On topological indices of nanostar dendrimers and polyomino chains

MUHAMMAD IMRAN*, SAKANDER HAYAT[a], MUHAMMAD KASHIF SHAFIQ[b]
Department of Mathematics, School of Natural Sciences (SNS), National University of Sciences and Technology (NUST), Sector H-12, Islamabad, Pakistan
[a]*Department of Mathematics, School of Natural Sciences (SNS), National University of Sciences and Technology (NUST), Sector H-12, Islamabad, Pakistan*
[b]*Department of Mathematics, Government College University, Faisalabad, Pakistan*

A numeric quantity which characterizes the whole structure of a graph is called a topological index. The concept of Randić $\chi(H)$, atom-bond connectivity (ABC) and geometric-arithmetic (GA) topological indices were established in chemical graph theory based on vertex degrees. Later on, other versions of ABC and GA indices were introduced and some of the versions of these indices are recently designed. Dendrimers are recognized as one of the major commercially available nanoscale building blocks, large and complex molecules with well defined chemical structure. The nanostar dendrimer is a part of a new group of macroparticles that appear to be photon funnels just like artificial antennas. A k-polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular $4k$-cycle of length one. In this article, we compute ABC, GA, and Randić indices of two important families of nanostar dendrimers. We also compute fourth version of atom-bond connectivity (ABC_4) index and fifth version of geometric-arithmetic (GA_5) index for graphs of 1 and 2-polyomino chains of 8-cycles.

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1. Introduction and preliminary results

Chemical graph theory is a branch of *mathematical chemistry* which applies graph theory to the mathematical model of chemical phenomenon. Topological indices is a subtopic of chemical graph theory, which correlates certain physico-chemical properties of of the underlying chemical compound. There are hundreds of papers on topological indices which have been published so far.

A topological index is a function "Top" from '$\sum$' to the set of real numbers, where '$\sum$' is the set of finite simple graphs with property that $Top(G) = Top(H)$ if both G and H are isomorphic. There is a lot of research which has been done on topological indices of different graph families so far, and is of much importance due to their chemical significance.

Nanobiotechnology is a rapidly advancing area of scientific and technological opportunity that applies the tools and processes of nanofabrication to build devices for studying biosystems. Dendrimers are one of the main objects of this new area of science. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers using a nanoscale fabrication process. Dendrimers are recognized as one of the major commercially available nanoscale building blocks, large and complex molecules with very well defined chemical structure. From a polymer chemistry point of view, dendrimers are nearly perfect monodisperse macromolecules with a regular and highly branched three dimensional architecture. They consist of three major architectural components: core, branches and end groups. New branches emitting from a central core are added in steps until a tree-like structure is created. The nanostar dendrimer is a part of a new group of macroparticles that appear to be photon funnels just like artificial antennas. These macromolecules and more precisely those containing phosphorus are used in the formation of nanotubes, micro and macrocapsules, nanolatex, coloured glasses, chemical sensors, modified electrodes and so on [1, 6]. A k-polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular $4k$-cycle of length one. In other words, it is an edge-connected union of cells [14].

In this article, H is considered to be simple connected graph with vertex set $V(H)$ and edge set $E(H)$, degree of vertex $a \in V(H)$ is d_a and $S_a = \sum_{b \in N_H(a)} d(b)$ where $N_H(a) = \{b \in V(H) \mid ab \in E(H)\}$. The notations used in this article are mainly taken from books [4, 13, 18].

The very first degree based topological index is Randić index [19] denoted by $\chi(H)$ and introduced by *Milan Randić* in 1975. Let H be a graph. The Randić index of H is defined as

$$\chi(H) = \sum_{ab \in E(H)} \frac{1}{\sqrt{d_a d_b}}$$

One of the well-known connectivity topological index is *atom-bond connectivity* (ABC) index introduced by *Estrada* et al. in [7]. For a graph H, the ABC index is defined as

$$ABC(H) = \sum_{ab \in E(H)} \sqrt{\frac{d_a + d_b - 2}{d_a d_b}}$$

Another well-known connectivity topological descriptor is *geometric-arithmetic* (GA) index which was introduced by *Vukičević* et al. in [15]. Consider a graph H, then its GA index is defined as

$$GA(H) = \sum_{ab \in E(H)} \frac{2\sqrt{d_a d_b}}{(d_a + d_b)}$$

The fourth version of ABC index is introduced by *Ghorbani* et al. [11] recently in 2010. Let H be a graph, then its ABC_4 index is defined as

$$ABC_4(H) = \sum_{ab \in E(H)} \sqrt{\frac{S_a + S_b - 2}{S_a S_b}}$$

Recently fifth version of GA index is proposed by *Graovac* et al. [12] in 2011. For a graph H, the its GA_5 index is defined as

$$GA_5(H) = \sum_{ab \in E(H)} \frac{2\sqrt{S_a S_b}}{(S_a + S_b)}$$

In this paper, we study certain degree based topological indices of two finite families of nanostar dendrimers and ABC_4 and GA_5 of k-polyomino chains with $k = 1,2$ of 8-cycles. These topological indices correlate certain physico-chemical properties of these nanostructures as well as describe the deep topologies of these macro molecules.

2. Main results

In this paper, we calculate ABC, GA, Randić, ABC_4 and GA_5 indices of two important classes of nanostar dendrimers and 1,2-polyomino chains of 8-cycles. In the following section, we compute these topological indices for nanostar dendrimers.

2.1 Nanostar dendrimers

Dendrimers are highly ordered branched macromolecules which have attracted much theoretical and experimental attention. The topological study of these macromolecules is a new subject of research [5, 17]. The aim of this section is to calculate analytical closed results of Randić, ABC, GA indices for two important classes of nanostar dendrimers. The first class of these macromolecules is named as $NS_1[n]$, where n is the defining parameter as shown in Fig. 1. The number of edges in this nanostar is $140(2)^n - 127$.

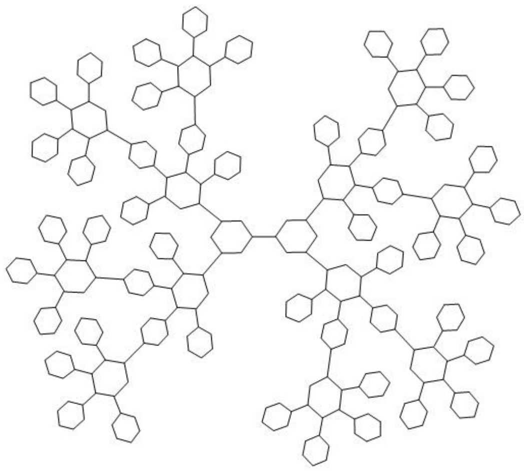

Fig. 1. The first type of nanostar dendrimer $NS_1[n]$ *with* $n = 2$.

Now we compute certain degree based topological indices for this class of nanostar dendrimers. We can clearly see that, there are three type of edges in graph of this nanostar dendrimer based on degrees of end vertices of each edge. Table 1 shows such a partition for $NS_1[n]$ for $n > 1$.

Table 1. Edge partition of nanostar dendrimer $NS_1[n]$, $n>1$ based on degrees of end vertices of each edge.

(d_a, d_b) where $ab \in E(H)$	(2,2)	(2,3)	(3,3)
Number of edges	12.2^n	$24.2^n - 12$	$6.2^n - 3$

In the following theorem, we compute the ABC index of $NS_1[n]$ nanostar dendrimer.

Theorem 2.1.1. Consider H be the graph of $NS_1[n]$ nanostar dendrimer, then its ABC index is equal to

$$ABC(H) = (18\sqrt{2}+4)2^n - 6\sqrt{2} - 2$$

Proof. Consider the graph of $NS_1[n]$ nanostar dendrimer. By using the edge partition based on the degrees of end vertices of each edge of graph of $NS_1[n]$ nanostar dendrimer given in Table 1, we compute the ABC index of $NS_1[n]$ nanostar dendrimer.Since

$$ABC(H) = \sum_{ab\in E(H)} \sqrt{\frac{d_a + d_b - 2}{d_a d_b}}$$

This gives that

$$ABC(NS_1[n]) = (12.2^n)\sqrt{\frac{2+2-2}{2\times 2}} + (24.2^n - 12)\sqrt{\frac{2+3-2}{2\times 3}} + (6.2^n - 3)\sqrt{\frac{3+3-2}{3\times 3}}$$

After simplification, we get

$$ABC(NS_1[n]) = (18\sqrt{2}+4)2^n - 6\sqrt{2} - 2$$

The GA index for $NS_1[n]$ nanostar dendrimer is computed in the following theorem.

Theorem 2.1.2. Consider the graph of $NS_1[n]$ nanostar dendrimer, then its GA index is equal to

$$GA(NS_1[n]) = (\frac{48\sqrt{6}}{5} + 18)2^n - 3 - \frac{24\sqrt{6}}{5}$$

Proof. Consider the graph of $NS_1[n]$ nanostar dendrimer. Since

$$GA(H) = \sum_{ab\in E(H)} \frac{2\sqrt{d_a d_b}}{d_a + d_b}$$

This directly implies from Table 3 that

$$GA(NS_1[n]) = (12.2^n)\frac{2\sqrt{2\times 2}}{2+2} + (24.2^n - 12)\frac{2\sqrt{2\times 3}}{2+3} + (6.2^n - 3)\frac{2\sqrt{3\times 3}}{3+3}$$

After simplification, we get

$$GA(NS_1[n]) = (\frac{48\sqrt{6}}{5} + 18)2^n - 3 - \frac{24\sqrt{6}}{5}$$

Now we compute Randić index for this family of nanostar dendrimers.

Theorem 2.1.3. Let the graph of $NS_1[n]$ nanostar dendrimer, then its Randi c′ index is

$$\chi(NS_1[n]) = (18\sqrt{2}+4)2^n - 6\sqrt{2} - 2$$

Proof. By using the partition given in Table 1 and applying the formula of the Randić index, we compute this index for $NS_1[n]$ nanostar dendrimer. Since

$$\chi(H) = \sum_{ab\in E(H)} \frac{1}{\sqrt{d_a d_b}}$$

This implies that

$$\chi(NS_1[n]) = (12.2^n)\frac{1}{\sqrt{2\times 2}} + (24.2^n - 12)\frac{1}{\sqrt{2\times 3}} + (6.2^n - 3)\frac{1}{\sqrt{3\times 3}}$$

After a bit calculation, we get

$$\chi(NS_1[n]) = (18\sqrt{2}+4)2^n - 6\sqrt{2} - 2$$

Now we consider the second type of nanostar dendrimers i.e. $NS_2[n]$, where n is the defining parameter as depicted in Fig 2. The vertex and edge cardinalities for graph of this nanostar dendrimer are $120.2^n - 108$ and $140.2^n - 127$ respectively. To compute topological indices for this nanostar, we need an edge partition based on degrees of end vertices of each edge. Table 2 shows such an edge partition for graph of this nanostar dendrimer.

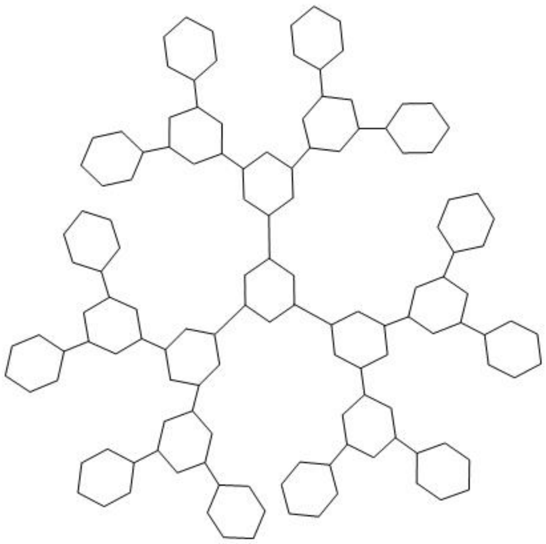

Fig. 2. The second type of nanostar dendrimer $NS_2[n]$ *with* $n = 2$.

Table 2. Edge partition of nanostar dendrimer $NS_2[n]$, $n > 1$ *based on degrees of end vertices of each edge.*

(d_a, d_b) where $ab \in E(H)$	(2,2)	(2,3)	(3,3)
Number of edges	$56.2^n - 48$	$48.2^n - 44$	$36.2^n - 35$

In the following theorem, we compute the ABC index of $NS_2[n]$ nanostar dendrimer.

Theorem 2.1.4. Let H be the graph of $NS_2[n]$ nanostar dendrimer, then its ABC index is equal to

$$ABC(H) = (52\sqrt{2} + 24)2^n - 46\sqrt{2} - \frac{70}{3}$$

Proof. Consider the graph of $NS_2[n]$ nanostar dendrimer. By using the edge partition based on the degrees of end vertices of each edge of graph of $NS_2[n]$ nanostar dendrimer given in Table 2, we compute the ABC index of $NS_2[n]$ nanostar dendrimer.Since

$$ABC(H) = \sum_{ab \in E(H)} \sqrt{\frac{d_a + d_b - 2}{d_a d_b}}$$

This gives that

$$ABC(NS_2[n]) = (56.2^n - 48)\sqrt{\frac{2+2-2}{2\times 2}} + (48.2^n - 44)\sqrt{\frac{2+3-2}{2\times 3}} + (36.2^n - 35)\sqrt{\frac{3+3-2}{3\times 3}}$$

After simplification, we get

$$ABC(NS_2[n]) = (52\sqrt{2} + 24)2^n - 46\sqrt{2} - \frac{70}{3}$$

The GA index for $NS_2[n]$ nanostar dendrimer is computed in the following theorem.

Theorem 2.1.5. Consider the graph of $NS_2[n]$ nanostar dendrimer, then its GA index is equal to

$$GA(NS_2[n]) = (\frac{96\sqrt{6}}{5} + 92)2^n - 83 - \frac{88\sqrt{6}}{5}$$

Proof. Consider the graph of $NS_2[n]$ nanostar dendrimer. Since

$$GA(H) = \sum_{ab \in E(H)} \frac{2\sqrt{d_a d_b}}{d_a + d_b}$$

This implies that

$$GA(NS_2[n]) = (56.2^n - 48)\frac{2\sqrt{2\times 2}}{2+2} + (48.2^n - 44)\frac{2\sqrt{2\times 3}}{2+3} + (36.2^n - 35)\frac{2\sqrt{3\times 3}}{3+3}$$

After simplification, we get

$$GA(NS_2[n]) = (\frac{96\sqrt{6}}{5} + 92)2^n - 83 - \frac{88\sqrt{6}}{5}$$

Now we compute Randić index for this family of nanostar dendrimers.

Theorem 2.1.6. Let the graph of $NS_1[n]$ nanostar dendrimer, then its Randić index is

$$\chi(NS_2[n]) = (8\sqrt{6} + 40)2^n - \frac{2}{2}\sqrt{6}3 - \frac{107}{3}$$

Proof. By using the partition given in Table 2 and applying the formula of the Randić index we can compute this index for $NS_2[n]$ nanostar dendrimer. Since

$$\chi(H) = \sum_{ab \in E(H)} \frac{1}{\sqrt{d_a d_b}}$$

This implies that

$$\chi(NS_2[n]) = (56.2^n - 48)\frac{1}{\sqrt{2\times 2}} + (48.2^n - 44)\frac{1}{\sqrt{2\times 3}} + (36.2^n - 35)\frac{1}{\sqrt{3\times 3}}$$

After a bit calculation, we get

$$\chi(NS_2[n]) = (8\sqrt{6}+40)2^n - \frac{2}{2}\sqrt{6}3 - \frac{107}{3}$$

2.2 Polyomino Chains of k -Cycles

A k -polyomino system is a finite 2 -connected plane graph such that each interior face (also called cell) is surrounded by a regular $4k$ -cycle of length one. In other words, it is an edge-connected union of cells [14]. In Fig. 3, one can see the polyomino chains of 8-cycles of two dimension. We use G_n to denote an n -dimensional graph of zig-zag chain of 8 -cycles.

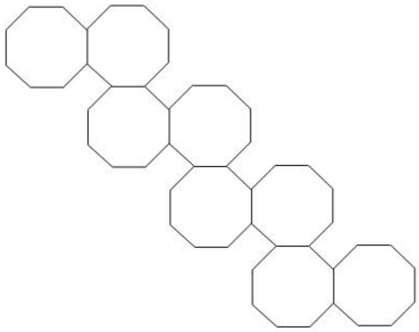

Fig. 3. The zig-zag chain of 8 -cycles, $n=2$.

Ghorbani et al. computed the ABC , GA and Randić index in [9]. In this section, we extend the results given in [9] to ABC_4 and GA_5 indices. To compute these indices, we need an edge partition of G_n based on degree sum of neighbors of end vertices of each edge. Table 3 shows such an edge partition of G_n . The vertex and edge cardinalities of G_n are $24n+2$ and $28n+1$ respectively.

Table 3. Cardinalities of different partite sets based on degrees of end vertices of each edge of graph of G_n .

(S_a, S_b) where $ab \in E(H)$	(5,4)	(4,4)	(5,7)	(5,8)	(7,8)	(8,8)
Number of edges	$8n$	$4n+4$	4	$8n-4$	2	$8n-5$

In the following theorem, a closed formula of ABC_4 for G_n is computed.

Theorem 2.2.1. Consider the graph of G_n nanotube, then its ABC_4 index is equal to

$$ABC_4(G_n) = (\frac{4\sqrt{35}}{5} + \sqrt{6} + \frac{2\sqrt{110}}{5} + \sqrt{14})n + \sqrt{6} + \frac{4\sqrt{14}}{7} + \frac{\sqrt{182}}{14} - \frac{\sqrt{110}}{5} - \frac{5\sqrt{14}}{8}$$

Proof. Consider the graph G_n . By using the edge partition based on the degrees of end vertices of each edge of graph of G_n given in Table 3, we compute the ABC_4 index.Since

$$ABC_4(H) = \sum_{ab \in E(H)} \sqrt{\frac{S_a + S_b - 2}{S_a S_b}}$$

This gives that

$$ABC(G_n) = (8n)\sqrt{\frac{5+4-2}{5\times 4}} + (4n+4)\sqrt{\frac{4+4-2}{4\times 4}} + (4)\sqrt{\frac{5+7-2}{5\times 7}} + (8n-4)\sqrt{\frac{5+8-2}{5\times 8}} + (2)\sqrt{\frac{7+8-2}{7\times 8}} + (8n-5)\sqrt{\frac{8+8-2}{8\times 8}}$$

After some calculation, we get

$$ABC_4(G_n) = (\frac{4\sqrt{35}}{5} + \sqrt{6} + \frac{2\sqrt{110}}{5} + \sqrt{14})n + \sqrt{6} + \frac{4\sqrt{14}}{7} + \frac{\sqrt{182}}{14} - \frac{\sqrt{110}}{5} - \frac{5\sqrt{14}}{8}$$

The GA_5 index for G_n is computed in the following theorem.

Theorem 2.2.2. Consider the graph of G_n , then its GA_5 index is equal to

$$GA(G_n) = (\frac{32\sqrt{5}}{9} + \frac{32\sqrt{10}}{13} + 12)n + \frac{2\sqrt{35}}{3} + \frac{8\sqrt{14}}{15} - \frac{16\sqrt{10}}{13} - 1$$

Proof. Table 3 shows the partition of edge set of graph of G_n based on the degrees of end vertices of each edge. Now we apply the formula of GA_5 index to compute this index.Since

$$GA_5(H)=\sum_{ab\in E(H)}\frac{2\sqrt{S_aS_b}}{S_a+S_b}$$

This implies that

$$GA(G_n)=(8n)\frac{2\sqrt{5\times 4}}{5+4}+(4n+4)\frac{2\sqrt{4\times 4}}{4+4}+(4)\frac{2\sqrt{5\times 7}}{5+7}+(8n-4)\frac{2\sqrt{5\times 8}}{5+8}+(2)\frac{2\sqrt{7\times 8}}{7+8}+(8n-5)\frac{2\sqrt{8\times 8}}{8+8}$$

After simplification, we get

$$GA(G_n)=(\frac{32\sqrt{5}}{9}+\frac{32\sqrt{10}}{13}+12)n+\frac{2\sqrt{35}}{3}+\frac{8\sqrt{14}}{15}-\frac{16\sqrt{10}}{13}-1$$

Now we compute ABC_4 and GA_5 indices for 2-polyomino system. We denote this graph as H_n i.e. n -dimensional 2-polyomino system . The vertex and edge cardinalities of H_n are $30n+2$ and $35n+1$ respectively. A 2-dimensional H_n is depicted in Fig. 4. There are seven types of edges based on degree sum of neighbors of end vertices of each edge in H_n. Table 4 shows such an edge partition of H_n.

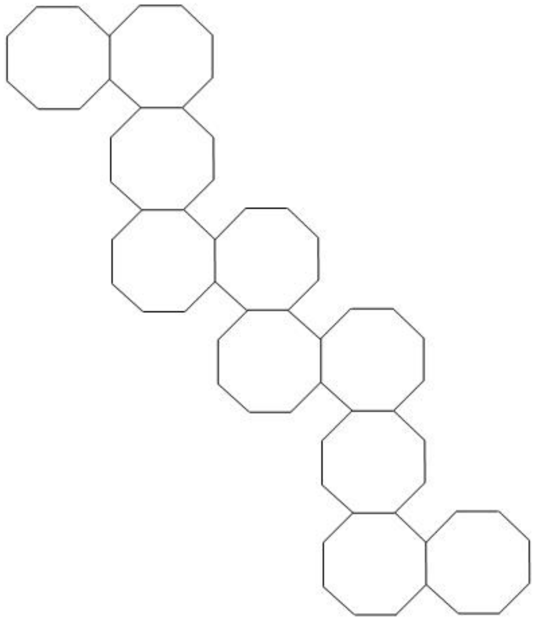

Fig. 4. The graph of 2 -polyomino system H_n with $n=2$.

Table 4. Edge partition of graph of H_n based on degree sum of vertices lying at unit distance from end vertices of each edge.

(S_a,S_b) where $ab\in E(H)$	(4,5)	(4,4)	(5,5)	(5,7)	(5,8)	(7,8)	(8,8)
Number of edges	$8n$	$4n+4$	$2n$	$4n+4$	$8n-4$	$2n+2$	$7n-5$

In following theorem, ABC_4 index of H_n is computed.

Theorem 2.2.3. Let the graph H_n with $n>1$, then its ABC_4 index is

$$ABC_4(H_n)=(\frac{4\sqrt{35}}{5}+\frac{4\sqrt{2}}{5}+\frac{4\sqrt{14}}{7}+\frac{2\sqrt{110}}{5}+\frac{\sqrt{182}}{14}+\frac{7\sqrt{14}}{8}+\sqrt{6})n$$

$$+\frac{4\sqrt{14}}{7}-\frac{\sqrt{110}}{5}+\frac{\sqrt{182}}{14}-\frac{5\sqrt{14}}{8}+\sqrt{6}$$

Proof. We use the edge partition of graph H_n based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 4 explains such a partition.Since

$$ABC_4(H)=\sum_{ab\in E(H)}\sqrt{\frac{S_a+S_b-2}{S_aS_b}}$$

This implies that

$$ABC_4(H_n)=(8n)\sqrt{\frac{4+5-2}{4\times 5}}+(4n+4)\sqrt{\frac{4+4-2}{4\times 4}}+(2n)\sqrt{\frac{5+5-2}{5\times 5}}+(4n+4)\sqrt{\frac{5+7-2}{5\times 7}}+(8n-4)\sqrt{\frac{5+8-2}{5\times 8}}+(2n+2)\sqrt{\frac{7+8-2}{7\times 8}}+(7n-5)\sqrt{\frac{8+8-2}{8\times 8}}$$

After an easy simplification, we get

$$ABC_4(H_n) = (\frac{4\sqrt{35}}{5} + \frac{4\sqrt{2}}{5} + \frac{4\sqrt{14}}{7} + \frac{2\sqrt{110}}{5} + \frac{\sqrt{182}}{14} + \frac{7\sqrt{14}}{8} + \sqrt{6})n$$
$$+ \frac{4\sqrt{14}}{7} - \frac{\sqrt{110}}{5} + \frac{\sqrt{182}}{14} - \frac{5\sqrt{14}}{8} + \sqrt{6}$$

Now we compute GA_5 index of H_n.

Theorem 2.2.4. For the graph H_n with $n > 1$, then its GA_5 index is

$$GA_5(H_n) = (\frac{32\sqrt{5}}{9} + \frac{2\sqrt{35}}{3} + \frac{32\sqrt{10}}{13} + \frac{8\sqrt{14}}{15} + 13)n + \frac{2\sqrt{35}}{3} - \frac{16\sqrt{10}}{13} + \frac{8\sqrt{14}}{15} - 1$$

Proof. The edge partition of H_n based on the degree sum of vertices lying at unit distance from end vertices of each edge is given in Table 4.Since

$$GA_5(H) = \sum_{ab\in E(H)} \frac{2\sqrt{S_a S_b}}{S_a + S_b}$$

This gives that

$$GA_5(H_n) = (8n)\frac{2\sqrt{4\times 5}}{4+5} + (4n+4)\frac{2\sqrt{4\times 4}}{4+4} + (2n)\frac{2\sqrt{5\times 5}}{5+5} + (4n+4)\frac{2\sqrt{5\times 7}}{5+7} + (8n-4)\frac{2\sqrt{5\times 8}}{5+8} + (2n+2)\frac{2\sqrt{7\times 8}}{7+8} + (7n-5)\frac{2\sqrt{8\times 8}}{8+8}$$

After an easy simplification, we get

$$GA_5(H_n) = (\frac{32\sqrt{5}}{9} + \frac{2\sqrt{35}}{3} + \frac{32\sqrt{10}}{13} + \frac{8\sqrt{14}}{15} + 13)n + \frac{2\sqrt{35}}{3} - \frac{16\sqrt{10}}{13} + \frac{8\sqrt{14}}{15} - 1$$

3.Conclusion and general remarks

In this paper, certain degree based topological indices, namely atomic-bond connectivity index (ABC), geometric-arithmetic index (GA) and Randić connectivity index for two important classes of nanostar dendrimers were studied for first time. By extending the results computed for polyomino system in [9], we also studied two new topological indices, namely fourth atomic-bond connectivity index ABC_4 and fifth geometric-arithmetic index GA_5 for k-polyomino system with $k = 1,2$.

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*Corresponding author: imrandhab@gmail.com