Iranian Journal of Mathematical Chemistry, Vol. 6, No.1, March 2015, pp. 29–39 **IJMC**

On the Distance Based Indices of H–phenylenic Nanotorus

ABBAS HEYDARI

Department of Science, Arak University of Technology, Arak, Iran

Correspondence should be addressed to a-heidari@iau-arak.ac.ir

Received 24 June 2014; Accepted 4 December 2014

ACADEMIC EDITOR: BIJAN TAERI

ABSTRACT Let G be a connected simple (molecular) graph. The distance $d(i, j)$ between two vertices i and j of G is equal to the length of a shortest path that connects i and j. In this paper we compute some distance based topological indices of H–phenylenic nanotorus. At first we obtain an exact formula for the Wiener index. As an application the Schultz index and modified Schultz index of this graph will be computed by using whose Wiener index. Finally, we compute eccentric connectivity index of this graph.

KEYWORDS Wiener index · Schultz index · modified Schultz index · eccentric connectivity index · H-phenylenic nanotorus.

1. INTRODUCTION

Let G be a simple connected graph with set vertex $V(G)$. For vertices i and j in $V(G)$, we denote by $d(i, j)$ the topological distance i.e., the number of edges on the shortest path, joining the two vertices of G. Since G is connected, $d(i, j)$ exists for all $i, j \in V(G)$. the degree of a vertex $i \in V(G)$ is the number of the vertices joining to i and denoted by $deg(i)$. The (i, j) entry of the adjacency matrix of G is denoted by $A(i, j)$. The Wiener index of G is defined as

$$W(G) = \frac{1}{2}\sum_{i,j\in V(G)} d(i, j). \tag{1}$$

The name Wiener index or Wiener number for the quantity defined in Equation *(1)* is usual in chemical literature, since Harold Wiener [1] in 1947, seemed to be the first to consider it. Wiener himself used the name path number, but denoted his quantity by W. Wiener's original definition was slightly different – yet equivalent – to (*1*). The definition of the Wiener index in terms of distances between vertices of a graph, such as in Equation (1), was first given by Hosoya [2]. For a review, historical details and further bibliography on the chemical applications of the Wiener index see [3–6].

Schultz [7] has introduced in 1989 a graph–theoretical descriptor for characterizing alkanes by an integer as follows:

$$S(G) = \sum_{\{i,j\}\subseteq V(G)} \deg(i)(d(i,j) + A(i,j)). \tag{2}$$

He named this descriptor the molecular topological index and denoted it by *MTI*. Later *MTI* became much better known under the name the Schultz index [8-9]. The Schultz index has been shown to be a useful molecular descriptor in the design of molecules with desired properties. Mathematical properties of *MTI* have also been studied [9–20].

Motivated by equations *(2)*, I. Gutman [21] defined the modification of Schultz index, i.e.,

$$S^*(G) = \sum_{\{i,j\}\subseteq V(G)} (\deg(i)\deg(j))d(i,j). \tag{3}$$

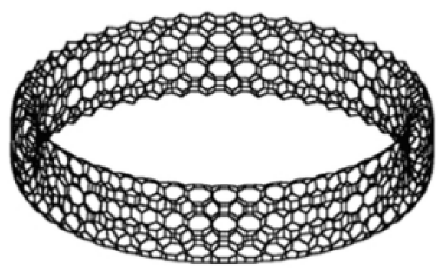

Figure 1. The Lattice of HPH(12,144).

which here we refer to as the modified Schultz index. Results in this direction can be found in Refs [21–22].

For a given vertex u of G its eccentricity $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. Hence,

$$\varepsilon(u) = Max_{v\in V(G)} d(u,v).$$

The eccentric connectivity index $\xi(G)$ of a graph G is defined as

$$\xi(G) = \sum_{v\in V(G)} \deg(v)\varepsilon(v). \tag{4}$$

The eccentric connectivity index has been found to have a low degeneracy and hence a significant potential of predicting biological activity of certain classes of chemical compounds [23–24].

Phenylenes (*PH*) are polycyclic conjugated systems composed of an alternating sequence of fused benzene and cyclobutadiene rings: C_6, C_4, C_6, … , C_6, C_4, C_6. Several properties (mathematical and physico-chemical) of *PH* are found to be closely related to the analogous properties of the corresponding hexagonal systems [26–28]. Fourmembered rings have been proposed for tessellating the sphere in generalized fullerenes and occur in the classical Archimedean polyhedra [29]. The Archimedean truncated cuboctahedron TCUOCT can be embedded, by a genus operation, on the toroidal surface. Its genus-1 transform $TCUOCT_{G1}$ shows the same distance degree sequence [30] (*DDS*) as the small phenylenic torus (*HPH* [*6*,*8*]).

Bahrami and Yazdani computed the *PI* index of H-Phenylenic tori (nanotorus) [31]. In this paper, we obtain an exact formula for the Wiener, Schultz, modified Schultz and the eccentric connectivity indices of H-phenylenic nanotorus.

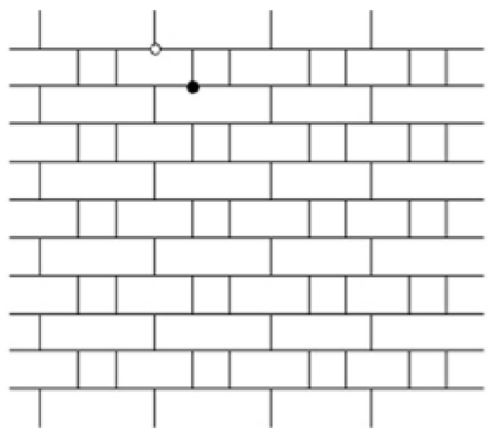

Figure 2. The Expanded Lattice of HPH(12,10).

2. RESULTS AND DISCUSSION

In this section we derive an exact formula for the Wiener index of graph H-phenylenic nanotorus where will be denoted by *HPH*(*m, n*). Then we compute the Schultz index of this graph, by using whose Wiener index. For this purpose at first we consider a coordinate representation for *HPH*(*m, n*) as shown in Figure 2 In this Figure *m* is a multiple of *3* and determines the number of rows of *HPH*(*m, n*). Also *n* is an even integer and denotes the number of horizontal rows the graph. One can consider two different types of vertices in *HPH*(*m, n*). At first the vertices such as the white vertex where whose below edge is deleted and secondly the vertices such as the black vertex where also beside parallel of whose below edge is deleted (see Figure 2).

The graph of *HPH*(*m, n*) can be embedded into $G = C_n \times C_m$, the Cartesian product of the cycle of order n and the cycle of order m (see Figure 3). Thus the Wiener index of *HPH*(*m*,*n*) can be computed by using the Wiener index of *G* and considering elimination some edges, resulting in an increase in the distance between vertices of *G* to obtain *HPH*(*m*,*n*). Recall that the Wiener index of *G* can be computed by well known formula for Cartesian product of two graphs [32] as follows:

$$W(G) = W(C_n \times C_m) = \frac{mn}{8}(m^2 + n^2).$$

Therefore it is sufficient that we compute increasing distance between some vertices of *HPH*(*m*,*n*) by deleting some of the edges of *G* to obtain this graph. By symmetry of the graph it is sufficient that we consider the white and the black vertices in *HPH*(*m*,*n*). At first we consider the white vertex. By deletion an edge of the *G*, the distance between two end vertices of this edge increase from *1* to *3*. Thus the distance between the white vertex on first row of *HPH*(*m*,*n*) and any other vertices of this graph may be increase or invariant. Now we consider the vertices of graph such that increase their distance to the white vertex. In the following sequence the number of those vertices of graph where are located on the *i*-th row of *HPH*(*m*,*n*) is calculated as

$$1,5,8,16,21,...$$

Therefore we define the sequence $\{S_i\}_{i=1}^{n}$ to obtain the members of the previous sequence as $S_1=1$ and for $2 \le i \le n$,

$$S_i = \begin{cases} S_{i-1} + 2i, & if \quad i \quad is \quad even \\ S_{i-1} + i, & if \quad i \quad is \quad odd. \end{cases}$$

Now suppose that $n<m$, the sum of members of $\{S_i\}_{i=1}^{n}$ determines increasing the distance between all of the vertices of the graph by deletion some of the edges of *G*. If $n \ge m$, then increasing distance between vertices of the graph must be computed by sum of the members of the sequence $\{S_i\}_{i=1}^{n}$ minus the summation of *n-m* first members of this sequence.

In continue we verify the black vertex of *HPH*(*m*,*n*). Similar to the white vertex the following sequence determines number of the vertices of *HPH*(*m*, *n*) such that the distance between those vertices and the black vertex increase by deletion some edges of *G* to obtain *HPH*(*m*,*n*).

$$2,4,10,14,24,30,...$$

It can easily be verified that the last sequence can be represented by $\{T_i\}_{i=1}^{n}$ where $T_1=2$ and for $2 \le i \le n$,

$$T_i = \begin{cases} T_{i-1} + i, & if \quad i \quad is \quad even \\ T_{i-1} + 2i, & if \quad i \quad is \quad odd. \end{cases}$$

Put $\alpha = \frac{1+(-1)^{\frac{n}{2}}}{2}$. In the following theorem the Wiener index of *HPH*(*m*,*n*) will be calculated by using the Wiener index of *G* and two previous sequences where determines the increasing distance between vertices of *G* by deletion some the edges of *G* to obtain *HPH*(*m*,*n*).

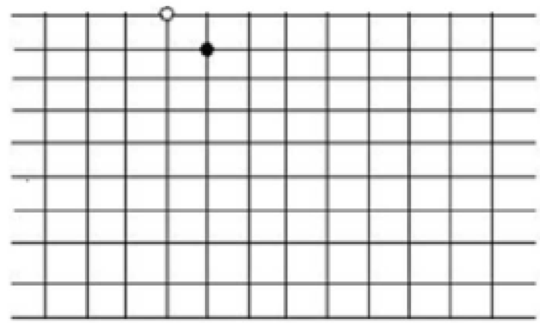

Figure 3. The Expanded Lattice of $C_{10} \times C_{12}$.

Theorem 1. The Wiener index of *HPH(m, n)* is computed as

$$W(H) = \begin{cases} \frac{n^2 m}{16}(2m(m+n)+n^2-4+\frac{4\alpha}{3}) & if \quad n < m \\ \frac{mn}{16}(5n^2m-nm^2+12n(2m-n-4)+m(m^2-12m+44)-48+\frac{4\alpha(m-4)}{3}) & if \quad n \geq m. \end{cases}$$

Proof. Let x and y denote the white and the black vertices of H = $HPH(m, n)$ respectively. If $G = C_n \times C_m$, put

$$R(x) = \sum_{v \in V(H)} d(x,v) - \sum_{v \in V(G)} d(x,v).$$

And

$$R(y) = \sum_{v \in V(H)} d(y,v) - \sum_{v \in V(G)} d(y,v).$$

Since number of the vertices of H where are same as x is equal to $\frac{|V(H)|}{3}$ and number of the vertices of H where are same as y is equal to $\frac{2|V(H)|}{3}$, thus

$$W(H) = W(G) + \frac{mn}{3} R(x) + \frac{2mn}{3} R(y).$$

By using *(3)* we have $R(x) = \sum_{i=1}^{\frac{m}{2}-1} S_i$. Therefore,

$$R(x) = \begin{cases} \frac{n(n^2-1)}{16}, & if \quad \frac{n}{2}-1 \quad is \quad even \\ \frac{n(n^2-8)}{16}, & if \quad \frac{n}{2}-1 \quad is \quad odd. \end{cases}$$

And by using *(4)*, $R(y) = \sum_{i=1}^{\frac{n}{2}-1} T_i$. Thus,

$$R(y)=\begin{cases}\dfrac{n(n^2-4)}{16}, & if \quad \dfrac{n}{2}-1 \quad is \quad even\\ \dfrac{n^3}{16} & , \quad if \quad \dfrac{n}{2}-1 \quad is \quad odd.\end{cases}$$

Now let $n < m$. If is $\frac{n}{2}-1$ an even integer we have

$$\begin{aligned}W(H) &= W(G)+\frac{mn}{3}R(x)+\frac{2mn}{3}R(y)\\ &= \frac{m^2n^2(m+n)}{8}+mn\frac{n(n^2-4)}{16}\\ &= \frac{n^2m}{16}(2mn+2m^2+n^2-4).\end{aligned}$$

If $\frac{n}{2}-1$ is an odd integer then

$$\begin{aligned}W(H) &= \frac{m^2n^2(m+n)}{8}+mn\frac{n(n^2-4)}{48}+2mn\frac{n^3}{48}\\ &= \frac{n^2m}{48}(6mn+6m^2+3n^2-8).\end{aligned}$$

Now suppose that $n \geq m$. In this case number of the vertices of $G = C_n \times C_m$ such that whose distance from *x* or *y* is increased for the *i*-th row of the graph must be revised if $i \geq n$. Because the members of sequences $\{S_i\}_{i=1}^n$ and $\{T_i\}_{i=1}^n$ must be less than *m* which is equal to number of the vertices on each row of *H*. Thus for $i \leq m$ number of the vertices of the graph such that whose distance from *x* and *y* has increase is computed as follows $\lambda(i) = S_i - S_{n-i+1}$ and $\mu(i) = T_i - T_{n-i+1}$ respectively. Thus if n/2 – 1 is an even integer then we have

$$R(x)=\frac{m-4}{16}(m^2-3mn-8n+3n^2+12n+12),$$

$$R(y)=\frac{m-4}{16}(m^2-3mn-8n+3n^2+12n+12).$$

And if n/2 – 1 is an odd integer then

$$R(x)=\frac{m-4}{16}(m^2-3mn-8n+3n^2+12n+8)$$

$$R(y)=\frac{m-4}{16}(m^2-3mn-8n+3n^2+12n+16).$$

Thus if n/2 – 1 is an even integer,

$$W(H)=W(G)+\frac{mn}{3}R(x)+\frac{2mn}{3}R(y)$$
$$=\frac{n^2m}{16}(5n^2m-nm^2-48n-12n^2$$
$$+24mn+m^3-12m^2+44m-48).$$

Now suppose that n/2 – 1 is an odd integer then

$$W(H)=\frac{mn}{16}(15n^2m-3nm^2-48n-36n^2$$
$$+72mn+3m^3-36m^2+136m-16).$$

This completes the proof. ■

In continue we compute the Schultz and modified Schultz indices of *HPH*(*m*, *n*) by using whose Wiener index of this graph.

Corollary 1. The Schultz index of *H=HPH(m,n)* is given as

$$S(H)=\begin{cases}\frac{3nm}{16}(2n^2m+2nm^2+n^3-(4-\frac{4\alpha}{3})n+24) & if \quad n<m\\ \frac{3mn}{16}(5n^2m-nm^2+12n(2m-n-4)+m(m^2-12m+44)-24+\frac{4\alpha(m-4)}{3}) & if \quad n\geq m.\end{cases}$$

Proof. Let $i\in V(H)$ be an arbitrary vertex of *H*. Since *deg(i)=3*, thus by using (*2*) the Schultz index of the graph is computed as

$$S(H)=\sum_{\{i,j\}\subseteq V(H)}\deg(i)(d(i,j)+A(i,j))$$
$$=3\sum_{\{i,j\}\subseteq V(H)}(d(i,j)+3\sum_{\{i,j\}\subseteq V(H)}A(i,j)$$
$$=3W(H)+3\,|\,E(H)\,|=3W(H)+\frac{9}{2}mn.$$

The results can be obtained by replacing the exact formula of the Wiener index of *H* where is obtained in Theorem 1. ■

In the following Corollary the modified Schultz index of *HPH(m,n)* will be calculated by using Theorem 1.

Corollary 2. The modified Schultz index of *H=HPH(m, n)* is given as

$$S^*(H)=\begin{cases}\frac{9n^2m}{16}(2m(m+n)+n^2-4+\frac{4\alpha}{3}) & if \quad n<m\\ \frac{9mn}{16}(5n^2m-nm^2+12n(2m-n-4)+m(m^2-12m+44)-48+\frac{4\alpha(m-4)}{3}) & if \quad n\geq m.\end{cases}$$

Proof. Let $i \in V(H)$ be an arbitrary vertex of *H*. Since *deg*(*i*) = *3*, thus by using (*3*) the modified Schultz index of the graph is computed as follows

$$S^*(H) = \sum_{\{i,j\} \subseteq V(H)} (\deg(i)\deg(j))\, d(i,j)$$
$$= 9 \sum_{\{i,j\} \subseteq V(H)} d(i,j) = 9W(H).$$

The results can be obtained by replacing the exact formula of the Wiener index of *HPH*(*m, n*) where is obtained in Theorem 1. ■

In continue the eccentric connectivity index of *HPH*(*m,n*) will be computed. To obtain maximum distance between $u \in V(H)$ and any other vertex of the graph we consider Figure (4). In this Figure the vertices on *HPH*(*m,n*) are verified in two different cases.

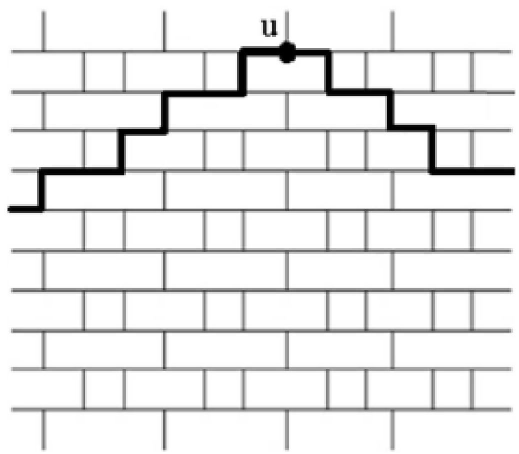

Figure 4.

At first the vertices where are located above of the black edges. Secondly the vertices where are located below of the black edges. Since *m* is a multiple of *3*, in order to obtain half of the horizontal rows of the graphs where is equal to *m/2*, we consider [*m/2*], the integer part of *m/2* in the following Theorem.

Theorem 2. The eccentric connectivity index of *H*=*HPH*(*m,n*) is computed as follows

$$\xi(H) = \begin{cases} 3mn([\frac{m}{2}] + \frac{n}{2}) & if \quad \frac{n}{2} \le \frac{m}{3} \\ 3mn([\frac{m}{2}] + n - \frac{m}{3}) & if \quad \frac{n}{2} > \frac{m}{3}. \end{cases}$$

Proof. By symmetry of the graph all of the vertices have equal eccentricity. Let $u \in V(H)$ be a vertex on the first row and column of the graph. If $v \in V(H)$ has maximum distance from *u* then *v* must be located on the (*n/2* + *1*)-th row of the graph.

On this row of the graph the vertex such that is located on column *m/2*-th column of the graph has maximum distance from *u*. If *v* is located up of the black edges in Figure 3 then $d(u,v)=[\frac{m}{2}]+\frac{n}{2}$. Thus if $\frac{m}{2}\geq\frac{n}{2}$ then we have $\varepsilon(u)=[\frac{m}{2}]+\frac{n}{2}$. Now suppose that $\frac{m}{2}<\frac{n}{2}$. In this case for each row where is located below of $\frac{m}{3}$–th row of the graph increase of distance from *u* is equal 2. So,

$$\varepsilon(u)=[\frac{m}{2}]+\frac{m}{3}+2(\frac{n}{2}-\frac{m}{3}).$$

By using (*3*) the eccentric connectivity of *HPH*(*m*,*n*) is computed as

$$\xi(H)=\sum_{v\in V(H)}\deg(v)\varepsilon(v)=3mn\varepsilon(v).$$

The results can be obtained by replacing the value of $\varepsilon(v)$ where calculated in previous paragraph in two different cases. ■

3. Experimental Section

In the following table for some value of *m* and *n* the Wiener, Schultz, modified Schultz and the eccentric connectivity indices of H-phenylenic nanotorus will be computed by using exact formulas where are computed in previous section.

Table 1.

n	*m*	*W(H)*	*S(H)*	$S^*(H)$	$\xi(H)$
4	6	800	2508	7200	360
4	12	4768	14520	42912	1152
4	18	14496	43812	788616	2376
6	6	2376	7290	21384	756
6	12	12528	37908	112752	1944
6	18	36288	109350	326592	3888
8	12	25984	78384	233856	2880
8	18	71808	216072	646272	5616
10	6	10800	32760	97200	1980
10	12	46800	140940	421200	4320
12	6	12528	37908	127752	2808
12	12	76992	231624	692928	6048
12	15	140376	354564	1263384	7560
12	18	239760	516192	2157840	9720

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