Journal of Mathematical Nanoscience 6 (1-2) (2016) 27–40

Journal of Mathematical Nanoscience

Available Online at: http://jmathnano.sru.ac.ir

Shahid Rajaee Teacher Training University

New version of degree-based topological indices of certain nanotube

Vijayalaxmi Shigehalli, Rachanna Kanabur *

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

Academic Editor: Ali Reza Ashrafi

Abstract. In this paper, we compute the geometric-arithmetic index (GA_1 index), SK index, SK_1 index and SK_2 index of H-naphtalenic nanotube and $TUC_4[m,n]$ nanotube. We also compute SK_3 index, GA_2 index for H-naphtalenic nanotube and $TUC_4[m,n]$ nanotube.

Keywords. geometric-arithmetic index (GA_1 index), SK index, SK_1 index, SK_2 index, SK_3 index, GA_2 index, H-naphtalenic nanotube, $TUC_4[m,n]$ nanotube.

1 Introduction

Let G be a simple connected graph in chemical graph theory. In mathematical 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 [5].

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 [8,17,21,22]. 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

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

$u \in V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [9].

2 Computing the topological indices of certain nanotube

Motivated by previous research on certain nanotube, here we introduce six new topological indices and compute their corresponding topological index value of certain nanotube [10,11,13,18–20].

Carbon nanotubes, long, thin cylinders of carbon, were discovered in 1991 by S. Iijima. These are large macromolecules that are unique for their size, shape, and remarkable physical properties. They can be thought of as a sheet of graphite (a hexagonal lattice of carbon) rolled into a cylinder. These intriguing structures have sparked much excitement in recent years and a large amount of research has been dedicated to their understanding. Currently, the physical properties are still being discovered and disputed. Nanotubes have a very broad range of electronic, thermal, and structural properties that change depending on their different kinds (defined by its diameter, length, chirality, or twist). To make things more interesting, besides having a single cylindrical wall (SWNTs), nanotubes can have multiple walls (MWNTs)–cylinders inside other cylinders. Recent work on computing topological indices of certain nanotube can be seen in [10,11,14].

The distance between two vertices a and b is denoted as $d_H(a,b)$ and is the length of shortest path between a and b in graph H. The length of shortest path between a and b is also called a-b geodesic. The longest path between any two vertices is called a-b detour.

In this paper, H is considered to be simple connected graph with vertex set $V(H)$ and edge set $E(H)$, da is the degree of vertex $a \in V(H)$ and

$$S_a = \sum_{b \in N_H(a)} d(b),$$

where $N_H = \{b \in V(H) \setminus ab \in E(H)\}$. The notations used in this paper, are mainly taken from books [4,21]. Now, we propose the following topological indices and compute their value for certain nanotube.

2.1 Geometric-arithmetic- (GA_1) index

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

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

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).

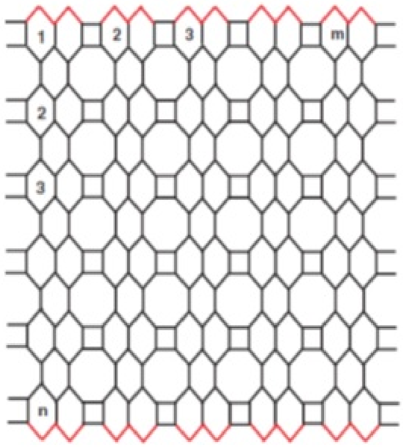

Figure 1. A 2D-lattice of H-naphtalenic nanotube $NPHX[m,n]$ showing the edge partition based on the degrees of end vertices of each edge.

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.

2.5 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 $S_G(u)$ and $S_G(v)$ are the summation of the degrees of all neighbours of vertices u and v in G.

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

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

2.6 Geometric-arithmetic (GA_2) index

Let $G = (V, E)$ be a molecular graph, and S_u is the degree of the vertex u, then GA_2 index of G is defined as

$$GA_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}},$$

where GA_2 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 $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v).

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

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

In this paper, we study certain degree based topological indices of H-naphtalenic nanotubes and $TUC_4[m,n]$ nanotube. These topological indices correlate certain physico-chemical properties of these nanotubes.

3 Main Results

In this paper, we study GA_1, SK, SK_1, SK_2, SK_3 and GA_2 indices of H-naphtalenic nanotube and $TUC_4[m,n]$ nanotube.

3.1 Results for H-naphtalenic nanotubes

In this section, we compute the certain topological indices for H-naphtalenic nanotubes. This nanotube is a trivalent decoration having sequence of C_6, C_6, C_4, C_6, C_6, C_4, ... in first row and a sequence of C_6, C_8, C_6, C_8, ... in other rows. In other words, the whole lattice is a plane tiling that can either cover a cylinder or a torus. These nanotubes are usually symbolized as $NPHX[m,n]$, in which m is the number of pair of hexagons in first row and n is the number of alternative hexagons in a column as depicted in Figure 1. Now we compute certain degree based topological indices for this class of nanotubes. We can clearly see that there are two type of edges in 2D-lattice of this nanotube, as shown by different colours in Figure 1, the colour red shows the edges ab and $d_a = 2$ and $d_b = 3$ and the colour black shows the edges ab with $d_a = d_b = 3$. Table 1 shows cardinalities of these two partite series of edge set of $NPHX[m,n]$ nanotube.

(d_a, d_b) where $a,b \in E(H)$	(2,3)	(3,3)
Number of edges	8m	15mn − 10m

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 $NPHX[m,n]$ nanotubes, then its GA_1 index is equal to*

$$GA_1(NPHX[m,n]) = (15n + 20 - 10\sqrt{6})m.$$

Proof. Consider the graph of $NPHX[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $NPHX[m,n]$ nanotube given in Table 1, we compute the GA_1 index of $NPHX[m,n]$ nanotube.

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

$$\begin{aligned} GA_1(NPHX(n)) &= 8m\left(\frac{2+3}{2\sqrt{6}}\right) + (15mn - 10m)\left(\frac{3+3}{2\sqrt{9}}\right) \\ &= \frac{20m}{\sqrt{6}} + 15mn - 10m \\ &= 15mn + \left(\frac{20}{\sqrt{6}} - 10\right)m \\ &= \left(15n + 20 - 10\sqrt{6}\right)m. \end{aligned}$$

□

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

$$SK(NPHX[m,n]) = (45n - 10)m.$$

Proof. Consider the graph of $NPHX[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $NPHX[m,n]$ nanotube given in Table 1, we compute the SK index of $NPHX[m,n]$ nanotube.

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

$$\begin{aligned} SK(NPHX(n)) &= 8m\left(\frac{2+3}{2}\right) + (15mn - 10m)\left(\frac{3+3}{2}\right) \\ &= 20m + 45mn - 30m \\ &= 45mn - 10m \\ &= (45n - 10)\,m. \end{aligned}$$

□

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

$$SK_1(NPHX[m,n]) = \frac{1}{2}(135n - 42)\, m.$$

Proof. Consider the graph of $NPHX[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $NPHX[m,n]$ nanotube given in Table 1, we compute the SK_1 index of $NPHX[m,n]$ nanotube.

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

$$\begin{aligned} SK_1(NPHX(n)) &= 8m\left(\frac{2\times 3}{2}\right) + (15mn - 10m)\left(\frac{3\times 3}{2}\right) \\ &= 24m + (15mn - 10m)\frac{9}{2} \\ &= \frac{1}{2}(48m + 135mn - 90m) \\ &= \frac{1}{2}(135n - 42)\, m. \end{aligned}$$

□

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

$$SK_2(NPHX[m,n]) = (135n - 40)\, m.$$

Proof. Consider the graph of $NPHX[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $NPHX[m,n]$ nanotube given in Table 1, we compute the SK_2 index of $NPHX[m,n]$ nanotube.

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

$$\begin{aligned} SK_2(NPHX(n)) &= 8m\left(\frac{2+3}{2}\right)^2 + (15mn - 10m)\left(\frac{3+3}{2}\right)^2 \\ &= 50m + 135mn - 90m \\ &= (135n - 40)\, m. \end{aligned}$$

Now we compute two important topological indices GA_2 and SK_3 for 2D-lattice of $NHPX[m,n]$ nanotube. There are six types of edges in $NHPX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge as depicted in Figure 2, in which different colours shows different partite sets of edge set of $NHPX[m,n]$

(S_a, S_b) where $u,v \in E(H)$	(6,7)	(6,8)	(8,8)	(7,9)	(8,9)	(9,9)
Number of edges	$4m$	$4m$	$2m$	$2m$	$4m$	$15mn - 18m$

Table 2. Edge partition of graph of $NHPX[m,n]$ nanotubes based on degree sum of vertices lying at unit distance from end vertices of each edge.

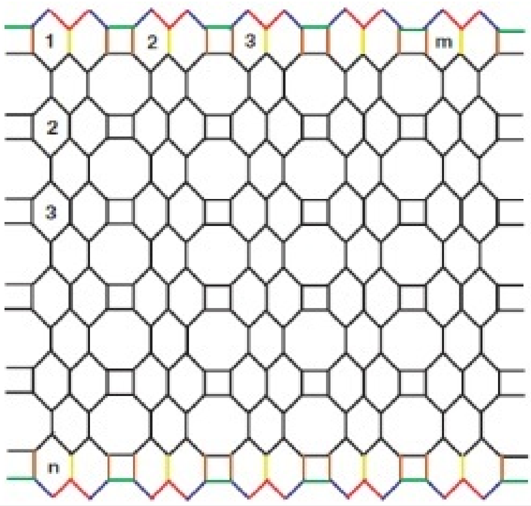

Figure 2. A graph of H-naphtalenic nanotube $NPHX[m,n]$ showing different partite sets based on the degree sum of neighbours of end vertices of each edge.

nanotube. In Figure 2, red colour shows the edges ab with $S_a = 6$ and $S_b = 7$, blue colour shows the type of edges ab with $S_a = 6$ and $S_b = 8$, green colour shows the type of edges ab with $S_a = S_b = 8$, yellow colour shows the type of edges ab with $S_a = 7$ and $S_b = 9$, brown colour shows the type of edges ab with $S_a = 8$ and $S_b = 9$ and black colour shows the partition having edges ab with $S_a = S_b = 9$.

In Table 2, cardinalities of such partite series of edge set of graph of $NHPX[m,n]$ nanotube are shown. In the following theorem, GA_2 index of $NHPX[m,n]$ nanotube and SK_3 index of $NHPX[m,n]$ nanotube is computed. □

Theorem 3.5. *Consider the graph of $NPHX[m,n]$ nanotube, then its GA_2 index is equal to*

$$GA_2(NPHX[m,n]) = \left(15n + \frac{26}{\sqrt{42}} + \frac{28}{\sqrt{48}} + \frac{16}{\sqrt{63}} + \frac{34}{\sqrt{72}} - 16\right) m.$$

Proof. We use the edge partition of graph of $NPHX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge. Now by using the partition given in Table 2 we can apply the formula of GA_2 index to compute this index for $NPHX[m,n]$ nanotube.

$$GA_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}}.$$

$$\begin{aligned} GA_2(NPHX(n)) &= 4m\left(\frac{6+7}{2\sqrt{42}}\right) + 4m\left(\frac{6+8}{2\sqrt{48}}\right) + 2m\left(\frac{8+8}{2\sqrt{64}}\right) + 2m\left(\frac{7+9}{2\sqrt{63}}\right) \\ &+ 4m\left(\frac{8+9}{2\sqrt{72}}\right) + (15mn-8m)\left(\frac{9+9}{2\sqrt{81}}\right) \\ &= \frac{26m}{\sqrt{42}} + \frac{28m}{\sqrt{48}} + 2m + \frac{16m}{\sqrt{63}} + \frac{34m}{\sqrt{72}} + 15mn - 18m \\ &= \left(15n + \frac{26}{\sqrt{42}} + \frac{28}{\sqrt{48}} + \frac{16}{\sqrt{63}} + \frac{34}{\sqrt{72}} - 16\right). \end{aligned}$$

□

Theorem 3.6. *Consider the graph of $NPHX[m,n]$ nanotube, then its SK_3 index is equal to*

$$SK_3(NPHX[m,n]) = (135n-42)\,m.$$

Proof. We use the edge partition of graph of $NPHX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge. Now by using the partition given in Table 2 we can apply the formula of SK_3 index to compute this index for $NPHX[m,n]$ nanotube.

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

$$\begin{aligned} SK_3(NPHX(n)) &= 4m\left(\frac{6+7}{2}\right) + 4m\left(\frac{6+8}{2}\right) + 2m\left(\frac{8+8}{2}\right) + 2m\left(\frac{7+9}{2}\right) + 4m\left(\frac{8+9}{2}\right) \\ &+ (15mn-8m)\left(\frac{9+9}{2}\right) \\ &= 26m + 28m + 16m + 34m + 135mn - 162m \\ &= (135n-42)\,m. \end{aligned}$$

3.2 Results for nanotubes coverd by C_4

In this section, we compute certain topological indices of nanotube covered only by C_4. The 2D-lattice of this family of nanotubes is a plane tiling of C_4. This tessellation of C_4 can either cover a cylinder or a torus. This family of nanotubes is denoted by $TUC_4[m,n]$, in which m is the number of squares in a row and n is the number of squares in a column as shown in Figure 4. A 3D representation of $TUC_4[m,n]$ nanotubes is depicted in Figure 3. There are three types of edges in 2D-lattice of $TUC_4[m,n]$ nanotube based on degrees of end vertices of each edge. Figure 3, explains such a partition of edges in which red coloured edges are the edges ab with $d_a = d_b = 3$, blue coloured edges are the edges ab with d_a =3, d_b = 4 and black coloured edges are the edges ab with $d_a = d_b = 4$. Table 3 shows the number of edges in each partite set. □

Theorem 3.7. *Consider the graph of $TUC_4[m,n]$ nanotubes, then its GA_1 index is equal to*

$$GA_1(TUC_4[m,n]) = \left(2n + \frac{7}{\sqrt{12}} - 1\right)(m+1).$$

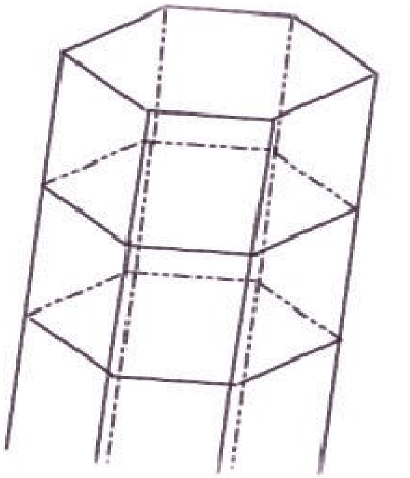

Figure 3. A $TUC_4[6,n]$ nanotube covered by C_4.

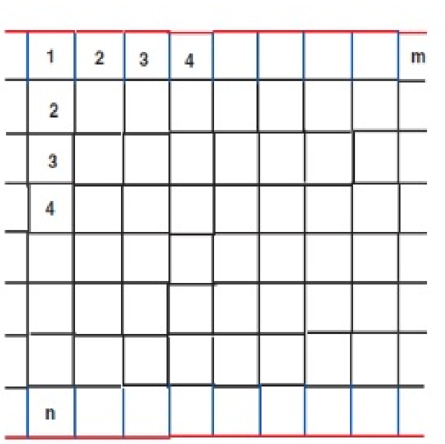

Figure 4. A graph of $TUC_4[m,n]$ nanotube showing the edge partition based on the degree of end vertices of each edge.

Proof. Consider the graph of $TUC_4[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $TUC_4[m,n]$ nanotube given in Table 3, we compute the GA_1 index of $TUC_4[m,n]$ nanotube.

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

$$\begin{aligned} GA_1\left(TUC_4\left[m,n\right]\right) &= \left(2m+2\right)\left(\frac{3+3}{2\sqrt{9}}\right) + \left(2m+2\right)\left(\frac{3+4}{2\sqrt{12}}\right) \\ &+ \left(m+1\right)\left(2n-3\right)\left(\frac{4+4}{2\sqrt{16}}\right) \\ &= \left(2m+2\right) + \left(2m+2\right)\left(\frac{7}{2\sqrt{12}}\right) + \left(m+1\right)\left(2n-3\right) \end{aligned}$$

(d_a, d_b) where $u,v \in E(H)$	(3,3)	(3,4)	(4,4)
Number of edges	$(2m+2)$	$(2m+2)$	$(m+1)(2n-3)$

Table 3. Cardinalities of different partite sets based on degrees of end vertices of each edge of graph of $TUC_4[m,n]$ nanotube.

$$\begin{aligned}
&= 2mn + \left(\frac{7}{2\sqrt{12}}\right) - m + \left(\frac{7}{2\sqrt{12}}\right) - 1 \\
&= \left(2n + \frac{7}{\sqrt{12}} - 1\right) - m + \frac{7}{12} - 1 + 2n \\
&= \left(2n + \frac{7}{\sqrt{12}} - 1\right)(m+1).
\end{aligned}$$

□

Theorem 3.8. *Consider the graph of $TUC_4[m,n]$ nanotubes, then its SK index is equal to*

$$SK(TUC_4[m,n]) = (8n+1)(m+1).$$

Proof. Consider the graph of $TUC_4[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $TUC_4[m,n]$ nanotube given in Table 3, we compute the SK index of $TUC_4[m,n]$ nanotube.

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

$$\begin{aligned}
SK(TUC_4[m,n]) &= (2m+2)\left(\frac{3+3}{2}\right) + (2m+2)\left(\frac{3+4}{2}\right) + (m+1)(2n-3)\left(\frac{4+4}{2}\right) \\
&= 6m + 6 + 7m + 7 + (2mn - 3m + 2n - 3)4 \\
&= (8n+1)m + 8n + 1 \\
&= (8n+1)(m+1).
\end{aligned}$$

□

Theorem 3.9. *Consider the graph of $TUC_4[m,n]$ nanotubes, then its SK_1 index is equal to*

$$SK_1(TUC_4[m,n]) = (16n-3)(m+1).$$

Proof. Consider the graph of $TUC_4[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $TUC_4[m,n]$ nanotube given in Table 3, we compute the SK_1 index of $TUC_4[m,n]$ nanotube.

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

$$\begin{aligned} SK_1\left(TUC_4\left[m,n\right]\right) &= (2m+2)\left(\frac{3\times 3}{2}\right) + (2m+2)\left(\frac{3\times 4}{2}\right) + (m+1)(2n-3)\left(\frac{4\times 4}{2}\right) \\ &= 9m+9+12m+12+(2mn-3m+2n-3)8 \\ &= (16n-3)m+16n+1 \\ &= (16n-3)(m+1). \end{aligned}$$

□

Theorem 3.10. *Consider the graph of $TUC_4[m,n]$ nanotubes, then its SK_2 index is equal to*

$$SK_2(TUC_4[m,n]) = \frac{1}{2}(64n-11)(m+1).$$

Proof. Consider the graph of $TUC_4[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $TUC_4[m,n]$ nanotube given in Table 3, we compute the SK_2 index of $TUC_4[m,n]$ nanotube.

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

$$\begin{aligned} SK_2(TUC_4[m,n])) &= (2m+2)\left(\frac{3+3}{2}\right)^2 + (2m+2)\left(\frac{3+4}{2}\right)^2 + (m+1)(2n-3)\left(\frac{4+4}{2}\right)^2 \\ &= (2m+2)9 + (2m+2)\left(\frac{49}{4}\right) + (2mn-3m+2n-3)16 \\ &= \frac{1}{2}(64mn-11m+64n-11) \\ &= \frac{1}{2}((64n-11)m+64n-11) \\ &= \frac{1}{2}(64n-11)(m+1). \end{aligned}$$

Now we compute GA_2 and SK_3 indices for two dimensional lattice of $TUC_4[m,n]$ nanotubes. There are five types of edges in the graph of $TUC_4[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each, as shown in Figure 5, in which red coloured edges are the edge ab with $S_a = S_b = 7$, blue coloured edges are the edge ab with $S_a = 7$ and $S_b = 15$, green coloured edges are the edge ab with $S_a = S_b = 15$, yellow coloured edges are the edge ab with $S_a = 15$ and $S_b = 16$, and black coloured edges are the edge ab with $S_a = S_b = 16$. Table 4 shows the cardinalities of these partite sets.

□

Theorem 3.11. *Let $TUC_4[m,n]$ nanotube be a graph with $(m \geq 1, n \geq 4)$, then its GA_2 index is*

$$GA_2(TUC_4[m,n]) = \left(2n-3+\frac{22}{\sqrt{105}}+\frac{31}{\sqrt{240}}\right)(m+1).$$

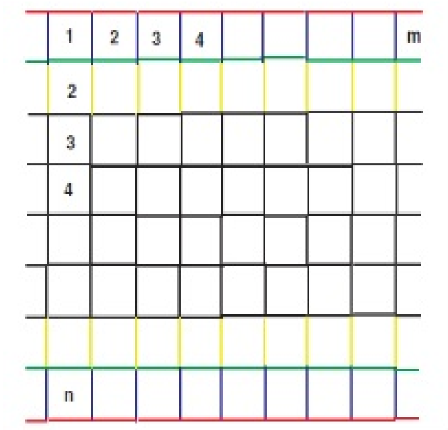

Figure 5. A graph of $TUC_4[m,n]$ nanotube showing the edge partition based on the degree sum of end vertices lying at unit distance from end vertices of each edge.

Table 4. Edge partition of graph of $TUC_4[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each edge.

(S_a, S_b) where $u,v \in E(H)$	(7,7)	(7,15)	(15,15)	(15,16)	(16,16)
Number of edges	$(2m+2)$	$(2m+2)$	$(2m+2)$	$(2m+2)$	$(m+1)(2n-7)$

Proof. We use the edge partition of graph of $TUC_4[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 4 we can apply the formula of GA_2 index to compute this index for $TUC_4[m,n]$ nanotube.

$$GA_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}}.$$

$$\begin{aligned} GA_2(TUC_4[m,n]) &= (2m+2)\left(\frac{7+7}{2\sqrt{49}}\right) + (2m+2)\left(\frac{7+15}{2\sqrt{105}}\right) + (2m+2)\left(\frac{15+15}{2\sqrt{225}}\right) \\ &+ (2m+2)\left(\frac{15+16}{2\sqrt{240}}\right) + (m+1)(2n-7)\left(\frac{16+16}{2\sqrt{256}}\right) \\ &= 2m+2+\frac{22m+22}{\sqrt{105}} + 2m+2+\frac{31m+31}{\sqrt{240}} + 2mn - 7m + 2n - 7 \\ &= 2mn - 3m + 2n - 3 + \frac{22m+22}{\sqrt{105}} + \frac{31m+31}{\sqrt{240}} \\ &= \left(2n-3+\frac{22}{\sqrt{105}}+\frac{31}{\sqrt{240}}\right)m + \left(2n-3+\frac{22}{\sqrt{105}}+\frac{31}{\sqrt{240}}\right) \\ &= \left(2n-3+\frac{22}{\sqrt{105}}+\frac{31}{\sqrt{240}}\right)(m+1). \end{aligned}$$

□

Theorem 3.12. *Let $TUC_4[m,n]$ nanotube be a graph with $(m \geq 1, n \geq 4)$, then its SK_3 index is*

$$SK_3(TUC_4[m,n]) = (32n-15)(m+1).$$

Proof. We use the edge partition of graph of $TUC_4[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge. Now by using the partition given in Table 4, we can apply the formula of GA_2 index to compute this index for $TUC_4[m,n]$ nanotube.

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

$$\begin{aligned} SK_3(TUC_4[m,n]) &= (2m+2)\left(\frac{7+7}{2}\right) + (2m+2)\left(\frac{7+15}{2}\right) + (2m+2)\left(\frac{15+15}{2}\right) \\ &+ (2m+2)\left(\frac{15+16}{2}\right) + (m+1)(2n-7)\left(\frac{16+16}{2}\right) \\ &= 14m + 14 + 22m + 22 + 30m + 30 + 31 + (2mn - 7m + 2n - 7)\,16 \\ &= 32mn - 15m + 32n - 15 \\ &= (32n-15)\,m + 32n - 15 \\ &= (32n-15)(m+1). \end{aligned}$$

□

Concluding Remarks: A generalized formula for geometric-arithmetic index (GA_1 index), SK index, SK_1 index, SK_2 index, SK_3 index, GA_2 index for H-naphtalenic nanotube and $TUC_4[m,n]$ nanotube is obtained without using a computer.

References

[1] S. M. Adhikari, A. Sakar and K. P. Ghatak, Simple theoretical analysis of the field emission from quantum wire effective mass superlattices of heavily doped materials, Quantum Matter. 2 (2013) 455–464.

[2] A. Bahramia and J. Yazdani, Padmakar-Ivan index of H-phenylinic nanotubes and Nanotorus, Digest Journal of Nanomaterials and Biostructures 3 (2008) 265–267.

[3] P. K. Bose, N. Paitya, S. Bhattacharya, D. De, S. Saha, K. M. Chatterjee, S. Pahari and K. P. Ghatak, Influence of light waves on the effective electron mass in quantum wells, wires, inversion layers and superlattices, Quantum Matter. 1 (2012) 89–126.

[4] M. V. Diudea, I. Gutman and J. Lorentz, Molecular Topology, Nova Science Publishers, Huntington, NY 2001.

[5] E. Estrada, L. Torres, L. Rodríguez and I Gutman, An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes, Indian J. Chem. 37A (1998) 849–855.

[6] K. P. Ghatak, S. Bhattacharya, A. Mondal, S. Debbarma, P. Ghorai and A. Bhattacharjiee, On the Fowler-Nordheim field emission from quantum-confined optoelectronic materials in the presence of light waves, Quantum Matter. 2 (1) (2013) 25–41.

[7] I. Gutman, Degree-based topological indices, Croat. Chem. Acta 86 (2013) 251–361.

[8] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total -electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535–538.

[9] F. Harary, Graph theory, Addison-Wesely, Reading mass, 1969.
[10] S. Hayat and M. Imarn, On degree based topological indices of certain nanotubes, J. Comput. Theor. Nanosci. 12 (8) (2015) 1–7.
[11] S. M. Hosamani, Computing Sanskruti index of certain nanostructures, J. Appl. Math. Comput. (2016) 1–9.
[12] A. Khrennikov, Einstein's dream-quantum mechanics as theory of classical random fields, Rev. Theor. Sci. 1 (2013) 34–57.
[13] K. Lavanya Lakshmi, A highly correlated topological index for polyacenes, Journal of Experimental Sciences 3 (4) (2012) 18–21.
[14] A. Madanshekaf and M. Moradi, The first geometric-arithmetic index of some nanostar dendrimers, Iran. J. Math. Chem. 5 (2014) 1–6.
[15] E. L. Pankratov and E. A. Bulaeva, optimal criteria to estimate temporal characteristics of diffusion process in a media with inhomogenous and nonstationary parameters. Analysis of influence of variation of diffusion coefficient on values of time characteristics, Rev. Theor. Sci. 1 (2013) 307–318.
[16] N. Paitya and K. P. Ghatak, Quantization and carrier mass, Rev. Theor. Sci. 1 (2013) 165–305.
[17] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (23) (1975) 6609–6615.
[18] V. S. Shegehalli and R. Kanabur, Geometric-arithmetic indices of some class of graph, J. Comp. Math. Sci. 6 (4) (2015) 194–199.
[19] V. S. Shegehalli and R. Kanabur, Geometric-arithmetic indices of path graph, J. Comp. Math. Sci. 6 (1) (2015) 19–24.
[20] V. S. Shegehalli and R. Kanabur, Computation of new degree-based topological indices of graphene, Journal of Mathematics, Hindawi Publications, (2016) http://dx.doi.org/10.1155/2016/4341919.
[21] N.Trinajstić, Chemical graph theory, CRC Press, Boca Raton, 1992.
[22] R. Todeschini and V. Consonni, Handbook of molecular descriptors, Wiley-VCH, Weinheim, 2000.