Computing topological indices of some hyper-branched macromolecules

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In this paper we calculate the number of Kekulé structures, anti-Kékule number and nullity of some families of nanostar dendrimers. In case when the nanostar dendrimer has no Kekulé structure, we give the size of a maximum matching in it. Furthermore, we investigate the first and fourth version of atom-bond connectivity index and first and fifth version of geometric-arithmetic index for these nano-structures.

(Received September 22, 2015; accepted November 25, 2016)

Keywords: Nanostar dendrimers, Nullity, Kékule structures, Anti-Kékule number, Atom-bond connectivity index, Geometric-arithmetic index

1. Introduction

In mathematical chemistry, we discuss and predict some important properties of a chemical structure by using mathematical techniques. Chemical graph theory is a branch of mathematical chemistry in which we apply tools from graph theory to mathematically model the chemical phenomenon. This theory plays a prominent role in the fields of chemical sciences.

Let G be an n-vertex molecular graph with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge set $E(G)$. The vertices of G correspond to atoms and an edge between two vertices corresponds to the chemical bond between these vertices. The hydrogen atoms are often omitted in a molecular graph. An edge in $E(G)$ with end-vertices u and v is denoted by uv. A subgraph H is said to be a spanning subgraph of G if $V(H)=V(G)$. A matching M in G is a subset of $E(G)$ such that no two edges in M have a commom end-vertex in G. A matching M is said to be perfect if each $v \in V(G)$ is incident with an edge in M. A vertex v of G is said to be M-saturated if an edge of the matching M is incident on v; otherwise, v is said to be M-unsaturated. A path in G is said to be an M-alternating path if its edges are alternately in M and $E(G)\setminus M$. An M-alternating path is said to be an M-augmenting path if its initial and terminal vertices are M-unsaturated.

The anti-Kekulé number of a connected graph G, denoted as $ak(G)$, is the smallest number of edges whose deletion from G gives a connected spanning subgraph without any Kekulé structure. Clearly, when G has no Kekulé structure then $ak(G)=0$. We define $ak(G)=\infty$ when it is not possible to find a connected spanning subgraph of G without any Kekulé structure. An edge e of the graph G is said to be a fixed single edge if it is not possible to find a perfect matching in G containing e.

Perfect matchings correspond to Kekulé structures in molecular graphs, which play an important role in analysis of the resonance energy and stability of hydro-carbon compounds [16]. It is well known that carbon compounds without Kekulé structures are unstable. The study of Kekulé structures of chemical compounds is very important as it may explain their physical and chemical properties [22].

The nanostar dendrimers are part of a new group of macromolecules that appear to be photon funnels 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, etc. [1, 10]. Nanostar dendrimers are one of the main objects of nanobiotechnology. They possess a well defined molecular topology. Their step-wise growth follows a mathematical progression. 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 [9, 23]. The number of Kekulé structures and some energy bounds of nanostar dendrimers were studied in [2,4].

Veljan and Vukičević [24] showed that the anti-Kekulé numbers of the infinite triangular, rectangular and hexagonal grids are 9, 6 and 4, respectively. Recently, the anti-Kekulé number of some nanotubes and nanocones were studied in [19].

In this paper, we compute Kekulé structures and anti-Kekulé number of some families of nanostar dendrimers. If the nanostar dendrimer has no Kekulé structure then we find the size of a maximum matching in it

(Section 3). The nullity of these nanostar dendrimers is also studied (Section 4). Furthermore, we compute the first and fourth version of atom-bond connectivity index and the first and fifth version of geometric-arithmetic index for these graphs (Section 5).

2. Some infinite families of nanostar dendrimers

In this section, we define four types of nanostar dendrimes and explain their generation with the help of figures. The first type of nanostar dendrimers $NS_1[n]$ is shown in Fig. 1. The order and size of $NS_1[n]$ nanostar dendrimers are $9\times 2^{n+2}-44$ and $10\times 2^{n+2}-50$, respectively.

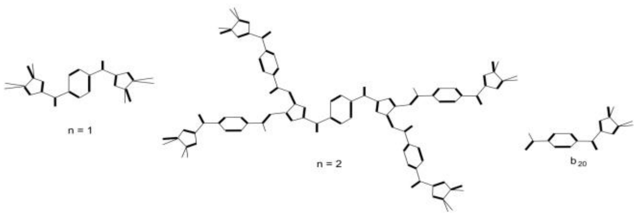

Fig. 1. $NS_1[n]$ with n=1 and n=2. The thick edges represent a matching. Here, b_{20} represents a branch of $NS_1[n]$ with 20 vertices.

The second type of nanostar dendrimers is denoted by $NS_2[n]$ and is shown in Fig. 2. The order and size of $NS_2[n]$ are 120×2^n-108 and 140×2^n-127, respectively.

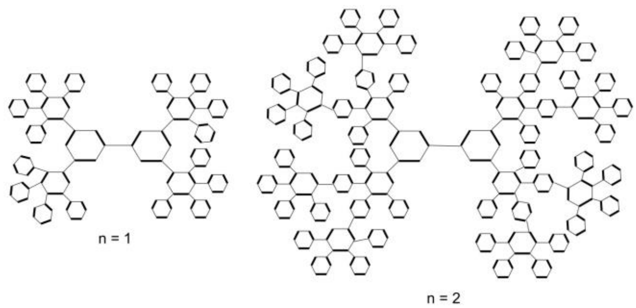

Fig. 2. $NS_2[n]$ with n=1 and n=2. The thick edges represent a matching.

We denote the molecular graph of polyphenylene nanostar dendrimers by $NS_3[n]$ shown in Fig. 3. The order and size of $NS_3[n]$ are $15\times 2^{n+3}$ - 95 and $35\times 2^{n+2}$ - 112, respectively.

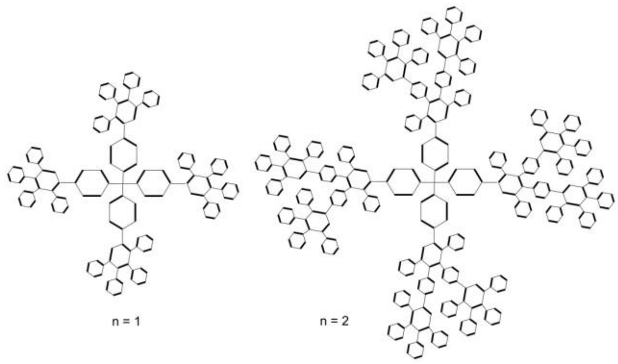

Fig. 3. $NS_3[n]$ with n=1 and 2. $NS_3[n]$ is also known as Polyphenylene dendrimer. The thick edges represent a matching.

The fourth type of nanostar dendrimers $NS_4[n]$ is shown in Fig. 4. Since $NS_4[n]$ is unicyclic graph, its order and size are same and are equal to $3\times 2^{n+1}+3$.

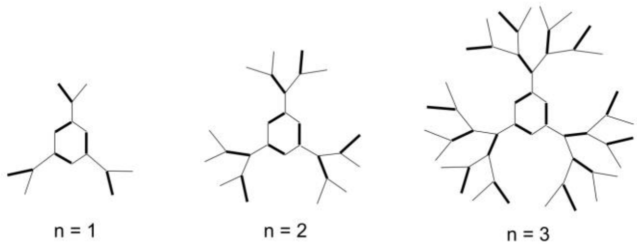

Fig. 4. $NS_4[n]$, with n = 1,2,3. The thick edges represent a matching.

Ashrafi and Mirzargar [1] studied the PI, Szeged and edge Szeged indices of $NS_4[n]$ nanostar dendrimers. Recently, in [3, 18] some researchers investigated m-order connectivity indices of $NS_3[n]$ nanostar dendrimers. The atom-bond connectivity index and geometric-arithmetic index of nanostar dendrimers $NS_2[n]$ and some polyomino chains were studied in [17]. Rostami and Shabanian [21] studied the first kind of geometric-arithmetic index of the nanostar dendrimers $NS_1[n]$ and $NS_2[n]$. Recently, Manuel et al. [20] studied the total-Szeged index of $NS_1[n]$ nanostar dendrimers. Ghorbani [12] studied the nullity of an infinite class of nanostar dendrimers.

There are four branches of $NS_2[n]$ emerging from two central hexagons and at each growth stage each branch contains five new hexagons. Since, the structure of this graph is symmetric, results obtained from one branch of G can be applied to the whole graph. Let M be a perfect matching in $NS_2[n]$. There are some observations about $NS_2[n]$ nanostars, which will help us in computing the number of Kekulé structures in $NS_2[n]$.

Observation 1. *For each positive integer* n *,* $NS_2[n]$ *has possibly following four types of hexagons:*

(i). Type (a): The hexagons with exactly one vertex of degree 3. Such a hexagon has degree sequence of the type

$(2,2,2,2,2,3)$. If the vertex of degree 3 is matched with a vertex outside this hexagon under a matching M, then at least one vertex of degree 2 will be M-unsaturated. Thus, such a matching M is not perfect.

(ii). Type (b): The hexagons with exactly two vertices of degree 3. Such hexagons have degree sequence of the form $(2,2,3,2,2,3)$. If one vertex of degree 3 is matched with a vertex outside this hexagon under a perfect matching M, then the other vertex of degree 3 is also matched under M with a vertex outside this hexagon.

(iii). Type (c): The hexagons with exactly three vertices of degree 3. Such hexagons have degree sequence of the form $(2,3,2,3,2,3)$. If a vertex of degree 3 is matched with a vertex outside this hexagon under a matching M, then at least one vertex of this hexagon will be M-unsaturated. Thus, such a matching M is not perfect.

(iv). Type (d): The hexagons with exactly five vertices of degree 3 such that it has two vertices of degree 3 having two distinct neighbours in two distinct hexagons of Type (b). Such a hexagon has degree sequence of the type $(2,3,3,3,3,3)$. If a vertex of degree 3 is matched with a vertex outside this hexagon under a matching M, then to have all vertices of this hexagon M-saturated, at least another vertex of degree 3 will be matched with a vertex outside this hexagon.

(v). Type-(e): The hexagons with exactly five vertices of degree 3 from which exactly four vertices have distinct neighbours in four different hexagons of Type-(a). Such a hexagon has degree sequence same as the degree sequence of a hexagon of Type-(d). To have all vertices of this hexagon M saturated, either none or exactly 2 or 4 vertices of degree 3 can be matched with vertices outside this hexagon. The later case leads to a contradiction by Case (i).

From Observation 1, we have the following lemma.

Lemma 2.1 *All those edges of* $NS_2[n]$ *whose end-vertices are in different hexagons are fixed single edges.*

Proof. From the structure of $NS_2[n]$, it is clear that there always exists a perfect matching. Let M be a perfect matching in $NS_2[n]$ and e' be an edge whose end-vertices are in different hexagons. We show that e' is a fixed single edge. On contrary suppose that $e' \in M$. Then we consider the following four cases.

Case 1. One end of e' is in a hexagon of Type (a) and other end is in a hexagon of Type (d) or Type (e). By Observation 1 (i), we have a contradiction.

Case 2. One end of e' is in a hexagon of Type (b) and other end is in a hexagon of Type (e). By Observation 1 (v), at least one vertex of degree 3 of a hexagon of Type (e) is matched with a vertex of a Type (a) hexagon. This, however, is not possible by Case 1.

Case 3. One end of e' is in a hexagon of Type (b) and other end is in a hexagon of Type (d). Then one can find an M-alternating path whose first edge is e and terminal edge is e', such that one end of e' is in a hexagon of Type (b) and other end is in a hexagon of Type (e). This is again not possible by Case 2.

Case 4. At least one end of e' is in a hexagon of Type (c). By Observation 1 (iii), this is not possible.

From the Cases 1–4, we find that all the edges with end-vertices in different hexagons of $NS_2[n]$ are fixed single edges.

3. The Kekulé structures and maximum matchings

In the following, we obtain some important short results about the Kekulé structures, maximum matchings and the anti-Kekulé number of nanostar dendrimers discussed in the previous section.

Theorem 3.1 *The nanostar* $NS_1[n]$ *has no Kekulé-structure.*

Proof. From Fig. 1, we see that there exists a pair of pendent vertices in $NS_1[n]$ which are adjacent to the same vertex. Such a pair of pendent vertices cannot be matched simultaneously under one matching. Thus, $NS_1[n]$ has no Kekulé structure.

Theorem 3.2 *The anti-Kekulé number of* $NS_1[n]$ *is* 0.

Proof. As $NS_1[n]$ has no Kekulé structure, the anti-Kekulé number of $NS_1[n]$ is obviously 0.

Theorem 3.3 *The size of a maximum matching in* $NS_1[n]$ *is* $2^{n+4}-21$.

Proof. For each n, let M_n be the matching in $NS_1[n]$ as shown in Fig. 1 with thick edges. For $n=1$, one can see that there is no M_1-augmenting path in $NS_1[1]$. Thus M_1 is a maximum matching and $|M_1| = 11 = 2^{1+4}-21$. Observe that $NS_1[2]$ is obtained from $NS_1[1]$ by connecting four identical branches with four pendent vertices of $NS_1[1]$ in the way as shown in Fig. 1. Let M_2 be the matching in $NS_1[2]$. Then it can be readily seen that there is no M_2-augmenting path in $NS_1[2]$. As the number of edges of M_2 in each branch B_{20} is 8, we have $|M_2| = (2^{1+4}-21)+4(8) = 2^{2+4}-21$. Similarly, if M_3 is a maximum matching in $NS_1[3]$ then $|M_3| = (2^{2+4}-21)+8(8) = 2^{3+4}-21$. In general, the size of a maximum matching in $NS_1[n]$ is $2^{n+4}-21$.

Theorem 3.4 *The number of Kekulé structures in $NS_2[n]$ is equal to $2^{5\times 2^{n+2}-18}$.*

Proof. From the structure of $NS_2[n]$, we see that all vertices of $NS_2[n]$ lie on vertex-disjoint hexagons. Thus a Kekulé structure can be easily obtained. Also, Lemma 2.1 implies that all the edges whose end-vertices are in different hexagons are fixed single edges. Thus, to prove the assertion, it is enough to find the Kekulé structures of hexagons of $NS_2[n]$.

For $n=1$, we see that there are $2+10(2)$ hexagons in $NS_2[1]$. For $n=2$, there are $2+10(2+2^2)$ hexagons in $NS_2[n]$. For $n=3$, there are $2+10(2+2^2+2^3)$ hexagons in $NS_2[n]$. Generalizing this, we see that there are $2+10\sum_{k=1}^{n}2^k=5\times 2^{n+2}-18$ hexagons in $NS_2[n]$. As each hexagon has exactly two Kekulé structures, there are $2^{5\times 2^{n+2}-18}$ Kekulé structures in $NS_2[n]$.

Theorem 3.5 *The anti-Kekulé number of $NS_2[n]$ is ∞.*

Proof. By Lemma 2.1, all edges whose end-vertices are in different hexagons are fixed single edges. Thus, in order to find the anti-Kekulé number of $NS_2[n]$, it is enough to remove the Kekulé structures of a single hexagon. However, the Kekulé structures of a hexagon can only be removed if two consecutive edges of the hexagon are deleted. From the structure of $NS_2[n]$, it is evident that deletion of any two edges of a hexagon gives us a disconnected subgraph. Therefore, the anti-Kekulé number of $NS_2[n]$ is ∞.

Theorem 3.6 *The nanostar $NS_3[n]$ has no Kekulé-structure.*

Proof. The proof follows from the fact that the order of the nanostar $NS_3[n]$ is odd.

Theorem 3.7 *The anti-Kekulé number of $NS_3[n]$ is 0.*

Proof. The proof is straightforward from Theorem 3.6.

Theorem 3.8 *The size of a maximum matching in $NS_3[n]$ is $15\times 2^{n+2}-48$.*

Proof. From the structure of $NS_3[n]$, it can be observed that all vertices of $NS_3[n]$, except one vertex, lie on hexagons. Let M be a matching in $NS_3[n]$ which consists of all vertex-disjoint edges of hexagons. Then

$|M|=\frac{1}{2}(|V(NS_3[n])|-1)=\frac{1}{2}(15\times 2^{n+3}-95-1)=15\times 2^{n+2}-48$. The matching M is shown with thick edges in Fig. 3. Clearly, M is a maximum matching.

Theorem 3.9 *The nanostar $NS_4[n]$ has no Kekulé-structure.*

Proof. The proof is similar to the proof of Theorem 3.1.

Theorem 3.10 *The anti-Kekulé number of $NS_4[n]$ is 0.*

Proof. The proof follows from Theorem 3.9.

Theorem 3.11 *The size of a maximum matching in $NS_4[n]$ is $2^{n+1}+1$ if $n\equiv 0 \pmod 2$ and $2^{n+1}+2$ otherwise.*

Proof. Let M be the matching in $NS_4[n]$ shown by thick edges in Fig. 4. One can observe that there is no M-augmenting path in $NS_4[n]$, for each $n=1,2,\cdots$. Thus M is a maximum matching. Now for $n=1$, we note that $|M|=6=2^{1+1}+2$. For $n=2$, we have $|M|=10=2^{2+1}+1$. For $n=3$, we have $|M|=18=2^{3+1}+2$. For $n=4$, we have $|M|=33=2^{4+1}+1$. Generalizing this, we get

$$|M|=\begin{cases}2^{n+1}+1 & n\equiv 0 \pmod 2\\ 2^{n+1}+2 & \textit{otherwise.}\end{cases}$$

4. The nullity of nanostar dendrimers

In this section, we calculate the nullity of nanostar dendrimers $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$. First we give some definitions and terminologies.

The adjacency matrix $A(G)=[a_{ij}]_{n\times n}$ of a graph G is defined by

$$a_{ij}=\begin{cases}1 & \text{if } v_iv_j\in E(G)\\ 0 & \text{otherwise}\end{cases}(\forall v_i,v_j\in V(G)).$$

The eigenvalues of the graph G are the eigenvalues of $A(G)$ and the spectrum of G is the multiset of eigenvalues of G. The nullity of graph G, denoted by $\eta(G)$, is the multiplicity of the eigenvalue zero in the spectrum of G. The graph G is singular if $\eta(G)=0$ and non-singular if $\eta(G)>0$. In [8], Collatz and Sinogowitz posed the problem of characterizing singular graphs. Since then, the theory of nullity of graphs has stimulated much research because of its noteworthy applications in chemistry. The role of nullity of graphs in chemistry was first recognized by Cvetkovic and Gutman [5]. The next lemma gives a formula for calculating the nullity of some bipartite graphs.

Lemma 4.1 (Cvetkovic, Gutman) *If a bipartite graph G with $n\geq 1$ vertices does not contain any cycle of length $4s$ $(s=1,2,...)$, then $\eta(G)=n-2m$, where*

m *is the size of its maximum matching.*

The following lemma is useful in finding nullity of graphs with pendent vertices.

Lemma 4.2 (Cvetkovic, Gutman) *Let v be a pendant vertex in a graph G and u be the vertex adjacent to v. Then $\eta(G)=\eta(G-u-v)$, where $G-u-v$ is the graph obtained from G by deleting the vertices u and v.*

The nullity of a path and cycle is given in the next lemma.

Lemma 4.3 (Cvetkovic, Gutman) *(i) The eigenvalues of the path P_n are of the form $2\cos(\frac{k\pi}{n+1})$, $k=1,\ldots,n$. According to this,*

$$\eta(P_n)=\begin{cases}1 & \text{if } n \text{ is odd}\\ 0 & \text{if } n \text{ is even.}\end{cases}$$

(ii) The eigenvalues of the cycle C_n are $2\cos(\frac{2k\pi}{n})$, $k=0,1,\ldots,n-1$. Thus

$$\eta(C_n)=\begin{cases}2 & \text{if } n\equiv 0 \pmod 4\\ 0 & \text{otherwise.}\end{cases}$$

Next lemma states that the nullity of a graph is equal to the sum of the nullities of its components.

Lemma 4.4 (Gutman, Borovicanin) *Let $G=\bigcup_{i=1}^{t} G_i$, where G_i, for each $i=1,\ldots,t$, are connected components of G. Then $\eta(G)=\sum_{i=1}^{t}\eta(G_i)$.*

Now, we present some results about the nullity of nanostar dendrimers $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$ by using Lemmas 4.1–4.4.

Theorem 4.1 *The nullity of $NS_1[n]$ is $2^{n+2}-2$.*

Proof. For $n=1$, applying Lemma 4.2 repeatedly on $NS_1[1]$, we obtain a subgraph $H_1=(3\times 2^1)K_1\cup C_6$ such that $\eta(NS_1[1])=\eta(H_1)$. By Lemma 4.3 and Lemma 4.4, we obtain $\eta(NS_1[1])=3\times 2^1+2^1-2$. For $n=2$, again applying Lemma 4.2 repeatedly on $NS_1[2]$, we obtain a subgraph $H_2=(3\times 2^2+2^2-2)K_1\cup(1+2^2)C_6$ such that $\eta(NS_1[2])=\eta(H_2)$. By Lemma 4.3 and Lemma 4.4, we obtain $\eta(NS_1[2])=3\times 2^2+2^2-2$. Generalizing this, we get $H_n=(3\times 2^n+2^n-2)K_1\cup(1+\sum_{k=2}^{n}2^k)C_6$ such that $\eta(NS_1[n])=\eta(H_n)=3\times 2^n+2^n-2=2^{n+2}-2$.

Theorem 4.2 *The nullity of $NS_2[n]$ is 0.*

Proof. The order of $NS_2[n]$ is $120\times 2^n-108$ and from Theorem 3.4 we know that $NS_2[n]$ has a Kekulé structure of size $\frac{120\times 2^n-108}{2}$. Since $NS_2[n]$ is a bipartite graph, using Lemma 4.1, we have $\eta(NS_2[n])=(120\times 2^n-108)-2(\frac{120\times 2^n-108}{2})=0$.

Theorem 4.3 *The nullity of $NS_3[n]$ is 1.*

Proof. From Theorem 3.8, the size of a maximum matching in $NS_3[n]$ is $15\times 2^{n+2}-48$. Since $NS_3[n]$ is a bipartite graph, applying Lemma 4.1 we get $\eta(NS_3[n])=15\times 2^{n+3}-95-2(15\times 2^{n+2}-48)=1$.

Theorem 4.4 *If $n\equiv 0(\text{mod } 2)$ then $\eta(NS_4[n])=2^{n+1}+1$, otherwise $\eta(NS_4[n])=2^{n+1}-1$.*

Proof. First note that $NS_4[n]$ is a bipartite graph. When $n\equiv 0(\text{mod } 2)$, then Theorem 3.11 and Lemma 4.1 give $\eta(NS_4[n])=3\times 2^{n+1}+3-2(2^{n+1}+1)=2^{n+1}+1$. Otherwise, we have $\eta(NS_4[n])=3\times 2^{n+1}+3-2(2^{n+1}+2)=2^{n+1}-1$.

5. Some degree based topological indices of nanostars dendrimers

This section deals with some degree based topological indices of nanostar dendrimers. Let H be a simple connected graph with vertex set $V(H)$ and edge set $E(H)$. Denote by d_v the degree of a vertex $v\in V(H)$ and define $S_u=\sum_{v\in N_H(u)}d_v$, where $N_H(u)=\{v\in V(H)\,|\,uv\in E(H)\}$. Introduced by Estrada et al. [11], the atom-bond connectivity index (ABC-index) is defined by

$$ABC(H)=\sum_{uv\in E(H)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}. \tag{1}$$

Recently, Ghorbani et al. [13] introduced the fourth version of ABC-index defined by

$$ABC_4(H)=\sum_{uv\in E(H)}\sqrt{\frac{S_u+S_v-2}{S_uS_v}}. \tag{2}$$

Another well-known connectivity topological descriptor is the geometric-arithmetic index (GA-index) which was introduced by Vukičević and Furtula [25] and is defined by

$$GA(H)=\sum_{uv\in E(H)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}. \qquad (3)$$

Graovac et al. [14] proposed the fifth version of GA -index which is defined by

$$GA_5(H)=\sum_{uv\in E(H)}\frac{2\sqrt{S_u S_v}}{S_u+S_v}. \qquad (4)$$

With each edge uv, we associate two pairs (d_u,d_v) and (S_u,S_v). The edge partition of $NS_1[n]$ nanostar dendrimers with respect to the degrees of the end-vertices of edges and with respect to the sum of degrees of the neighbours of end-vertices of edges is given by Table 1 and Table 2, respectively. A similar (d_u,d_v) and (S_u,S_v) -type edge partitions of $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$ nanostar dendrimers are given by Tables 3-7.

Table 1: (d_u,d_v) *-type edge partition of* $NS_1[n]$.

(d_u,d_v)	**Number of edges**
(1,3)	$2^{n+2}-6$
(1,4)	2^{n+2}
(2,2)	$2^{n+2}-6$
(2,3)	$9\times 2^{n+1}-28$
(2,4)	2^{n+1}
(3,3)	$7\times 2^{n}-10$
(4,4)	2^{n}

Table 2: (S_u,S_v) *-type edge partition of* $NS_1[n]$.

(S_u,S_v)	**Number of edges**
(3,6)	$2^{n+1}-4$
(3,7)	$2^{n+1}-2$
(4,8)	2^{n+2}
(5,5)	$2^{n+2}-6$
(5,7)	$2^{n+3}-12$
(6,6)	$2^{n+1}-4$
(6,7)	$2^{n+3}-16$
(7,7)	$7\times 2^{n}-6$
(7,8)	2^{n+1}
(8,8)	2^{n}

Table 3: (S_u,S_v) *-type edge partition of NS2[n].*

(S_u,S_v)	**Number of edges**
(4,4)	$3\times 2^{n+3}-16$
(4,5)	$3\times 2^{n+3}-16$
(5,5)	$2^{n+3}-16$
(5,7)	$5\times 2^{n+3}-48$
(6,8)	$2^{n+3}-8$
(7,6)	12
(7,7)	1
(7,8)	$2^{n+3}-8$
(7,9)	$3\times 2^{n+2}-12$
(8,9)	$2^{n+3}-8$
(9,9)	$2^{n+3}-8$

Table 4: (d_u,d_v) *-type edge partition of NS3[n].*

(d_u,d_v)	**Number of edges**
(2,2)	$7\times 2^{n+3}-40$
(2,3)	$11\times 2^{n+2}-32$
(3,3)	$10\times 2^{n+2}-44$
(3,4)	4

Table 5: (S_u,S_v) *-type edge partition of NS3[n]n≥3.*

(S_u,S_v)	**Number of edges**
(4,4)	$3\times 2^{n+3}-16$
(4,5)	$3\times 2^{n+3}-16$
(5,5)	$2^{n+3}-8$
(5,7)	$5\times 2^{n+3}-40$
(5,8)	8
(6,8)	$2^{n+3}-8$
(7,8)	$2^{n+3}-8$
(7,9)	$3\times 2^{n+2}-12$
(8,9)	$2^{n+3}-8$
(8,12)	4
(9,9)	$2^{n+3}-8$

Table 6: (d_u,d_v) *-type edge partition of NS4[n].*

(d_u,d_v)	**Number of edges**
(1,3)	3×2^{n}
(2,3)	6
(3,3)	$3\times 2^{n}-3$

Table 7: (S_u, S_v) *-type edge partition of* $NS_4[n]$, $n \geq 3$.

(S_u, S_v)	**Number of edges**
(5,3)	3×2^n
(5,9)	$3\times 2^{n-1}$
(7,6)	6
(7,9)	3
(9,9)	$3\times 2^{n-1}-6$

5.1 Results for ABC and ABC_4-index

Now we compute the ABC and ABC_4-indices of the nanostar dendrimers $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$ using the edge partitions shown in Tables 1-7.

Theorem 5.1 *The atom-bond connectivity index of* $NS_1[n]$ *is given by*

$$ABC(NS_1[n]) = (12+\frac{19}{12}\sqrt{3})2^{1/2+n} + (2\sqrt{3}+\frac{14}{3})2^n - 2\sqrt{6} - 17\sqrt{2} - \frac{20}{3}.$$

Proof. Using equation (1), and the edge partition in Table 1, we have

$$ABC(NS_1[n]) = (2^{n+2}-6)\sqrt{\frac{1+3-2}{3}} + (2^{n+2})\sqrt{\frac{1+4-2}{4}} + (2^{n+2}-6)\sqrt{\frac{2+2-2}{4}} + (9\times 2^{n+1}-28)\sqrt{\frac{2+3-2}{6}} + (2^{n+1})\sqrt{\frac{2+4-2}{8}} + (7\times 2^n - 10)\sqrt{\frac{3+3-2}{9}} + (2^n)\sqrt{\frac{4+4-2}{16}}.$$

After simplification, we get the desired result.

$$ABC(NS_1[n]) = (12+\frac{19}{12}\sqrt{3})2^{1/2+n} + (2\sqrt{3}+\frac{14}{3})2^n - 2\sqrt{6} - 17\sqrt{2} - \frac{20}{3}.$$

The atom-bond connectivity index of $NS_2[n]$ is calculated by Hayat et al. [17]. In the next theorem, we calculate atom-bond connectivity index of $NS_3[n]$.

Theorem 5.2 *The atom-bond connectivity index of* $NS_3[n]$ *is given by*

$$ABC(NS_3[n]) = 50(2^{1/2+n}) + \frac{80}{3}(2^n) - \frac{88}{3} + \frac{2}{3}\sqrt{15} - 36\sqrt{2}.$$

Proof. Using equation (1), and the edge partition in Table 4, we have

$$ABC(NS_3[n]) = (7\times 2^{n+3}-40)\sqrt{\frac{2+2-2}{4}} + (11\times 2^{n+2}-32)\sqrt{\frac{2+3-2}{6}} + (10\times 2^{n+2}-44)\sqrt{\frac{3+3-2}{9}} + (4)\sqrt{\frac{3+4-2}{12}}.$$

After simplification we get

$$ABC(NS_3[n]) = 50(2^{1/2+n}) + \frac{80}{3}(2^n) - \frac{88}{3} + \frac{2}{3}\sqrt{15} - 36\sqrt{2}.$$

Theorem 5.3 *The atom-bond connectivity index of* $NS_4[n]$ *is given by*

$$ABC(NS_4[n]) = 2^{1/2+n}\sqrt{3} + 2^{n+1} + 3\sqrt{2} - 2.$$

Proof. Using equation (1) and the edge partition in Table 6, we have

$$ABC(NS_4[n]) = (3\times 2^n)\sqrt{\frac{1+3-2}{3}} + (6)\sqrt{\frac{2+3-2}{6}} + (3\times 2^n - 3)\sqrt{\frac{3+3-2}{9}}.$$

After simplification we get

$$ABC(NS_4[n]) = 2^{1/2+n}\sqrt{3} + 2^{n+1} + 3\sqrt{2} - 2.$$

Theorem 5.4 *The fourth atom-bond connectivity index of* $NS_1[n]$ *is given by*

$$ABC_4(NS_1[n]) = (2^{n+1}-4)\sqrt{\frac{7}{18}} + (2^{n+1}-2)\sqrt{\frac{8}{21}} + (2^{n+2})\sqrt{\frac{5}{16}} + (2^{n+2}-6)\sqrt{\frac{8}{25}} + (2^{n+3}-12)\sqrt{\frac{2}{7}} + (2^{n+1}-4)\sqrt{\frac{5}{18}} + (2^{n+3}-16)\sqrt{\frac{11}{42}} + (7\times 2^n - 6)\sqrt{\frac{12}{49}} + (2^{n+1})\sqrt{\frac{13}{56}} + (2^n)\sqrt{\frac{7}{32}}.$$

Proof. Using equation (2) and the edge partition in Table 2, we have

$$ABC_4(NS_1[n]) = (2^{n+1}-4)\sqrt{\frac{3+6-2}{18}} + (2^{n+1}-2)\sqrt{\frac{3+7-2}{21}} + (2^{n+2})\sqrt{\frac{4+8-2}{32}} + (2^{n+2}-6)\sqrt{\frac{5+5-2}{25}} + (2^{n+3}-12)\sqrt{\frac{5+7-2}{35}} + (2^{n+1}-4)\sqrt{\frac{6+6-2}{36}} + (2^{n+3}-16)\sqrt{\frac{6+7-2}{42}} + (7\times 2^n-6)\sqrt{\frac{7+7-2}{49}} + (2^{n+1})\sqrt{\frac{7+8-2}{56}} + (2^n)\sqrt{\frac{8+8-2}{64}}.$$

After simplification we get

$$ABC_4(NS_1[n]) = (2^{n+1}-4)\sqrt{\frac{7}{18}} + (2^{n+1}-2)\sqrt{\frac{8}{21}} + (2^{n+2})\sqrt{\frac{5}{16}} + (2^{n+2}-6)\sqrt{\frac{8}{25}} + (2^{n+3}-12)\sqrt{\frac{2}{7}} + (2^{n+1}-4)\sqrt{\frac{5}{18}} + (2^{n+3}-16)\sqrt{\frac{11}{42}} + (7\times 2^n - 6)\sqrt{\frac{12}{49}} + (2^{n+1})\sqrt{\frac{13}{56}} + (2^n)\sqrt{\frac{7}{32}}.$$

Theorem 5.5 *The fourth atom-bond connectivity index of* $NS_2[n]$ *is given by*

$$ABC_4(NS_2[n]) = (3\times 2^{n+3}-16)\sqrt{\frac{3}{8}} + (3\times 2^{n+3}-16)\sqrt{\frac{7}{20}} + (2^{n+3}-16)\sqrt{\frac{8}{25}} + (5\times 2^{n+3}-48)\sqrt{\frac{10}{35}} + (2^{n+3}-8)\sqrt{\frac{1}{4}} + (12)\sqrt{\frac{11}{42}} + (1)\sqrt{\frac{12}{49}} + (2^{n+3}-8)\sqrt{\frac{13}{56}} + (3\times 2^{n+2}-12)\sqrt{\frac{2}{9}} + (2^{n+3}-8)\sqrt{\frac{5}{24}} + (2^{n+3}-8)\sqrt{\frac{16}{81}}.$$

Proof. Using equation (2) and the edge partition in Table 3, we have

$$ABC_4(NS_2[n]) = (3\times 2^{n+3}-16)\sqrt{\frac{4+4-2}{16}} + (3\times 2^{n+3}-16)\sqrt{\frac{4+5-2}{20}} + (2^{n+3}-16)\sqrt{\frac{5+5-2}{25}} + (5\times 2^{n+3}-48)\sqrt{\frac{5+7-2}{35}} + (2^{n+3}-8)\sqrt{\frac{6+8-2}{48}} + (12)\sqrt{\frac{7+6-2}{42}} + (1)\sqrt{\frac{7+7-2}{49}}$$

$$+(2^{n+3}-8)\sqrt{\frac{7+8-2}{56}}+(3\times 2^{n+2}-12)\sqrt{\frac{7+9-2}{63}}+(2^{n+3}-8)\sqrt{\frac{8+9-2}{72}}+(2^{n+3}-8)\sqrt{\frac{9+9-2}{81}}.$$

After simplification we get

$$ABC_4(NS_2[n])=(3\times 2^{n+3}-16)\sqrt{\frac{3}{8}}+(3\times 2^{n+3}-16)\sqrt{\frac{7}{20}}+(2^{n+3}-16)\sqrt{\frac{8}{25}}+(5\times 2^{n+3}-48)\sqrt{\frac{10}{35}}+$$
$$(2^{n+3}-8)\sqrt{\frac{1}{4}}+(12)\sqrt{\frac{11}{42}}+(1)\sqrt{\frac{12}{49}}+(2^{n+3}-8)\sqrt{\frac{13}{56}}+(3\times 2^{n+2}-12)\sqrt{\frac{2}{9}}+(2^{n+3}-8)\sqrt{\frac{5}{24}}+(2^{n+3}-8)\sqrt{\frac{16}{81}}.$$

Theorem 5.6 *The fourth atom-bond connectivity index of* $NS_3[n]$ *is given by*

$$ABC_4(NS_3[n])=(3\times 2^{n+3}-16)\sqrt{\frac{3}{8}}+(3\times 2^{n+3}-16)\sqrt{\frac{7}{20}}+(2^{n+3}-8)\sqrt{\frac{8}{25}}+(5\times 2^{n+3}-40)\sqrt{\frac{2}{7}}+(8)\sqrt{\frac{11}{40}}+$$
$$(2^{n+3}-8)\sqrt{\frac{1}{4}}+(2^{n+3}-8)\sqrt{\frac{13}{56}}+(3\times 2^{n+2}-12)\sqrt{\frac{2}{9}}+(2^{n+3}-8)\sqrt{\frac{5}{24}}+(4)\sqrt{\frac{3}{16}}+(2^{n+3}-8)\sqrt{\frac{16}{81}}.$$

Proof. Using equation (2) and the edge partition in

Table 5, we have

$$ABC_4(NS_3[n])=(3\times 2^{n+3}-16)\sqrt{\frac{4+4-2}{16}}+(3\times 2^{n+3}-16)\sqrt{\frac{4+5-2}{20}}+(2^{n+3}-8)\sqrt{\frac{5+5-2}{25}}$$
$$+(5\times 2^{n+3}-40)\sqrt{\frac{5+7-2}{35}}+(8)\sqrt{\frac{5+8-2}{40}}+(2^{n+3}-8)\sqrt{\frac{6+8-2}{48}}+(2^{n+3}-8)\sqrt{\frac{8+7-2}{56}}$$
$$+(3\times 2^{n+2}-12)\sqrt{\frac{7+9-2}{63}}+(2^{n+3}-8)\sqrt{\frac{8+9-2}{72}}+(4)\sqrt{\frac{8+12-2}{96}}+(2^{n+3}-8)\sqrt{\frac{9+9-2}{81}}.$$

After simplification we get

$$ABC_4(NS_3[n])=(3\times 2^{n+3}-16)\sqrt{\frac{3}{8}}+(3\times 2^{n+3}-16)\sqrt{\frac{7}{20}}+(2^{n+3}-8)\sqrt{\frac{8}{25}}+(5\times 2^{n+3}-40)\sqrt{\frac{2}{7}}+(8)\sqrt{\frac{11}{40}}$$
$$+(2^{n+3}-8)\sqrt{\frac{1}{4}}+(2^{n+3}-8)\sqrt{\frac{13}{56}}+(3\times 2^{n+2}-12)\sqrt{\frac{2}{9}}+(2^{n+3}-8)\sqrt{\frac{5}{24}}+(4)\sqrt{\frac{3}{16}}+(2^{n+3}-8)\sqrt{\frac{16}{81}}.$$

Theorem 5.7 *The fourth atom-bond connectivity index of* $NS_4[n]$ *is given by*

$$ABC_4(NS_4[n])=(3\times 2^{n})\sqrt{\frac{2}{5}}+(3\times 2^{n-1})\sqrt{\frac{4}{15}}+(3\times 2^{n-1}-6)\sqrt{\frac{16}{81}}+(6)\sqrt{\frac{11}{42}}+(3)\sqrt{\frac{2}{9}}.$$

Proof. Using equation (2) and the edge partition in Table 7, we have

$$ABC_4(NS_4[n])=(3\times 2^{n})\sqrt{\frac{5+3-2}{15}}+(3\times 2^{n-1})\sqrt{\frac{5+9-2}{45}}+(6)\sqrt{\frac{7+6-2}{42}}+(3)\sqrt{\frac{7+9-2}{63}}$$
$$+(3\times 2^{n-1}-6)\sqrt{\frac{9+9-2}{81}}.$$

After simplification we get

$$ABC_4(NS_4[n]) = (3\times 2^n)\sqrt{\frac{2}{5}} + (3\times 2^{n-1})\sqrt{\frac{4}{15}} + (3\times 2^{n-1}-6)\sqrt{\frac{16}{81}} + (6)\sqrt{\frac{11}{42}} + (3)\sqrt{\frac{2}{9}}.$$

5.2 Results for GA and GA_5 -index

Now, we compute the GA and GA_5 -indices of the nanostar dendrimers $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$ using the edge partitions shown in Tables 1-7.

Theorem 5.8 *The geometric-arithmetic index of* $NS_3[n]$ *is given by*

$$GA(NS_3[n]) = 96(2^n) + \frac{88}{5}(2^{1/2+n})\sqrt{3} - \frac{64}{5}\sqrt{6} + \frac{16}{7}\sqrt{3} - 84.$$

Proof. Using equation (3) and the edge partition in Table 4, we have

$$GA(NS_3[n]) = (7\times 2^{n+3}-40)\frac{2\sqrt{4}}{2+2} + (11\times 2^{n+2}-32)\frac{2\sqrt{6}}{2+3} + (10\times 2^{n+2}-44)\frac{2\sqrt{9}}{3+3} + (4)\frac{2\sqrt{12}}{3+4}.$$

After simplification we get

$$GA(NS_3[n]) = 96(2^n) + \frac{88}{5}(2^{1/2+n})\sqrt{3} - \frac{64}{5}\sqrt{6} + \frac{16}{7}\sqrt{3} - 84.$$

Theorem 5.9 *The geometric-arithmetic index of* $NS_4[n]$ *is given by*

$$GA(NS_4[n]) = 3\sqrt{3}(2^{-1+n}) + 3(2^n) + \frac{12}{5}\sqrt{6} - 3.$$

Proof. Using equation (3) and the edge partition in Table 6, we have

$$GA(NS_4[n]) = (3\times 2^n)\frac{2\sqrt{3}}{1+3} + (6)\frac{2\sqrt{6}}{2+3} + (3\times 2^n - 3)\frac{2\sqrt{9}}{3+3}.$$

After simplification we get

$$GA(NS_4[n]) = 3\sqrt{3}(2^{-1+n}) + 3(2^n) + \frac{12}{5}\sqrt{6} - 3.$$

Theorem 5.10 *The fifth geometric-arithmetic index of* $NS_1[n]$ *is given by*

$$GA_5(NS_1[n]) = 14\times 2^n + (2^{n+1}-4)\frac{2\sqrt{18}}{9} + (2^{n+1}-2)\frac{\sqrt{21}}{5} + (2^{n+2})\frac{\sqrt{32}}{6} + (2^{n+3}-12)\frac{\sqrt{35}}{6}$$
$$+(2^{n+3}-16)\frac{2\sqrt{42}}{13} + (2^{n+1})\frac{2\sqrt{56}}{15} - 16.$$

Proof. Using equation (4) and the edge partition in Table 2, we have

$$GA_5(NS_1[n]) = (2^{n+1}-4)\frac{2\sqrt{18}}{3+6} + (2^{n+1}-2)\frac{2\sqrt{21}}{3+7} + (2^{n+2})\frac{2\sqrt{32}}{4+8} + (2^{n+2}-6)\frac{2\sqrt{25}}{5+5} + (2^{n+3}-12)\frac{2\sqrt{35}}{5+7}$$
$$+(2^{n+1}-4)\frac{2\sqrt{36}}{6+6} + (2^{n+3}-16)\frac{2\sqrt{42}}{6+7} + (7\times 2^n - 6)\frac{2\sqrt{49}}{7+7} + (2^{n+1})\frac{2\sqrt{56}}{7+8} + (2^n)\frac{2\sqrt{64}}{8+8}.$$

After simplification we get

$$GA_5(NS_1[n]) = 14\times 2^n + (2^{n+1}-4)\frac{2\sqrt{18}}{9} + (2^{n+1}-2)\frac{\sqrt{21}}{5} + (2^{n+2})\frac{\sqrt{32}}{6} + (2^{n+3}-12)\frac{\sqrt{35}}{6}$$
$$+(2^{n+3}-16)\frac{2\sqrt{42}}{13} + (2^{n+1})\frac{2\sqrt{56}}{15} - 16.$$

Theorem 5.11 *The fifth geometric-arithmetic index of* $NS_2[n]$ *is given by*

$$GA_5(NS_2[n]) = 5\times 2^{n+3} + (3\times 2^{n+3} - 16)\frac{2\sqrt{20}}{9} + (5\times 2^{n+3} - 48)\frac{\sqrt{35}}{6} + (2^{n+3} - 8)\frac{\sqrt{48}}{7} + (12)\frac{2\sqrt{42}}{13}$$
$$+(2^{n+3} - 8)\frac{2\sqrt{56}}{15} + (3\times 2^{n+2} - 12)\frac{\sqrt{63}}{8} + (2^{n+3} - 8)\frac{2\sqrt{72}}{17} - 39.$$

Proof. Using equation (4) and the edge partition in Table 3, we have

$$GA_5(NS_2[n]) = (3\times 2^{n+3} - 16)\frac{2\sqrt{16}}{4+4} + (3\times 2^{n+3} - 16)\frac{2\sqrt{20}}{4+5} + (2^{n+3} - 16)\frac{2\sqrt{25}}{5+5} + (5\times 2^{n+3} - 48)\frac{2\sqrt{35}}{5+7} +$$
$$(8)\frac{2\sqrt{40}}{5+8} + (2^{n+3} - 8)\frac{2\sqrt{48}}{8+6} + (12)\frac{2\sqrt{42}}{7+6} + (1)\frac{2\sqrt{49}}{7+7} + (2^{n+3} - 8)\frac{2\sqrt{56}}{7+8} +$$
$$(3\times 2^{n+2} - 12)\frac{2\sqrt{63}}{7+9} + (2^{n+3} - 8)\frac{2\sqrt{72}}{8+9} + (2^{n+3} - 8)\frac{2\sqrt{81}}{9+9}.$$

After simplification we get

$$GA_5(NS_2[n]) = 5\times 2^{n+3} + (3\times 2^{n+3} - 16)\frac{2\sqrt{20}}{9} + (5\times 2^{n+3} - 48)\frac{\sqrt{35}}{6} + (2^{n+3} - 8)\frac{\sqrt{48}}{7} + (12)\frac{2\sqrt{42}}{13}$$
$$+(2^{n+3} - 8)\frac{2\sqrt{56}}{15} + (3\times 2^{n+2} - 12)\frac{\sqrt{63}}{8} + (2^{n+3} - 8)\frac{2\sqrt{72}}{17} - 39.$$

Theorem 5.12 *The fifth geometric-arithmetic index of* $NS_3[n]$ *is given by*

$$GA_5(NS_3[n]) = 5\times 2^{n+3} + (3\times 2^{n+3} - 16)\frac{2\sqrt{20}}{9} + (5\times 2^{n+3} - 40)\frac{\sqrt{35}}{6} + (8)\frac{2\sqrt{40}}{13} + (2^{n+3} - 8)\frac{\sqrt{48}}{7}$$
$$+(2^{n+3} - 8)\frac{2\sqrt{56}}{15} + (3\times 2^{n+2} - 12)\frac{\sqrt{63}}{8} + (2^{n+3} - 8)\frac{2\sqrt{72}}{17} + (4)\frac{\sqrt{96}}{10} - 32.$$

Proof. Using equation (4) and the edge partition in Table 5, we have

$$GA_5(NS_3[n]) = (3\times 2^{n+3} - 16)\frac{2\sqrt{16}}{4+4} + (3\times 2^{n+3} - 16)\frac{2\sqrt{20}}{4+5} + (2^{n+3} - 8)\frac{2\sqrt{25}}{5+5} + (5\times 2^{n+3} - 40)\frac{2\sqrt{35}}{5+7} +$$
$$(8)\frac{2\sqrt{40}}{5+8} + (2^{n+3} - 8)\frac{2\sqrt{48}}{8+6} + (2^{n+3} - 8)\frac{2\sqrt{56}}{7+8} + (3\times 2^{n+2} - 12)\frac{2\sqrt{63}}{7+9} + (2^{n+3} - 8)\frac{2\sqrt{72}}{8+9} +$$
$$(4)\frac{2\sqrt{96}}{8+12} + (2^{n+3} - 8)\frac{2\sqrt{81}}{9+9}.$$

After simplification we get

$$GA_5(NS_3[n]) = 5\times 2^{n+3} + (3\times 2^{n+3} - 16)\frac{2\sqrt{20}}{9} + (5\times 2^{n+3} - 40)\frac{\sqrt{35}}{6} + (8)\frac{2\sqrt{40}}{13} + (2^{n+3} - 8)\frac{\sqrt{48}}{7} +$$
$$(2^{n+3} - 8)\frac{2\sqrt{56}}{15} + (3\times 2^{n+2} - 12)\frac{\sqrt{63}}{8} + (2^{n+3} - 8)\frac{2\sqrt{72}}{17} + (4)\frac{\sqrt{96}}{10} - 32.$$

Theorem 5.13 *The fifth geometric-arithmetic index of*

$NS_4[n]$ *is given by*

$$GA_5(NS_4[n]) = 3\times 2^{n-1} + (3\times 2^n)\frac{\sqrt{15}}{4} + (3\times 2^{n-1})\frac{\sqrt{45}}{7} + (6)\frac{2\sqrt{42}}{13} + (3)\frac{\sqrt{63}}{8} - 6.$$

Proof. Using equation (4) and the edge partition in Table 7, we have

$$GA_5(NS_4[n]) = (3\times 2^n)\frac{2\sqrt{15}}{5+3} + (3\times 2^{n-1})\frac{2\sqrt{45}}{5+9} + (6)\frac{2\sqrt{42}}{7+6} + (3)\frac{2\sqrt{63}}{7+9} + (3\times 2^{n-1} - 6)\frac{2\sqrt{81}}{9+9}.$$

After simplification we get

$$GA_5(NS_4[n]) = 3\times 2^{n-1} + (3\times 2^n)\frac{\sqrt{15}}{4} + (3\times 2^{n-1})\frac{\sqrt{45}}{7} + (6)\frac{2\sqrt{42}}{13} + (3)\frac{\sqrt{63}}{8} - 6.$$

6. Conclusion

In this paper, we consider four infinite families of nanostar dendrimers $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$. We compute the number of Kekulé structures and anti-Kekulé number of these nanostar dendrimers. In case, the nanostar dendrimer has no Kekulé structure, we give the size of a maximum matching in it. Furthermore, we compute the ABC, ABC_4, GA and GA_5-indices of these nanostar dendrimers using the edge partitions shown in Tables 1-7. It would be interesting to study some distance based topological indices of these families of nanostar dendrimers.

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