Scientific paper

Some Connectivity Indices and Zagreb Index of Polyhex Nanotubes

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Received: 10-02-2012

Abstract

Several topological indices are investigated in polyhex nanotubes: Randić connectivity index, sum-connectivity index, atom-bond connectivity index, geometric-arithmetic index, First and Second Zagreb indices and Zagreb polynomials. Formulas for calculating the above topological descriptors in polyhex zigzag $TUZC_6[m,n]$ and armchair $TUAC_6[m,n]$ nanotube families are given.

Keywords: Polyhex Nanotubes, Randić connectivity index, Sum-connectivity index, Geometric-arithmetic index, Atom-bond connectivity index, Zagreb polynomial.

1. Introduction

Let G is an arbitrary simple, connected, graph, with the vertex set $V(G)$ and edge set $E(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of molecules while the edges represent chemical bonds.[1,2] Numbers encoding certain structural features of organic molecules and derived from the corresponding molecular graph, are called *graph invariants* or more commonly *topological indices*. One of the oldest graph invariants is the *Wiener index*, $W(G)$, introduced by the chemist *Harold Wiener*[2] in 1947. It is defined as the sum of topological distances $d(u,v)$ between any two atoms in the molecular graph

$$W(G) = \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} d(u,v)$$

The *Hosoya polynomial* of G is defined as

$$H(G,x) = \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} x^{d(u,v)}$$

where summation runs over all the unordered pairs u,v of distinct vertices in G. The Hosoya polynomial was introduced by *Haruo Hosoya* in 1988.[4,5]

An important topological index introduced more than thirty years ago by *I. Gutman* and *N. Trinajstić* is the *First Zagreb index* $Zg_1(G)$.[6–8] It is defined as the sum of squares of the vertex degrees d_u and d_v of vertices u and v in G

$$Zg_1(G) = \sum_{v\in V(G)} (d_v)^2 = \sum_{e=uv\in E(G)} (d_u + d_v)$$

Some basic properties of $Zg_1(G)$ can be found in some recent papers.[6,7,9,10]

Another topological index is the *Second Zagreb index* $Zg_2(G)$ and it is defined as[11,12]

$$Zg_2(G) = \sum_{e=uv\in E(G)} (d_u \times d_v)$$

According to the above Zagreb indices, the *First Zagreb polynomial* $Zg_1(G,x)$ and the *Second Zagreb polynomial* $Zg_2(G,x)$ have been defined. They are defined as[13–17]

$$Zg_1(G,x) = \sum_{e=uv\in E(G)} x^{d_u + d_v}$$

and

$$Zg_1(G,x) = \sum_{e=uv\in E(G)} x^{d_u d_v}$$

Milan Randić proposed in 1975 a structural descriptor called the *branching index*[1] that later became the well-known *Randić connectivity index*; it is defined on the ground of vertex degrees

$$\chi(G)=\sum_{e=uv\in E(G)}\frac{1}{\sqrt{d_u d_v}}$$

In 2008, *B. Zhou* and *N. Trinajstić*[18,19] proposed another connectivity index, named the *Sum-connectivity index X(G)*

$$X(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u+d_v}}$$

Recently, *D. Vukičević* and *B. Furtula*[27] introduced a topological index named the *Geometric-Arithmetic index GA(G)*

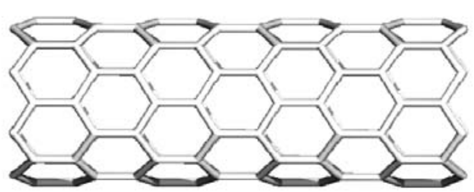
$$GA(G)=\sum_{e=uv\in E(G)}\frac{2d_u d_v}{\sqrt{d_u+d_v}}$$

Furtula also introduced a connectivity index named the *Atom-Bond Connectivity index ABC(G).*[15,19,20] The above authors gave the lower and upper bounds for the *GA* index, determined the trees with the minimum, the second and the third minimum, as well as the second and the third maximum *GA* indices.[20] The Atom-Bond Connectivity index is defined as

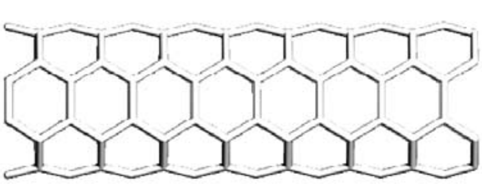
$$ABC(G)=\sum_{e=uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}.$$

Predicting physico-chemical properties such as entropy, enthalpy of vaporization, enthalpy of formation and a centric factor, was proved[20,21] to be better by *GA* index than by the Randić connectivity index.

In this paper, we investigate the above presented topological indices in two families of polyhex nanotubes: *zigzag* $TUZC_6$ (or HC_6) and *armchair* $TUAC_6$ (or VC_6), respectively (see Figure 1).



$TUZC_6[8,7]$



$TUAC_6[8,7]$

Figure 1. The 3D Lattice of Zigzag (up) and Armchair (down) polyhex nanotubes.

2. Main Results and Discussion

Let denote the number of hexagons in the first row/column of the 2D-lattice of HC_6 (Figure 2) and VC_6 (Figure 3) by *m* and n, respectively. For other related research and historical details, see refs.[17,22–29] Before presenting the main results, let us introduce some definitions.

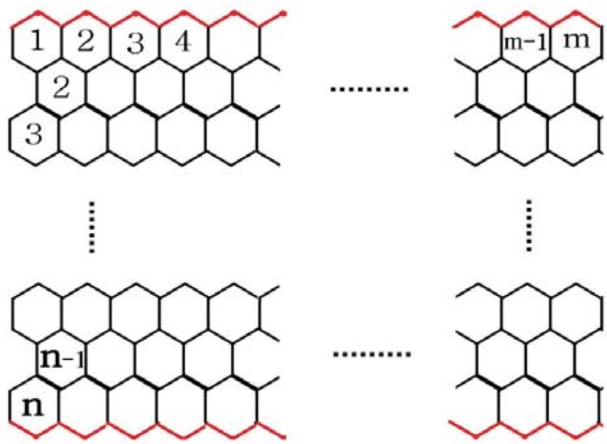


Figure 2. The 2-Dimensional Lattice of $G=HC_6[m,n]$.

Definition 2.1. Let *G* and d_v $(1\le d_v\le n\text{-}1)$ be a simple connected molecular graph and the vertex degrees of vertices/atom *v* in *G*. We divide the vertex set *V(G)* and edge set *E(G)* of *G* into several partitions based on d_v ($\forall v \in$ ((G)) as follows

$$\forall k,\delta\le k\le\Delta,\quad V_k=\{v\in V(G)\,|\,d_v=k\},$$

$$\forall i,2\delta\le i\le 2\Delta\quad E_i=\{e=uv\in E(G)\,|\,d_v+d_u=i\}$$

$$\forall j,\delta^2\le j\le\Delta^2,\quad E_j^*=\{e=uv\in E(G)\,|\,d_v\times d_u=j\}$$

where δ and Δ are the minimum and maximum, respectively, of d_v for all $v\in V$(G).

In polyhex nanotubes, the degree of an arbitrary vertex/atom of a molecular graph is equal to 1, 2 or 3. Therefore, we have three partitions of *V(G)*

$$V_3=\{v\in V(G)\,|\,d_v=3\}$$

$$V_2=\{v\in V(G)\,|\,d_v=2\}$$

$$V_2=\{v\in V(G)\,|\,d_v=2\}$$

Since the hydrogen atoms in molecular graphs (i.e., vertices of degree 1) are often omitted, thus we will ignore the vertex set V_1. Next, the three partitions of *E(G)* are as follows

$$E_6=E_9^*=\{u,v\in V(G)\,|\,d_u=d_v=3\}$$

$$E_5=E_6^*=\{u,v\in V(G)\,|\,d_u=3\&d_v=2\}$$

$$E_4=E_4^*=\{u,v\in V(G)\,|\,d_u=d_v=2\}$$

By these preliminaries, we have following theorems.

Theorem 1. Let G be the zigzag nanotubes $HC_6[m,n]$ ($\forall m,n \in \mathbb{N}$) the following indices are calculated by formulas:

Randić Connectivity index

$$\chi(HC_6[m,n]) = mn + 2m\left(\frac{\sqrt{6}-1}{3}\right)$$

Sum-Connectivity index

$$X(HC_6[m,n]) = \left(\frac{\sqrt{6}}{2}\right)mn + \left(\frac{4\sqrt{5}}{5} - \frac{\sqrt{6}}{3}\right)m$$

Atom-Bond Connectivity index

$$ABC(HC_6[m,n]) = 2mn + 2m\left(\sqrt{2} - \frac{2}{3}\right)$$

Geometric-Arithmetic index

$$GA(HC_6[m,n]) = 9\sqrt{6}mn + 6m\left(\frac{8\sqrt{5}}{5} - \sqrt{6}\right).$$

Proof. Consider the zigzag nanotubes $G=HC_6[m,n]$ (Figure 2). The number of vertices in this nanotube is equal to $|V(HC_6[m,n])| = 2m(n+1)$ ($\forall m,n \in \mathbb{N}$) Since $|V_2| = m + m$ and $|V_3| = 2mn$, thus $|E(HC_6[m,n])| = 2(2m) + 3(2m)/2 = 3mm + 2m$.

We marked the edges of E_5, E_6^* by red color and the edges of E_6, E_9^* by black color in Figure 2. The size of set E_5 (or E_6^*) is equal to $2|V_2| = 4m$ and the size of set E_6 (or E_9^*) is equal to $3mn - 2m$. Then, we have following computations, for all $m,n \geq 1$.

$$\begin{aligned}\chi(HC_6[m,n]) &= \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u d_v}} \\ &= \sum_{u_1v_1\in E_9^*} \frac{1}{\sqrt{d_{u_1}d_{v_1}}} + \sum_{u_2v_2\in E_6^*} \frac{1}{\sqrt{d_{u_2}d_{v_2}}} \\ &= \frac{|E_9^*|}{\sqrt{9}} + \frac{|E_6^*|}{\sqrt{6}} = \frac{3mn-2m}{\sqrt{9}} + \frac{4m}{\sqrt{6}} \\ &= mn + 2m\left(\frac{\sqrt{6}-1}{3}\right),\end{aligned}$$

$$\begin{aligned}X(HC_6[m,n]) &= \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\ &= \sum_{u_1v_1\in E_6} \frac{1}{\sqrt{d_{u_1}+d_{v_1}}} + \sum_{u_2v_2\in E_5} \frac{1}{\sqrt{d_{u_2}+d_{v_2}}} \\ &= \frac{|E_6|}{\sqrt{6}} + \frac{|E_5|}{\sqrt{5}} = \frac{3mn-2m}{\sqrt{6}} + \frac{4m}{\sqrt{5}} \\ &= \left(\frac{\sqrt{6}}{2}\right)mn + \left(\frac{4\sqrt{5}}{5} - \frac{\sqrt{6}}{3}\right)m,\end{aligned}$$

$$\begin{aligned}ABC(HC_6[m,n]) &= \sum_{e=uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ &= |E_6|\sqrt{\frac{6-2}{9}} + |E_5|\sqrt{\frac{5-2}{6}} \\ &= (3mn-2m)\sqrt{\frac{4}{9}} + 4m\sqrt{\frac{3}{6}}n \\ &= 2mn + 2m\left(\sqrt{2} - \frac{2}{3}\right),\end{aligned}$$

$$\begin{aligned}GA(HC_6[m,n]) &= \sum_{e=uv\in E(G)} \frac{2d_u d_v}{\sqrt{d_u+d_v}} \\ &= |E_9^*|\frac{18}{\sqrt{6}} + |E_6^*|\frac{12}{\sqrt{5}} \\ &= (3mn-2m)\left(\frac{18}{\sqrt{6}}\right) + 4m\left(\frac{12}{\sqrt{5}}\right) \\ &= 9\sqrt{6}mn + 6m\left(\frac{8\sqrt{5}}{5} - \sqrt{6}\right).\end{aligned}$$

Thus, the proof of Theorem 1 is completed.

Theorem 2. Let G be the zigzag nanotubes $HC_6[m,n]$. Then,

(a) The First Zagreb polynomial of G is of the form $Zg_1(HC_6[m,n],x) = (3mn - 2m)\,x^6 + 4\,mx^5$ while the First Zagreb index is $Zg_1(HC_6[m,n]) = 18mn + 8m$.

(b) The Second Zagreb polynomial of G is equal to $Zg_2(HC_6[m,n],y) = (3mn - 2m)\,y^9 + 4my^6$ and the Second Zagreb index is $Zg_2(HC_6[m,n]) = 27mn + 6m$.

Proof. Let rewrite the Zagreb polynomials according to Definition 2.1 as

$$Zg_1(G,x) = \sum_{e=uv\in E(G)} x^{d_u+d_v} = \sum_{uv\in E_6} x^6 + \sum_{uv\in E_5} x^5$$

$$Zg_2(G,y) = \sum_{e=uv\in E(G)} y^{d_u+d_v} = \sum_{uv\in E_9^*} y^9 + \sum_{uv\in E_6^*} y^6.$$

Next, $|E_6| = |E_9^*| = 3mn - 2m$ and $|E_5| = |E_6^*| = 4m$ (see the proof of Theorem 1). Thus, the Zagreb polynomials of $HC_6[m,n]$ can be written immediately. Thus, the First and Second Zagreb polynomials of $HC_6[m,n]$ are equal to

$$Zg_1(HC_6[m,n],x) = (3mn - 2m)\,x^6 + 4mx^5,$$

$$Zg_2(HC_6[m,n],y) = (3mn - 2m)\,y^9 + 4my^6.$$

The corresponding Zagreb indices are calculated as the first derivative of the above polynomials, in $x = 1$,

$$Zg_1(HC_6[m,n]) = \left.\frac{\partial Zg_1(G,x)}{\partial x}\right|_{x=1} = (3mn - 2m)\times 6 + 4m\times 5 = 18mn + 8m,$$

$$Zg_2(HC_6[m,n]) = \left.\frac{\partial Zg_2(G,y)}{\partial y}\right|_{y=1} = (3mn - 2m) \times 9 + 4m \times 6 = 27mn + 6m.$$

Thus proving the Theorem 2.

Theorem 3. Consider the armchair polyhex nanotubes $H=VC_6[m,n]$ ($\forall m,n \in \mathbb{N}$) the following indices are calculated by formulas:

Randić Connectivity index

$$\chi(VC_6[m,n]) = \left(n + \frac{\sqrt{6}-1}{3} + \frac{1}{2}\right)m$$

Sum-Connectivity index

$$X(VC_6[m,n]) = \left(\frac{\sqrt{6}n}{2} + \frac{2\sqrt{5}}{5} - \frac{\sqrt{6}}{6} + \frac{1}{2}\right)m$$

Atom-Bond Connectivity index

$$ABC(VC_6[m,n]) = \left(2n + \frac{3\sqrt{2}}{2} - \frac{2}{3}\right)m$$

Geometric-Arithmetic index

$$GA(VC_6[m,n]) = \left(9\sqrt{6}n + \frac{24\sqrt{5}}{5} - 3\sqrt{6} + 4\right)m$$

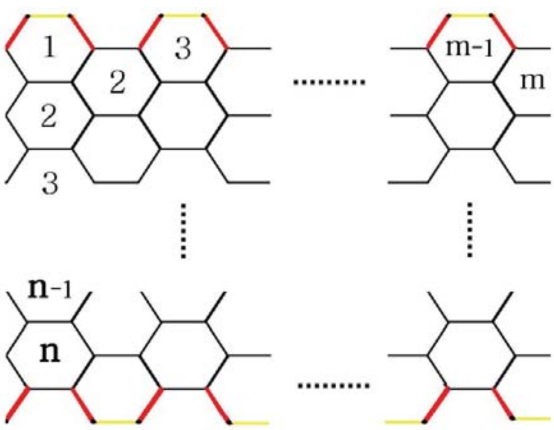


Figure 3. The 2-Dimensional Lattice of $H=VC_6[m,n]$.

Proof. Let H be armchair polyhex nanotubes $VC_6[m,n]$ ($m,n \in \mathbb{N}$) There are $2m(n+1)$ vertices in the graph $H = VC_6[m,n]$. According to Figure 3, $|V_2| = 2\,m/2 + 2\,m/2 = 2m$ and $|V_3| = 2mn$. This implies that for every armchair polyhex $H = VC_6[m,n]$ nanotubes the number of edge is $|E(VC_6[m,n])| = 2(2m) + 3(2m)/2 = 3mm + 2m$.

In Figure 3, we marked the members of E_4, E_4^* by yellow color, the members of E_5, E_6^* by red color and the members of E_6, E_9^* by black color. Then, the size of sets E_4 (or E_4^*), E_5 (or E_9^*) and E_6 (or E_9^*) are equal to $m/2 + m/2$, $2m$ $(= 2|E_4|)$ and $3mn$-m, respectively.

Thus, the formulas for the topological indices in $H=VC_6[m,n]$ ($\forall m,n \in \mathbb{N}$) will be

$$\chi(VC_6[m,n]) = \sum_{e=uv\in E(H)} \frac{1}{\sqrt{d_u d_v}}$$
$$= \sum_{u_1v_1\in E_9^*} \frac{1}{\sqrt{d_{u_1} d_{v_1}}} + \sum_{u_2v_2\in E_6^*} \frac{1}{\sqrt{d_{u_2} d_{v_2}}} + \sum_{u_3v_3\in E_4^*} \frac{1}{\sqrt{d_{u_3} d_{v_3}}}$$
$$= \frac{|E_9^*|}{\sqrt{9}} + \frac{|E_6^*|}{\sqrt{6}} + \frac{|E_4^*|}{\sqrt{4}}$$
$$= \left(\frac{3mn-m}{3}\right) + \frac{\sqrt{6}}{6}(2m) + \frac{m}{2}$$
$$= mn + \left(\frac{\sqrt{6}-1}{3} + \frac{1}{2}\right)m$$

$$X(VC_6[m,n]) = \sum_{e=uv\in E(H)} \frac{1}{\sqrt{d_u d_v}}$$
$$= \sum_{u_1v_1\in E_6} \frac{1}{\sqrt{d_{u_1} d_{v_1}}} + \sum_{u_2v_2\in E_5} \frac{1}{\sqrt{d_{u_2} d_{v_2}}} + \sum_{u_3v_3\in E_4} \frac{1}{\sqrt{d_{u_3} d_{v_3}}}$$
$$= \frac{|E_6|}{\sqrt{6}} + \frac{|E_5|}{\sqrt{5}} + \frac{|E_4|}{\sqrt{4}}$$
$$= \frac{3mn-m}{\sqrt{6}} + \frac{2m}{\sqrt{5}} + \frac{m}{2}$$
$$= \frac{\sqrt{6}}{2}mn + \left(\frac{2\sqrt{5}}{5} - \frac{\sqrt{6}}{6} + \frac{1}{2}\right)m$$

$$ABC(VC_6[m,n]) = |E_6|\sqrt{\frac{6-2}{9}} + |E_5|\sqrt{\frac{5-2}{6}} + |E_4|\sqrt{\frac{4-2}{4}}$$
$$= |E_6|\left(\frac{2}{3}\right) + (|E_5| + |E_4|)\left(\frac{\sqrt{2}}{2}\right)$$
$$= \left(\frac{6mn-2m}{3}\right) + 3m\frac{\sqrt{2}}{2}$$
$$= 2mn + \left(\frac{3\sqrt{2}}{2} - \frac{2}{3}\right)m$$

$$GA(VC_6[m,n]) = |E_9^*|\frac{18}{\sqrt{6}} + |E_6^*|\frac{12}{\sqrt{5}} + |E_5^*|\frac{8}{\sqrt{4}}$$
$$= 3\sqrt{6}(3mn - m) + 2m\left(\frac{12\sqrt{5}}{5}\right) + 4m$$
$$= 9\sqrt{6}mn + \left(\frac{24\sqrt{5}}{5} - 3\sqrt{6} + 4\right)m$$

So, the proof of Theorem 3 is completed.

Theorem 4. Let H be $VC_6[m,n]$ armchair polyhex nanotubes. Then:

(c) The First Zagreb polynomial of H is equal to

$$Zg_1(VC_6[m,n],t) = (3mn - m)t^6 + (2m)t^5 + (m)t^4$$

while the First Zagreb index is $Zg_1(VC_6[m,n]) = 18mn + 8m$.

(d) The Second Zagreb polynomial of H is equal to

$$Zg_2(VC_6[m,n],z) = (3mn - m)z^9 + (2m)^{6} + (m)z^4$$

and the Second Zagreb index is $Zg_2(VC_6[m,n]) = 27mn + 7m$.

Proof. The proof is analogous to the proof of Theorem 2.

3. Conclusions

Two families of polyhex nanotubes, zigzag ($TUZC_6$) and armchair ($TUAC_6$), respectively, have been investigated here, and formulas for computing their Randić connectivity index, Sum-Connectivity index, Atom-Bond Connectivity index, Geometric-Arithmetic index, First Zagreb index, Second Zagreb index and the corresponding Zagreb polynomials have been derived.

4. Acknowledgments

The author is thankful to Prof. *Mircea V. Diudea* from Faculty of Chemistry and Chemical Engineering Babes-Bolyai University (Romania) for helpful comments and suggestions.

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Povzetek

Predpostavimo da je G poljuben preprosto povezan graf z množico vozlišč V(G) in množico robov E(G). Kemijska teorija grafov predstavlja pomembno vejo splošne teorije grafov. Pri kemijskih grafih vozlišča predstavljajo atome v molekuli, robovi pa kemijske vezi. Po drugi strani pa je tudi izračunavanje indeksov povezanosti v molekulskih grafih pomembna veja v teoriji kemijskih grafov.

V prispevku smo se osredotočili na Randićev indeks povezanosti, indeks povezanosti atom-vez, prvi Zagreb indeks, drugi Zagreb indeks in Zagreb polinom za cik-cak nanocevke $TUZC_6$ in poliheksagonalne nanocevke $TUAC_6$. Predstavljeni so molekulski grafi cik-cak nanocevk $TUZC_6$ in poliheksagonalnih nanocevk $TUAC_6$, ki predstavljajo pomembno družino nanocevk, saj jih sestavljajo šesterokotni obroči (heksagoni).