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 \( TUA_{C_6} \) \( [m, n] \) family is given.

Keywords. molecular graph, arithmetic-geometric index (\( AG_2 \) index), \( SK_3 \) index, sanskruti index, armchair polyhex nanotube.

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 theory 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 $TUAC_6[m,n]$.](image)

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

$E_5 = \{ u,v \in V(TUAC_6[m,n]) | d_u = d_v = 3 \}$,

$E_5 = \{ u,v \in V(TUAC_6[m,n]) | d_u = 3, and d_v = 2 \}$, 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 $u$, $w$; $d_u = 2$ 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 \( TUAC_6[m,n] \) armchair polyhex nanotube based on degree sum of vertices lying at unit distance from end vertices of each edge.

<table>
<thead>
<tr>
<th>((S_u, S_v), \text{ where } u,v \in E(H))</th>
<th>(5,5)</th>
<th>(5,8)</th>
<th>(8,8)</th>
<th>(8,9)</th>
<th>(9,9)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>( m )</td>
<td>( 2m )</td>
<td>( m )</td>
<td>( 2m )</td>
<td>( 9mn - 4m )</td>
</tr>
</tbody>
</table>

**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

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

**Theorem 3.2.** Let \( G \) be the armchair nanotube \( TUAC_6[m,n] \). Then the SK3 index of \( G \) is equal to

\[ SK_3(G) = (81n + 7)m. \]

**Proof.**

\[
SK_3(G) = \sum_{u,v \in E(G)} \frac{SG(u) + SG(v)}{2}. 
\]

This implies that

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

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

\[ S(G) = (1167.75n - 75.58)m. \]

**Proof.**

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

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This implies that
\[
S(TUAC_6[m,n]) = (5.5) \left( \frac{25}{5+5-2} \right)^3 + (5.8) \left( \frac{40}{5+8-2} \right)^3 + (8.8) \left( \frac{64}{8+8-2} \right)^3
\]
\[
+ (8.9) \left( \frac{72}{8+9-2} \right)^3 + (9.9) \left( \frac{81}{9+9-2} \right)^3
\]
\[
= m \left( \frac{25}{8} \right)^3 + 2m \left( \frac{40}{11} \right)^3 + m \left( \frac{64}{14} \right)^3 + 2m \left( \frac{72}{15} \right)^3
\]
\[
+ (9mn - 4m) \left( \frac{81}{16} \right)^3
\]
\[
= m (3.125)^3 + 2m (3.6363)^3 + m (4.5714)^3 + 2m (4.8)^3
\]
\[
+ (9mn - 4m) (5.0625)^3
\]
\[
= (1167.75n - 75.58) m.
\]

**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.

**References**


