International Letters of Chemistry, Physics and Astronomy *Online: 2014-03-12*
ISSN: 2299-3843, Vol. 30, pp 74-80
doi:10.18052/www.scipress.com/ILCPA.30.74

The second-connectivity and second-sum-connectivity indices of Armchair Polyhex Nanotubes *TUAC$_6$[m,n]*

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ABSTRACT

The m-connectivety and m-sum connectivity indices of G are defined as to be ${}^{m}\chi(G)=\sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}d_{i_2}\dots d_{i_{m+1}}}}$ and ${}^{m}X(G)=\sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+\dots+d_{i_{m+1}}}}$, where $v_{i_1}v_{i_2}..v_{i_{m+1}}$ runs over all paths of length m in G and d_i is the degree of vertex v_i. In this paper, we give explicit formulas for the second-connectivity and second-sum-connectivity indices of an infinite class of Armchair Polyhex Nanotubes *TUAC$_6$[m,n]*.

Keywords: Molecular Graph; Armchair Polyhex Nanotubes; m-connectivety index; m-sum connectivity index

1. INTRODUCTION

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. $|V(G)| = n$, $|E(G)| = e$ are the number of vertices and edges. The *m-connectivity index* of G is defined as

$${}^{m}\chi(G)=\sum_{v_{i_1}v_{i_2}..v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}d_{i_2}..d_{i_{m+1}}}},$$

where $v_{i_1}v_{i_2}..v_{i_{m+1}}$ runs over all paths of length m in G and d_i is the degree of vertex v_i. In particular, 1-connectivity and 2-connectivity indices are defined as

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

and

$$^{2}\chi(G)=\sum_{v_{i_1}v_{i_2}v_{i_3}}\frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}}}$$

The 1-connectivity index (now called *Randić index*) introduced by *Milan Randić* in 1975 [1], where *uv* ranging over all pairs of adjacent vertices of *G*.

A closely related variant of the Randić connectivity index called the *sum-connectivity index* was introduced by *B. Zhou* and *N. Trinajstić* [2-7] in 2008 as the sum over all edges of the graph of the terms $(d_u+d_v)^{-1/2}$,

$$X(G)=\sum_{v_u v_v}\frac{1}{\sqrt{d_u+d_v}}$$

where d_u and d_v are the degrees of the vertices *u* and *v*, respectively.

Also, the *m-sum connectivity index* of *G* is defined as

$$^{m}X(G)=\sum_{v_{i_1}v_{i_2}..v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+\ldots+d_{i_{m+1}}}}$$

where $v_{i_1}v_{i_2}..v_{i_{m+1}}$ runs over all paths of length *m* in *G*.

In particular, *2-sum-connectivity index* is equale to

$$^{2}X(G)=\sum_{v_{i_1}v_{i_2}v_{i_3}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+d_{i_3}}}$$

For more study about the m-connectivity index, the readers may consult [8-20] and references cited therein and some mathematical properties of the (general) sum-connectivity were given in [19-26].

In this paper, we give explicit formulas for the second-connectivity and second-sum-connectivity indices of an infinite class of Armchair Polyhex Nanotubes *$TUAC_6[m,n]$*.

2. RESULTS AND DISCUSSION

Consider the molecular graph Armchair Polyhex Nanotubes $TUAC_6$ and let we denote the number of hexagons in the first row/column of the 2D-lattice of $TUAC_6[m,n]$ (Figure 1) by *m* and *n*, respectively. For other related research and historical details, see the paper series [27-35] and the general representation of this nano structure is shown in Figure 1 and Figure 2.

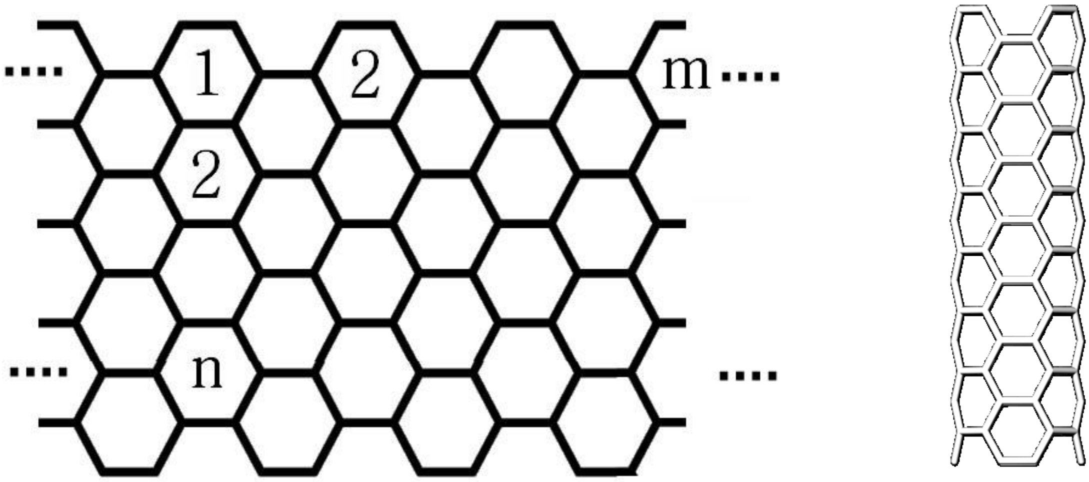

Figure 1. The 2D Lattice (left) and 3D Lattice (right) of Armchair polyhex nanotubes of $TUAC_6[m,n]$.

The vertices/atoms and edges/bonds sets of the Armchair Polyhex Nanotubes $TUAC_6[m,n]$ are equale to $|V(TUAC_6[m,n])| = 2m(n+1)$ and $|E(TUAC_6[m,n])| = 3mn+2m$, respectively. Since $|V_2| = |\{v \in V(G)|\ d_v = 2\}| = 2m+2m$ and $|V_3| = \{v \in V(G)|\ d_v = 3\}| = 2mn.$

Let we define d_{ijk} as a number of 2-edges paths with 3 vertices of degree i, j and k, respectively. It is obvious, $d_{ijk} = d_{kji}$ and an edge $e = v_iv_j$ is equale to d_{didj}.

Now, from Figure 2, we see that for every vertex in V_2, there is a 2-edges path d_{223} (The red path in Figure 2) and also there are two 2-edges paths d_{233} (The yellow path in Figure 2).

From Figure 1, (the 2-dimensional lattice of Armchair Polyhex Nanotubes $TUAC_6[m,n]$, $\forall m,n > 1$), it's easy to see that the number of 2-edges paths in $TUAC_6[m,n]$ is equale to $6mn+4m$. Since there are six 2-edges paths for all hexagon or cycle C_6 in $TUAC_6[m,n]$ and also there is an addition 2-edges path for every member of V_2. In other words,

$$d^2(TUAC_6[m,n]) = \underbrace{6 \times mn}_{\text{cycles } C_6} + \underbrace{4m}_{V_2}$$

So, from Figure 2, one can see that for all other vertices in V_3, there are $d^2(TUAC_6[m,n]) - 4m - 2 \times 4m = 6mn - 8m$ 2-edges paths d_{333} (We marked these 2-edges paths by black color in Figure 2).

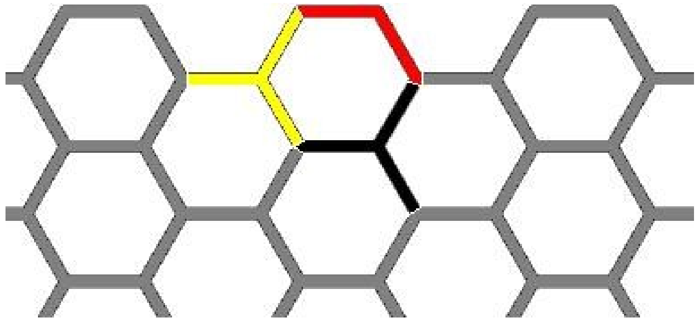

Figure 2. Examples of 2-edges paths d_{223} , d_{233} and d_{333} of $TUAC_6[m,n]$.

Now, by using above mentions, we have the second-connectivity index of *Armchair Polyhex Nanotubes* $TUAC_6[m,n]$ as

$$^{2}\chi(TUAC_6[m,n]) = \sum_{v_{i_1}v_{i_2}v_{i_3}} \frac{1}{\sqrt{d_{i_1}\times d_{i_2}\times d_{i_3}}}$$

$$= \frac{d_{223}}{\sqrt{2\times2\times3}} + \frac{d_{233}}{\sqrt{2\times3\times3}} + \frac{d_{333}}{\sqrt{3\times3\times3}}$$

$$= \frac{4m}{2\sqrt{3}} + \frac{8m}{3\sqrt{2}} + \frac{6mn-8m}{3\sqrt{3}}$$

$$= \left(\frac{6n\sqrt{3}-2\sqrt{3}+12\sqrt{2}}{9}\right)m$$

and also the 2-sum-connectivity index of $TUAC_6[m,n]$, $\forall m,n > 1$ is equale to

$$^{2}X(TUAC_6[m,n]) = \sum_{v_{i_1}v_{i_2}v_{i_3}} \frac{1}{\sqrt{d_{i_1}+d_{i_2}+d_{i_3}}}$$

$$= \frac{d_{223}}{\sqrt{2+2+3}} + \frac{d_{233}}{\sqrt{2+3+3}} + \frac{d_{333}}{\sqrt{3+3+3}}$$

$$= \frac{4m\sqrt{7}}{7} + \frac{4m\sqrt{2}}{2} + \frac{6mn-8m}{3}$$

$$= \left(2n + \frac{24\sqrt{7} + 84m\sqrt{2} - 112}{42} \right) m$$

Finally, from reference [16], we know that the first-connectivity index (Randić index) and first-sum-connectivity index of Armchair Polyhex Nanotubes $TUAC_6[m,n]$ are equale to

$$\chi(TUAC_6[m,n]) = \left(n + \frac{2\sqrt{6}+1}{6} \right) m$$

and

$$X(TUAC_6[m,n]) = \left(\frac{\sqrt{6}n+1}{2} + \frac{2\sqrt{5}}{5} - \frac{\sqrt{6}}{6} \right) m$$

3. CONCLUSION

In this report, we study some properties of two connectivity indices of (molecular) graphs that called second-connectivity and second-sum-connectivity indices and were defined as

$$^{2}\chi(G) = \sum_{v_{i_1} v_{i_2} v_{i_3}} \frac{1}{\sqrt{d_{i_1} d_{i_2} d_{i_3}}}$$

and

$$^{2}X(G) = \sum_{v_{i_1} v_{i_2} v_{i_3}} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3}}}$$

where $v_{i_1} v_{i_2} .. v_{i_{m+1}}$ runs over all paths of length m in G and d_i is the degree of vertex v_i.

In continue, closed analytical formulas for these connectivity indices of a physico chemical structure of Hexagonal nanotubes are given. This nano structure is Armchair Polyhex Nanotubes $TUAC_6[m,n]$. The structures of Armchair Polyhex Nanotubes $TUAC_6[m,n]$ consist of several Hexagon C_6.

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(Received 01 March 2014; accepted 07 March 2014)