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On the higher randić indices of nanotubes

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ABSTRACT

The Randić connectivity index of the graph G is defined by M. Randić as $\chi(G)=\sum_{e=v_1v_2\in E(G)}(d_1d_2)^{-1/2}$. *The sum-connectivity index X(G) of a graph G is the sum of* $(d_u+d_v)^{-1/2}$ *of all edges uv of G, where* d_u *and* d_v *are the degrees of the vertices u and v in G. This index was recently introduced by B. Zhou and N. Trinajstić. The general m-connectivety and general m-sum connectivity indices of G are defined as* ${}^m\chi(G)=\sum_{v_{i_1}v_{i_2}..v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}d_{i_2}..d_{i_{m+1}}}}$ *and* ${}^mX(G)=\sum_{v_{i_1}v_{i_2}..v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+...+d_{i_{m+1}}}}$, *where* $v_{i_1}v_{i_2}..v_{i_{m+1}}$ *runs over all paths of length m in G. In this paper, we give a closed formula of the third-connectivity index and third-sum-connectivity index of Nano structure "*$TUC_4C_8(S)$ *Nanotubes".*

Keywords: Molecular Graph, Nano structure, $TUC_4C_8(S)$ Nanotubes, Randić index, Sum-connectivity index, Higher Randić Indices.

INTRODUCTION

All graphs considered in this paper are finite, undirected and simple. For terminology and notation not defined here we follow those in [1-3]. For a graph $G=(V(G);E(G))$ with vertex set $V(G)$ and edge set $E(G)$, the *weight* of an edge $e=uv\in E(G)$ is defined to be $w_e=(d_u+d_v)^{-1/2}$, where d_u and d_v are the degrees of the vertices u and v in G, respectively.

The *Randić* connectivity indexof a graph G is the sum of the weights w'_e, where for $e=uv\in E(G)$ $w'_e=(d_vd_u)^{-1/2}$ and *Randić* connectivity index is equal to [4]:

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

The Randić connectivity index is a graphic invariant much studied in both mathematical and chemical literature; for details see a survey book written by *Li* and *Gutman* [5] and the references cited therein.

In [12], the Randić connectivity index is called the *product connectivity index* [6, 7], whereas the sum of edge weights studied in this paper is called the *sum-connectivity index* Zhou by *B. Zhou* and *N.Trinajstić* and is equal to [6-10]:

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

The *Higher Randić index or m-connectivity index* of a graph *G* is defined as

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

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

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

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.

For more study about the *Higher Randić* and the *m-sum-connectivity index*, the readers may consult in the paper serices [11-24].

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

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

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

And also, the 2-sum-connectivity and 3-sum-connectivity indices are defined as

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

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

In this paper, we study closed formulas of the third-connectivity and third-sum-connectivity indices of Nano structure "$TUC_4C_8(S)$ Nanotubes". Readers can see the 3-dimensional (cylinder) and 2-dimensional lattices of *G* $TUC_4C_8[r,s]$ nanotube in Figures 1 and 2. In addition, for further study and more historical details, see the paper series [25-34].

RESULTS AND DISCUSSION

In this section, we compute the general form of the 3-connectivety and 3-sum connectivity indices for the famous $TUC_4C_8(S)$ Nanotubes as:

Theorem 1. Let $TUC_4C_8[r,s]$ be the Nanotubes $TUC_4C_8(S)$ ($\forall r,s\in \mathbb{N}-\{1\}$). Then, the *3- connectivity* and *3-sum connectivity* indices of $TUC_4C_8[r,s]$ are equal to

$$^{3}\chi(TUC_4C_8[r,s])=\frac{40}{9}rs+\frac{\left(1+2\sqrt{6}\right)}{3}r$$

$$^{3}X(TUC_4C_8[r,s])=2r\left(\frac{20s-9}{\sqrt{12}}+\frac{5}{\sqrt{11}}+\frac{2}{\sqrt{10}}\right).$$

Proof of Theorem 1: Consider the Nano structure "Nanotubes $TUC_4C_8(S)$". If we enumerate all octagons of $TUC_4C_8(S)$ (any cycle C_8) and all quadrangles(cycle C_4) in the first row of the 2D-lattice of $TUC_4C_8(S)$ (Figure 1) by number *1,2,...,r* and enumerate all octagons in the first column by *1,2,...,s*, then there exists *mn* numbers of these octagons in $TUC_4C_8(S)$, so we demnote Nanotubes $TUC_4C_8(S)$ by $TUC_4C_8[r,s]$ ($\forall r,s\in \mathbb{N}$-{1}).

This implies that in general case of Nanotubes $TUC_4C_8[r,s]$, the number of vertices of $TUC_4C_8(S)$ as degrees 2 and 3 are equal to $|V_2|=2r+2r$ and $|V_3|=8rs$. And there are $8rs+4r$ vertices/atoms and $|E(TUC_4C_8[r,s])|=½[2(4r)+3(8rs)]=12rs+4r$ edges/bonds.

Now, let we denote d_{ijk} as a number of 2-edges paths with 3 vertices of degree *i*, *j* and *k*, respectively. Obviously, $d_{ijk} = d_{kji}$ and an edge $e=v_iv_j$ is equale to $d_{didj.}$ And denote d_{ijkl} as a number of 3-edges paths with 4 vertices of degree *i*, *j*, *k* and *l*, respectively.

Now, from the general case of the 2-dimensional lattice of Nanotubes $TUC_4C_8[r,s]$ in Figure 1, one can see that we have five categorizes *A, B, C, D* and *X* of vertices of $TUC_4C_8[r,s]$. Since there are many types of *3-edges paths* for every vertices in $V(TUC_4C_8[r,s])$; we show that these five categorizes of vertices (*A, B, C, D* and *X*) and their 3-edges paths types in following tabal.

Figure 1. The 3-Dimensional lattice of $TUC_4C_8[r,s]$ Nanotube

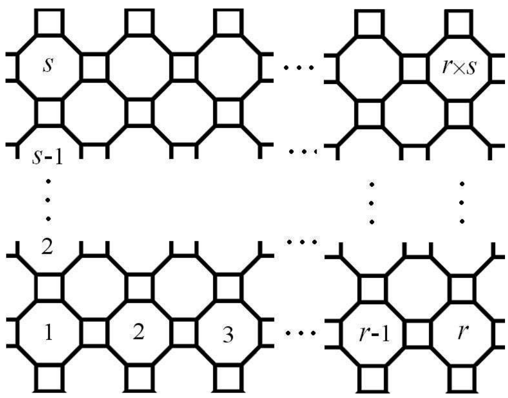
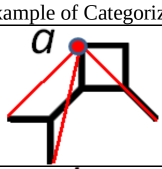
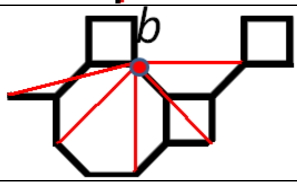
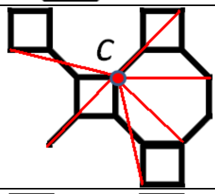
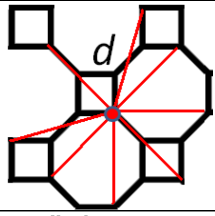


Figure 2. The 2-dimensional lattice of $TUC_4C_8[r,s]$ Nanotube

Table 1. All five categorizes of vertices (*A, B, C, D* and *X*) and their 3-edges paths in *$TUC_4C_8[r,s]$* Nanotubes $\forall r,s\in \mathbb{N}-\{1\}$

Categorizes	Size of Categorizes	Example of Categorizes	d_{2233}	d_{2333}	d_{3333}
A	$\|V_2\|=4r$		1	3	0
B	$4r$		0	0	6
C	$4r$		1	1	6
C	$4r$		0	1	9
X	$8rs+4r-4(4r)$ $=8rs-12r$	All other vertices	0	0	10

Thus, by using the results in Table 1, one can compute the third-connectivity index of $TUC_4C_8[r,s]$ Nanotubes ($\forall r,s\in \mathbb{N}-\{1\}$) as follow.

$$^3\chi(TUC_4C_8[r,s])=\sum_{v_{i_1}v_{i_2}v_{i_3}v_{i_4}}\frac{1}{\sqrt{d_{i_1}\times d_{i_2}\times d_{i_3}\times d_{i_4}}}$$

$$=\tfrac{1}{2}\times\left(\sum_{a\in A}\frac{1}{\sqrt{d_a d_2 d_3 d_4}}+\sum_{b\in B}\frac{1}{\sqrt{d_b d_2 d_3 d_4}}+\sum_{c\in C}\frac{1}{\sqrt{d_c d_2 d_3 d_4}}+\sum_{d\in D}\frac{1}{\sqrt{d_d d_2 d_3 d_4}}+\sum_{x\in X}\frac{1}{\sqrt{d_X d_2 d_3 d_4}}\right)$$

$$=\tfrac{1}{2}\times\left[4r\left(\frac{1}{\sqrt{2\times2\times3\times3}}+\frac{3}{\sqrt{2\times3\times3\times3}}\right)+4r\left(\frac{6}{\sqrt{3\times3\times3\times3}}\right)+4r\left(\frac{1}{\sqrt{2\times2\times3\times3}}+\frac{1}{\sqrt{2\times3\times3\times3}}+\frac{6}{\sqrt{3\times3\times3\times3}}\right)\right.$$
$$\left.+4r\left(\frac{1}{\sqrt{2\times3\times3\times3}}+\frac{9}{\sqrt{3\times3\times3\times3}}\right)+(8rs-12r)\frac{10}{\sqrt{3\times3\times3\times3}}\right]$$

$$=\tfrac{1}{2}\times\left[4r\left(\frac{1+\sqrt{6}}{6}\right)+4r\left(\frac{2}{3}\right)+4r\left(\frac{1}{6}+\frac{\sqrt{6}}{18}+\frac{6}{9}\right)+4r\left(\frac{\sqrt{6}}{18}+1\right)+(8rs-12r)\frac{10}{9}\right]$$

$$=2r\left(\frac{3+3\sqrt{6}}{18}\right)+2r\left(\frac{12}{18}\right)+4r\left(\frac{15+\sqrt{6}}{18}\right)+2r\left(\frac{18+\sqrt{6}}{18}\right)+(4rs-6r)\frac{20}{18}$$

$$=2r\left(\frac{3+3\sqrt{6}}{18}\right)+2r\left(\frac{12}{18}\right)+4r\left(\frac{15+\sqrt{6}}{18}\right)+2r\left(\frac{18+\sqrt{6}}{18}\right)+(4rs-6r)\frac{20}{18}$$

$$=\frac{80rs+6r+2r\sqrt{6}}{18}$$

Therefore $^3\chi(TUC_4C_8[r,s])=\frac{40}{9}rs+\frac{(1+2\sqrt{6})}{3}r$.■

On the other hands, the 3-sum-connectivity index of Nanotubes $TUC_4C_8[r,s]$ ($\forall r,s\in \mathbb{N}-\{1\}$) is equale to

$$^{3}X(TUC_4C_8[r,s])=\sum_{v_{i_1}v_{i_2}v_{i_3}v_{i_4}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+d_{i_3}+d_{i_4}}}$$

$$=\tfrac{1}{2}\left(\sum_{a\in A}\frac{1}{\sqrt{d_a+d_2+d_3+d_4}}+\sum_{b\in B}\frac{1}{\sqrt{d_b+d_2+d_3+d_4}}+\sum_{c\in C}\frac{1}{\sqrt{d_c+d_2+d_3+d_4}}+\sum_{d\in D}\frac{1}{\sqrt{d_d+d_2+d_3+d_4}}+\sum_{x\in X}\frac{1}{\sqrt{d_x+d_2+d_3+d_4}}\right)$$

$$=2r\left[\left(\frac{1}{\sqrt{2+2+3+3}}+\frac{3}{\sqrt{2+2+3+3}}\right)+\left(\frac{6}{\sqrt{3+3+3+3}}\right)+\left(\frac{1}{\sqrt{2+2+3+3}}+\frac{1}{\sqrt{2+3+3+3}}+\frac{6}{\sqrt{3+3+3+3}}\right)\right.$$
$$\left.+\left(\frac{1}{\sqrt{2+3+3+3}}+\frac{9}{\sqrt{3+3+3+3}}\right)+(2s\text{-}3)\frac{10}{\sqrt{3+3+3+3}}\right]$$

$$=2r\left[\left(\frac{1}{\sqrt{10}}+\frac{3}{\sqrt{11}}\right)+\left(\frac{6}{\sqrt{12}}\right)+\left(\frac{1}{\sqrt{10}}+\frac{1}{\sqrt{11}}+\frac{6}{\sqrt{12}}\right)+\left(\frac{1}{\sqrt{11}}+\frac{9}{\sqrt{12}}\right)+(2s\text{-}3)\frac{10}{\sqrt{12}}\right]$$

Thus $^{3}X(TUC_4C_8[r,s])=2r\left(\frac{2}{\sqrt{10}}+\frac{5}{\sqrt{11}}+\frac{20s-9}{\sqrt{12}}\right)$.

Now the proof is complete. ■

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