

The General Connectivity and General Sum-Connectivity Indices of Nano Structures

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ABSTRACT

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $\forall v_i \in V(G)$, d_i denotes the degree of v_i in G . The *Randić* connectivity index of the graph G is defined as [1-3] $\chi(G) = \sum_{e=uv \in E(G)} (d_u d_v)^{-1/2}$. The sum-connectivity index is defined as $X(G) = \sum_{e=uv \in E(G)} (d_u + d_v)^{-1/2}$. The sum-connectivity index is a new variant of the famous *Randić* connectivity index usable in quantitative structure-property relationship and quantitative structure-activity relationship studies.

The *general m-connectivity* and *general m-sum connectivity* indices of G are defined as ${}^m\chi(G) = \sum_{v_i v_{i_2} \dots v_{i_m} \in \mathcal{V}_m} \frac{1}{\sqrt{d_{i_1} d_{i_2} \dots d_{i_m}}}$ and ${}^mX(G) = \sum_{v_i v_{i_2} \dots v_{i_m} \in \mathcal{V}_m} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + \dots + d_{i_m}}}$, where \mathcal{V}_m runs over all paths of length m in G . In this paper, we introduce a closed formula of the third-connectivity index and third-sum-connectivity index of Nano structure "Armchair Polyhex Nanotubes $TUAC_6[m,n]$ " ($m, n \geq 1$).

Keywords: Molecular Graph; Nano structure; Armchair Polyhex Nanotubes; *Randić* connectivity index; (general) *m-connectivity index*; (general) *m-sum-connectivity index*

1. INTRODUCTION

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, d_v denotes the degree of v in G . The distance between the vertices u and v , denoted by $d(u,v)$, is the length of the shortest path joining them. Also, if e is an edge of G , connecting the vertices u and v , then we write $e=uv$ and say " u and v are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices. Molecular graphs and especially Nano structures are simple connected graphs such that its vertices correspond to the atoms and the edges to the bonds.

The *Randić* connectivity index (or product-connectivity index [2, 3]) of the graph G is defined as [1]

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

The *Randić* connectivity index is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies, e.g., [4-6].

Its mathematical properties as well as those of its generalizations have been studied extensively as summarized in the books [7,8].

Various variants of *Randić* connectivity index have been proposed in the literature, see, e.g., [1-10]. One new such variant is the sum-connectivity index. The sum-connectivity index introduced by *B. Zhou* and *N. Trinajstić* in 2008, and it is defined as [3, 11-15]

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

The (general) *m*-connectivity index is defined as

$${}^m\chi(G) = \sum_{v_1 v_2 \dots v_{m+1}} \frac{1}{\sqrt{d_{i_1} d_{i_2} \dots d_{i_{m+1}}}}$$

where $v_1 v_2 \dots v_{m+1}$ runs over all paths of length *m* in *G* and d_i is the degree of vertex v_i . For more study about the (general) *m*-sum-connectivity index, the readers may consult in the paper series [16-37] and books [38, 39].

In particular, 2-connectivity and 3-connectivity indices are defined as

$${}^2\chi(G) = \sum_{v_1 v_2 v_3} \frac{1}{\sqrt{d_{i_1} d_{i_2} d_{i_3}}}$$

And

$${}^3\chi(G) = \sum_{v_1 v_2 v_3 v_4} \frac{1}{\sqrt{d_{i_1} d_{i_2} d_{i_3} d_{i_4}}}$$

The (general) *m*-sum-connectivity index is defined as

$${}^mX(G) = \sum_{v_1 v_2 \dots v_{m+1}} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + \dots + d_{i_{m+1}}}}$$

In particular, 2-sum-connectivity and 3-sum-connectivity indices are defined as

$${}^2X(G) = \sum_{v_1 v_2 v_3} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3}}}$$

And

$${}^3X(G) = \sum_{v_1 v_2 v_3 v_4} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3} + d_{i_4}}}$$

In this paper, we obtain closed formulas of the third-connectivity index and third-sum-connectivity index of Nano structure "Armchair Polyhex Nanotubes $TUAC_6[m,n]$ " ($m, n \geq 1$).

2. RESULTS AND DISCUSSION

The aim of this section is to compute the general m -connectivity and general m -sum connectivity indices for the famous Polyhexagon Nano structure. Consider the Nano structure "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. According to the structure of $TUAC_6[m,n]$, we see that the vertex/atom set of the Armchair Polyhex Nanotubes $TUAC_6[m,n]$ is equal to $|V(TUAC_6[m,n])|=2m(n+1)$.

Also, we have two partitions $|V_2|=|\{v \in V(G) | d_v=2\}|=2m+2m$ and $|V_3|=|\{v \in V(G) | d_v=3\}|=2mn$ for vertices/atoms of $TUAC_6[m,n]$. Therefore the edge/bond set of $TUAC_6[m,n]$ is equal to $|E(TUAC_6[m,n])| = \frac{1}{2}(3 \times 2mn + 2 \times 4m) = 3mn + 2m$. For more details of this Polyhexagon Nano structure, see the paper series [29, 40-48] and see Figure 1 and Figure 2.

Let we define an edge $e=v_i v_j$ is equal to $d_{ij}=1$ and d_{ijk} as a number of 2-edges paths with 3 vertices of degree i, j and k , and d_{ijkl} as a number of 3-edges paths with 4 vertices of degree i, j, k and l , respectively. Obviously, $d_{ij}=d_{ji}$, $d_{ijk}=d_{kji}$ and $d_{ijkl}=d_{lkji}$.

Now, from the structure of Armchair polyhex nanotubes of $TUAC_6[m,n]$ in Figure 1, one can see that we have five categorizes A, B, C, D and E of vertices of $TUAC_6[m,n]$. And also from Figure 2, (the 2-dimensional lattice of Armchair Polyhex Nanotubes $TUAC_6[m,n]$, $\forall m, n > 1$), we see that there are many types of 3-edges paths for every vertices in $V(TUAC_6[m,n])$. These five categorizes and their 3-edges paths types are shown in Figure 3, ..., 6.

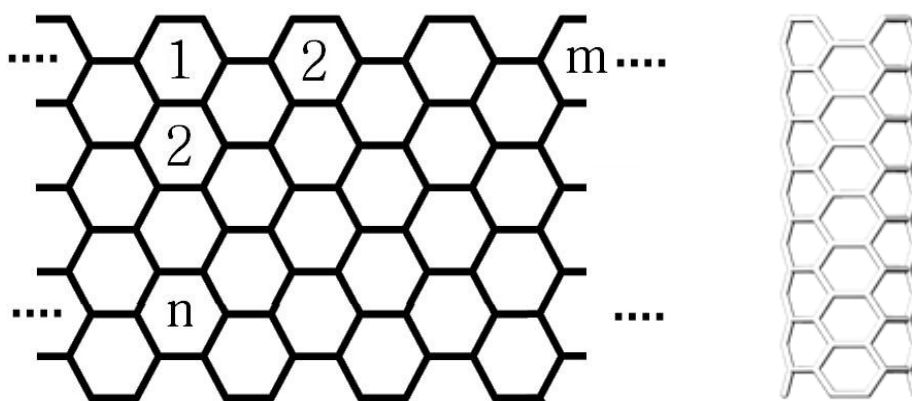


Figure 1. The 2D Lattice (left) and 3D Lattice (right) of Armchair polyhex nanotubes of $TUAC_6[m,n]$.

From Figure 2,3, one can see that for all vertices in categorizes A , there are 6 number of 3-edges paths, such that 2 of these 3-edges paths are diameters of cycles C_6 and 4 others are non-diameter.

From Figure 4, for all vertices in categorizes B , there are 8 number of 3-edges paths, such that 2×2 of them are diameters of cycles C_6 and 4 of them are non-diameter.

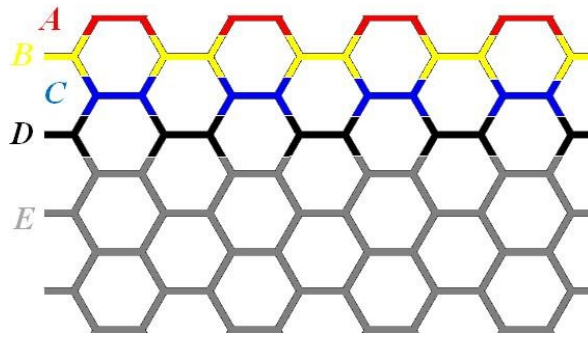


Figure 2. Five categorizes A, B, C, D and E of vertices of $TUAC_6[m,n]$.

$\forall v \in C$ of $V(TUAC_6[m,n])$, we have 11 3-edges paths, such that there are 3×2 diameters of cycles C_6 and 5 non-diameter 3-edges paths (see Figure 5).

From Figure 6, for all vertices in categorizes D ($\forall v \in D \subset V(TUAC_6[m,n])$), there are 3×3 number of 3-edges paths (diameters of cycles C_6), and 6 number of 3-edges paths (non-diameter).

Alternatively, for all other vertices in categorizes E , there are 3×3 number of 3-edges paths (diameters of cycles C_6), and 6 number of 3-edges paths (non-diameter), see Figure 2.

On based the definition of all categorizes of $V(TUAC_6[m,n])$, It's easy to see that

$$V(TUAC_6[m,n]) = A \cup B \cup C \cup D$$

And from Figure 2, $|A| = |V_2| = 2 \times 2m$, $|B| = 2 \times 2m$ and $|C| = 2 \times 2m = |D|$. Obviously, $|E| = |V(TUAC_6[m,n])| - |A| - |B| - |C| - |D| = 2mn + 2m - 4(4m) = 2mn - 14m$.

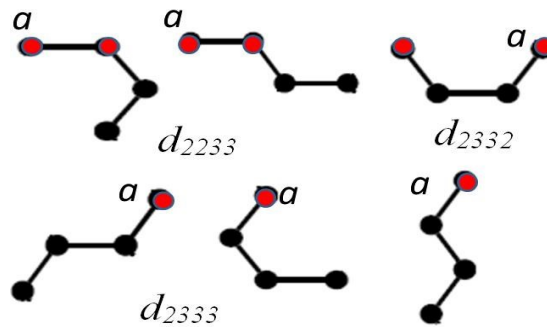


Figure 3. All 3-edges paths of $V(TUAC_6[m,n])$, that start on vertices in set A .

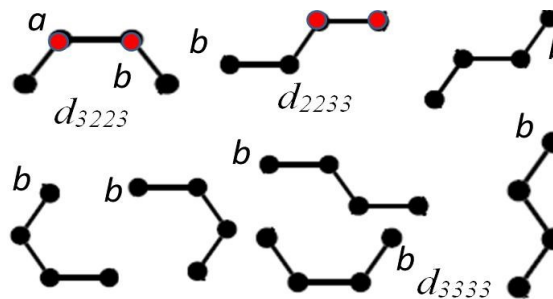


Figure 4. All 3-edges paths of $V(TUAC_6[m,n])$, that start on vertices in set B .

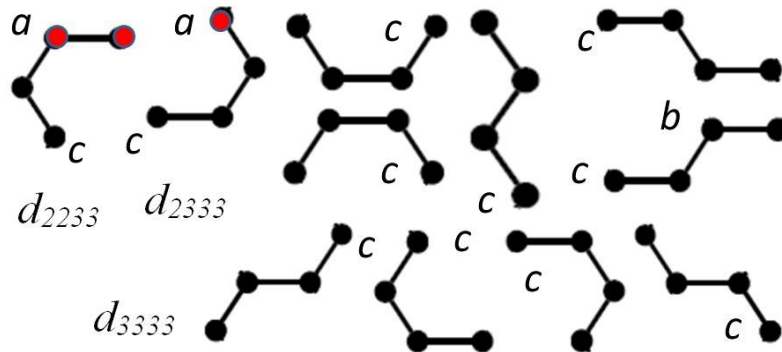


Figure 5. All 3-edges paths of $V(TUAC_6[m,n])$, that start on vertices in set C .

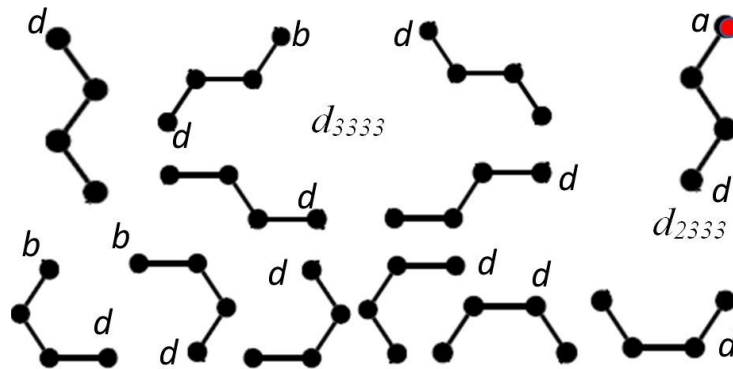


Figure 6. All 3-edges paths of $V(TUAC_6[m,n])$, that start on vertices in set D .

Now, by using the results from Figures 2,3,..6, the third-connectivity index of *Armchair Polyhex Nanotubes* $TUAC_6[m,n]$ as

$$\begin{aligned}
 {}^3\chi(TUAC_6[m,n]) &= \sum_{v_{i_1}v_{i_2}v_{i_3}v_{i_4}} \frac{1}{\sqrt{d_{i_1} \times d_{i_2} \times d_{i_3} \times d_{i_4}}} \\
 &= \frac{1}{2} \times \left(\sum_{v_a \in A} \frac{1}{\sqrt{d_a d_2 d_3 d_4}} + \sum_{v_b \in B} \frac{1}{\sqrt{d_b d_2 d_3 d_4}} + \sum_{v_c \in C} \frac{1}{\sqrt{d_c d_2 d_3 d_4}} + \sum_{v_d \in D} \frac{1}{\sqrt{d_d d_2 d_3 d_4}} \right) \\
 &= \frac{1}{2} \times \left(4m \left(\frac{2}{\sqrt{2 \times 2 \times 3 \times 3}} + \frac{1}{\sqrt{2 \times 3 \times 3 \times 2}} + \frac{3}{\sqrt{2 \times 3 \times 3 \times 3}} \right) + 4m \left(\frac{1}{\sqrt{3 \times 2 \times 2 \times 3}} + \frac{1}{\sqrt{2 \times 2 \times 3 \times 3}} + \frac{6}{\sqrt{3 \times 3 \times 3 \times 3}} \right) \right. \\
 &\quad \left. + 4m \left(\frac{1}{\sqrt{2 \times 2 \times 3 \times 3}} + \frac{2}{\sqrt{2 \times 3 \times 3 \times 3}} + \frac{8}{\sqrt{3 \times 3 \times 3 \times 3}} \right) + 4m \left(\frac{1}{\sqrt{2 \times 3 \times 3 \times 3}} + \frac{11}{\sqrt{3 \times 3 \times 3 \times 3}} \right) + (2mn - 14m) \frac{12}{\sqrt{3 \times 3 \times 3 \times 3}} \right) \\
 &= \frac{1}{2} \left(4m \left(\frac{9+3\sqrt{6}}{18} \right) + 4m + 4m \left(\frac{19+2\sqrt{6}}{18} \right) + 4m \left(\frac{22+\sqrt{6}}{18} \right) + (2mn-14m) \frac{4}{3} \right) \\
 &= 2m \left(\frac{9+3\sqrt{6}}{18} + \frac{18}{18} + \frac{19+2\sqrt{6}}{18} + \frac{22+\sqrt{6}}{18} + \frac{12(n-7)}{18} \right)
 \end{aligned}$$

Thus

$${}^3\chi(TUAC_6[m,n]) = 2m \left(\frac{6n+3\sqrt{6}-8}{9} \right)$$

Also, by using above mentions, the 3-sum-connectivity index of $TUAC_6[m,n]$, $\forall m,n > 1$ is equal to

$$\begin{aligned}
 {}^3X(TUAC_6[m,n]) &= \sum_{v_i v_i v_i v_i} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3} + d_{i_4}}} = \frac{1}{2} \times \\
 &\left(\sum_{v_a \in A} \frac{1}{\sqrt{d_a + d_2 + d_3 + d_4}} + \sum_{v_b \in B} \frac{1}{\sqrt{d_b + d_2 + d_3 + d_4}} + \sum_{v_c \in C} \frac{1}{\sqrt{d_c + d_2 + d_3 + d_4}} + \sum_{v_d \in D} \frac{1}{\sqrt{d_d + d_2 + d_3 + d_4}} \right) \\
 &= \frac{1}{2} \times \left(4m \left(\frac{3}{\sqrt{2+2+3+3}} + \frac{3}{\sqrt{2+3+3+3}} \right) + 4m \left(\frac{2}{\sqrt{2+2+3+3}} + \frac{6}{\sqrt{3+3+3+3}} \right) + 4m \right. \\
 &\left. \left(\frac{1}{\sqrt{2+2+3+3}} + \frac{2}{\sqrt{2+3+3+3}} + \frac{8}{\sqrt{3+3+3+3}} \right) + 4m \left(\frac{1}{\sqrt{2+3+3+3}} + \frac{11}{\sqrt{3+3+3+3}} \right) + (2mn-14m) \frac{12}{\sqrt{3+3+3+3}} \right) \\
 &= \frac{1}{2} \left(4m \left(\frac{3}{\sqrt{10}} + \frac{3}{\sqrt{11}} \right) + 4m \left(\frac{2}{\sqrt{10}} + \frac{6}{\sqrt{12}} \right) + 4m \left(\frac{1}{\sqrt{10}} + \frac{2}{\sqrt{11}} + \frac{8}{\sqrt{12}} \right) + 4m \left(\frac{1}{\sqrt{11}} + \frac{11}{\sqrt{12}} \right) + (2mn-14m) \frac{11}{\sqrt{12}} \right)
 \end{aligned}$$

Therefore

$${}^3X(TUAC_6[m,n]) = 2m \left(\frac{6}{\sqrt{10}} + \frac{6}{\sqrt{11}} + \frac{6n-17}{\sqrt{12}} \right)$$

3. CONCLUSION

In this paper we have established some properties of two connectivity indices in terms of a physico chemical structure of Hexagonal nanotubes. In this report, we compute a closed formula of the 3-connectivity and 3-sum-connectivity indices of Nano structure "Armchair Polyhex Nanotubes $TUAC_6[m,n]$ " ($m,n \geq 1$). It may be useful to give the connectivity indices in terms of other Hexagonal (C_6) molecular graphs

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