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An Exact Expression for the Wiener Index of a Polyhex Nanotorus

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Abstract

The Wiener index of a graph G is defined as $W(G) = 1/2\sum_{\{x,y\}\subseteq V(G)}d(x,y)$, where V(G) is the set of all vertices of G and for $x,y \in V(G)$, d(x,y) denotes the length of a minimal path between x and y. In this paper an algorithm for computing the distance matrix of a polyhex nanotorus T = T[p,q] is given. Using this matrix, we obtain an exact expression for the Wiener index of T. We prove that:

$$W(T) = \begin{cases} \dfrac{pq^2}{24}(6p^2 + q^2 - 4) & q < p \\ \dfrac{p^2q}{24}(3q^2 + 3pq + p^2 - 4) & q \geq p \end{cases}.$$

INTRODUCTION

The first use of a graph invariant for the correlation of the measured properties of molecules with their structural features was made in 1947 by the chemist Harold Wiener. In that year, he introduced the notion of path number of a graph as the sum of the distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds[1]. Next Hosoya[2] named such graph invariants, topological index. With hundreds of topological indices one would expect that most molecules could be well characterized and their physicochemical properties correlated with the available descriptors. We encourage the reader to consult Refs. [3-9] and references therein, for further study on the topic.

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We now recall some algebraic definitions that will be used in the paper. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-shapes of which are represented by V(G) and E(G), respectively. If e is an edge of G, connecting the vertices u and v then we write e=uv. The distance between a pair of vertices u and w of G is denoted by d(u,w). Wiener index of a graph G is defined as $W(G) = 1/2\sum_{\{x,y\}\subseteq V(G)} d(x,y)$.

In a series of papers, Diudea and coauthors [10-16] studied the topological indices of some chemical graphs related to nanostructures. They also computed the Wiener index of some nanotubes. In this paper we continue this program to find an exact expression for the Wiener index of a polyhex nanotorus.

Our notation is standard and mainly taken from [10,11] and [17]. Throughout this paper T = T[p,q] denotes an arbitrary polyhex torus in terms of its circumference (q) and its length (p), see Figure 1.

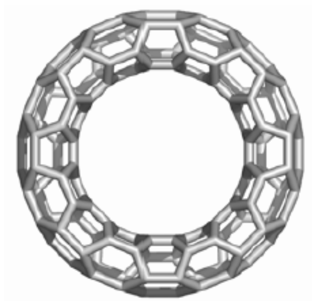

Figure 1. A Polyhex Nanotorus (This figure is taken from a paper by John and Diudea [18]).

The main result of this paper is as follows:

Theorem. Suppose T = T[p,q] is a polyhex nanotorus. Then we have:

$$W(T) = \begin{cases} \dfrac{pq^2}{24}(6p^2 + q^2 - 4) & q < p \\ \dfrac{p^2q}{24}(3q^2 + 3pq + p^2 - 4) & q \geq p \end{cases}.$$

MAIN RESULT

In this section, the Wiener index of the graph T = T[p,q] were computed, in which T = T[p,q] denotes an arbitrary polyhex nanotorus, in the terms of their circumference p and their length q. We first notice that p and q must be even. To compute the Wiener index of this graph, we assume that u_{ij} denotes the (i,j)-entry of the 2-dimansional lattice of T, Figure 2.

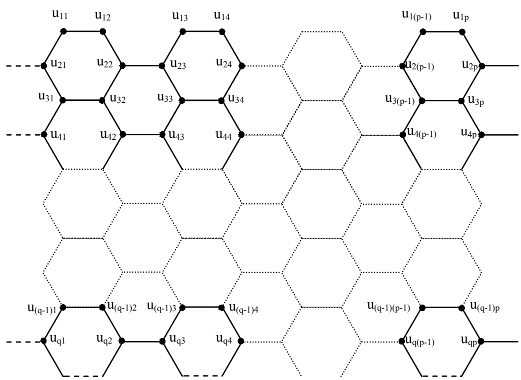

Figure 2. A 2-Dimensional Lattice for T[p,q].

To compute the Wiener index of T[p,q], we first calculate the molecular symmetry group of T. Let D_{2n} be the dihedral group of order 2n, $n \geq 3$. This group can be presented by $D_{2n} = \langle x , y \mid x^n = y^2 = 1, y^{-1}xy = x^{-1}\rangle$.

Proposition 1. The point group of T[p,q] is isomorphic to D_p.

Proof. Suppose $V_1, V_2, \ldots, V_p$ are hexagons of the first row of 2-dimensional lattice of T and $\sigma = (1,2,\ldots,p)$. Then σ determines a permutation x of the molecular symmetry group G of T. Moreover, the reflection about the horizontal plane will be another element y of the group G. Now it is easy to see that the group G is generated by x and y. This group satisfies the relations $x^p = e$, $y^2 = e$ and $x^{-1}yx = x^{-1}$ and so it is a dihedral group of order 2p, as desired. ■

The following result gives an exact expression for the Wiener index of T, in the case that p = q.

Proposition 2. $W(T[p,p]) = \frac{7}{24}p^5 - \frac{1}{6}p^3$.

Proof. Suppose $A_{ij} = \sum_{x\in V(T)} d(x,u_{ij})$. Then it is easy to see that $W(T) = 1/2\sum_{1\le i,j\le n} A_{ij}$. From the 2-dimensional lattice of T, one can see that for every ordered pair (i,j) and (r,s), $1 \le i,j,r,s \le p$, $A_{ij} = A_{rs}$. Hence $W(T) = (p^2/2)A_{11}$. Therefore for computing W(T) it is enough to calculate A_{11}. Define $X_{p,p} = [y_{i,j}]$ and $x_p = \sum_{i,j} y_{i,j}$, where $y_{i,j} = d(u_{11},u_{ij})$. We will find an inductive method for computing $X_{p,p}$. To do this, we consider the 2-dimensional lattice of T[p-2,p-2] and define $X_{p-2,p-2} = [x_{i,j}]$, similar to $X_{p,p}$. Obviously, This lattice is a part of the 2-dimensional lattice of T[p,p] and we have:

$$y_{i,j} = \begin{cases} x_{i,j} & i \le \frac{p}{2} \ \& \ j \le \frac{p}{2} \\ x_{i-2,j} & i > \frac{p}{2} + 2 \ \& \ j \le \frac{p}{2} \\ x_{i,j-2} & i \le \frac{p}{2} \ \& \ j > \frac{p}{2} + 2 \\ x_{i-2,j-2} & i > \frac{p}{2} \ \& \ j > \frac{p}{2} \end{cases}$$

Therefore, $X_{p,p}$ and $X_{p-2,p-2}$ are essentially different only in the two rows and columns. These are (p/2 + 1)–th and (p/2 + 2)–th rows and columns. If V denotes the (p/2+1)–th row of the matrix $X_{p,p}$ then by symmetries of a torus, $V - [1\ 1\ \ldots\ 1]$ is the (p/2+2)–th row of the matrix $X_{p,p}$. On the other hand, from 2-dimensional lattice of T we have $V = [\frac{p}{2}\ \frac{p}{2}+1 \ldots p\ p\text{-}1 \ldots \frac{p}{2}+1\ ]$. In the same way, we can calculate the (p/2+1)–th and (p/2 +2)–th columns of $X_{p,p}$.We have:

$$\begin{array}{lll} x_{\frac{n}{2}+1-2i,\frac{n}{2}+1} = x_{\frac{p}{2}+1,\frac{p}{2}+1} \ , & x_{\frac{p}{2}-2i,\frac{p}{2}+1} = x_{\frac{p}{2}+2,\frac{p}{2}+1} & : -\frac{p}{4} \le i \le \frac{p}{4} \\ x_{\frac{n}{2}+1-2i,\frac{n}{2}+2} = x_{\frac{p}{2}+1,\frac{p}{2}+2} \ , & x_{\frac{p}{2}-2i,\frac{p}{2}+2} = x_{\frac{p}{2}+2,\frac{p}{2}+2} & : -\frac{p}{4} \le i \le \frac{p}{4} \end{array}.$$

These equations imply that $x_p = x_{p-2} + (7/2)p^2 - 7p + 4$. But this recurrence relation is linear and so $x_p = A + B$ in which A is the general solution of its associated homogeneous equation and B is one particular solution for the main equation. By a well-known method for solving such equations, we have $x_p = A + B(-1)^p + (7/12)\, p^3 - (4/12)p$. But p is even, so $x_p = C + (7/12)p^3 - (4/12)p$. We now apply the primary condition $x_4 = 36$ to prove that $x_p = (7/12)p^3 - (4/12)p$. Therefore $W(T) = (p^2/2)A_{11} = (7/24)p^5 - (1/6)p^3$, which completes the proof. ■

Corollary. Suppose $q < p$, $X_{q,q} = [x_{ij}]$ and $Y_{p,p} = [a_{ij}]$. Then we have:

$$x_{i,j} = \begin{cases} a_{i,j} & \text{if } i \le \frac{q}{2}+1 \ ,\ j \le \frac{q}{2}+1 \\ a_{p-q+i,j} & \text{if } i > \frac{q}{2}+1 \ ,\ j \le \frac{q}{2}+1 \end{cases} ; x_{i,j} = \begin{cases} a_{i,p-q+j} & \text{if } i \le \frac{q}{2}+1 \ ,\ j > \frac{q}{2}+1 \\ a_{p-q+i,p-q+j} & \text{if } i > \frac{q}{2}+1 \ ,\ j > \frac{q}{2}+1 \end{cases}.$$

The previous corollary states that for every even integers p and q, q < p, we can construct $X_{q,q}$ from $X_{p,p}$. In fact, the matrix $X_{q,q}$ is constructed from $X_{p,p}$ by eliminating $((q/2) + 2)$–th, …, $(p-(q/2)+1)$–th rows and columns.

We present another method to compute the matrix $X_{p,p} = [x_{ij}]$, p is even. Define two $(p/2 +1) \times p$ matrices $A = [a_{ij}]$ and $B = [b_{ij}]$ as follows:

$$a_{1,j} = \begin{cases} a_{1,j-1}+1 \\ a_{1,j-1}-1 \end{cases} \quad , \quad a_{2,j} = \begin{cases} a_{1,j}+1 & \text{if} \quad j \text{ is even and } j \le (p/2)+1 \\ a_{1,j}-1 & \text{if} \quad j \text{ is even and } j > (p/2)+1 \end{cases},$$

$$a_{2,j} = \begin{cases} a_{2,j-1}+1 \\ a_{2,j-1}-1 \end{cases} \quad , \quad a_{1,j} = \begin{cases} a_{2,j}+1 & \text{if} \quad j \text{ is odd and } j \le (p/2)+1 \\ a_{2,j}-1 & \text{if} \quad j \text{ is odd and } j > (p/2)+1 \end{cases},$$

$$a_{1,1} = 0 \quad , \quad a_{2,1} = 1 \text{ and } a_{i,j} = \begin{cases} a_{1,j} & \text{if} \quad i > 3 \ \&\ i \text{ is odd} \\ a_{2,j} & \text{if} \quad i > 3 \ \&\ i \text{ is even} \end{cases},$$

$$b_{\frac{p}{2}+1,j} = \begin{cases} \frac{p}{2}+j-1 & \text{if} \quad j \le \frac{p}{2}+1 \\ \frac{3p}{2}-j+1 & \text{if} \quad j > \frac{p}{2}+1 \end{cases}, \ b_{i,j} = b_{i+1,j}-1.$$

Using similar argument as Propositions 2, we can prove in the first (p/2)+1 rows of the matrix $X_{p,p}$, $x_{ij} = \mathrm{Max}\{a_{ij}, b_{ij}\}$. Moreover, if $i > p/2 + 1$ then $x_{i,j} = x_{p-i+2,j}$. On the other hand, these calculations show that the maximum entry of $X_{p,p}$ is p and there are p/2 entries in this matrix with value of p and n+1 entries with value of p–1. Finally, the entries of main diagonal of $X_{p,p}$ is as follows:

$$x_{i,i} = \begin{cases} 2(i-1) & \text{if} \quad i \le (n/2)+1 \\ 2(n-i+1) & \text{if} \quad i > (n/2)+1 \end{cases}.$$

We now consider the general case that $p \neq q$. We have the following result:

Proposition 3. If $p \neq q$ then we have:

$$W(T) = \begin{cases} \frac{pq^2}{24}(6p^2 + q^2 - 4) & q < p \\ \frac{p^2 q}{24}(3q^2 + 3pq + p^2 - 4) & q > p \end{cases}.$$

Proof. Using a similar argument as Proposition 1, it is enough to calculate A_{11}. Define $X_{p,q} = [x_{i,j}]$, where $x_{i,j} = d(u_{11},u_{ij})$. By symmetries of a torus, Proposition 1, for $i > 1 + q/2$ we have $x_{i,j} = x_{q-i+2,j}$ and so it is enough to compute only the first $1 + q/2$ rows of $X_{p,q}$. Our argument consider two separate cases that $p < q$ and $p > q$.

Case 1. $p > q$. Consider the matrix $X_{p,p}$ constructed in Proposition 1 and assume that $A_1, A_2, \ldots, A_p$ are the rows of $X_{p,p}$. To calculate the matrix $X_{p,q}$, we must omit the rows $A_{2+(q/2)}, A_{3+(q/2)}, \ldots, A_{p-(q/2)+1}$ from $X_{p,p}$. In fact, $X_{p,q} = [A_1,\ldots,A_{1+(q/2)},A_{p-(q/2)+2}, \ldots, A_p]^t$ and if $X_{p,p} = [a_{i,j}]$ then we have:

$$x_{ij} = \begin{cases} a_{i,j} & i \le \frac{q}{2}+1 \\ a_{p-q+i,j} & i > \frac{q}{2}+1 \end{cases}.$$

Suppose $R = [A_{2+(q/2)}, \ldots, A_{p-(q/2)+1}]^t$ and S, Y are the sum of entries in the matrices $X_{p,p}$ and R, respectively. Then $W(T) = (pq/2)(S-Y)$. But, in the proof of Proposition 2 we prove that $S = (7/12)p^3 - (4/12)p$ and so it is enough to compute Y. Define two sequences X_r and S_r as the sum of $(n/2-r+2)$–th, $(n/2-r+3)$–th, …., and $(n/2+r+1)$-th rows of the matrix $X_{p,p}$, and, the sum of entries of $X_{p,r}$, respectively, in which $S_0 = S$, $X_0 = X$ and $r < p$ is an even positive integer. Then $Y = X_{(p-q)/2}$. By the proof of Proposition 2, $X_1 = (p/2)(3p-2)$ and we have:

$$\begin{aligned} X_1 - X_0 &= (p/2)(3p-2), \\ X_2 - X_1 &= (p/2)(3p-2) - 4((p/2)-1), \\ X_3 - X_2 &= X_2 - X_1 - 4((p/2)-2), \\ &\vdots \\ X_r - X_{r-1} &= X_{r-1} - X_{r-2} - 4((p/2)-(r-1)). \end{aligned}$$

These equations imply that $X_r = X_{r-1} - 2pr + 2p + 2r^2 - 2r + (3/2)p^2 - p$, which is a simple linear recurrence relation. Hence, $X_r = (1/3)r(r+1)(2r+1) - (p + 1)r^2 + ((3/2)p^2 - 1)r$ and with substituting $r = (p-q)/2$, we have $Y = \frac{p-q}{12}[7p^2 + q^2 + pq - 4]$.

Therefore $W(T) = (pq^2/24)(6p^2 + q^2 - 4)$, as desired.

Case 2. q > p. Using similar argument as the Case 1 and eliminating some columns we have:

$$x_{i,j} = \begin{cases} a_{i,j} & \text{if} \quad j \le \frac{n}{2}+1 \\ a_{i,m-n+j} & \text{if} \quad j > \frac{n}{2}+1 \end{cases},$$

where as before, $X_{p,q} = [x_{i,j}]$ and $X_{p,p} = [a_{i,j}]$. Then a similar argument as Case 1 shows that $W(T) = (qp^2/24)(3q^2 + 3pq + p^2 - 4)$, which completes the proof. ■

We now ready to state our main result. We have:

Theorem. Suppose $T = T[p,q]$ is a polyhex nanotorus. Then we have:

$$W(T) = \begin{cases} \frac{pq^2}{24}(6p^2 + q^2 - 4) & q < p \\ \frac{p^2q}{24}(3q^2 + 3pq + p^2 - 4) & q \ge p \end{cases}.$$

Proof. The proof is follows from Propositions 1–3. ■

In the end of this paper we compute the matrix $X_{18,18}$ from $X_{16,16}$. We can calculate the matrix $X_{16,16}$, by our second method our by induction, Proposition 1. Then $X_{18,18}$ is constructed by Proposition 1.

$$X_{16,16} = \begin{bmatrix} 0 & 1 & 4 & 5 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 4 & 3 \\ 1 & 2 & 3 & 6 & 7 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 6 & 5 & 2 \\ 2 & 3 & 4 & 5 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 4 & 3 \\ 3 & 4 & 5 & 6 & 7 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 6 & 5 & 4 \\ 4 & 5 & 6 & 7 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 6 & 5 \\ 5 & 6 & 7 & 8 & 9 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 8 & 7 & 6 \\ 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 16 & 15 & 12 & 11 & 10 & 9 & 8 & 7 \\ 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 14 & 13 & 12 & 11 & 10 & 9 & 8 \\ 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 & 15 & 14 & 13 & 12 & 11 & 10 & 9 \\ 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 14 & 13 & 12 & 11 & 10 & 9 & 8 \\ 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 16 & 15 & 12 & 11 & 10 & 9 & 8 & 7 \\ 5 & 6 & 7 & 8 & 9 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 8 & 7 & 6 \\ 4 & 5 & 6 & 7 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 6 & 5 \\ 3 & 4 & 5 & 6 & 7 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 6 & 5 & 4 \\ 2 & 3 & 4 & 5 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 4 & 3 \\ 1 & 2 & 3 & 6 & 7 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 6 & 5 & 2 \end{bmatrix}$$

$$X_{18,18} = \begin{bmatrix} 0 & 1 & 4 & 5 & 8 & 9 & 12 & 13 & 16 & \boldsymbol{17} & \boldsymbol{16} & 15 & 12 & 11 & 8 & 7 & 4 & 3 \\ 1 & 2 & 3 & 6 & 7 & 10 & 11 & 14 & 15 & \boldsymbol{18} & \boldsymbol{17} & 14 & 13 & 10 & 9 & 6 & 5 & 2 \\ 2 & 3 & 4 & 5 & 8 & 9 & 12 & 13 & 16 & \boldsymbol{17} & \boldsymbol{16} & 15 & 12 & 11 & 8 & 7 & 4 & 3 \\ 3 & 4 & 5 & 6 & 7 & 10 & 11 & 14 & 15 & \boldsymbol{18} & \boldsymbol{17} & 14 & 13 & 10 & 9 & 6 & 5 & 4 \\ 4 & 5 & 6 & 7 & 8 & 9 & 12 & 13 & 16 & \boldsymbol{17} & \boldsymbol{16} & 15 & 12 & 11 & 8 & 7 & 6 & 5 \\ 5 & 6 & 7 & 8 & 9 & 10 & 11 & 14 & 15 & \boldsymbol{18} & \boldsymbol{17} & 14 & 13 & 10 & 9 & 8 & 7 & 6 \\ 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 16 & \boldsymbol{17} & \boldsymbol{16} & 15 & 12 & 11 & 10 & 9 & 8 & 7 \\ 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & \boldsymbol{18} & \boldsymbol{17} & 14 & 13 & 12 & 11 & 10 & 9 & 8 \\ 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 & \boldsymbol{17} & \boldsymbol{16} & 15 & 14 & 13 & 12 & 11 & 10 & 9 \\ \boldsymbol{9} & \boldsymbol{10} & \boldsymbol{11} & \boldsymbol{12} & \boldsymbol{13} & \boldsymbol{14} & \boldsymbol{15} & \boldsymbol{16} & \boldsymbol{17} & \boldsymbol{18} & \boldsymbol{17} & \boldsymbol{16} & \boldsymbol{15} & \boldsymbol{14} & \boldsymbol{13} & \boldsymbol{12} & \boldsymbol{11} & \boldsymbol{10} \\ \boldsymbol{8} & \boldsymbol{9} & \boldsymbol{10} & \boldsymbol{11} & \boldsymbol{12} & \boldsymbol{13} & \boldsymbol{14} & \boldsymbol{15} & \boldsymbol{16} & \boldsymbol{17} & \boldsymbol{16} & \boldsymbol{15} & \boldsymbol{14} & \boldsymbol{13} & \boldsymbol{12} & \boldsymbol{11} & \boldsymbol{10} & \boldsymbol{9} \\ 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & \boldsymbol{18} & \boldsymbol{17} & 14 & 13 & 12 & 11 & 10 & 9 & 8 \\ 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 16 & \boldsymbol{17} & \boldsymbol{16} & 15 & 12 & 11 & 10 & 9 & 8 & 7 \\ 5 & 6 & 7 & 8 & 9 & 10 & 11 & 14 & 15 & \boldsymbol{18} & \boldsymbol{17} & 14 & 13 & 10 & 9 & 8 & 7 & 6 \\ 4 & 5 & 6 & 7 & 8 & 9 & 12 & 13 & 16 & \boldsymbol{17} & \boldsymbol{16} & 15 & 12 & 11 & 8 & 7 & 6 & 5 \\ 3 & 4 & 5 & 6 & 7 & 10 & 11 & 14 & 15 & \boldsymbol{18} & \boldsymbol{17} & 14 & 13 & 10 & 9 & 6 & 5 & 4 \\ 2 & 3 & 4 & 5 & 8 & 9 & 12 & 13 & 16 & \boldsymbol{17} & \boldsymbol{16} & 15 & 12 & 11 & 8 & 7 & 4 & 3 \\ 1 & 2 & 3 & 6 & 7 & 10 & 11 & 14 & 15 & \boldsymbol{18} & \boldsymbol{17} & 14 & 13 & 10 & 9 & 6 & 5 & 2 \end{bmatrix}$$

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