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Computing Degree-Based Topological Indices of Polyhex Nanotubes

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Abstract. Recently, Shigehalli and Kanabur [17] have put forward for new degree based topological indices, namely Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index and SK_2 index of a molecular graph G. In this paper, we obtain the explicit formulae 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

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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 Arithmetic-Geometric (AG_1) Index

Let $G = (V, E)$ be a molecular graph, and d_u is the degree of the vertex u. Then AG_1 index of G is defined as

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}},$$

Where AG_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

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

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.

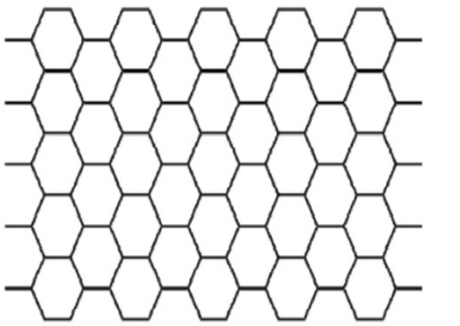

Figure 1. Graph of armchair polyhex $TUAC_6[5,9]$ nanotube

(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-Naphtalenic nanotubes based on degrees of end vertices of each edge.

Theorem 3.1. *Consider the graph of $TUAC_6[m,n]$ nanotubes, then its AG_1 index is equal to*

$$AG_1(TUAC_6[m,n]) = \left(3n + \frac{10}{\sqrt{6}}\right) m.$$

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 Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}}.$$

This implies that

$$\begin{aligned} AG_1(TUAC_6) &= (2,2)\left(\frac{2+2}{2\sqrt{4}}\right) + (2,3)\left(\frac{2+3}{2\sqrt{6}}\right) + (3,3)\left(\frac{3+3}{2\sqrt{9}}\right) \\ &= 2m\,(1) + (4m)\left(\frac{5}{2\sqrt{6}}\right) + (3mn-2m)\,(1) \\ &= 3mn + \frac{10m}{\sqrt{6}} \\ &= \left(3n + \frac{10}{\sqrt{6}}\right) m. \end{aligned}$$

□

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

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

□

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

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

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

□

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.

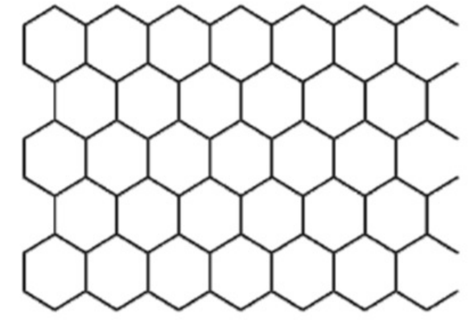

Figure 2. Graph of zigzag edge polyhex TUZC6 [7, 5] nanotube.

(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-dimentional graph of $TUZC_6$ nanotube with respect to degree of end vertices of edges.

Theorem 3.5. *Consider the graph of $TUZC_6[m,n]$ nanotubes, then its AG_1 index is equal to*

$$AG_1(TUAC_6[m,n]) = 3mn + \left(\frac{10}{\sqrt{6}} - 2\right)m.$$

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 Arithmetic-Geometric index of G which is expressed as

$$AG_1(H) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}}.$$

This implies that

$$\begin{aligned} AG_1(TUZC_6) &= (2,3)\left(\frac{2+3}{2\sqrt{6}}\right) + (3,3)\left(\frac{3+3}{2\sqrt{9}}\right) \\ &= (4m)\left(\frac{5}{2\sqrt{6}}\right) + (3mn - 2m)(1) \\ &= \frac{10m}{\sqrt{6}} + 3mn - 2m \\ &= 3mn + \left(\frac{10}{\sqrt{6}} - 2\right)m. \end{aligned}$$

□

Theorem 3.6. *Consider the graph of $TUZC_6[m,n]$ 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

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

□

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

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

This implies that

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

□

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 Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, SK_2 index for Polyhex Nanotubes is obtained without using computer.

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