



Computing degree-based topological indices of polyhex nanotubes

Vijayalaxmi Shigehalli, Rachanna Kanabur *

Department of Mathematics, Rani Channamma University, Belagavi - 591156, Karnataka, India

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Abstract. Recently, Shigehalli and Kanabur [17] have put forward for new degree based topological indices, namely geometric-arithmetic index (GA_1 index), SK index, SK_1 index and SK_2 index of a molecular graph G . In this paper, we obtain the explicit formulas of these indices for polyhex nanotube without the aid of a computer.

Keywords. chemical graph, degree-based topological indices, polyhex nanotube.

1 Introduction

A topological index of a chemical compound is an integer, derived following a certain rule, which can be used to characterize the chemical compound and predict certain physio-chemical properties like boiling point, molecular weight, density and refractive index and so forth [2, 19].

A molecular graph $G = (V, E)$ is a simple graph having $n = |V|$ vertices and $m = |E|$ edges. The vertices $v_i \in V$ represent non-hydrogen atoms and the edges $(v_i, v_j) \in E$ represent covalent bonds between the corresponding atoms. In particular, hydrocarbons are formed only by carbon and hydrogen atom and their molecular graphs represent the carbon skeleton of the molecule [2, 19].

Molecular graphs are a special type of chemical graphs, which represent the constitution of molecules. They are also called constitutional graphs. When the constitutional graph of a

*Corresponding author (Email address: rachukanabur@gmail.com).

molecule is represented in a two-dimensional basis it is called structural graph [2, 19].

All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by $d_u(G)$ and is the number of vertices that are adjacent to u . The edge connecting the vertices u and v is denoted by uv [5].

2 Computing the topological indices of polyhex nanotube

Motivated by previous research on polyhex nanotube [4, 6, 8–10, 12, 15–17], here we compute the values of four new topological indices of polyhex nanotube.

2.1 Geometric-arithmetic (GA_1) index

Let $G = (V, E)$ be a molecular graph, and d_u is the degree of the vertex u . Then GA_1 index of G is defined as

$$GA_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) \cdot d_G(v)}}$$

Where GA_1 index is considered for distinct vertices. The above equation is the sum of the ratio of the arithmetic mean and geometric mean of u and v , where $d_G(u)$ (or $d_G(v)$) denotes the degree of the vertex u (or v).

2.2 SK Index

The SK index of a graph $G = (V, E)$ is defined as

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}$$

where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G .

2.3 SK_1 Index

The SK_1 index of a graph $G = (V, E)$ is defined as

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) \cdot d_G(v)}{2}$$

where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G .

2.4 SK_2 Index

The SK_2 index of a graph $G = (V, E)$ is defined as

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2$$

where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G .

3 Main Results

3.1 Armchair polyhex nanotubes

Consider the armchair polyhex nanotubes $G = TUAC_6[m, n]$, where m denotes number of hexagons in first row and n denotes the number of rows. The number of vertices/atoms of armchair polyhex nanotubes is equal to

$$|V(TUAC_6[m, n])| = 2m(n + 2),$$

and the number of edges/bonds is

$$|E(TUAC_6[m, n])| = 3mn + 4m.$$

There are three different kinds of edges of G depending on the degree of terminal vertices of edges.

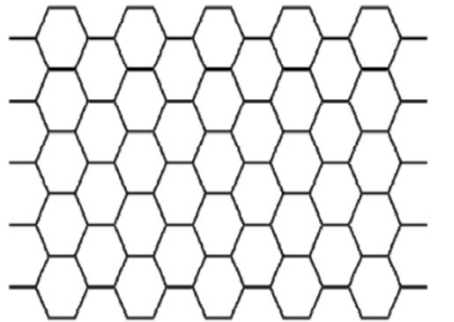


Figure 1. Graph of armchair polyhex $TUAC_6[5, 9]$ nanotube.

| (d_a, d_b) where $a, b \in E(H)$ | (2,2) | (2,3) | (3,3) |
|------------------------------------|-------|-------|----------|
| Number of edges | 2m | 4m | 3mn – 2m |

Table 1. Edge partition of 2D-lattice of H-naphthalenic nanotubes based on degrees of end vertices of each edge.

Theorem 3.1. Consider the graph of $TUAC_6[m, n]$ nanotubes, then its GA_1 index is equal to

$$GA_1(TUAC_6[m, n]) = \left(3n + \frac{10}{\sqrt{6}} \right) m.$$

Proof. Consider the $TUAC_6[m, n]$ nanotube. The number of vertices in $TUAC_6[m, n]$ are $2m(n + 2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn + 4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the geometric-arithmetic index of G which is expressed as

$$GA_1(G) = \sum_{u, v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}}.$$

This implies that

$$\begin{aligned} GA_1(TUAC_6) &= (2,2) \left(\frac{2+2}{2\sqrt{4}} \right) + (2,3) \left(\frac{2+3}{2\sqrt{6}} \right) + (3,3) \left(\frac{3+3}{2\sqrt{9}} \right) \\ &= 2m(1) + (4m) \left(\frac{5}{2\sqrt{6}} \right) + (3mn - 2m)(1) \\ &= 3mn + \frac{10m}{\sqrt{6}} \\ &= \left(3n + \frac{10}{\sqrt{6}} \right) m. \end{aligned}$$

□

Theorem 3.2. Consider the graph of $TUAC_6[m, n]$ nanotubes, then its SK index is equal to

$$SK(TUAC_6[m, n]) = (9n + 8) m.$$

Proof. Consider the $TUAC_6[m, n]$ nanotube. The number of vertices in $TUAC_6[m, n]$ are $2m(n + 2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn + 4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK index of G which is expressed as

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}.$$

This implies that

$$\begin{aligned} SK(TUAC_6[m, n]) &= (2,2) \left(\frac{2+2}{2} \right) + (2,3) \left(\frac{2+3}{2} \right) + (3,3) \left(\frac{3+3}{2} \right) \\ &= 2m(2) + 4m \left(\frac{5}{2} \right) + (3mn - 2m)(3) \\ &= 4m + 10m + 9mn - 6m \\ &= (9n + 8) m. \end{aligned}$$

□

Theorem 3.3. Consider the graph of $TUAC_6[m, n]$ nanotubes, then its SK_1 index is equal to

$$SK_1(TUAC_6[m, n]) = \left(\frac{27n}{2} - 7 \right) m.$$

Proof. Consider the $TUAC_6[m, n]$ nanotube. The number of vertices in $TUAC_6[m, n]$ are $2m(n + 2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn + 4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}.$$

This implies that

$$\begin{aligned} SK_1(TUAC_6[m,n]) &= (2,2) \binom{2 \times 2}{2} + (2,3) \binom{2 \times 3}{2} + (3,3) \binom{3 \times 3}{2} \\ &= 2m(2) + 4m \binom{6}{2} + (3mn - 2m) \binom{9}{2} \\ &= 4m + 12m + \frac{27mn}{2} - 9m \\ &= \left(\frac{27n}{2} - 7\right)m. \end{aligned}$$

□

Theorem 3.4. Consider the graph of $TUAC_6[m,n]$ nanotubes, then its SK_2 index is equal to

$$SK_2(TUAC_6[m,n]) = (27n + 15)m.$$

Proof. Consider the $TUAC_6[m,n]$ nanotube. The number of vertices in $TUAC_6[m,n]$ are $2m(n + 2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn + 4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK_2 index of G which is expressed as

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2.$$

$$\begin{aligned} SK_2(TUAC_6[m,n]) &= (2,2) \left(\frac{2+2}{2}\right)^2 + (2,3) \left(\frac{2+3}{2}\right)^2 + (3,3) \left(\frac{3+3}{2}\right)^2 \\ &= 2m(4) + 4m \binom{25}{4} + (3mn - 2m) \binom{36}{4} \\ &= 8m + 25m + 27mn - 18m \\ &= (27n + 15)m. \end{aligned}$$

□

3.2 Zigzag-edge polyhex nanotubes

Consider the armchair polyhex nanotubes $H = TUZC_6[m,n]$, where m denotes number of hexagons in first row and n denotes the number of rows. The number of vertices/atoms of zigzag-edge polyhex nanotubes is equal to

$$|V(TUZC_6[m,n])| = 2m(n + 2),$$

and the number of edges/bonds is

$$|E(TUZC_6[m,n])| = 3mn + 4m.$$

There are two different kinds of edges of H depending on the degree of terminal vertices of edges.

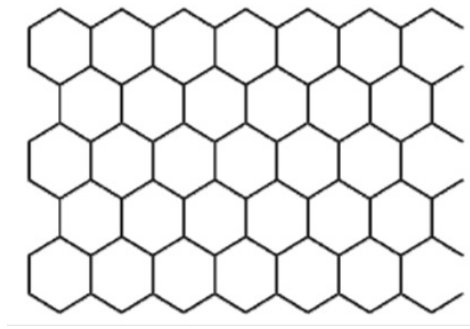


Figure 2. Graph of zigzag edge polyhex TUZC6 [7, 5] nanotube.

| | | |
|------------------------------------|-------|------------|
| (d_a, d_b) where $a, b \in E(H)$ | (2,3) | (3,3) |
| Number of edges | $4m$ | $3mn - 2m$ |

Table 2. Edge partition of 2-dimensional graph of TUZC₆ nanotube with respect to degree of end vertices of edges.

Theorem 3.5. Consider the graph of TUZC₆[m, n] nanotubes, then its GA_1 index is equal to

$$GA_1(TUAC_6[m, n]) = 3mn + \left(\frac{10}{\sqrt{6}} - 2\right) m.$$

Proof. Consider the TUZC₆[m, n] nanotube. The number of vertices in TUZC₆[m, n] are $2m(n + 2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn + 4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the geometric-arithmetic index of G which is expressed as

$$GA_1(H) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) \cdot d_G(v)}}.$$

This implies that

$$\begin{aligned} GA_1(TUZC_6) &= (2,3) \left(\frac{2+3}{2\sqrt{6}}\right) + (3,3) \left(\frac{3+3}{2\sqrt{9}}\right) \\ &= (4m) \left(\frac{5}{2\sqrt{6}}\right) + (3mn - 2m) (1) \\ &= \frac{10m}{\sqrt{6}} + 3mn - 2m \\ &= 3mn + \left(\frac{10}{\sqrt{6}} - 2\right) m. \end{aligned}$$

□

Theorem 3.6. Consider the graph of TUZC₆[m, n] nanotubes, then its SK index is equal to

$$SK(TUZC_6[m, n]) = 9mn + 4m.$$

Proof. Consider the $TUZC_6[m, n]$ nanotube. The number of vertices in $TUZC_6[m, n]$ are $2m(n + 2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn + 4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK index of G which is expressed as

$$SK(H) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}.$$

This implies that

$$\begin{aligned} SK(TUAC_6[m, n]) &= (2, 3) \binom{2+3}{2} + (3, 3) \binom{3+3}{2} \\ &= 4m \binom{5}{2} + (3mn - 2m) (3) \\ &= 10m + 9mn - 6m \\ &= 9mn + 4m. \end{aligned}$$

□

Theorem 3.7. Consider the graph of $TUZC_6[m, n]$ nanotubes, then its SK_1 index is equal to

$$SK_1(TUZC_6[m, n]) = \left(\frac{27n}{2} + 3 \right) m.$$

Proof. Consider the $TUZC_6[m, n]$ nanotube. The number of vertices in $TUZC_6[m, n]$ are $2m(n + 2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn + 4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK_1 index of G which is expressed as

$$SK_1(H) = \sum_{u,v \in E(G)} \frac{d_G(u) \cdot d_G(v)}{2}.$$

This implies that

$$\begin{aligned} SK_1(TUZC_6[m, n]) &= (2, 3) \binom{2 \times 3}{2} + (3, 3) \binom{3 \times 3}{2} \\ &= 4m \binom{6}{2} + (3mn - 2m) \binom{9}{2} \\ &= 12m + \frac{27mn}{2} - 9m \\ &= \frac{27mn}{2} + 3m \\ &= \left(\frac{27n}{2} + 3 \right) m. \end{aligned}$$

□

Theorem 3.8. Consider the graph of $TUZC_6[m, n]$ nanotubes, then its SK_2 index is equal to

$$SK_2(TUZC_6[m, n]) = (27n + 7) m.$$

Proof. Consider the $TUZC_6[m, n]$ nanotube. The number of vertices in $TUZC_6[m, n]$ are $2m(n + 2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn + 4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK_2 index of G which is expressed as

$$SK_2(H) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2.$$

$$\begin{aligned} SK_2(TUZC_6[m, n]) &= (2,3) \left(\frac{2+3}{2} \right)^2 + (3,3) \left(\frac{3+3}{2} \right)^2 \\ &= 4m \left(\frac{25}{4} \right) + (3mn - 2m) \left(\frac{36}{4} \right) \\ &= 25m + 27mn - 18m \\ &= 27mn + 7m \\ &= (27n + 7) m. \end{aligned}$$

□

Concluding Remarks: A generalized formula for geometric-arithmetic index (GA_1 index), SK index, SK_1 index, SK_2 index for polyhex nanotubes is obtained without using computer.

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