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DETOUR MATRIX AND DETOUR INDEX OF SOME NANOTUBES

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Let Gbe a graph. The matrix DD = [dd_{ij}], in which ddij is defined as the length of the longest path between vertices i and j is called the detour matrix of G. In this paper exact formulae for the detour index of armchair polyhex and $TUC_4C_8(R)$ nanotubes with exactly one row are computed.

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1. Introduction

Carbon nanotubes are molecular-scale tubes of graphitic carbon with outstanding properties. They are among the stiffest and strongest fibres known, and have remarkable electronic properties and many other unique characteristics. For these reasons they have attracted huge academic and industrial interest, with thousands of papers on nanotubes being published every year. Commercial applications have been rather slow to develop, however, primarily because of the high production costs of the best quality nanotubes.

Graph theory was successfully provided the chemist with a variety of very useful tools, namely, the topological index. A topological index is a numeric quantity from the structural graph of a molecule. The term "topological index" was first proposed by Hosoya[1] for characterizing the topological nature of a graph. The first topological index was proposed in 1947 by the chemist Harold Wiener.[2] Topological index is an integer quite easily obtained from a graph by a specified recipe. It can be used to evaluate structural similarity and diversity. Its main role is to work as a numerical molecular descriptor in QSAR/QSPR model.

There are hundreds of molecular descriptors. For example, the program CODESSA evaluates some 400 graph theoretical descriptors and quantum chemical parameters for molecules to be considered in a structure-property-activity study.[3]

A graph is a mathematical object and can be represented either in a geometrical or algebraic way. In the algebraic way, we consider a matrix named, adjacency matrix of the graph under consideration. This matrix is defined as $A = [a_{ij}]$, where $a_{ij} = 1$, for an adjacent pair v_i and v_j, and 0 otherwise. Here $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $E(G) = \{e_1, e_2, \ldots, e_m\}$ are the set of all vertices and edges of G, respectively. If G is given, then A is uniquely determined, and vice versa.

The detour matrix $DD = [dd_{ij}]$ can be defined for G with entries $dd_{ii} = 0$ and dd_{ij}, $i \neq j$, as the maximum distance between vertices v_i and v_j. If a graph G is given, the matrix D can be reproduced. The detour matrix was introduced in graph theory some time ago by F. Harary[4] for describing the connectivity in directed graphs. The detour matrix, in contrast to the distance matrix that records the length of the shortest path between vertices, records the length of the

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longest distance between each pair of vertices. The detour index is defined as the sum of entries in matrix has recently received some attention in the chemical literature.

The most important works on the geometric structures of nanotubes, nanotori and their topological indices was done by Diudea and his co-authors.[5-11] One of the present authors (ARA) computed the Wiener, PI and Szeged indices of some nanotubes.[12-17]

The aim of this paper is to compute the detour matrix and then detour index of some special case of armchair polyhex and $TUC_4C_8(R)$ nanotubes, Figure 1. For a real number x, [x] denotes the greatest integer ≤ x. Our notation is standard and is taken mainly from the standard books of graph theory.

2. Main Results

In this section, the detour index of an armchair polyhex nanotube and a $TUC_4C_8(R)$ nanotube with exactly one row are computed, Figures 1 and 2.

Theorem A. Suppose T is the benzenoid chain of Figure 1. Then the $(6i+r,6j+s)^{th}$ entry of Detour matrix of T, $1 \le r,s \le 6$, is as follows:

	6j+1	**6j+2**	**6j+3**	**6j+4**	**6j+5**	**6j+6**
6i+1	4(j-i)	4(j-i)+5	4(j-i)+5	4(j-i)+4	4(j-i)+4	4(j-i)+3
6i+2	4(j-i)+1	4(j-i)+6	4(j-i)+6	4(j-i)+5	4(j-i)+5	4(j-i)+4
6i+3	4(j-i)+1	4(j-i)+6	4(j-i)+6	4(j-i)+5	4(j-i)+5	4(j-i)+4
6i+4	4(j-i)+2	4(j-i)+7	4(j-i)+7	4(j-i)+6	4(j-i)+6	4(j-i)+5
6i+5	4(j-i)+2	4(j-i)+7	4(j-i)+7	4(j-i)+6	4(j-i)+6	4(j-i)+4
6i+6	4(j-i)+3	4(j-i)+2	4(j-i)+2	4(j-i)+1	4(j-i)+1	4(j-i)

Proof. We first compute the length of a maximum path between the vertex labelled 6i+1 and a vertex of the $(k+1)^{th}$ hexagon. To do this, it is enough to compute the length of a maximum path between 6i+1 and u = 6k+2, v = 6k+4 and w = 6k+6, Figure 1. Then we can see that the following are maximum path between, 6i+1 and x, x ∈ {u, v, w}:
6i+1-u: 6i+1, 6i+2, 6i+4, 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6, 6k+4, 6k+2,
6i+1-v: 6i+1, 6i+2, 6i+4, 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6, 6k+4,
6i+1-w: 6i+1, 6i+2, 6i+4, 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6.

Then $dd_{(6i+1)u} = 4(k-i)+5$, $dd_{(6i+1)v} = 4(k-i)+4$ and $dd_{(6i+1)w} = 4(k-i)+3$. By symmetry of this graph, $dd_{(6i+1)x} = dd_{(6i+1)u}$ and $dd_{(6i+1)y} = dd_{(6i+1)v}$. On the other hand the length of a maximum path between 6i+1 and 6k+1 is 4(k-i). This completes the entries of the r^{th} row, r ≡ 1 (mod 6). By symmetry, it is enough to compute the length of a maximum path between r and s, r ∈ {2,4,6} and s ∈ {6k+2,6k+4,6k+6}. The following are a maximum path between, r and s, r ∈ {6i+2, 6i+4, 6i+6} and s ∈ {6k+2,6k+4,6k+6}:

6i+2-u: 6i+2, 6i+1, 6i+3, 6i+5, 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6, 6k+4, 6k+2,
6i+2-v: 6i+2, 6i+1, 6i+3, 6i+5, 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6, 6k+4,
6i+2-w: 6i+2, 6i+1, 6i+3, 6i+5, 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6.
6i+4-u: 6i+4, 6i+2, 6i+1, 6i+3, 6i+5, 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6, 6k+4, 6k+2,
6i+4-v: 6i+4,6i+2, 6i+1, 6i+3, 6i+5, 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6, 6k+4,
6i+4-w: 6i+4,6i+2, 6i+1, 6i+3, 6i+5, 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6.
6i+6-u: 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6, 6k+4, 6k+2,
6i+6-v: 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6, 6k+4,
6i+6-w: 6i+6, 6i+7,…, 6k+1, 6k+3, 6k+5, 6k+6.
This completes calculation of detour matrix. ■

Corollary. If T is the benzenoid chain of Figure 1, then $dd(T) = 3p(8p^2 + 24p – 11)$.

Proof. The proof is straightforward and follows from Theorem 1. ■

Theorem B. Suppose S is an armchair polyhex nanotube with exactly one row and p hexagons. Then the $(6i+r,6j+s)^{th}$ entry of detour matrix of T, $1 \le s \le 6$ and $r \in \{1,2,4,6\}$, is as follows:

	6j+1	**6j+2, 6j+3**	**6j+4, 6j+5**	**6j+6**	**p**
6i+1	4(p-j+i)	4(p-j+i)+1	4(p-j+i)+2	4(p-j+i)-3	j-i ≤ [p/2]
6i+1	4(j-i)	4(j-i)+5	4(j-i)+4	4(j-i)+3	j-i ≥ [p/2]
6i+2	4(p-j+i)+5	4(p-j+i)+6	4(p-j+i)+7	4(p-j+i)+2	j-i ≤ [p/2]
6i+2	4(j-i)+1	4(j-i)+6	4(j-i)+5	4(j-i)+4	j-i ≥ [p/2]
6i+4	4(p-j+i)+4	4(p-j+i)+5	4(p-j+i)+6	4(p-j+i)+1	j-i ≤ [p/2]
6i+4	4(j-i)+2	4(j-i)+7	4(j-i)+6	4(j-i)+5	j-i ≥ [p/2]
6i+6	4(p-j+i)+3	4(p-j+i)+4	4(p-j+i)+5	4(p-j+i)	j-i ≤ [p/2]
6i+6	4(j-i)+3	4(j-i)+2	4(j-i)+1	4(j-i)	j-i ≥ [p/2]

Proof. Suppose S has exactly p hexagon. Consider two cases that $k \le [p/2]$ and $k \ge [p/2]$. We first assume that $k \le [p/2]$. To compute the length of a maximum path between u and 6i+r, $r \in \{1, 2, 4, 6\}$, it is enough to calculate the length of a maximum path between r and u−6i.

Suppose u = 6k+2 is a vertex in the $(k+1)^{th}$ hexagon of S, Figure 2. Then 1,6p+5,6p+3,6p+1,6p,…..,6k+6,6k+5,6k+3,6k+1,6k+2 is a maximum path between 1 and u and so $dd_{1-u} = 4(p-k)$. For u = 6k+4 and 6k+6, we have the following maximum paths between 1 and u, respectively:

1,6p+5,6p+3,6p+1,6p,…,6k+6,6k+5,6k+3,6k+1,6k+2,6k+4,
1,6p+5,6p+3,6p+1,6p,…,6k+6.

These paths has lengths 4(p-k)+5 and 4(p-k) + 4, respectively. For u = 6k+1, clearly there exists a maximum path of length 4(p-k). Choose r = 2. Then 2,4,6,5,3,1,6p+5,6p+3,6p+1,6p,…,6k+6,6k+5,6k+3,6k+1 is a maximum path of length 4(p-k)+5 between r and 6k+1. To calculate the length of a maximum path between 2 and 6k+2, 6k+4 and 6k+6, its is enough to consider above path between 2 and 6k+1 and then add a maximum path between 6k+1 and 6k+s, $s \in \{2, 4, 6\}$. Therefore $dd_{2-(6k+2)} = 4(p-k) + 6$, $dd_{2-(6k+4)} = 4(p-k) + 5$ and $dd_{2-(6k+6)} = 4(p-k) + 4$. If r =4, 6 then 4, 6, 5, 3, 1, 6p+5, 6p+3, 6p+1, 6p,…, 6k+6, 6k+5, 6k+3, 6k+1 and 6, 5, 3, 1, 6p+5, 6p+3, 6p+1, 6p, …, 6k+6, 6k+5, 6k+3, 6k+1 are maximum paths between r and 6k+1, respectively. By our argument above, $dd_{4-(6k+1)} = 4(p-k) + 2$, $dd_{4-(6k+2)} = 4(p-k) + 7$, $dd_{4-(6k+4)} = 4(p-k) + 6$, $dd_{4-(6k+6)} = 4(p-k) + 5$, $dd_{6-(6k+1)} = 4(p-k) + 3$, $dd_{6-(6k+2)} = 4(p-k) + 2$, $dd_{6-(6k+4)} = 4(p-k) + 1$ and $dd_{6-(6k+6)} = 4(p-k)$. If $k \ge [p/2]$ then the maximum paths of Theorem A completes our argument. ■

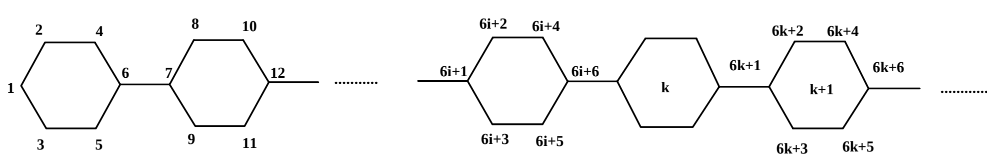

Fig. 1. A Chain of Hexagons.

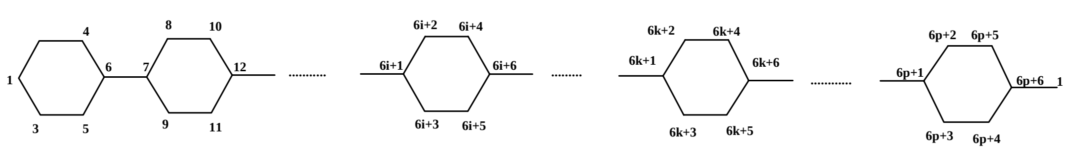

Fig.2. A Polyhex Armchair Nanotube with Exactly One Row and p Hexagons.

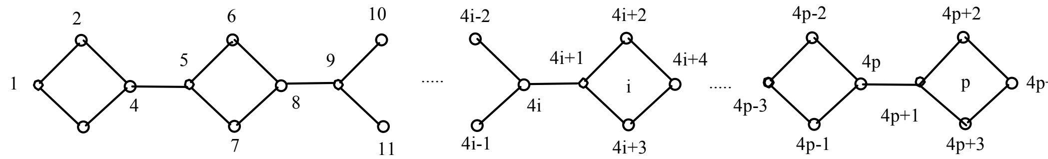

Fig. 3. A Chain of Rhombs.

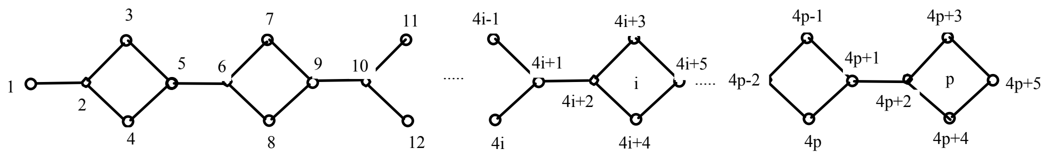

Fig. 4. The $TUC_4C_8(R)$ Nanotube with Exactly One Row.

Corollary. If T is an armchair polyhex nanotube then we have:

$$dd(T) = \begin{cases} 2p(27p^2 + 30p - 34) & 2 \mid p \\ p(54p^2 + 60p - 67) & 2 \nmid p \end{cases}$$

Theorem C. Suppose G is the graph of Figure 3. Then the Detour matrix of G is as follows:

	4j+1	**4j+2, 4j+3**	**4j+4**
4i+1	3(j-i)	3(j-i)+3	3(j-i)+2
4i+2, 4i+3	3(j-i)+1	3(j-i)+4	3(j-i)+3
4i+4	3(j-i)+1	3(j-i)+4	3(j-i)+3

Proof. We first compute the length of a maximum path between the vertex labelled 4i+1 and a vertex of the $(k+1)^{th}$ rhomb of G. To do this, it is enough to compute the length of a maximum path between 4i+1 and u = 4k+1, v = 4k+2 and w = 4k+4, Figure 3. Then we can see that the following are maximum path between, 4i+1 and x, $x \in \{u, v, w\}$:

4i+1-u: 4i+1, 4i+2, 4i+4,…, 4k+1,
4i+1-v: 4i+1, 4i+2, 4i+4,…, 4k+1, 4k+2,
4i+1-w: 4i+1, 4i+2, 4i+4, 4…, 4k+1, 4k+2, 4k+4.

Then $dd_{(4i+1)u} = 3(k\text{-}i)$, $dd_{(4i+1)v} = 3(k\text{-}i)+3$ and $dd_{(4i+1)w} = 3(k\text{-}i)+2$. On the other hand, the following are maximum path between, 4i+2 and x, $x \in \{u, v, w\}$:

4i+2-u: 4i+2, 4i+1, 4i+3, 4i+4,…, 4k+1,
4i+2-v: 4i+2, 4i+1, 4i+3, 4i+4,…, 4k+1, 4k+2,
4i+2-w: 4i+2, 4i+1, 4i+3, 4i+4, 4…, 4k+1, 4k+2, 4k+4.

So $dd_{(4i+2)u} = 3(k\text{-}i)+1$, $dd_{(4i+2)v} = 3(k\text{-}i)+4$ and $dd_{(4i+2)w} = 3(k\text{-}i)+3$. Finally, the following are maximum path between, 4i+4 and x, $x \in \{u, v, w\}$:

4i+4-u: 4i+4,…, 4k+1,
4i+4-v: 4i+4,…, 4k+1, 4k+2,
4i+4-w: 4i+4, …, 4k+1, 4k+2, 4k+4.

Therefore, $dd_{(4i+4)u} = 3(k\text{-}i)\text{-}2$, $dd_{(4i+4)v} = 3(k\text{-}i)+1$ and $dd_{(4i+4)w} = 3(k\text{-}i)$. This completes the proof. ■

Corollary. If G is the graph shown in figure 3 then $dd(G) = 8p(p^2 + 2p - 1)$.

Theorem D. Suppose H is a $TUC_4C_8(R)$ nanotube with exactly one row. Then the Detour index of H is as follows:

$$dd(T) = \begin{cases} p(18p^2 + 10p - 15) & 2 \nmid p \\ 2p(9p^2 + 5p - 8) & 2 \mid p \end{cases}.$$

Proof. We first compute the length of a maximum path between vertices 1 and 2 with u = 4k+1 and v = 4k+2, Figure 4. We have the following four maximum paths between these vertices:

1-u: 1,4p+4, 4p+3, 4p+1,…, 4k+4,4k+3,4k+1,
1-v: 1,4p+4, 4p+3, 4p+1,…, 4k+4, 4k+3,4k+1,4k+2,
2-u: 2,4,3,1,4p+4, 4p+3,…, 4k+4,4k+3,4k+1,
2-v: 2,4,3,1,4p+4, 4p+3,…, 4k+4,4k+3,4k+1, 4k+2.

If p is odd then we have the following values for the length of a maximum path between 1 and x:

	2	3,4	5	…	4i+2	4i+3,4i+4	4i+5	…
1	3p-1	3p	3p-3	…	3(p-i)-1	3(p-i)	3(p-i)-3	…

	4t+2	4t+3,4t+4	4t+5	…	4j+2	4j+3, 4j+4	4j+5	…
1	(3p+1)/2	(3p+5)/2	(3p+3)/2	…	3j+1	3j+4	3j+3	…

where t = (p-3)/2. On the other hand,

	1	2,5	4	…	4i+2	4i+3,4i+4	4i+5	…
3	3p	3p-1	3p	…	3(p-i)	3(p-i)+1	3(p-i)-3	…

	4t+2	4t+3,4t+4	4t+5	…	4j+2	4j+3, 4j+4	4j+5	…
3	(3p-7)/2	(3p-1)/2	(3p-3)/2	…	3j+1	3j+4	3j+3	…

Using these and similar calculation for the case of p even, we conclude the result. ■

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