^1_{n-4})	9
(x^4_{n-3}, x^1_{n-1})	3	(x^6_{n-4}, x^1_{n-3})	7	(x^6_{n-5}, x^1_{n-3})	8
(x^4_{n-3}, x^1_{n-5})	6	(x^6_{n-4}, x^1_{n-2})	6	(x^6_{n-5}, x^1_{n-2})	7
(x^4_{n-3}, x^1_{n-4})	5	(x^6_{n-4}, x^1_{n-1})	5	(x^6_{n-5}, x^1_{n-1})	6
(x^5_{n-6}, x^1_{n-5})	9	(x^6_{n-6}, x^1_{n-5})	10	(x^6_{n-3}, x^1_{n-2})	5
(x^5_{n-6}, x^1_{n-4})	8	(x^6_{n-6}, x^1_{n-4})	9	(x^6_{n-3}, x^1_{n-1})	4
(x^5_{n-6}, x^1_{n-3})	8	(x^6_{n-6}, x^1_{n-3})	9	(x^6_{n-3}, x^1_{n-5})	8
(x^5_{n-4}, x^1_{n-3})	7	(x^3_{n-2}, x^1_{n-1})	3	(x^6_{n-3}, x^1_{n-4})	7

Now, we compute the distance matrix of vertices of the inner cap with the vertices of the tube and the vertices of the outer cap. It is enough to compute them for the vertices a_1, a_6, a_{11}. All of them are reported in Table 4 and 5. Finally, the matrices A and B are distance matrices of the inner and the outer cap, respectively.

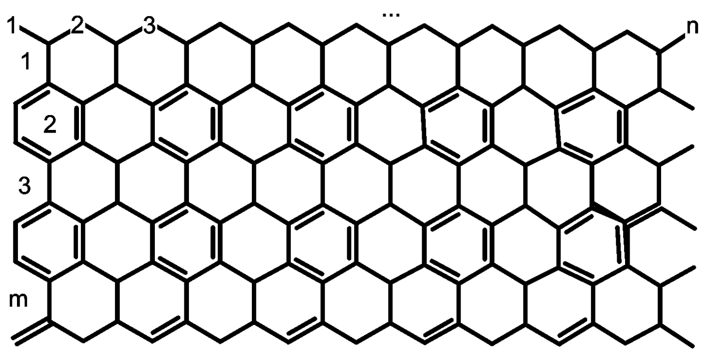

Figure 2. 2- D graph of zig−zag nanotube $NT(5,n)$, for $m = 5$, $n = 10$.

Table 4. Distances between the vertex a_1 with the vertices of the zig−zag nanotube $NT(10,n)$ and the vertices of the outer cap.

Vertices	$d(x,y)$	The shortest path between them
(a_1,x_i^1)	$i+2$	$a_1 \to a_6 \to a_{11} \to x_1^1 \to \cdots \to x_i^1$
(a_1,x_i^2)	$i+3$	$a_1 \to a_2 \to a_7 \to a_{12} \to x_1^2 \to \cdots \to x_i^2$
(a_1,x_i^3)	$i+3$	$a_1 \to a_2 \to a_7 \to a_{13} \to x_1^3 \to \cdots \to x_i^3$
(a_1,x_i^4)	$i+4$	$a_1 \to a_2 \to a_7 \to a_{13} \to a_{14} \to x_1^4 \to \cdots \to x_i^4$
(a_1,x_i^5)	$i+4$	$a_1 \to a_2 \to a_3 \to a_8 \to a_{15} \to x_1^5 \to \cdots \to x_i^5$
(a_1,x_i^5)	$i+4$	$a_1 \to a_5 \to a_4 \to a_9 \to a_{16} \to x_1^6 \to \cdots \to x_i^6$
(a_1,x_{n-3}^1)	$n-1$	$a_1 \to a_6 \to a_{11} \to x_1^1 \to \cdots \to x_{n-3}^1$
(a_1,x_{n-3}^2)	n	$a_1 \to a_2 \to a_7 \to a_{12} \to x_1^2 \to \cdots \to x_{n-3}^2$
(a_1,x_{n-2}^1)	n	$a_1 \to a_6 \to a_{11} \to x_1^1 \to \cdots \to x_{n-2}^1$
(a_1,x_{n-1}^1)	$n+1$	$a_1 \to a_6 \to a_{11} \to x_1^1 \to \cdots \to x_{n-1}^1$
(a_1,x_{n-3}^3)	n	$a_1 \to a_2 \to a_7 \to a_{13} \to x_1^3 \to \cdots \to x_{n-3}^3$
(a_1,x_{n-3}^4)	$n+1$	$a_1 \to a_2 \to a_7 \to a_{13} \to a_{14} \to x_1^4 \to \cdots \to x_{n-3}^4$
(a_1,x_{n-2}^2)	$n+1$	$a_1 \to a_2 \to a_7 \to a_{13} \to x_1^3 \to \cdots \to x_{n-2}^2$
(a_1,x_{n-1}^2)	$n+2$	$a_1 \to a_2 \to a_7 \to a_{13} \to x_1^3 \to \cdots \to x_{n-1}^1$
(a_1,x_{n-3}^5)	$n+1$	$a_1 \to a_2 \to a_3 \to a_8 \to a_{15} \to x_1^5 \to \cdots \to x_{n-3}^5$
(a_1,x_{n-3}^6)	$n+1$	$a_1 \to a_2 \to a_3 \to a_8 \to a_{15} \to x_1^5 \to \cdots \to x_{n-3}^6$
(a_1,x_{n-2}^3)	$n+2$	$a_1 \to a_2 \to a_3 \to a_8 \to a_{15} \to x_1^5 \to \cdots \to x_{n-2}^3$
(a_1,x_{n-1}^3)	$n+3$	$a_1 \to a_2 \to a_3 \to a_8 \to a_{15} \to x_1^5 \to \cdots \to x_{n-1}^3$

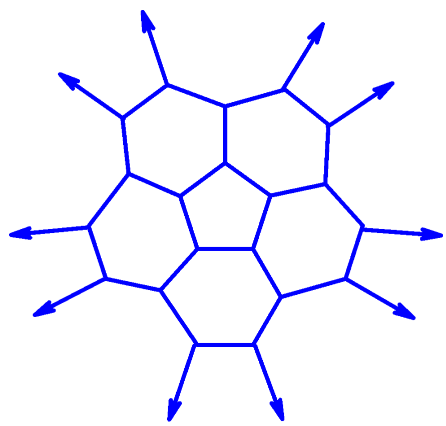

Figure 3. Cap B.

Table 5. Distances between the vertices a_6 and a_{11} with the vertices of the zig−zag nanotube $NT(10,n)$ and the vertices of the outer cap.

Vertices	$d(x,y)$	Vertices	$d(x,y)$
(a_6,x_i^1)	$i+1$	(a_{11},x_i^1)	i
(a_6,x_i^2)	$i+2$	(a_{11},x_i^2)	$i+1$
(a_6,x_i^3)	$i+3$	(a_{11},x_i^3)	$i+2$
$(a_6,x_i^4) i \neq 1$	$i+4$	$(a_{11},x_i^4) i \neq 1,2$	$i+3$
(a_6,x_1^4)	6	(a_{11},x_1^4)	5
(a_6,x_i^5)	$i+5$	(a_{11},x_2^4)	5
(a_6,x_i^6)	$i+5$	$(a_{11},x_i^5) i \neq 1,2$	$i+4$
(a_6,x_{n-3}^1)	$n-2$	(a_{11},x_1^5)	6
(a_6,x_{n-3}^2)	$n-1$	(a_{11},x_2^5)	6
(a_6,x_{n-2}^1)	$n-1$	$(a_{11},x_i^6) i \neq 1,2,3$	$i+5$
(a_6,x_{n-1}^1)	n	(a_{11},x_1^6)	7
(a_6,x_{n-3}^3)	n	(a_{11},x_2^6)	8
(a_6,x_{n-3}^4)	$n+1$	(a_{11},x_3^6)	9
(a_6,x_{n-2}^2)	$n+1$	(a_{11},x_{n-3}^1)	$n-3$
(a_6,x_{n-1}^2)	$n+1$	(a_{11},x_{n-3}^2)	$n-2$
(a_6,x_{n-3}^5)	$n+2$	(a_{11},x_{n-2}^1)	$n-2$
(a_6,x_{n-3}^6)	$n+2$	(a_{11},x_{n-1}^1)	$n-1$
(a_6,x_{n-2}^3)	$n+3$	(a_{11},x_{n-3}^3)	$n-1$
(a_6,x_{n-1}^3)	$n+2$	(a_{11},x_{n-3}^4)	n
-	-	(a_{11},x_{n-2}^2)	n
-	-	(a_{11},x_{n-1}^2)	n
-	-	(a_{11},x_{n-3}^5)	$n+1$
-	-	(a_{11},x_{n-3}^6)	$n+2$
-	-	(a_{11},x_{n-2}^3)	$n+2$
-	-	(a_{11},x_{n-1}^3)	$n+1$

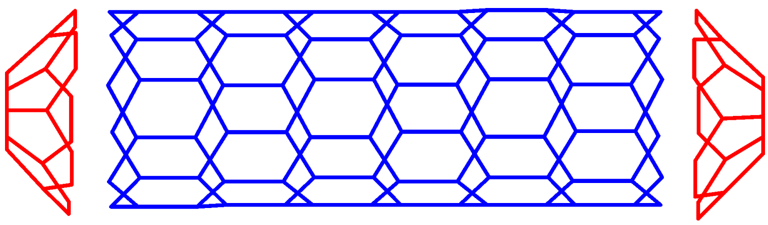

Figure 4. Fullerene A_{10n} constructed by combining two copies of B and the zig-zag nanotube $NT(5,n)$.

$$A=\begin{pmatrix}
0&1&2&2&1&1&2&3&3&2&2&3&3&4&4&4&4&3&3&2\\
1&0&1&2&2&2&1&2&3&3&3&2&2&3&3&4&4&4&4&3\\
2&1&0&1&2&3&2&1&2&3&4&3&3&2&2&3&3&4&4&4\\
2&2&1&0&1&3&3&2&1&2&4&4&4&3&3&2&2&3&3&4\\
1&2&2&1&0&2&3&3&2&1&3&4&4&4&4&3&3&2&2&3\\
1&2&3&3&2&0&3&4&4&3&1&2&4&5&5&5&5&4&2&1\\
2&1&2&3&3&3&0&3&4&4&2&1&1&2&4&5&5&5&5&4\\
3&2&1&2&3&4&3&0&3&4&5&4&2&1&1&2&4&5&5&5\\
3&3&2&1&2&4&4&3&0&3&5&5&5&4&2&1&1&2&4&5\\
2&3&3&2&1&3&4&4&3&0&4&5&5&5&5&4&2&1&1&2\\
2&3&4&4&3&1&2&5&5&4&0&1&3&4&6&6&6&5&3&2\\
3&2&3&4&4&2&1&4&5&5&1&0&2&3&5&6&6&6&4&3\\
3&2&3&4&4&4&1&2&5&5&3&2&0&1&3&4&6&6&6&5\\
4&3&2&3&4&5&2&1&4&5&4&3&1&0&2&3&5&6&6&6\\
4&3&2&3&4&5&4&1&2&5&6&5&3&2&0&1&3&4&6&6\\
4&4&3&2&3&5&5&2&1&4&6&6&4&3&1&0&2&3&5&6\\
4&4&3&2&3&5&5&4&1&2&6&6&6&5&3&2&0&1&3&4\\
3&4&4&3&2&4&5&5&2&1&5&6&6&6&4&3&1&0&2&3\\
3&4&4&3&2&2&5&5&4&1&3&4&6&6&6&5&3&2&0&1\\
2&3&4&4&3&1&4&5&5&2&2&3&5&6&6&6&4&3&1&0
\end{pmatrix}$$

$$B=\begin{pmatrix}
0&2&3&5&6&6&6&4&3&1&1&4&5&5&2&2&3&4&4&3\\
2&0&1&3&4&6&6&6&5&3&1&2&5&5&4&2&3&4&4&3\\
3&1&0&2&3&5&6&6&6&4&2&1&4&5&5&3&2&3&4&4\\
5&3&2&0&1&3&4&6&6&6&4&1&2&5&5&3&2&3&4&4\\
6&4&3&1&0&2&3&5&6&6&5&2&1&4&5&4&3&2&3&4\\
6&6&5&3&2&0&1&3&4&6&5&4&1&2&5&4&3&2&3&4\\
6&6&6&4&3&1&0&2&3&5&5&5&2&1&4&4&4&3&2&3\\
4&6&6&6&5&3&2&0&1&3&5&5&4&1&2&4&4&3&2&3\\
3&5&6&6&6&4&3&1&0&2&4&5&5&2&1&3&4&4&3&2\\
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4&4&4&4&3&3&2&2&3&3&3&3&2&1&2&2&2&1&0&1\\
3&3&4&4&4&4&3&3&2&2&2&3&3&2&1&1&2&2&1&0
\end{pmatrix}$$

References

[1] P. W. Fowler and D. E. Manolopoulos, An Atlas of Fullerenes, Oxford Univ. Press, Oxford, 1995.
[2] M. Ghorbani and T. Ghorbani, Computing the Wiener index of an infinite class of fullerenes, Studia Ubb Chemia. 58 (2013) 43–50.
[3] M. Ghorbani, Computing Wiener index of C_{24n} fullerenes, J. Comput. Theor. Nanosci. 12 (2015) 1847–1851.
[4] M. Ghorbani and M. Songhori, Computing Wiener index of C_{12n} fullerenes, Ars Combin. 130 (2017) 175–180.
[5] H. W. Kroto, J. E. Fichier and D. E. Cox, The Fullerene, Pergamon Press, Inc, New York, 1993.
[6] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69 (1947) 17–20.