



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 family 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 the graphs in this paper are simple 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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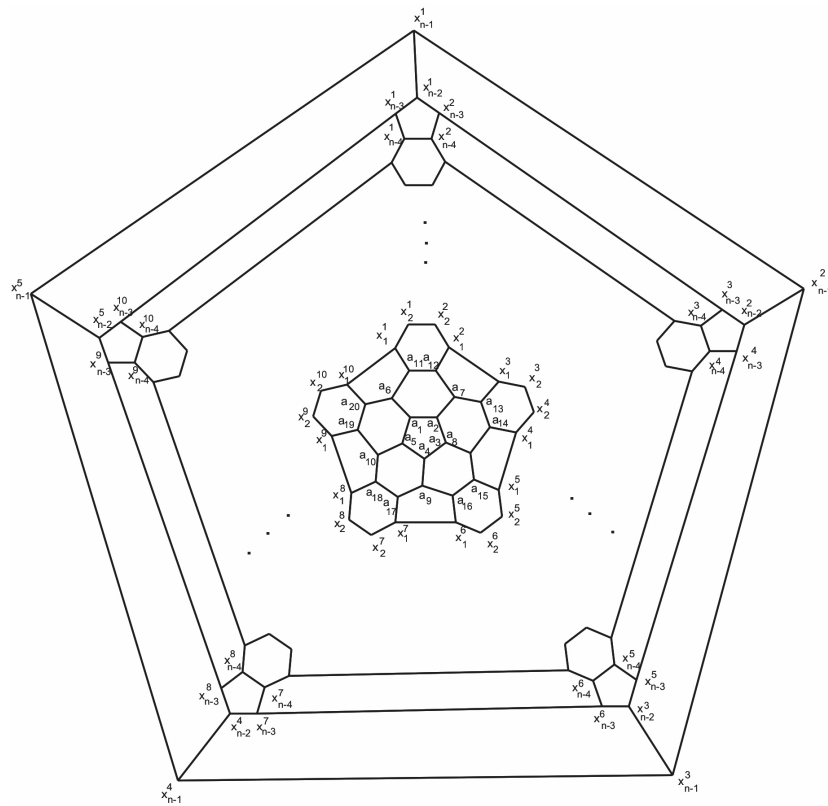


Figure 1. The fullerene graph A_{10n} .

2 Main Results

A zig-zag nanotube with m rows and n columns of hexagons is denoted by $NT(m, n)$, shown in Figure 2. By combining a nanotube $NT(5, n)$ 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} , shown in Figure 1. For computing the distance matrix of A_{10n} , first we compute the distance between two arbitrary vertices of nanotube $NT(5, n)$. To do this, we can divide the set of vertices of $NT(5, n)$ to $n - 4$ subsets as shown in Figure 1. The vertices of the i -th layer ($1 \leq i \leq n - 4$) labeled by x_i^1, \dots, x_i^{10} .

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 $x_i^j \rightarrow x_{i+1}^j \rightarrow \dots \rightarrow x_r^j$ 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 $d(x_i^j, x_r^{j+1}) = 3$ if i is odd and 1, otherwise. Now Suppose that j is even. Then, $d(x_i^j, x_r^{j+1}) = 1$ if i is odd and 3, otherwise. Note that, its 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 Table 1. Other are reported in Table 2.

Table 1.

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

Table 2.

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 cases:

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

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

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

Case 2. Let $r > i$ and Suppose $2 \leq r \leq n - 4$ and $1 \leq i \leq n - 5$. The path $x_r^3 \rightarrow x_{r-1}^3 \rightarrow x_{r-1}^2 \rightarrow x_i^1$ 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 we have

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

Now, suppose that r is odd. Again we have two cases:

Case 1. Let $r < i$ and Suppose $1 \leq r \leq n - 5$ and $1 \leq i \leq n - 3$. The path $x_r^3 \rightarrow x_r^2 \rightarrow x_i^1$ 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 $1 \leq r \leq n - 3$. Similarity, if $i = n - 2$, then $d(x_r^3, x_{n-2}^1) = 1 + |r - i|$. If $i = n - 1$, by regarding the path $x_r^3 \rightarrow x_{n-1}^2 \rightarrow x_{n-1}^1$ we have $d(x_r^3, x_{n-1}^1) = 1 + |r - i|$.

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

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

• Let $j = 4$. We find the distance between the vertices x_r^4 and x_i^1 .

First, suppose that r is even. We have two cases:

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

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

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

Case 2. Let $r > i$ and Suppose $2 \leq r \leq n - 4$ and $1 \leq i \leq n - 5$. The path $x_r^4 \rightarrow x_r^3 \rightarrow x_{r-1}^3 \rightarrow x_{r-1}^2 \rightarrow x_i^1$ 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 we have

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

If $r = n - 2$ and $1 \leq i \leq n - 4$, The path $x_r^2 \rightarrow x_{r-1}^3 \rightarrow x_{r-1}^2 \rightarrow x_{r-2}^2 \rightarrow x_{r-2}^1 \rightarrow x_i^1$ 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 $r = n - 1$ and $1 \leq i \leq n - 3$, The path $x_r^2 \rightarrow x_r^1 \rightarrow x_{r-1}^1 \rightarrow x_{r-2}^1 \rightarrow x_i^1$ 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 cases:

Case 1. Let $r < i$ and $1 \leq r \leq n - 7$ and $1 \leq i \leq n - 3$. The path $x_r^4 \rightarrow x_{r+1}^4 \rightarrow x_{r+1}^3 \rightarrow x_{r+2}^3 \rightarrow x_{r+2}^2 \rightarrow x_i^1$ 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 we have

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

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 $r > i$ and Suppose $3 \leq r \leq n - 5$ and $1 \leq i \leq n - 6$. The path $x_r^4 \rightarrow x_{r-1}^4 \rightarrow x_{r-1}^3 \rightarrow x_{r-2}^3 \rightarrow x_{r-2}^2 \rightarrow x_i^1$ 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 we have

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

Similar to above if $r = n - 3$ and $1 \leq i \leq n - 6$ then if $r - 2 = i$, then $d(x_r^4, x_i^1) = 7$ and otherwise we have $d(x_r^4, x_i^1) = 5 + |(r - 2) - i|$.

• 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 cases:

Case 1. Let $r < i$ and $2 \leq r \leq n - 8$ and $1 \leq i \leq n - 3$. The path $x_r^5 \rightarrow x_{r+1}^5 \rightarrow x_{r+1}^4 \rightarrow x_{r+2}^4 \rightarrow x_{r+2}^3 \rightarrow x_{r+3}^3 \rightarrow x_{r+3}^2 \rightarrow x_i^1$ 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 we have

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

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 $x_r^5 \rightarrow x_{r-1}^5 \rightarrow x_{r-1}^4 \rightarrow x_{r-2}^4 \rightarrow x_{r-2}^3 \rightarrow x_{r-3}^3 \rightarrow x_{r-3}^2 \rightarrow x_i^1$ 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 we have

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

If $r = n - 4$ and $1 \leq i \leq n - 6$, then similar to above 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 cases:

Case 1. Let $r < i$ and $1 \leq r \leq n - 7$ and $1 \leq i \leq n - 3$. The path $x_r^5 \rightarrow x_r^4 \rightarrow x_{r+1}^4 \rightarrow x_{r+1}^3 \rightarrow x_{r+2}^3 \rightarrow x_{r+2}^2 \rightarrow x_i^1$ 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 we have

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

Let $1 \leq r \leq n - 5$. 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 $r > i$ and $3 \leq r \leq n - 5$ and $1 \leq i \leq n - 6$. The path $x_r^5 \rightarrow x_r^4 \rightarrow x_{r-1}^4 \rightarrow x_{r-1}^3 \rightarrow x_{r-2}^3 \rightarrow x_{r-2}^2 \rightarrow x_i^1$ 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 we have

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

If $r = n - 3$ and $1 \leq i \leq n - 6$, then similar to above if $r - 2 = i$, then $d(x_r^5, x_i^1) = 8$ and otherwise we have

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

- 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 cases:

Case 1. Let $r < i$ and $2 \leq r \leq n - 4$ and $1 \leq i \leq n - 3$. The path $x_r^6 \rightarrow x_r^5 \rightarrow x_{r+1}^5 \rightarrow x_{r+1}^4 \rightarrow x_{r+2}^4 \rightarrow x_{r+2}^3 \rightarrow x_{r+3}^3 \rightarrow x_{r+3}^2 \rightarrow x_i^1$ 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 we have

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

Let $2 \leq r \leq n - 6$. If $i = n - 2$, by regarding the path $x_r^6 \rightarrow x_{n-1}^3 \rightarrow x_{n-1}^2 \rightarrow x_{n-1}^1 \rightarrow x_{n-2}^1$ 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 $r > i$ and $4 \leq r \leq n - 6$ and $1 \leq i \leq n - 7$. The path $x_r^6 \rightarrow x_r^5 \rightarrow x_{r-1}^5 \rightarrow x_{r-1}^4 \rightarrow x_{r-2}^4 \rightarrow x_{r-2}^3 \rightarrow x_{r-3}^3 \rightarrow x_{r-3}^2 \rightarrow x_i^1$ 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 we have

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

Similarity, if $r = n - 4$ and $1 \leq i \leq n - 6$, if $r - 3 = i$, then $d(x_r^6, x_i^1) = 10$ and otherwise we have

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

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

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

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

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

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

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

suppose $r + 4 < i$, The path $x_r^6 \rightarrow x_r^7 \rightarrow x_{r+1}^7 \rightarrow x_{r+1}^8 \rightarrow x_{r+2}^8 \rightarrow x_{r+2}^9 \rightarrow x_{r+3}^9 \rightarrow x_{r+3}^{10} \rightarrow x_{r+4}^{10} \rightarrow x_{r+4}^1 \rightarrow x_i^1$ is the shortest path between vertices x_r^6 and x_i^1 . So we have

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

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 $x_r^6 \rightarrow x_{r+1}^6 \rightarrow x_{r+1}^5 \rightarrow x_{r+2}^5 \rightarrow x_{r+2}^4 \rightarrow x_{r+3}^4 \rightarrow x_{r+3}^3 \rightarrow x_{r+4}^3 \rightarrow x_{r+4}^2 \rightarrow x_i^1$ 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 1. Let $r > i$ and $3 \leq r \leq n - 5$ and $1 \leq i \leq n - 6$. suppose $r - 3 \geq i$, The path $x_r^6 \rightarrow x_r^7 \rightarrow x_{r-1}^7 \rightarrow x_{r-1}^8 \rightarrow x_{r-2}^8 \rightarrow x_{r-2}^9 \rightarrow x_{r-3}^9 \rightarrow x_{r-3}^{10} \rightarrow x_{r-4}^{10} \rightarrow x_{r-4}^1 \rightarrow x_i^1$ 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 $d(x_r^6, x_i^1) = 10$.

Similarity, if $r = n - 3, 1 \leq i \leq n - 6$ and $r - 3 \geq i$, then $d(x_r^6, x_i^1) = 9 + |(r - 4) - i|$. and 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 $r = n - 1, 1 \leq i \leq n - 2$, then $d(x_{n-1}^6, x_i^1) = r + 2 - i$.

The other cases are reported in the table 3.

Table 3.

Vertices	$d(x,y)$	Vertices	$d(x,y)$	Vertices	$d(x,y)$
(x_{n-3}^3, x_{n-2}^1)	2	(x_{n-4}^5, x_{n-2}^1)	6	(x_{n-4}^6, x_{n-5}^1)	9
(x_{n-3}^3, x_{n-1}^1)	3	(x_{n-4}^5, x_{n-1}^1)	5	(x_2^6, x_1^1)	9
(x_{n-4}^1, x_{n-3}^1)	4	(x_{n-4}^5, x_{n-5}^1)	8	(x_1^6, x_1^1)	8
(x_{n-4}^4, x_{n-3}^1)	5	(x_2^5, x_1^1)	8	(x_1^6, x_2^1)	9
(x_{n-2}^2, x_{n-1}^1)	2	(x_{n-5}^5, x_{n-4}^1)	7	(x_1^6, x_3^1)	9
(x_{n-2}^2, x_{n-3}^1)	4	(x_{n-5}^5, x_{n-3}^1)	7	(x_1^6, x_4^1)	11
(x_{n-1}^2, x_{n-2}^1)	2	(x_{n-3}^5, x_{n-2}^1)	5	(x_1^6, x_5^1)	9
(x_{n-5}^4, x_{n-4}^1)	6	(x_{n-3}^5, x_{n-1}^1)	4	(x_{n-3}^6, x_{n-2}^1)	5
(x_{n-5}^4, x_{n-3}^1)	6	(x_{n-3}^5, x_{n-5}^1)	7	(x_{n-5}^6, x_{n-2}^1)	7
(x_{n-3}^4, x_{n-2}^1)	4	(x_{n-3}^5, x_{n-4}^1)	6	(x_{n-5}^6, x_{n-4}^1)	9
(x_{n-3}^4, x_{n-1}^1)	3	(x_{n-4}^6, x_{n-3}^1)	7	(x_{n-5}^6, x_{n-3}^1)	8
(x_{n-3}^4, x_{n-5}^1)	6	(x_{n-4}^6, x_{n-2}^1)	6	(x_{n-5}^6, x_{n-2}^1)	7
(x_{n-3}^4, x_{n-4}^1)	5	(x_{n-4}^6, x_{n-1}^1)	5	(x_{n-5}^6, x_{n-1}^1)	6
(x_{n-6}^5, x_{n-5}^1)	9	(x_{n-6}^6, x_{n-5}^1)	10	(x_{n-3}^6, x_{n-2}^1)	5
(x_{n-6}^5, x_{n-4}^1)	8	(x_{n-6}^6, x_{n-4}^1)	9	(x_{n-3}^6, x_{n-1}^1)	4
(x_{n-6}^5, x_{n-3}^1)	8	(x_{n-6}^6, x_{n-3}^1)	9	(x_{n-3}^6, x_{n-5}^1)	8
(x_{n-4}^5, x_{n-3}^1)	7	(x_{n-2}^3, x_{n-1}^1)	3	(x_{n-3}^6, x_{n-4}^1)	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.

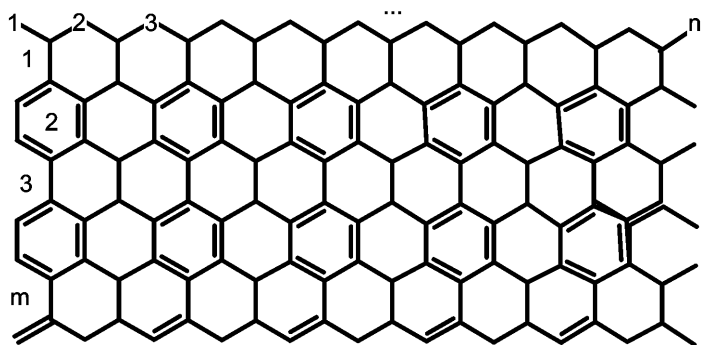


Figure 2. 2- D graph of zig zag nanotube $NT(5, n)$, for $m = 5, n = 10$.

Table 4.

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

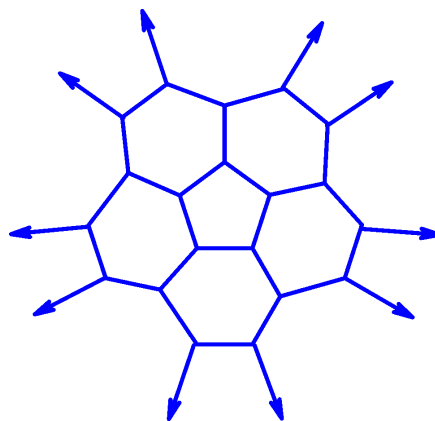


Figure 3. Cap B.

Table 5.

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)	$n + 1$

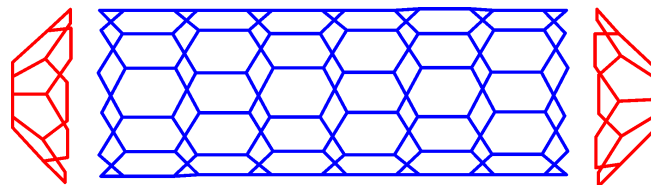


Figure 4. Fullerene A_{10n} constructed by combining two copies of B and the zig-zag nanotube $NT(5, n)$.

$$\mathbf{A} = \begin{pmatrix}
 01221123322334444332 \\
 10122212333223344443 \\
 21012321234332233444 \\
 22101332124443322334 \\
 12210233213444433223 \\
 1233203443124555421 \\
 2123330344211245554 \\
 32123430345421124555 \\
 33212443035554211245 \\
 23321344304555542112 \\
 23443125540134666532 \\
 32344214551023566643 \\
 32344412553201346665 \\
 43234521454310235666 \\
 43234541256532013466 \\
 44323552146643102356 \\
 44323554126665320134 \\
 34432455215666431023 \\
 34432255413466653201 \\
 23443145522356664310
 \end{pmatrix}$$

$$\mathbf{B} = \begin{pmatrix}
 02356664311455223443 \\
 20134666531255423443 \\
 31023566642145532344 \\
 53201346664125532344 \\
 64310235665214543234 \\
 66532013465412543234 \\
 66643102355521444323 \\
 46665320135541244323 \\
 35666431024552134432 \\
 13466653202554134432 \\
 11245555420344312332 \\
 42112455553034421233 \\
 55421124554303432123 \\
 55554211244430333212 \\
 24555542113443023321 \\
 22334444331233201221 \\
 33223344442123310122 \\
 44332233443212321012 \\
 44443322333321222101 \\
 33444433222332112210
 \end{pmatrix}$$

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