



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 in [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, Geometric-Arithmetic index (AG_2 index), SK_3 index, Sanskruti index and 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. 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, and 12]. This theory had an important effect on the development of the chemical sciences.

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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 $d_u(G)$ equal 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, we compute 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

In armchair polyhex nanotube $G = TUAC_6$ (Figure1) suppose m and n denote the number of hexagons in the first row /column of the 2D-lattice of $TUAC_6[m, n]$ (Figure 2), respectively. The number of vertices/atoms in this nanotube is $|V(TUAC_6[m, n])| = 2m(n + 1)$, $m, n \in E(G)$ and obviously the number of edges/bonds is $|E(TUAC_6[m, n])| = 3mn + 2m$.

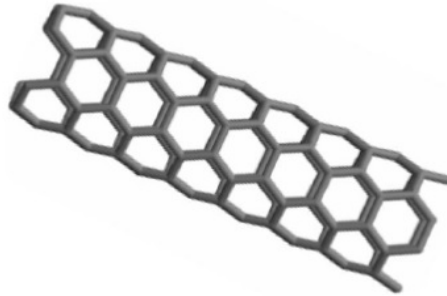


Figure 1. The 3D lattice of Armchair polyhex nanotubes $TUAC_6[m, n]$.

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

$$E_6 = \{u, v \in V(TUAC_6[m, n]) / d_u = d_v = 3\}$$

$$E_5 = \{u, v \in V(TUAC_6[m, n]) / d_u = 3, \text{ and } d_v = 2\} \text{ and}$$

$$E_4 = \{u, v \in V(TUAC_6[m, n]) / d_u = d_v = 2\}.$$

From Figure 2, it is easy to see that the size of edge/bond partitions E_4 , E_5 and E_6 are equal to m , $2m$ and $3mn - m$, respectively. From Figure 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), $S_a = 3 \times 3 = 9$.

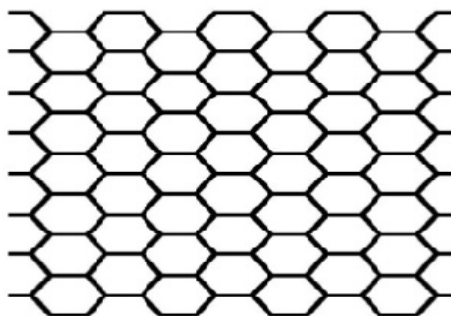


Figure 2. The 2D lattice of Armchair polyhex nanotubes $TUAC_6[m, n]$.

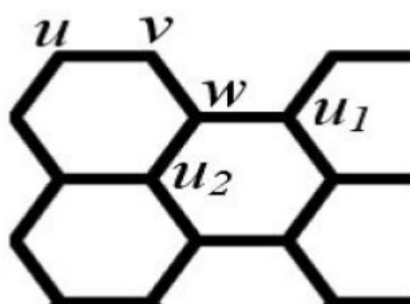


Figure 3. The particular of 2D lattice of Armchair polyhex $TUAC_6[m, n]$.

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

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

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

(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	$2m$	$9mn - 4m$

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.

Theorem 3.1. Let G be the armchair nanotube TUAC₆[m, n], for all $m, n \in E(G)$. Then the AG_2 index of G is

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

Proof. We know

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

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 $TUAC_6[m, n]$, for all $m, n \in E(G)$. Then the SK_3 index of G is

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

Proof. We have

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

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 $TUAC_6[m, n]$, for all $m, n \in E(G)$. Then the Sanskruti index of G is

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

Proof. It is easy to see that

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

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 of $TUAC_6[m,n]$ armchair polyhex nanotube without using computer.

References

- [1] A. Bahramia and J. Yazdani, Padmakar-Ivan Index of H-Phenylinic Nanotubes and Nanotore, Digest Journal of Nanomaterials and Biostructures 3 (2008) 265-267.
- [2] A. Iranmanesh and A. R. Ashrafi, Balaban index of an armchair polyhex $TUC_4C_8(R)$ and $TUC_4C_8(S)$ nanotorus, Journal of Computational and Theoretical Nanoscience 4 (3) (2007) 514-517.
- [3] F. Harary, Graph theory, Addison-Wesely, Reading mass, 1969.
- [4] H. Deng, The PI Index of $TUAC_6[2p,q]$, MATCH Communications in Mathematical and in Computer Chemistry 55 (2006) 461-476.
- [5] I. Gutman, Degree-based topological indices, Croat. Chem. Acta. 86 (2013) 251-361.
- [6] I. Gutman and N. Trinajstic, Graph theory and molecular orbital. Total π -electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535-538.
- [7] M. Eliahi and B. Taeri, Distance in Armchair Polyhex Nanotubes, MATCH Communications in Mathematical and in Computer Chemistry 62 (2009) 295-310.
- [8] M. V. Diudea, I. Gutman and J. Lorentz, Molecular Topology, Nova, Huntington (2001).
- [9] M. R. Farahani, On The Fourth Atom-Bond Connectivity Index Of Armchair Polyhex Nanotubes, Proc. Rom. Acad. Series B. 15 (1) (2013) 3-6.
- [10] M. R. Farahani, Some Connectivity Indices and Zagreb Index of Polyhex Nanotubes, Acta Chimica Slovenica. 59 (4) (2012) 779-783.
- [11] M. V. Diudea, M. Stefu, B. P. Z. and P. E. John, Armchair Polyhex Nanotubes, Croatica Chemica Acta 77 (2004) 111-115.
- [12] N. Trinajstic, Chemical Graph theory, CRC Press, Boca Raton, 1992.
- [13] S. Yousefi and A. R. Ashrafi, Distance Matrix and Wiener Index of Armchair Polyhex Nanotubes, Studia Univ. Babeş-Bolyai. Chemia. 53 (4) (2008) 111-116.
- [14] S. M. Hosamani, Computing Sanskrit index of certain nanostructures, J. Appl. Math. Comput. (2016) 1-9.

- [15] S. M. Hosamani and I. Gutman, Zagreb indices of transformation graphs and total transformation graphs, *Appl. Math. Comput.* 247 (2014) 1156-1160.
- [16] V. S. Shigehalli and R. Kanabur, Computation of New Degree-Based Topological Indices of Graphene, *Journal of Mathematics* (2016).
- [17] V. S. Shigehalli and R. Kanabur, Computing Degree-Based Topological Indices of Polyhex Nanotubes, *Journal of Mathematical Nanoscience* 6 (1-2) (2016) 59- 68.
- [18] V. S. Shegehalli and R. Kanabur, New Version of Degree-Based Topological Indices of Certain nanotube, *Journal of Mathematical Nano science* 6 (1-2) (2016) 29-39.
- [19] V. S. Shegehalli and R. Kanabur, Arithmetic-Geometric indices of Path Graph, *Journal of Computer and Mathematical sciences* 6 (1) (2015) 19-24.