

Multiplicative Wiener index of zigzag polyhex nanotubes

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The multiplicative Wiener index, $\pi(G)$, is equal to the product of the distances between all pairs of vertices of the underlying molecular graph G . In this paper we compute this index for zigzag polyhex nanotubes.

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1. Introduction

Wiener index is one of the most popular molecular-graph-based structure-descriptors used in QSPR and QSAR studies [1, 2]. We recall that topological indices are numeral values, assigned to a molecule according to its size and structure and are used to study the relation between the structure of molecule and its chemical, physical and biological properties [2, 3]. Wiener index was the first proposed by Wiener [4] as an aid to determining the boiling point of paraffin. It is equal to the sum of the distances between all pairs of vertexes of a (molecular) graph. From that time, various applications of Wiener index in many fields of chemistry were represented [1, 2, 5-7]. Recently Gutman et al. [8], parallel to Wiener index, have introduced multiplicative Wiener index equal to the product of distances between all pairs of vertexes. They studied basic properties of this index and its possible physicochemical applications. Also for a variety of classes of isomeric alkanes, monocycloalkanes, bicycloalkanes, benzenoid hydrocarbons, and phenylenes a very good (either linear or slightly curvilinear) correlation between Wiener and multiplicative Wiener indices [9]. For nanotubes, the big size of corresponding graphs makes the calculations complicated. Many of topological indices of these molecules are obtained (See [10-23]). In this paper we calculate the multiplicative Wiener index of zigzag polyhex nanotubes (See Fig. 1).

2. Main results and discussion

Let G be a concerned simple graph (i.e. G has no loops, multiple or directed edges) with set of vertices $V(G) = \{v_1, \dots, v_n\}$. The distance matrix $D(G)$ of G is a square matrix of order n , whose entry d_{ij} is the distance, the number of edges of a shortest path, between the vertices v_i and v_j in G . The Wiener index of G , $W(G)$, is equal to the sum of distances between all pairs of vertexes of G . By the above notations:

$$W(G) = \sum_{i < j} d_{ij}.$$

The multiplicative Wiener index, $\pi(G)$, is equal to the product of distances between all pairs of vertexes of G

$$\pi(G) = \prod_{i < j} d_{ij} \quad (1)$$

For a vertex $u \in V(G)$ we define

$$\pi(u) = \prod_{u \neq v \in V(G)} d(u, v) \quad (2)$$

Then it is easy to see

$$\pi(G)^2 = \prod_{u \in V(G)} \pi(u) \quad (3)$$

Throughout this paper $G = \text{TUHC}_6 [2p, q]$, (see Fig. 1), denotes an arbitrary zigzag polyhex nanotorus in terms of the circumference $2p$ and the length q (see Fig 1). Also we choose a coordinate label for vertices of G , as shown in Fig. 2. Note that G is a bipartite graph. We recall that a graph G is bipartite if the vertices can be colored with white and black so that adjacent vertices have different color.

The product of distances of one white vertex of level 0 to the all vertices of level k , $k=1, 2, \dots, q-1$, is given as:

$$w_k = \prod_{r=1}^{2p} d(x_{02}, x_{kr}) = \prod_{r=1}^{2p} d(x_{01}, x_{kr}) = \begin{cases} \frac{(k+p)!(k+p-1)!(2k)^{k+1}(2k+1)^k}{((2k)!)^2} & \text{If } 1 \leq k < p \\ (2k+1)^p (2k)^p & \text{If } p \leq k. \end{cases} \quad (4)$$

Also

$$w_0 = p!(p-1)! \quad (5)$$

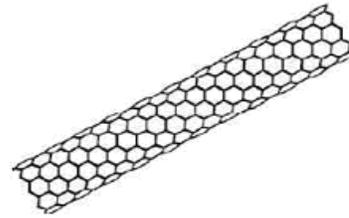


Figure 1. A TUHC₆[2p, q] nanotube

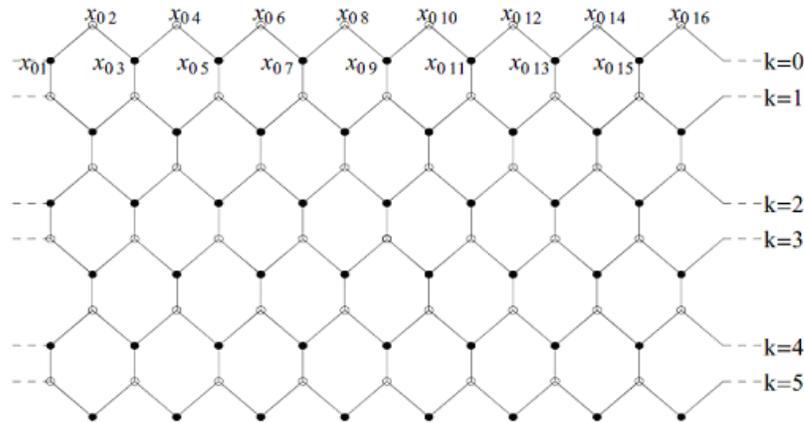


Fig. 2. A TUHC₆ [2p,q] Lattice with p = 8 and q = 6.

Similarly, the product of distances of one black to the all vertex of level 0 to all vertices of level k, k=1, 2, ..., q-1, is given as:

$$b_k = \prod_{r=1}^{2p} d(x_{01}, x_{kr}) = \prod_{r=1}^{2p} d(x_{03}, x_{kr}) = \begin{cases} \frac{(k+p)!(k+p-1)!(2k)^{k+1}(2k-1)^k}{(2k!)^2} & \text{If } 1 \leq k < p \\ (2k-1)^p (2k)^p & \text{If } p \leq k \end{cases} \quad (6)$$

and

$$b_0 = p!(p-1)! \quad (7)$$

Therefore

$$\begin{aligned} \pi(x_{02}) = \pi(x_{04}) = \dots &= w_0 w_1 \dots w_{q-1} \\ \pi(x_{01}) = \pi(x_{03}) = \dots &= b_0 b_1 \dots b_{q-1} \end{aligned} \quad (8)$$

We consider the tube can be built up from two halves collapsing at level 1. The bottom part is the graph $G_1 = \text{TUH}C_6 [2p, q-1]$ and we can consider x_{11} as one of the white vertices in the first row of the graph G_1 . According to (7), we have

$$\pi(x_{11}) = \pi(x_{13}) = \dots = w_0 w_1 \dots w_{q-2} \quad (9)$$

The top part is graph $G_2 = \text{TUH}C_6 [2p, 2q-1]$ and level 1 of graph G is the first its row and x_{11} is such a black vertex of G_2 . Therefore by (7) $\pi_{G_1}(x_{11}) = \pi_{G_1}(x_{13}) = \dots = b_0 b_1$. Since $w_0 = b_0$ and $\pi_G(x_{11}) = \frac{\pi_{G_1}(x_{11}) \pi_{G_2}(x_{11})}{b_0}$, we have $\pi(x_{11}) = w_0 \dots w_{q-2} b_1$, hence

$$\pi(x_{11}) = \pi(x_{13}) = \dots = w_0 \dots w_{q-2} b_1 \quad (10)$$

Similarly for x_{12} we obtain

$$\pi(x_{12}) = \pi(x_{14}) = \dots = b_0 \dots b_{q-2} w_1 \quad (11)$$

By repeating tis argument we obtain

(I) If $0 \leq j \leq q-1$ and j is an odd number, then

$$\begin{aligned} \pi(x_{j1}) = \pi(x_{j3}) = \dots &= w_0 \dots w_{q-(j+1)} b_1 \dots b_j \\ \pi(x_{j2}) = \pi(x_{j4}) = \dots &= b_0 \dots b_{q-(j+1)} w_1 \dots w_j \end{aligned}$$

(II) If $0 \leq j \leq q-1$ and j is an even number, then

$$\begin{aligned} \pi(x_{j1}) = \pi(x_{j3}) = \dots &= b_0 \dots b_{q-(j+1)} w_1 \dots w_j \\ \pi(x_{j2}) = \pi(x_{j4}) = \dots &= w_0 \dots w_{q-(j+1)} b_1 \dots b_j \end{aligned}$$

For all $0 \leq j \leq q-1$, put

$$g(j) = b_0 \dots b_{q-(j+1)} w_1 \dots w_j$$

$$f(j) = w_0 \dots w_{q-(j+1)} b_1 \dots b_j.$$

Then

$$\pi(G)^2 = \prod_{x_j \in V(G)} \pi(x_j) = \prod_{j=0}^{q-1} (f(j)g(j))^p. \tag{12}$$

Let

$$y(k) = \frac{[(k+p)!(k+p-1)!(2k)^{k+1}]^2 (4k^2-1)^k}{(2k!)^4}$$

$$z(k) = (4k^2-1)^p (2k)^{2p}$$

In the case of short tubes, $0 < q \leq p$, the expansion of (12) leads to

$$\pi(p, q) = \{(p-1)!p!\}^{pq} \sqrt{\prod_{j=0}^{q-1} [\prod_{k=1}^{q-(j+1)} y(k) \prod_{k=1}^j y(k)]^p}$$

while in the case of long tubes, $q \geq p$, the multiplicative Wiener index is evaluated by

$$\pi(p, q) = \{(p-1)!p!\}^{pq} \sqrt{\prod_{j=p}^{q-1} [\prod_{k=1}^j y(k) \prod_{k=1}^{q-(j+1)} y(k)]^p} \times \sqrt{\prod_{j=0}^{p-1} [\prod_{k=1}^{p-1} y(k) \prod_{k=1}^j y(k) \prod_{k=p}^{q-(j+1)} z(k)]^p} \times \sqrt{\prod_{j=p}^{q-1} [\prod_{k=1}^{p-1} y(k) \prod_{k=1}^{q-(j+1)} y(k) \prod_{k=p}^j z(k)]^p}.$$

Tables 1 and 2 list some values for $\text{Ln}(\pi(p, q))$ of some nanotubes.

Table 1. Multiplicative Wiener index, $q \leq p$.

p	q	Ln(π(p, q))	p	q	Ln(π(p, q))
9	9	25899.55249	10	10	41602.78343
9	8	19850.36335	10	8	25233.42172
9	7	14700.30240	10	6	13315.26686
9	6	10409.86108	10	5	8907.405569
9	5	6936.600751	10	4	5463.243832
9	4	4234.422084	10	3	2923.435223
9	2	933.5155788	10	2	1221.245332

Table 2. Multiplicative wiener index, $q \geq p$.

p	q	Ln(π(p, q))	p	q	Ln(π(p, q))
3	3	139.4518204	4	4	589.4823124
3	8	1738.867497	4	8	3243.433761
3	16	9620.665755	4	16	17430.13104686
5	5	1722.471202	6	6	4051.648489
5	10	9043.692945	6	12	20658.81545
5	15	23799.89256	6	18	53627.92843
5	20	933.5155788	6	24	105125.2455
7	7	8256.866198	8	8	15193.43107
7	14	41255.75023	8	16	74784.45046
7	21	106047.1987	8	24	190799.4903
7	28	206644.7223	8	32	370085.6996

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