THE SECOND AND SECOND-SUM-CONNECTIVITY INDICES OF TUC4C8(S) NANOTUBES

M. R. FARAHANI[a*], H.M.A. SIDDIQUI[b], SH. BABY[b], M. IMRAN[c], M. K. SIDDIQUI[d]
[a]*Department of Applied Mathematics, Iran University of Science and Technology, Narmak, 16844, Tehran, Iran*
[b]*Department of Mathematics, Government College University Faisalabad (GCUF), Pakistan*
[c]*School of Natural Sciences, National University of Sciences and Technology, Sector H-12, P.O. 44000, Islamabad, Pakistan*
[d]*Department of Mathematics, Comsats Institute of Information Technology Sahiwal, Pakistan.*

Let G be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. The m-connectivity index ${}^m\chi_\alpha(G)$ of an organic molecule whose molecular graph G is the sum of the weights $\left(d_{i_1}d_{i_2}...d_{i_{m+1}}\right)^\alpha$ where $i_1, i_2, ..., i_{m+1}$ runs over all paths of length m in G and d_i is the degree of vertex v_i. In this paper, we compute the second-connectivity and second-sum-connectivity indices of $TUC_4C_8(S)$ Nanotubes for the first time.

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1. Introduction

Let G be a simple connected graph with vertex set $V(G)=\{v_1,v_2,...v_n\}$ and d_i denotes the degree (number of first neighbors) of vertex v_i in G. The *m-connectivity index* of G is defined as

$${}^m\chi_\alpha(G) = \sum_{v_{i_1}v_{i_2}...v_{i_{m+1}}} \left(d_{i_1}d_{i_2}...d_{i_{m+1}}\right)^\alpha$$

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

In particular, the connectivity index of an organic molecule whose molecular graph is G is defined (see [1]) as

$${}^1\chi_\alpha(G) = \sum_{e=uv\in E(G)} \left(d_u d_v\right)^\alpha$$

The *m-sum connectivity index* of G is defined as

$${}^mX_\alpha(G) = \sum_{v_{i_1}v_{i_2}...v_{i_{m+1}}} \left(d_{i_1}+d_{i_2}+...+d_{i_{m+1}}\right)^\alpha$$

*Corresponding author: mrfarahani88@gmail.com

where $v_{i_1}v_{i_2}..v_{i_{m+1}}$ runs over all paths of length *m* in *G*. In particular, the first-sum connectivity index of molecular graph *G* is defined as

$$^1X_\alpha(G) = \sum_{e=uv\in E(G)} \left(d_u d_v\right)^\alpha$$

The famous version of *m- connectivity* and *m-sum connectivity* indices of G are *Randić connectivity index* [1], and *sum-connectivity index* [2-8]. These indices are equal to

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

And

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

In 1975, *Randić* introduced the respective structure-descriptor in [1] for $\alpha=-½$ (which he called the *branching index*, and is now also called the *Randić index*) in his study of alkanes. The *Randić connectivity* index has been closely correlated with many chemical properties (see [9]).

Mathematical properties of the *m- connectivity* and *m-sum connectivity* indices for general graphs can be found in [10-29].

In the present paper, we compute the second-connectivity and second-sum-connectivity indices of $TUC_4C_8(S)$ Nanotubes for the first time.

2. Results and discussion

In this section, we will consider second-connectivity and second-sum-connectivity indices of $TUC_4C_8(S)$ Nanotubes.

If we enumerate all octagons of $TUC_4C_8(S)$ (any cycle C_8) and all quadrangles (cycle C_4) in the first row 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 $TUC_4C_8(S)$. And the number of vertices of $TUC_4C_8(S)$ as degrees 2 and 3 are equal to $|V_2|=2r+2r$ and $|V_3|=8rs-2r$.

And these imply that in general case of Nanotubes $TUC_4C_8[r,s]$ have $8rs+2r$ vertices/atoms and

$$|E(TUC_4C_8[r,s])| = \frac{2(4r)+3(8rs-2r)}{2} = 12rs+r \text{ edges/bonds.}$$

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 [30-40].

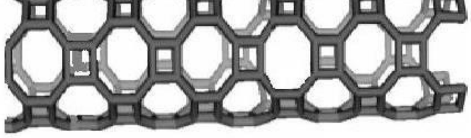

Fig. 1. The 3-dimensional (cylinder) Lattice of Nanotubes $TUC_4C_8(S)$.

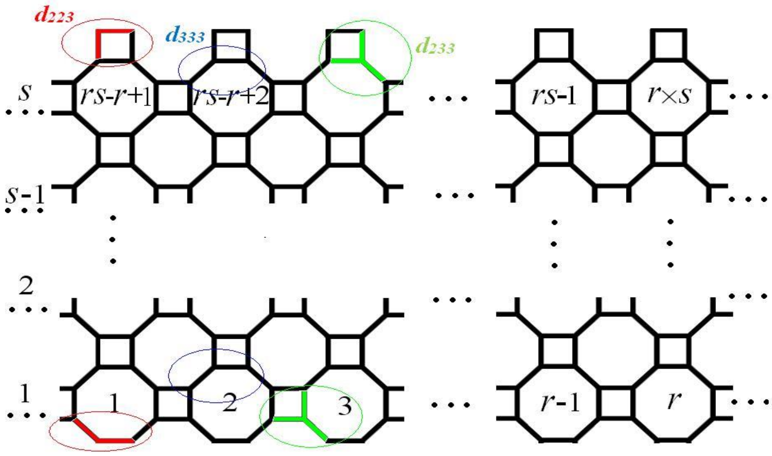

Fig. 2. The 2-dimensional Lattice of Nanotubes $TUC_4C_8[r,s]$.

Theorem 1. Let $TUC_4C_8[r,s]$ be the Nanotubes $TUC_4C_8(S)$ ($\forall r,s\in \mathbb{N}-\{1\}$). Then, the *2-connectivity* and *2-sum connectivity* indices of $TUC_4C_8[r,s]$ are equal to

$$^{2}\chi(TUC_4C_8[r,s])=\left(\frac{24\sqrt{3}s+17\sqrt{3}+12\sqrt{2}}{9}\right)r$$

$$^{2}X(TUC_4C_8[r,s])=\left(8s+\frac{4\sqrt{7}}{7}+\frac{11}{3}+2\sqrt{2}\right)r$$

Corollary 1. $\forall m,n\in\mathbb{N}-\{1\}$, consider the Nanotubes $TUC_4C_8[r,s]$, then

$$^{2}\chi(TUC_4C_8[r,s])\approx(4.62s+5.16)r$$
$$^{2}X(TUC_4C_8[r,s])\approx 8r(s+1)$$

Proof of Theorem 1: Let we define 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 equal to d_{didj}.

Now, from the structure of Nanotubes $TUC_4C_8[r,s]$ in Figure 2, one can see that for every vertex in V_2, there is one 2-edges path $\mathbf{d_{223}}$ (The red path in Figure 2) and also there are two 2-edges paths $\mathbf{d_{233}}$ (The green path in Figure 2). Obviously, all other2-edges paths in Nanotubes $TUC_4C_8[r,s]$ are $\mathbf{d_{333}}$ (The blue path in Figure 2).

Here, by according to from the structure of Nanotubes $TUC_4C_8[r,s]$ in Figure 2 and using above results, we can compute the second-connectivity index of $TUC_4C_8[r,s]$ as follows:

$$^{2}\chi(TUC_4C_8[r,s])=\sum_{v_{i_1}v_{i_2}v_{i_3}}\frac{1}{\sqrt{d_{i_1}\times d_{i_2}\times d_{i_3}}}$$
$$=\frac{d_{223}}{\sqrt{2\times2\times3}}+\frac{d_{233}}{\sqrt{2\times3\times3}}+\frac{d_{333}}{\sqrt{3\times3\times3}}$$
$$=\frac{|V_2|}{2\sqrt{3}}+\frac{2|V_2|}{3\sqrt{2}}+\frac{1}{2}\left(\frac{3|V_2|+5|V_2|+6(|V_3|-2|V_2|)}{3\sqrt{3}}\right)$$
$$=\frac{(4r)}{2\sqrt{3}}+\frac{2(4r)}{3\sqrt{2}}+\frac{3(4r)+5(4r)+6(8rs-2r-8r)}{2\times3\sqrt{3}}$$
$$=\frac{2r\sqrt{3}}{3}+\frac{4r\sqrt{2}}{3}+\left(\frac{24rs+11r}{9}\right)\sqrt{3}$$

$$=\left(\frac{24\sqrt{3}s+17\sqrt{3}+12\sqrt{2}}{9}\right)r$$

$$\approx(4.6188009s+5.1572694)r \approx(4.62s+5.16)r.$$

and also by using above mentions the 2-sum-connectivity index of $TUAC_6[m,n]$ $(\forall m,n>2)$ is equal to

$$^2X(TUC_4C_8[r,s])=\sum_{v_{i_1}v_{i_2}v_{i_3}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+d_{i_3}}}$$

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

$$=\frac{(4r)}{\sqrt{7}}+\frac{(8r)}{2\sqrt{2}}+\frac{1}{2}\left(\frac{48rs+22r}{3}\right)$$

$$=\left(\frac{4\sqrt{7}}{7}+2\sqrt{2}+8s+\frac{11}{3}\right)r$$

$$\approx(8s+1.5118578+2.828427+3.666666)r \approx 8r(s+1).$$

Here, these completes the proof of the Theorem1.

3. Conclusion

In this report, we present some properties of two connectivity indices of molecular graphs, called ”Second-connectivity and Sum-connectivity indices” and a closed formulas for these connectivity indices of the structure of Nanotubes $TUC_4C_8(S)$ are computed.

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