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On certain degree-based topological indices of armchair polyhex nanotubes

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Abstract. Recently [18], Shigehalli and Kanabur have introduced two new topological indices namely, AG_2 index and SK_3 index. Hosamani [14], has studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G. In this paper, formula for computing the armchair polyhex nanotube $TUAC_6[m,n]$ family is given.

Keywords: molecular graph, arithmetic-geometric index (AG_2 index), SK_3 index, sanskruti index, armchair polyhex nanotube
Mathematics Subject Classification (2010): 05C09.

1 Introduction

Let G be a simple connected graph in chemical graph theory. In mathematics chemistry, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. And also a connected graph is a graph such that there is a path between all pairs of vertices. Note that hydrogen atoms are often omitted [3, 12].

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [6, 8, 12]. This the-

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ory had an important effect on the development of the chemical sciences.

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 [3]. Motivated by previous research on armchair polyhex nanotubes. Here we computed the topological index value of armchair polyhex nanotubes [2,4,7,9,10,11,13,16,17,18].

2 Computing the topological indices of certain nanotubes

The armchair polyhex nanotubes $G = TUAC_6$(Fig. 1) suppose m and n denote the number of hexagons in the first row/column of the 2D-lattice of $TUAC_6[m,n]$ (Fig. 2), respectively. Thus the number of vertices/atoms in this nanotube is equal to $|V(TUAC_6[m,n])| = 2m(n+1)$, $m,n \in E(G)$ and obviously the number of edges/bonds is $|E(TUAC_6[m,n])| = 3mn + 2m$.

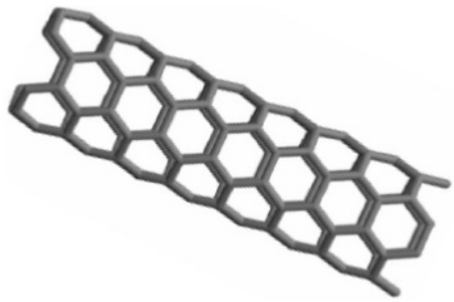

Figure 1. The 3D lattice of Armchair polyhex nanotubes $TUAC_6[m,n]$.

There are two partitions $V_2 = \{v \in V(G)/d_v = 2\}$ and $V_3 = \{v \in V(G)/d_v = 3\}$ of $V(TUAC_6[m,n])$, since the degree of an arbitrary vertex/atom of a molecular graph armchair polyhex is equal to 2 or 3. Next, these partitions imply that $E(TUAC_6[m,n])$ can be divided in three partitions

$E_6 = \{u,v \in V(TUAC_6[m,n]) | d_u = d_v = 3\}$,
$E_5 = \{u,v \in V(TUAC_6[m,n]) | d_u = 3, \textit{ and } d_v = 2\}$, and
$E_4 = \{u,v \in V(TUAC_6[m,n]) | d_u = d_v = 2\}$.

From Fig. 2, it is easy to see that the size of edge/bond partitions E_4, E_5 and E_6 are equal to are equal to m, $2m$ and $3mn - m$, respectively. From Fig. 3, one can see that for every atom/vertex $v \in V_2$, $S_v = 2 + 3 = 5$, since for its adjacent vertices u, w; $d_u = 2 \textit{ and } d_w = 3$ ($u \in V_2$, $w \in V_3$) and obviously $S_u = 5$. Whereas $S_w = 2 \times 3 + 2$, since for $N(w) = \{u_1, u_2, v\}$, the degree of vertices/atoms u_1, u_2 equal to three. Also, for all other vertices a (which belong to V_3), $S_a = 3 \times 3 = 9$.

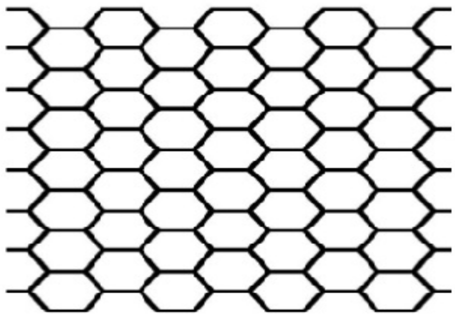

Figure 2. The 2D lattice of Armchair polyhex nanotubes $TUAC_6[m,n]$.

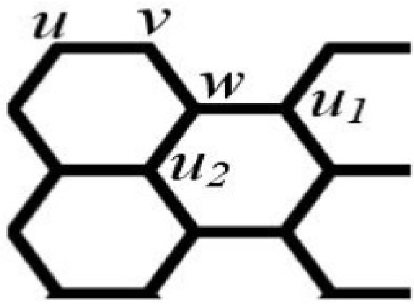

Figure 3. The particular of 2D lattice of Armchair polyhex $TUAC_6[m,n]$.

2.1 Arithmetic-Geometric (AG_2) Index

Let $G = (V, E)$ be a molecular graph, and $S_G(u)$ is the degree of the vertex u, then AG_2 index of G is defined as

$$AG_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}},$$

where $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G.

$$S_G(u) = \sum_{u,v \in E(G)} d_G(u),$$

and

$$N_G(u) = \{v \in V(G) | uv \in E(G)\}.$$

2.2 SK_3 Index

The SK_3 index of a graph $G = (V, E)$ is defined as

$$SK_3(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2},$$

where $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G.

$$S_G(u) = \sum_{u,v \in E(G)} d_G(u),$$

and

$$N_G(u) = \{v \in V(G) | uv \in E(G)\}.$$

2.3 Sanskruti Index

Recently, Hosamani [18], studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G.

$$S(G) = \sum_{uv \in E(G)} \left(\frac{S_G(u) S_G(v)}{S_G(u) + S_G(v) - 2} \right)^3,$$

where $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G.

$$S_G(u) = \sum_{u,v \in E(G)} d_G(u),$$

and

$$N_G(u) = \{v \in V(G) | uv \in E(G)\}.$$

3 Main results

Table 1. Edge partition of graph of $TUAC6[m,n]$ armchair polyhex nanotube based on degree sum of vertices lying at unit distance from end vertices of each edge.

(S_u, S_v), where $u,v \in E(H)$	(5,5)	(5,8)	(8,8)	(8,9)	(9,9)
Number of edges	m	$2m$	m	$2m$	$9mn - 4m$

Theorem 3.1. *Let G be the armchair nanotube $TUAC_6[m,n]$ $\forall\ m,n \in E(G)$. Then the AG_2 index of G is equal to*

$$AG_2(G) = (9n - 2.0588)\, m.$$

Proof.

$$AG_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}}.$$

This implies that

$$\begin{aligned}
AG_2(TUAC_6[m,n]) &= (5,5)\left(\frac{5+5}{2\sqrt{25}}\right) + (5,8)\left(\frac{5+8}{2\sqrt{40}}\right) + (8,8)\left(\frac{8+8}{2\sqrt{64}}\right) \\
&+ (8,9)\left(\frac{8+9}{2\sqrt{72}}\right) + (9,9)\left(\frac{9+9}{2\sqrt{81}}\right) \\
&= m\,(1) + (2m)\left(\frac{13}{2\sqrt{40}}\right) + (m)\,(1) + (2m)\left(\frac{17}{2\sqrt{72}}\right) + (9mn-4m)\,(1) \\
&= 9mn - 2m + \frac{13m}{\sqrt{40}} + \frac{17m}{\sqrt{72}} \\
&= \left(9n - 2 + \frac{13}{\sqrt{40}} + \frac{17}{\sqrt{72}}\right) m \\
&= (9n - 2.0588)\, m.
\end{aligned}$$

Theorem 3.2. *Let G be the armchair nanotube $TUAC_6[m,n]$ $\forall\ m,n \in E(G)$. Then the SK_3 index of G is equal to*

$$SK_3(G) = (81n + 7)\, m.$$

Proof.

$$SK_3(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2}.$$

This implies that

$$\begin{aligned}
SK_3(TUAC_6[m,n]) &= (5,5)\left(\frac{5+5}{2}\right) + (5,8)\left(\frac{5+8}{2}\right) + (8,8)\left(\frac{8+8}{2}\right) \\
&+ (8,9)\left(\frac{8+9}{2}\right) + (9,9)\left(\frac{9+9}{2}\right) \\
&= m\,(5) + (2m)\left(\frac{13}{2}\right) + (m)\,(8) + (2m)\left(\frac{17}{2}\right) + (9mn-4m)\,(9) \\
&= 5m + 13m + 8m + 17m + 81mn - 36m \\
&= 81mn + 7m \\
&= (81n + 7)\, m.
\end{aligned}$$

Theorem 3.3. *Let G be the armchair nanotube $TUAC_6[m,n]$ $\forall\ m,n \in E(G)$. Then the Sanskruti index of G is equal to*

$$S(G) = (1167.75n - 75.58)\, m.$$

Proof.

$$S(G) = \sum_{uv \in E(G)} \left(\frac{S_G(u) S_G(v)}{S_G(u) + S_G(v) - 2}\right)^3.$$

This implies that

$$\begin{aligned}
S(TUAC_6[m,n]) &= (5,5)\left(\frac{25}{5+5-2}\right)^3 + (5,8)\left(\frac{40}{5+8-2}\right)^3 + (8,8)\left(\frac{64}{8+8-2}\right)^3 \\
&+ (8,9)\left(\frac{72}{8+9-2}\right)^3 + (9,9)\left(\frac{81}{9+9-2}\right)^3 \\
&= m\left(\frac{25}{8}\right)^3 + 2m\left(\frac{40}{11}\right)^3 + m\left(\frac{64}{14}\right)^3 + 2m\left(\frac{72}{15}\right)^3 \\
&+ (9mn-4m)\left(\frac{81}{16}\right)^3 \\
&= m\,(3.125)^3 + 2m\,(3.6363)^3 + m\,(4.5714)^3 + 2m\,(4.8)^3 \\
&+ (9mn-4m)\,(5.0625)^3 \\
&= (1167.75n - 75.58)\,m.
\end{aligned}$$

Conclusion

In this paper, we have computed the value of AG_2 index, SK_3 index and Sanskruti index for $TUAC_6[m,n]$ armchair polyhex nanotube without using computer.

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