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HARARY INDEX OF ZIGZAG POLYHEX NANOTORUS

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The Harary index, H = H(G), of a molecular graph G is based on the concept of reciprocal distance and is defined, in parallel to the Wiener index, as the half-sum of the off-diagonal elements of the molecular distance matrix of G. In this paper we compute the Harary index of zigzag polyhex nanotorus.

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1. Introduction

One of considerable topics in chemistry is surveying the quantitative structure-property relationship between the structure of a molecule and chemical, physical and biological properties of it(QSPR). For this purpose, the form of molecule must be coded according to numbers. A common method, for coding the molecule structure, is to assign a graph to the molecule, where the vertices are atoms of molecule and edges are chemical bonds between the atoms. According to this graph, we can assign various numeral values (topological indices), polynomials, matrices and extra to the molecules which are usually invariant under automorphism of graphs (See [1-3]). A novel topological index for the characterization of chemical graphs, derived from the reciprocal distance matrix and named the Harary index in honor of Professor Frank Harary, has independently been defined by Plavšić et al. [4] and Ivanciuc et al. [5] in 1993. The Harary index and the related indices have shown a modest success in structure-property correlations,[3-8] but the use of these indices in combination with other descriptors appears to be very efficacious in improving the QSPR models[8]. For nanotubes and nanotorus, the big size of corresponding graphs makes the calculations complicated. Diudea [9-13] was the first chemist which considered the problem of computing topological indices of nanostructures. Various topological indices have been calculated for these molecules up to this time [13-22]. In this paper, we represent a calculation for Harary index of G=HC_6 [p,q], an zigzag polyhex nanotorus.

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. In 1947 chemist Harold Wiener [23] developed the most widely known topological descriptor, the Wiener index, and used in to determine physical properties of types of alkanes known as paraffins. 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:

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

Harary index, a parallel of Wiener index, is reasonably well-correlated with many physical and chemical properties of organic compounds, and chemists are hence interested in computing it for a variety of classes of graphs. This index, $H(G)$ is defined the half of the summation of the inverse of the distances of the vertices of the graph G according to the expression:

$$H(G) = \sum_{i<j} \frac{1}{d_{ij}} \ .$$

Throughout this paper G=HC_6 [p,q], (see Figure 1), denotes an arbitrary zigzag polyhex nanotorus in terms of the circumference p and the length q. The aim of our work is finding an exact expression for the Harary index of the zigzag polyhex nanotorus. For this purpose we choose a coordinate label for vertices of G as shown in Figure 2. Note that G has pq vertices.

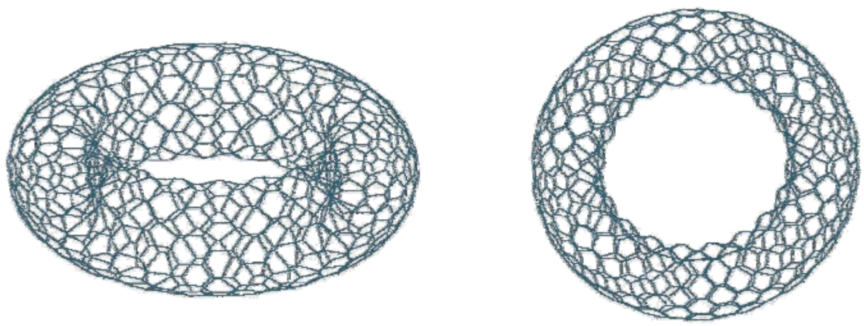

Fig. 1. HC$_6$[20,40]: Side view; Top view

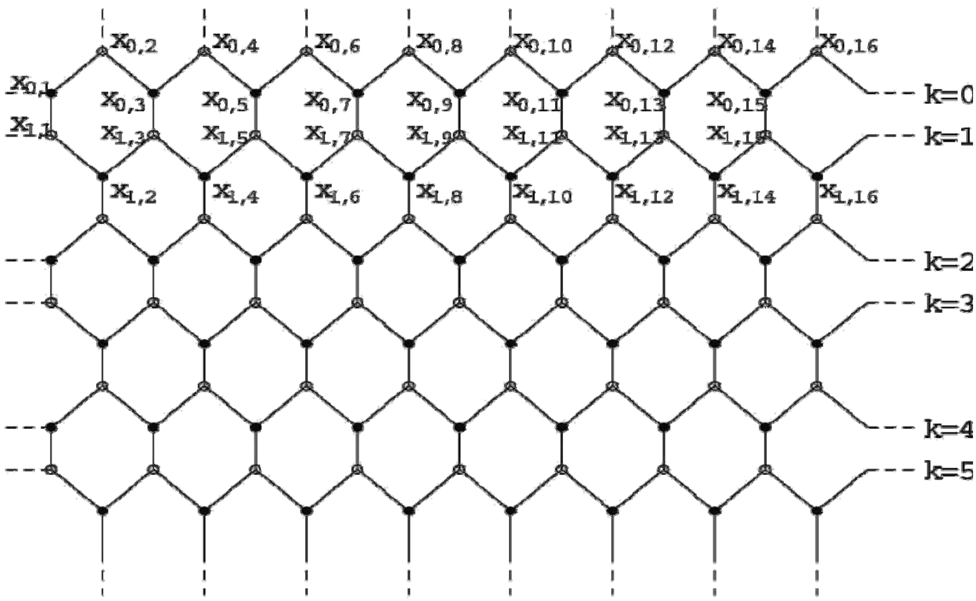

Fig. 2. A zigzag polyhex nanotorus lattice with p=16 and q=6.

Let p=2c and q=2d. We begin our work with the following lemma about G.

Theorem 1. Let $u \in V(G)$ is a white vertex on level 0. Then the sum of the inverses of the distances between u and all vertices on level k, level 0≤k<d, is denoted by w_k is

I: k=0 $$w_0 = 2\sum_{j=2}^{c} \frac{1}{j-1} + \frac{1}{c};$$

II: k <c $$w_k = 2\sum_{j=k+2}^{c} \frac{1}{k+j-1} + \frac{k+1}{2k} + \frac{k}{2k+1};$$

III: d>k ≥c $$w_k = c\frac{1}{2k+1} + c\frac{1}{2k}.$$

Also if u be a black vertex on level 0 then the sum of the inverses of the distances between u and all vertices on level k, 0≤k<d, is denoted by b_k is

I: k=0 $$b_0 = 2\sum_{j=2}^{c} \frac{1}{j-1} + \frac{1}{c};$$

II: k <c $$b_k = 2\sum_{j=k+2}^{c} \frac{1}{k+j-1} + \frac{k+1}{2k} + \frac{k}{2k-1};$$

III: d>k ≥c $$b_k = c\frac{1}{2k-1} + c\frac{1}{2k}.$$

Proof: We compute b_k. Since G is symmetric, it is suffices we consider x_{01}. At first note that the lattice is symmetric (with respect to the line joining x_{01} to x_{11}). We distinguish three cases**:**

Case 1: d>k ≥c and k is even. In this case for all 1 ≤ j ≤ c + 1, we have

$$d(x_{01}, x_{kj}) = \begin{cases} 2k-1 & \text{if } j \text{ is even} \\ 2k & \text{if } j \text{ is odd.} \end{cases}$$

Now by considering these vertices and their symmetric vertices we obtain c vertices having distance 2k-1 from x_{01}, and c vertices having 2k distance from x_{01}. Therefore

$$b_k = c\frac{1}{2k-1} + c\frac{1}{2k}.$$

Case 2: d>k ≥c and k is even. In this case for all 1 ≤ j ≤ c + 1, we have

$$d(x_{01}, x_{kj}) = \begin{cases} 2k & \text{if } j \text{ is even} \\ 2k-1 & \text{if } j \text{ is odd.} \end{cases}$$

Now by considering these vertices and their symmetric vertices we obtain c vertices having distance 2k-1 from x_{01}, and c vertices having 2k distance from x_{01}. Therefore

$$b_k = c\frac{1}{2k-1} + c\frac{1}{2k}.$$

Case 3: k<c. Then $d(x_{01}, x_{kc}) = k + c$. For all j's, such that $c+1 \le j$ and $k+1 < j$, we have

$$d(x_{01}, x_{kj}) = k + j - 1.$$

Thus the sum of the inverse of the distances between x_{01} and x_{kj} (for all j's, such that c+1≤j and k+1<j) and their symmetric vertices is

$$S_1 = 2\sum_{j=k+2}^{c} \frac{1}{k+j-1} + \frac{1}{k+c}.$$

Hence if k=0 then $b_0 = 2\sum_{j=2}^{c} \frac{1}{j-1} + \frac{1}{c}$. Also if 1≤j≤k+1, then

$$d(x_{01},x_{kj})=\begin{cases}2k & \text{if } \ k-j \ \text{ is odd}\\ 2k-1 & \text{if } \ k-j \ \text{ is even.}\end{cases}$$

Therefore the product of the distances between x_{01} and x_{kj} (for all j such that$1\le j\le k+1$) and their symmetric vertices is

$$S_2=(k+1)\frac{1}{2k}+k\frac{1}{2k-1}.$$

So

$$b_k=S_1+S_2=2\sum_{j=k+2}^{c}\frac{1}{k+j-1}+\frac{k+1}{2k}+\frac{k}{2k-1}.$$

Result 1. The inverse of the distances of one white or black vertex of level 0 to all vertices on level d is

$$w_d=b_d=\sum_{x\in\text{level } d}\frac{1}{d(x_{01},x)}$$

$$=\begin{cases}2\sum_{j=d+2}^{c}\frac{1}{d+j-1}+\frac{d+1}{2d}+\frac{d}{2d-1} & \text{if } \ d<c\\ \frac{c}{2d-1}+\frac{c}{2d} & \text{if } d\ge c.\end{cases}$$

Proof: Since G is symmetric (with respect to the line joining x_{01} to x_{11}), it is sufficient to prove the assertion for x_{01} and x_{02}. For x_{01}, the proof is exactly the proof of Result 1. We consider the tori that can be built up from two halves collapsing at level 0. In the top part x_{02} is such as a black vertex so by the proof of Result 1, we can calculate b_d.

Result 2. For each $u\in V(G)$ we have

$$\sum_{u\neq v\in V(G)}\frac{1}{d(u,v)}=b_o+b_1+\ldots b_d+w_1+\cdots+w_{d-1}.$$

Proof: At first note that the lattice is symmetric (with respect to the level k). So it is suffices to consider x_{01} and x_{02}. For other black (white) vertices the argument is similar. Now we begin with x_{01}. Let $B_1=\{k\mid 0\le k\le d\}$ and $B_2=\{k\mid d<k\le q-1\}$. Then we have

$$\sum_{x_{01}\neq v\in V(G)}\frac{1}{d(x_{01},v)}=\sum_{x_{01}\neq v\in B_1}\frac{1}{d(x_{01},v)}+\sum_{v\in B_2}\frac{1}{d(x_{01},v)}$$

But

$$\sum_{x_{01}\neq v\in B_1}\frac{1}{d(x_{01},v)}=\sum_{x_{01}\neq v\in level\,0}\frac{1}{d(x_{01},v)}+\sum_{v\in level\,1}\frac{1}{d(x_{01},v)}+\cdots+\sum_{v\in level\,\text{d}}\frac{1}{d(x_{01},v)}$$

$$=b_o+b_1+\cdots+b_d.$$

For computing the last sum we consider the tori that can be built up from two halves collapsing at level 0. The top part is formed of the lines of B_2 that x_{01} are such as a black vertex. So by a changing index and using the proof of the Theorem 1, we obtain that

$$\sum_{v\in B_2}\frac{1}{d(x_{01},v)}=\sum_{x_{01}\neq v\in level\ \text{q-1}}\frac{1}{d(x_{01},v)}+\sum_{v\in level\ \text{q-2}}\frac{1}{d(x_{01},v)}+\cdots+\sum_{v\in level\ \text{d+1}}\frac{1}{d(x_{01},v)}$$

$$=w_1+w_2+\cdots+w_{d-1}.$$

This completes the proof.

Since HC_6 [p,q] has pq vertices then by result 2 we have

Theorem 2. The Harary index of G=HC_6 [p,q] is given by

$$H(G) = \frac{pq}{2}(b_o + b_1 + \ldots b_d + w_1 + \cdots + w_{d-1}). \qquad (1)$$

Let $\gamma = \lim it_{n\to\infty}(\sum_{i=1}^{n}\frac{1}{i} - \ln(n))$, $\Psi(x) = \frac{\Gamma'(x)}{\Gamma(x)}$ and $\Gamma(x) = \int_0^\infty t^{x-1}e^{-t}dt$ be the Gamma function. We recall that γ is Euler-Mascheroni constant and has the numerical value 0.577215665. Also $\sum_{i=1}^{n}\frac{1}{i} - \gamma = \Psi(n+1)$.

The expansion of (1) leads us to

Corollary Let p=2c and q=2d.
If p>q then

$$H(c,d) = 2\text{cd}\{(\text{-4d}+2)\text{Ln}(2) + \gamma - [2d\Psi(\text{d}) - \Psi(\text{d}+\frac{1}{2})] + \frac{8cd + 8d^2 - 5d - 1 - 5c}{2(c+d)} + $$
$$+ 2\sum_{k=1}^{d}[2\Psi(\text{c}+\text{k}) - \Psi(\text{k}+\frac{1}{2})]\} - \frac{2d^2 + c^2}{c+d}.$$

If p≤q then

$$H(c,d) = 2\text{cd}\{\text{Ln}(2)(\text{-4c - 6}) + \gamma - \text{c}\Psi(\text{c}+\frac{1}{2}) - \text{c}\Psi(\text{d}) - 2\Psi(\text{c}) + 3\text{c}\Psi(\text{c}) - \text{c}\Psi(\text{d}+\frac{1}{2}) - \Psi(\text{c}+\frac{1}{2}) +$$
$$\text{4c - 3} + 2\sum_{\text{k}=1}^{\text{c-1}}[2\Psi(\text{k}+\text{c}) - \Psi(\text{k}+\frac{1}{2})]\} + \text{c}^2 \text{ - 2d}.$$

3. Exprimental

In Table 1 and 2 by using the corollary we obtain Harary index for some p and q.

Table 1 (Haray index q<p)

p	q	H(p,q)	p	q	H(p,q)
4	2	19.33333333	80	40	217256.3782
6	2	37.50000000	80	50	304789.1989
6	4	121.4000000	80	60	399637.3809
8	2	58.26666667	10	4	269.1904762
100	10	30786.21784	10	6	514.8928571
100	14	54569.42075	10	8	799.0634921
100	20	98864.91179	12	10	1489.168831
100	40	301078.1339	12	8	1064.704762
100	50	425296.0531	14	6	858.8666667

Table 2 (Harary index q≥p)

p	q	H(p,q)	p	q	H(p,q)
2	4	15.66666667	6	12	602.4935065
2	6	28.40000000	8	12	991.2900433
4	8	167.2761905	10	12	1442.307359
6	8	343.1714286	10	14	1790.704740
20	40	24006.76951	8	14	1225.633256
22	40	28197.54348	200	2000	187253760.6
100	200	3064297.789	400	2000	638715743.8
100	400	7514893.08	600	2000	1291594754.
100	500	9951475.66	1000	2000	3077940141.

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