Some topological indices of V –Phenylenic nanotube and nanotori

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In this paper, several topological indices are investigated in linear [n]-phenylenic, lattice of $C_4C_6C_8[p,q]$, $TUC_4C_6C_8[p,q]$ nanotube and $C_4C_6C_8[p,q]$ nanotori: Randić connectivity index, Sum-connectivity index, Harmonic index, augmented Zagreb index and Zagreb polynomials.

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1. Introduction

In the whole paper, G is a simple graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. The vertices in G are connected by an edge if there exists an edge $uv \in E(G)$ connecting the vertices u and v in G such that $u,v \in V(G)$. For any $u \in V(G)$, d_u represents the number of edges incident to u, called the degree of the vertex u in G. In chemical graphs, the vertices of the graph correspond to the atoms of molecules while the edges represent chemical bonds [1]. Numbers encoding certain structural features of organic molecules and derived from the corresponding molecular graph, are called graph invariants or more commonly topological indices. The connectivity index introduced in 1975 by Milan Randić [2], has shown this index to reflect molecular branching. Randić index (Randić molecular connectivity index) was defined as $\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u d_v}}$.

In 2009, Zhou and Trinajstić [3] proposed another connectivity index, named the Sum-connectivity index $X(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_{u+}d_v}}$. The Harmonic index of graph G is defined [4, 5] as $H(G)=\sum_{uv\in E(G)}\frac{2}{d_u+d_v}$. The augmented Zagreb index (AZI index for short) of G proposed by Furtula et al. [6] is defined as $\mathrm{AZI(G)}=\sum_{uv\in E(G)}\left(\frac{d_u d_v}{d_u+d_{v-2}}\right)^3$. Recently, Fath-Tabar[7]put forward the first and the second Zagreb polynomials of the graph G, defined respectively as $\mathrm{ZG_1(G,x)}=\sum_{uv\in E(G)}x^{d_u+d_v}$ and $\mathrm{ZG_2(G,x)}=\sum_{uv\in E(G)}x^{d_u d_v}$, where x is a dummy variable. The aim of this paper is to compute some topological indices of linear [n]-phenylenic, lattice of $C_4C_6C_8[p,q]$, $TUC_4C_6C_8[p,q]$ nanotube and $C_4C_6C_8[p,q]$ nanotori. In recent years, there has been considerable interest in general problems of determining topological indices [8-14].

2. Main results and discussion

The aim of this section, at first, is to compute some topological indices of the molecular graph of linear [n]-phenylenic as depicted in Fig. 1.

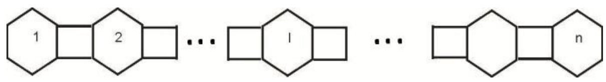

Fig. 1. The molecular graph of a linear [n]-phenylenic.

Remark 2.1 It is easy to see that $\mathrm{T}=\mathrm{T}[n]$ has $6n$ vertices and $8n-2$ edges. We partition the edges of T into three subsets $E_1(\mathrm{T})$, $E_2(\mathrm{T})$ and $E_3(\mathrm{T})$. Table 1 shows the number of three types of edges.

Table 1. The number of three types of edges of the graph T

(d_u,d_v) where $uv\in E(T)$	Total Number of Edges
$E_1=[2,2]$	6
$E_2=[2,3]$	$4n-4$
$E_3=[3,3]$	$4n-4$

From this table, we give an explicit computing formula for some indices of a linear [n]-phenylenic, as shown in above graph.

Theorem 2.2 *Consider the graph* T *of a linear* [n]-*phenylenic. Then*

(i) $\chi(T)=\sum_{uv\in E(T)}\frac{1}{\sqrt{d_u d_v}}=\frac{|E_1|}{\sqrt{4}}+\frac{|E_2|}{\sqrt{6}}+\frac{|E_3|}{\sqrt{9}}=\frac{6}{2}+\frac{4n-4}{\sqrt{6}}+\frac{4n-4}{3}=\left(\frac{4+2\sqrt{6}}{3}\right)n+\frac{5-2\sqrt{6}}{3}.$

(ii) $X(T)=\sum_{uv\in E(T)}\frac{1}{\sqrt{d_u+d_v}}=\frac{|E_1|}{\sqrt{4}}+\frac{|E_2|}{\sqrt{5}}+\frac{|E_3|}{\sqrt{6}}=\frac{6}{2}+\frac{4n-4}{\sqrt{5}}+\frac{4n-4}{\sqrt{6}}=4\left(\frac{\sqrt{5}}{5}+\frac{\sqrt{6}}{6}\right)n+(3-\frac{4\sqrt{5}}{5}-\frac{2\sqrt{6}}{3}).$

(iii) $H(T)=\sum_{uv\in E(T)}\frac{2}{d_u+d_v}=\frac{2|E_1|}{4}+\frac{2|E_2|}{5}+\frac{2|E_3|}{6}=\frac{2(6)}{4}+\frac{2(4n-4)}{5}+\frac{2(4n-4)}{6}=\frac{44}{15}n+\frac{1}{15}.$

(iv) $AZI(T)=\sum_{uv\in E(T)}\left(\frac{d_u d_v}{d_u+d_v-2}\right)^3=|E_1|\left(\frac{4}{2}\right)^3+|E_2|\left(\frac{6}{3}\right)^3+|E_3|\left(\frac{9}{4}\right)^3=(6)\left(\frac{4}{2}\right)^3+(4n-4)$

$$\left(\frac{6}{3}\right)^3+(4n-4)\left(\frac{9}{4}\right)^3=\frac{1241}{16}n-\frac{473}{16}.$$

In continue of this section, we see the following figures.

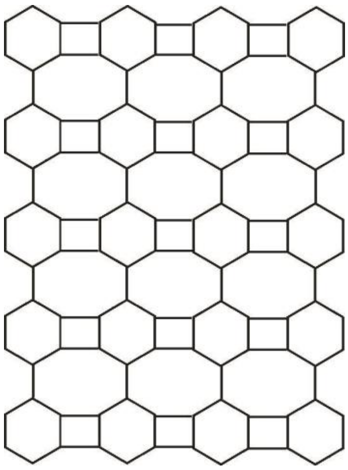

Fig. 2. The 2-D graph lattice of $C_4C_6C_8[4,5]$

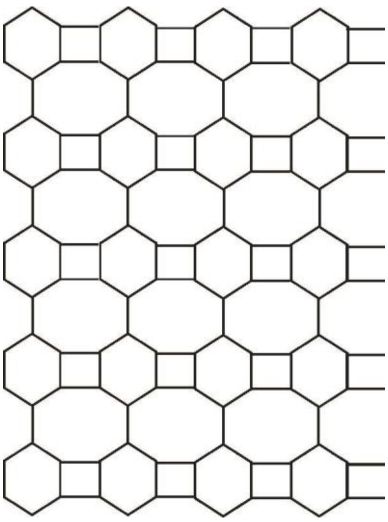

Fig. 3. The 2-D graph lattice $TUC_4C_6C_8[4,5]$ nanotube

Remark 2.3 [15] We now consider the molecular graph $G=C_4C_6C_8[p,q]$, Fig. 2. It is easy to see that $|V(G)|=6pq$ and $|E(G)|=9pq-2q-p$. We partition the edges of G into three subsets $E_1(\mathrm{G})$, $E_2(\mathrm{G})$ and $E_3(\mathrm{G})$. The number of three types of edges is shown in Table 2.

Table 2. The number of three types of edges of the graph G

(d_u,d_v) where $uv\in E(G)$	Total Number of Edges
$E_1=[2,2]$	2q + 4
$E_2=[2,3]$	4p + 4q − 8
$E_3=[3,3]$	9pq − 8q − 5p + 4

From this table, we give an explicit computing of some indices of G (Fig. 2).

Theorem 2.4 *Consider the graph G of lattice $C_4C_6C_8[p,q]$. Then*

(i) $\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u d_v}}=\frac{|E_1|}{\sqrt{4}}+\frac{|E_2|}{\sqrt{6}}+\frac{|E_3|}{\sqrt{9}}=\frac{2q+4}{2}+\frac{4p+4q-8}{\sqrt{6}}+\frac{9pq-8q-5p+4}{3}=3pq+\left(\frac{2\sqrt{6}-5}{3}\right)(p+q)+\frac{10-4\sqrt{6}}{3}.$

(ii) $X(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u+d_v}}=\frac{|E_1|}{\sqrt{4}}+\frac{|E_2|}{\sqrt{5}}+\frac{|E_3|}{\sqrt{6}}=\frac{2q+4}{2}+\frac{4p+4q-8}{\sqrt{5}}+\frac{9pq-8q-5p+4}{\sqrt{6}}=\frac{3\sqrt{6}}{2}pq+\left(\frac{4\sqrt{5}}{5}-\frac{5\sqrt{6}}{6}\right)p+\left(1+\frac{4\sqrt{5}}{5}-\frac{4\sqrt{6}}{3}\right)q+(2+\frac{2\sqrt{6}}{3}-\frac{8\sqrt{5}}{5}).$

(iii) $H(G)=\sum_{uv\in E(G)}\frac{2}{d_u+d_v}=\frac{2|E_1|}{4}+\frac{2|E_2|}{5}+\frac{2|E_3|}{6}=\frac{2(2q+4)}{4}+\frac{2(4p+4q-8)}{5}+\frac{2(9pq-8q-5p+4)}{6}=3pq-\frac{1}{15}(p+q)+\frac{2}{15}.$

(iv) $\mathrm{AZI(G)}=\sum_{uv\in E(G)}\left(\frac{d_u d_v}{d_u+d_v-2}\right)^3=|E_1|\left(\frac{4}{2}\right)^3+|E_2|\left(\frac{6}{3}\right)^3+|E_3|\left(\frac{9}{4}\right)^3=(2\mathrm{q}+4)\left(\frac{4}{2}\right)^3+(4\mathrm{p}+4\mathrm{q}-8)\left(\frac{6}{3}\right)^3+(9\mathrm{pq}-8\mathrm{q}-5\mathrm{p}+4)\left(\frac{9}{4}\right)^3=\frac{6561}{64}pq-\frac{1597}{64}p-\frac{345}{8}q+\frac{217}{16}.$

Remark 2.5 We now consider the molecular graph $K=TUC_4C_6C_8[p,q]$, Fig. 3. It is easy to see that $|V(K)|=6pq$ and $|E(K)|=9pq-p$. We partition the edges of nanotube K into two subsets $E_1(\mathrm{K})$, $E_2(\mathrm{K})$ and compute the total number of edges for the 2-dimensional of graph K (Table 3).

Table 3. The number of two types of edges of the graph K

(d_u,d_v) where $uv\in E(K)$	Total Number of Edges
$E_1=[2,3]$	$4p$
$E_2=[3,3]$	$9pq-5p$

In the following theorem we compute some indices of K (Fig. 3).

Theorem 2.6 *Consider the graph* K *of* $TUC_4C_6C_8[p,q]$ *nanotube. Then*

(i) $\chi(K)=\sum_{uv\in E(K)}\frac{1}{\sqrt{d_ud_v}}=\frac{|E_1|}{\sqrt{6}}+\frac{|E_2|}{\sqrt{9}}=\frac{4p}{\sqrt{6}}+\frac{9pq-5p}{\sqrt{9}}=3pq+\left(\frac{2\sqrt{6}-5}{3}\right)p.$

(ii) $X(K)=\sum_{uv\in E(K)}\frac{1}{\sqrt{d_u+d_v}}=\frac{|E_1|}{\sqrt{5}}+\frac{|E_2|}{\sqrt{6}}=\frac{4p}{\sqrt{5}}+\frac{9pq-5p}{\sqrt{6}}=\frac{3\sqrt{6}}{2}pq+\left(\frac{4\sqrt{5}}{5}-\frac{5\sqrt{6}}{6}\right)p.$

(iii) $H(K)=\sum_{uv\in E(K)}\frac{2}{d_u+d_v}=\frac{2|E_1|}{5}+\frac{2|E_2|}{6}=\frac{2(4p)}{5}+\frac{2(9pq-5p)}{6}=3pq-\frac{1}{15}p.$

(iv) $\mathrm{AZI(K)}=\sum_{uv\in E(K)}\left(\frac{d_ud_v}{d_u+d_v-2}\right)^3=|E_1|\left(\frac{6}{3}\right)^3+|E_2|\left(\frac{9}{4}\right)^3=(4\mathrm{p})\left(\frac{6}{3}\right)^3+(9pq-5p)\left(\frac{9}{4}\right)^3=\frac{6561}{64}pq-\frac{1597}{64}.$

In the end of this paper, we can see the molecular graph of $L=C_4C_6C_8[p,q]$ nanotorus in the Fig. 4. It is easily seen that |E(L)|=9pq.

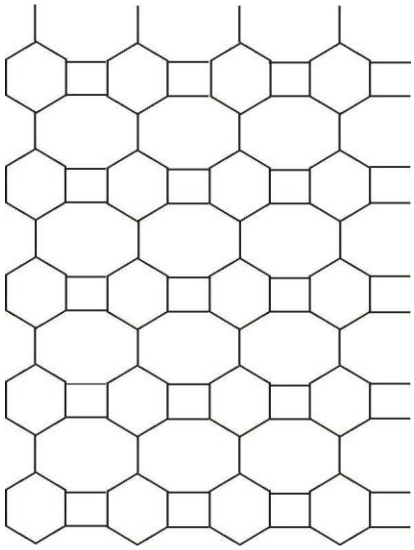

Fig. 4. The 2-D graph lattice of $C_4C_6C_8[4,5]$ *nanotori.*

Lemma 2.7 *For an arbitrary graph G,*

(a) $\chi(G)=\frac{1}{k}|E(G)|$ *if and only if G be a k-regular graph.*

(b) $X(G)=\frac{1}{\sqrt{2k}}|E(G)|$ *if and only if G be a k-regular graph.*

(c) $H(G)=\frac{1}{k}\,|E(G)|$ *if and only if G be a k-regular graph.*

Proof. It is easy to check according to Fig. 4.

Note 2.8 *By using Lemma 2.7, consider the Fig. 4. One can see that the graph is 3-regular, so*$\chi(L)=3pq$, $X(L)=\frac{3\sqrt{6}}{2}pq, H(L)=3pq$.

Theorem 2.9 *The first and second Zagreb polynomials of above graphs are equal to:*

(i) $\mathrm{ZG_1(G,x)=(9pq-8q-5p+4)x^6+(4p+4q-8)x^5+(2q+4)x^4}$,

(ii) $\mathrm{ZG_2(G,x)=(9pq-8q-5p+4)x^9+(4p+4q-8)x^6+(2q+4)x^4}$,

(iii) $\mathrm{ZG_1(K,x)=(9pq-5p)x^6+(4p)x^5}$,

(iv) $\mathrm{ZG_2(K,x)=(9pq-5p)x^9+(4p)x^6}$,

(v) $\mathrm{ZG_1(L,x)=(9pq)x^6}$,

(vi) $\mathrm{ZG_2(L,x)=(9pq)x^9}$.

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