Wiener and Schultz indices of V-Naphtalenic Nanotori

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The Wiener and Schultz indices of a molecule graph are two graph invariants in which based on distances in a connected graph. In this paper computation of the Wiener index of V-naphtalenic nanotori is purposed. As application the Schultz index of this graph will be calculated by using the Wiener index.

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1. Introduction

A topological index is a numeric quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. It most be structural invariant, i.e., it most not depends on the labeling or pictorial representation of the graph. Topological indices play an important role in structure property and structure activity studies, particularly when multivariate regression analysis, artificial neural networks, and pattern recognition are used as statistical tools.

Let G be an undirected connected graph without loops or multiple edges. The sets of vertices and edges of G are denoted by $V(G)$ and $E(G)$, respectively. 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 vertices $i, j \in V(G)$. The Wiener index of G is defined as follow [1]:

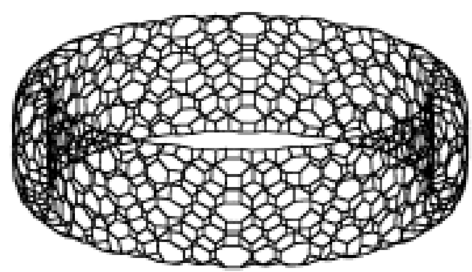
$$W(G) = \sum_{\{i,j\} \subseteq V(G)} d(i, j). \qquad (1)$$

Schultz [2] has introduced in 1989 a graph theoretical descriptor for characterizing alkanes by an integer number as follow:

$$MTI(G) = \sum_{i,j \in V(G)} \deg(i)(d(i, j) + A(i, j)). \qquad (2)$$

Where $deg(i)$ denotes vertex degree of I and $A(i,j)$ denotes the (i,j) entry of adjacency matrix of G. 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 [3-5]. 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 [6-8]. Therefore, further studies on mathematical and computational properties of the Schultz index and on its relation to other molecular descriptors are desirable. Recently computing topological indices of nanostructures have been the object of many papers [9-14]. Novel naphthylenic tori, generated by suitable modifications (that include the leapfrog procedure) of a square net embedded on the torus, are characterized by the ring spiral code, Wiener polynomial and spectral data. The wiener polynomial and wiener index of H-naphtalenic tori was computed by Diudea [15].



A V-Naphtalenic Nanotori for m=12 and n=100.

In this paper we obtain an exact formula for computation the Wiener and Schultz indices of V-naphtalenic nanotori.

2. Results and discussion

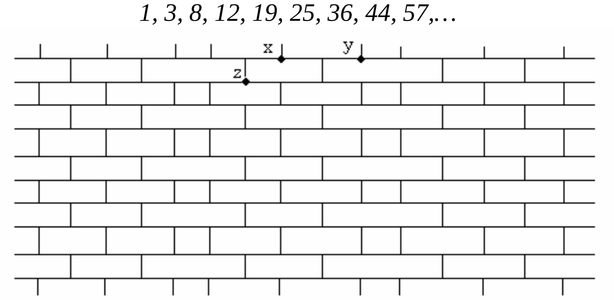
In this section at first we derive an exact formula for calculation the Wiener index of the graph V-naphtalenic nanotori. Then we compute the Schultz index of this graph, by using the obtained results for the Wiener index of V-naphtalenic nanotori. For this purpose we consider a coordinate representation of the graph as is shown in Fig. *2*. In this representation m and n denote the number of horizontal and vertical rows of vertices of the graph. Thus *m* must be multiple of *5* and *n* be even integer. We denote this lattice by *VNP(m, n)*. One can consider three different types of vertices in *VNP(m,n)* such as *x*, *y* and *z*.

The lattice *VNP(m, n)* can be embedded in to $G = C_m \times C_n$, the Cartesian product of the cycle of order *m* and the cycle of order *n* (see Fig. 3). Thus the Wiener index of *VNP(m,n)* can be computed by using Wiener index of *G* and considering deleting of some edges to obtain the lattice *VNP(m, n)* where increase the distance between some vertices of *VNP(m, n)*. The wiener index of *G* can be computed by well known formula for Cartesian product of two graphs [16] as follow:

$$W(C_m \times C_n) = \begin{cases} \dfrac{m^2n^2(m+n)}{8} & if \quad m \quad is \quad even \\ \dfrac{m^2n^2(m+n)-mn^2}{8} & if \quad m \quad is \quad odd. \end{cases} \qquad (3)$$

Therefore to calculation of the Wiener index of *VNP(m, n)* it is sufficient that increasing of the distance between vertices of the graph is computed if some of the edges of *G* are deleted to obtain *VNP(m, n)*. By symmetry of the graph it's sufficient that increasing of the distance between vertices *x* ,*y*, *z* and all of the other vertices of *VNP(m, n)* is calculated. Because other vertices of the graph are same as vertices *x*, *y* and *z*. At first we consider vertex *x* of *VNP(m, n)*. By deletion an edge of the graph, the distance between two end vertices of this edge increase from *1* to *3*. So the distance between *x* on the first row of *VNP(m, n)* and all of the other vertices of the graph may be increase or invariant. Thus the vertices of the graph in which their distance from *x* is changed must be indicated. The number of those vertices where are placed on the *i*-th row of the graph can be calculated as follow:

1, 3, 8, 12, 19, 25, 36, 44, 57,…



The extended lattice of VNP(15,10)

This sequence can represented as $\{S_i\}_{i=1}^{n}$ where $S_1=1$ and for $i \geq 2$

$$S_i = \begin{cases} S_{i-1} + i & if \quad i \quad is \quad even \\ S_{i-1} + \dfrac{3i+1}{4} & if \quad 4 \mid i-3 \\ S_{i-1} + \dfrac{3i-1}{4} & if \quad 4 \mid i-1. \end{cases}$$

Now we consider vertex *y* of *VNP(m, n)*. Similar to vertex *x* the following sequence indicate the number of vertices in which their distances from vertex *y* increase by deletion some edges of *G* to obtain *VNP(m, n)*.

2, 4, 8, 12, 20, 26, 36, 44, 58, 67,…

This sequence can be represented as $\{T_i\}_{i=1}^{n}$ where $T_1=2$ and for $i \geq 2$

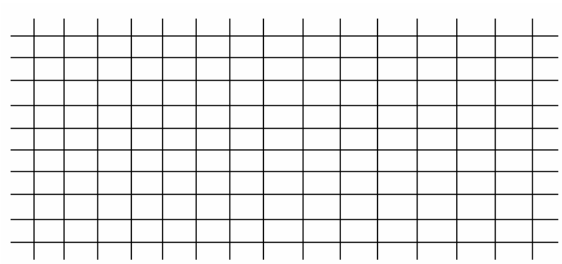
$$T_i = \begin{cases} T_{i-1} + i & if \quad i \quad is \quad even \\ T_{i-1} + \dfrac{3i-1}{4} & if \quad 4 \mid i-3 \\ T_{i-1} + \dfrac{3i+1}{4} & if \quad 4 \mid i-1. \end{cases}$$

At least we consider vertex *z* of the graph *VNP(m, n)*. The following sequence indicate the number of vertices of *VNP(m, n)* where their distance form *z* increase by deletion some edges of *G* to obtain *VNP(m, n)*.

1, 4, 7, 13, 18, 27, 34, 46, 55,…

This sequence can be represented as follow:

$$R_i = \begin{cases} R_{i-1} + \dfrac{3i}{2} & if \quad i \quad is \quad even \\ T_{i-1} + i & if \quad i \quad is \quad odd. \end{cases}$$



Extended lattice of $C_{10} \times C_{15}$

In continue the wiener index of the graph will be computed by using above sequences. To consideration two cases even or odd for m, put $\alpha=\frac{1-(-1)^m}{2}$. If *[r]* denotes the integer part of rational number r the Wiener index of *VNP(m, n)* is calculated in term of m and n.

Theorem 1. Let $n\le m$. The Wiener index of *H=VNP(m, n)* is computed as

$$W_1=\frac{mn}{120}(15mn(m+n)+(168-15\alpha)n-336+[\frac{n-2}{8}](336n-1728)-[\frac{n-2}{8}]^2(2640-216n+1152[\frac{n-2}{8}])$$
$$-[\frac{n-2}{4}](544-240n)-[\frac{n-2}{4}]^2(960-192n-512[\frac{n-2}{4}])+96[\frac{n}{8}](n+1)-[\frac{n}{8}]^2(816-216n+1152[\frac{n}{8}])).$$

If $n>m$ then

$$W_2=W1+\frac{mn}{120}([\frac{n-m}{8}](1056+336(m-n))-[\frac{n-m}{8}]^2(2208+216(m-n)+1152[\frac{n-m}{8}])+$$
$$[\frac{n-m}{4}](64+240(m-n))-[\frac{n-m}{4}]^2(576+192(m-n)+512[\frac{n-m}{4}])-[\frac{n-m+2}{8}](288-96(m-n))$$
$$+[\frac{n-m+2}{8}]^2(384+216(m-n)+1152[\frac{n-m+2}{8}])+120\alpha+168((1+48\alpha)m-(1+63\alpha)n).$$

Proof: Let $\delta(x)=\sum_{v\in V(H)}d_H(v,x)-\sum_{v\in V(G)}d_G(v,x)$, $\delta(y)=\sum_{v\in V(H)}d_H(v,y)-\sum_{v\in V(G)}d_G(v,y)$ and $\delta(z)=\sum_{v\in V(H)}d_H(v,z)-\sum_{v\in V(G)}d_G(v,z)$ for vertices x, y and z of H. Since the number of vertices of H where are same as x is $\frac{mn}{5}$ and number of vertices where are same as y or z is $\frac{2mn}{5}$ thus

$$W(H)=W(G)+\frac{mn}{5}(\delta(x)+2\delta(y)+2\delta(z)).\quad (4)$$

Now let $S_i^*=\sum_{j=1}^{i}S_j$, $T_i^*=\sum_{j=1}^{i}T_j$ and $R_i^*=\sum_{j=1}^{i}R_j$. If $n\le m$ then

$$S_i^*=\sum_{j=0}^{[\frac{i+3}{4}]-1}(6i+1)+\sum_{j=0}^{[\frac{i+1}{4}]-1}(6i+5)+\sum_{j=0}^{[\frac{i}{2}]-1}(2i+2)=[\frac{i+3}{4}](3[\frac{i+3}{4}]-2)+[\frac{i+1}{4}](3[\frac{i+1}{4}]+2)+[\frac{i}{2}]([\frac{i}{2}]+1).$$

$$T_i^*=\sum_{j=0}^{[\frac{i+3}{4}]-1}(6i+2)+\sum_{j=0}^{[\frac{i+1}{4}]-1}(6i+4)+\sum_{j=0}^{[\frac{i}{2}]-1}(2i+2)=[\frac{i+3}{4}](3[\frac{i+3}{4}]-1)+[\frac{i+1}{4}](3[\frac{i+1}{4}]+1)+[\frac{i}{2}]([\frac{i}{2}]+1).$$

$$R_i^*=\sum_{j=0}^{[\frac{i}{2}]}3i+\sum_{j=0}^{[\frac{i+1}{2}]}(2i-1)=\frac{3}{2}[\frac{i}{2}]([\frac{i}{2}]+1)+[\frac{i+1}{2}]^2.$$

By using (3) the Wiener index of G is computed as $W(G)=\frac{m^2n^2(m+n)-\alpha mn^2}{8}$. So by using *(4)* the Wiener index of H can be obtained as

$$W_1=W(G)+\frac{mn}{5}\sum_{i=1}^{\frac{n}{2}-1}(S_i^*+2T_i^*+2R_i^*)=\frac{mn}{120}(15mn(m+n)+(168-15\alpha)n-336+[\frac{n-2}{8}](336n-1728)$$
$$-[\frac{n-2}{8}]^2(2640-216n+1152[\frac{n-2}{8}])-[\frac{n-2}{4}](544-240n)-[\frac{n-2}{4}]^2(960-192n-512[\frac{n-2}{4}])+$$
$$96[\frac{n}{8}](n+1)-[\frac{n}{8}]^2(816-216n+1152[\frac{n}{8}])).$$

Now suppose $n>m$. In this case the Wiener index of H calculated as follow

$$W_2=W(G)+\frac{mn}{5}(\sum_{i=1}^{\frac{n}{2}-1}(S_i^*+2T_i^*+2R_i^*)-\sum_{i=1}^{\frac{n-m}{2}-1}(S_i^*+2T_i^*+2R_i^*))=W1+\frac{mn}{120}([\frac{n-m}{8}](1056+$$
$$336(m-n))-[\frac{n-m}{8}]^2(2208+216(m-n)+1152[\frac{n-m}{8}])+[\frac{n-m}{4}](64+240(m-n))-[\frac{n-m}{4}]^2$$
$$(576+192(m-n)+512[\frac{n-m}{4}])-[\frac{n-m+2}{8}](288-96(m-n))+[\frac{n-m+2}{8}]^2(384+216(m-n)$$
$$+1152[\frac{n-m+2}{8}])+120\alpha+168((1+48\alpha)m-(1+63\alpha)n).$$

This completes the proof.

In the following Corollary the Schultz index of *VNP(m,n)* nanotori will be calculated by using the Wiener index of this graph where is computed in Theorem *1*.

Corollary 1. The Schultz index of *H=VNP(m,n)* is computed as follow

$$MTI(H)=6W(H)+9mn$$

Proof: Let for $i\in V(H)$, deg *(i)* denotes the vertex degree of i. Thus *deg(i)=3* for all of the vertices of *H*. So by using *(2)* the Schultz index of the graph is calculated as

$$MTI(H)=\sum_{i,j\in V(H)}\deg(i)(d_H(i,j)+A(i,j))=3\sum_{i,j\in V(H)}d_H(i,j)+3\sum_{i,j\in V(H)}A(i,j)$$
$$=3\times2\times W(G)+3\times2\times|E(G)|=6W(H)+9mn.$$

This completes the proof.

3. Experimental section

In the Table *1* we obtain the Wiener and Schultz indices of V-naphtalenic nanotori for some values of m and n by using Theorem *1* and Corollary *1*.

Table 1. The number of Wiener and Schultz indices of V-Naphtalenic Nanotori.

m	*n*	*W(H)*	*MTI(H)*	*m*	*n*	*W(H)*	*MTI(H)*
5	2	85	600	15	4	8688	52668
5	4	496	3156	15	8	44352	267192
5	6	1503	9432	15	12	124992	751572
5	8	3408	20808	15	16	273216	1641456
5	10	6505	39480	15	20	513360	3082860
10	2	600	3780	20	10	160080	962280
10	6	7824	47484	20	20	965600	5797200
10	10	30040	181140	20	30	3037920	18232920
10	14	77056	463596	30	20	2498400	14995800
10	20	215120	1292520	30	30	7336440	44026740

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