

Computing some degree-based topological indices of a hetrofunctional dendrimer

NAZIA NAZIR, RASHID FAROOQ, MEHAR ALI MALIK*

School of Natural Sciences, National University of Sciences and Technology, H-12, Islamabad, Pakistan

In this paper, we compute the nullity and number of Kekulé structures in a class of hetrofunctional dendrimers (HFD)ei. When there is no Kekulé structure in a dendrimer, we find the size of a maximum matching in it. Furthermore, we compute the first and fourth version of atom-bond connectivity index, first and fifth version of geometric-arithmetic index and Randić index of this dendrimer.

(Received December 11, 2015; accepted June 09, 2016)

Keywords: Nanostar dendrimers, Nullity, Matching, Atom-bond connectivity index, Geometric-arithmetic index, Randić index

1. Introduction

The word “dendrimer” is originated from two distinct Greek words "dendri" (branch) and "meros" (part). The first dendrimer was introduced in the late 1970's by German scientists E. Bhuleier, W. Wehner and F. VÖgtle [2]. Dendrimers form a class of polymeric macromolecules. They are uni-molecular micelle in nature with special physico-chemical properties which make them suitable for biological and drug delivery applications [13]. The applications of nanostar dendrimers are not restricted to drug delivery or diagnosis, they are now extended to gene delivery, solubilization, targeting and other biomedical applications. The graphical structure of a chemical compound can be viewed in terms of a graph, commonly known as a molecular graph, where atoms and their covalent bonds are respectively considered as the vertices and edges of the graph.

Let G be an n -vertex molecular graph of a hetrofunctional dendrimer with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. An edge in $E(G)$ with end-vertices u and v is denoted by uv . The order and size of G are respectively the cardinalities $|V(G)|$ and $|E(G)|$. A subgraph H of a graph G is called a spanning subgraph of G if $V(H) = V(G)$. A (u, v) -path on m vertices in G is a path with vertex set $\{u = v_0, v_1, \dots, v_{m-1} = v\}$ and edge set $\{v_{i-1}v_i \mid 1 \leq i \leq m-1\}$. A subgraph H of a graph G is said to be induced if H contains all the edges between its vertices which are present in G . A subset $M \subseteq E(G)$ is called a matching if no two edges in M share an end-vertex. A vertex $v \in V(G)$ is said to be M -saturated if v is incident with an edge in M . Otherwise,

v is said to be M -unsaturated. A matching M in a graph G is called perfect if it saturates all the vertices of G . A path in G is said to be M -alternating if its edges alternately lie in M and $E(G) \setminus M$. An M -alternating path is called M -augmenting if both of its end-vertices are M -unsaturated. In molecular graphs, perfect matchings correspond to Kekulé structures which play an important role in analysis of the resonance energy and stability of hydro-carbon compounds [12]. The organic compounds without any Kekulé structure are known to be chemically unstable. Thus study of Kekulé structures of chemical compounds is very important as it explains their physico-chemical properties [15].

The anti-Kekulé number of a connected graph G , denoted by $ak(G)$, is the minimum number of edges which must be deleted from G to obtain a connected subgraph that does not contain any Kekulé structure. Obviously, when a graph G does not contain any Kekulé structure then $ak(G) = 0$. If it is not possible to find a connected spanning subgraph of G without any Kekulé structure then $ak(G) = \infty$.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The adjacency matrix $A(G) = [a_{ij}]_{n \times n}$ of the graph G is defined by

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

The spectrum of $A(G)$ is the multiset of eigenvalues of $A(G)$. The eigenvalues and spectrum of a graph G are the eigenvalues and spectrum of $A(G)$. The nullity $\eta(G)$ of graph G is the multiplicity of the eigenvalue zero in the spectrum of G . A graph G is singular if

$\eta(G) > 0$ and non-singular otherwise. In [6], 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].

Farooq et al. [8] considered a class of hetrofunctional dendrimer, denoted by $D[n]$, and computed some eccentricity based topological indices. In this paper, we consider the same class $D[n]$ of hetrofunctional dendrimers and compute some degree based topological indices. Furthermore, we compute nullity and the number of Kekulé structures in $D[n]$. When there is no Kekulé structure, we compute size of the maximum matchings of the dendrimers in $D[n]$.

2. A hetrofunctional dendrimer $D[n]$

In this section, we study the molecular graph of a class of hetrofunctional dendrimers (HFD) which is grown at the n th stage ($n \geq 1$) and is denoted by $D[n]$. The molecular graph of $D[n]$ is shown in Fig. 1. This dendrimer is an HFD(ei)-G3-e(allyl) 16-i-(hydroxyl) 28 molecule which is an HFD with internal hydroxyle and peripheral allyl group. The graphs corresponding to different growth stages are shown in Fig. 2–3. It is evident that $D[n]$ is a unicyclic graph, thus $|V(D[n])| = |E(D[n])|$. Its order is given by

$$|V(D[n])| = \begin{cases} 16 \times 2^{t+1} + 8 \times 2^t - 38 & \text{if } n = 2t, t \geq 1 \\ 24 \times 2^{t+1} - 38 & \text{if } n = 2t + 1, t \geq 0. \end{cases}$$

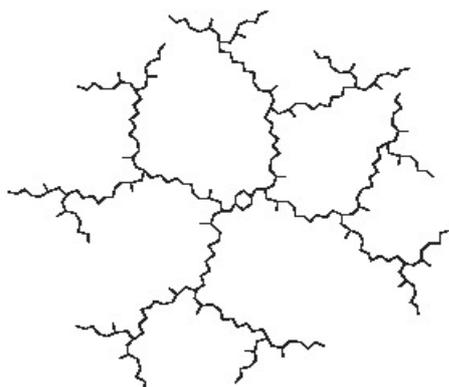


Fig. 1: $D[n]$ with $n = 6$.

3. The Kekulé structures and maximum matchings in $D[n]$

In this next section, we find the number of Kekulé structures in the graph of the dendrimer $D[n]$. When there is no Kekulé structure in $D[n]$, we find a maximum matching in it and give the size of this maximum matching for any stage $n (\geq 1)$.

We first give the following lemma.

Lemma 3.1 For $n = 1$, there are two Kekulé structures in $D[n]$.



Fig. 2. Two distinct perfect matchings in $D[n]$ with $n = 1$, where thick edges represent a matching.

Proof. Consider the matchings represented by the thick edges in Fig. 2-(a) and Fig. 2-(b). There is only one hexagon in $D[1]$ and a hexagon has exactly two Kekulé structures. Thus $D[1]$ has two Kekulé structures.

In the next lemma, we show that $D[n]$ contains no Kekulé structure when n exceeds 1.

Lemma 3.2 For $n \geq 2$, $D[n]$ has no Kekulé structure.

Proof. From the structure of $D[n]$, we see that if n is even then $D[n]$ contains a path P_7 whose end vertices have degree 1 in $D[n]$. Denote by v_1, v_2, \dots, v_7 the vertices of P_7 . Then $d(v_1) = d(v_7) = 1$, $d(v_2) = 3$ and all other internal vertices of P_7 has degree 2 in $D[n]$. If M is a perfect matching in $D[n]$ then $v_1 v_2 \in M$. Since $1 \leq d(v_i) \leq 2$ for $i \in \{3, 4, \dots, 7\}$, P_7 has one M -unsaturated vertex which contradicts the fact that M is a perfect matching.

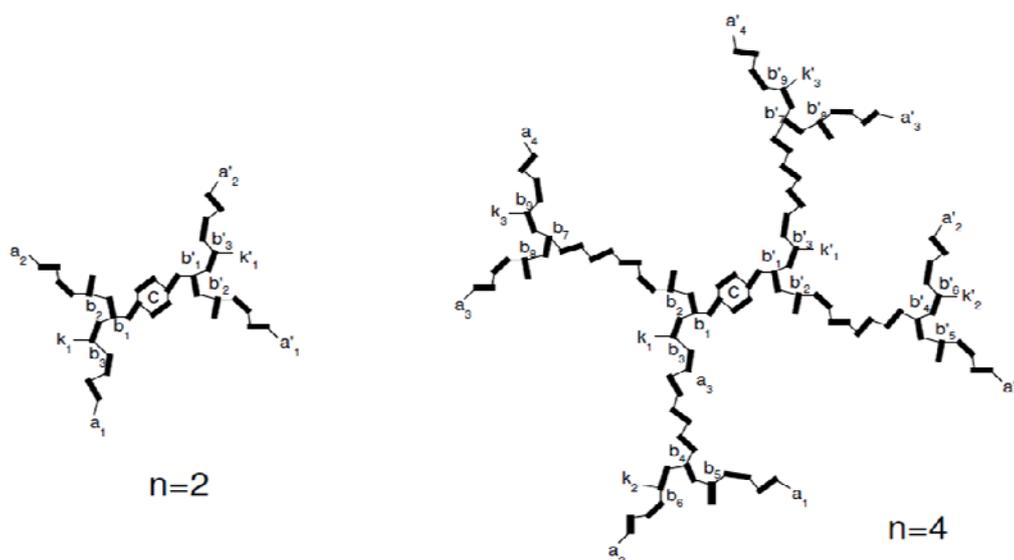


Fig. 3. $D[n]$ with $n = 2$ and $n = 4$. The thick edges represent a matching. Here b_{21} represents a branch of $D[n]$ with 21 vertices.

If n is odd then $D[n]$ contains a path P_{11} . By similar arguments as given above, one can show that

$D[n]$ has no perfect matching. Thus $D[n]$ has no Kekulé structure for $n > 1$.

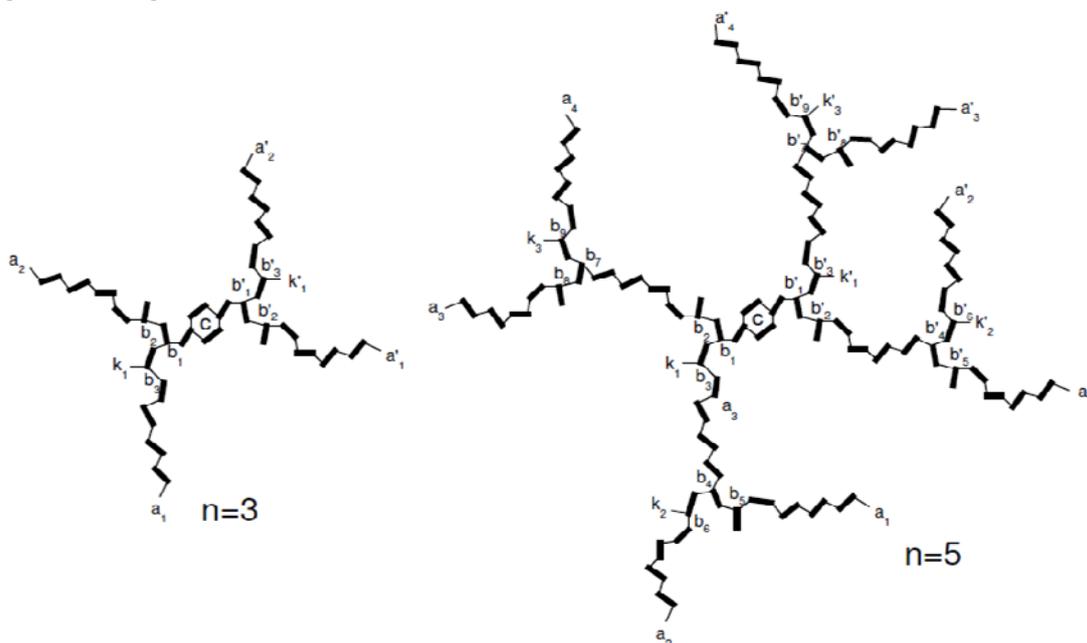


Fig. 4. $D[n]$ with $n = 3$ and $n = 5$. The thick edges represent a matching M .

Observation 1: Consider a tree T_n on n -vertices, $n \geq 7$, shown in Fig. 5 such that
 (i) $d(x, y)$ and $d(z, w)$ are odd.
 (ii) $d(y, z)$ is even.

Then from the construction of T_n , we can easily see that the size of a maximum matching in T_n is $\lfloor \frac{n}{2} \rfloor - 1$.



Fig. 5. A tree T_n , $n \geq 7$.

Observation 2: Let T_{n_1} and T_{n_2} be two trees that satisfies (i) and (ii) of Observation 1, where $n_1, n_2 \geq 7$. We join T_{n_1} with T_n at vertex x and T_{n_2}

with T_n at vertex w and the resulting tree, say $T_{n+n_1+n_2}$, is shown in Fig. 6. Then the size of a maximum matching in $T_{n+n_1+n_2}$ is $\left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{n_1}{2} \right\rfloor + \left\lfloor \frac{n_2}{2} \right\rfloor - 3$.

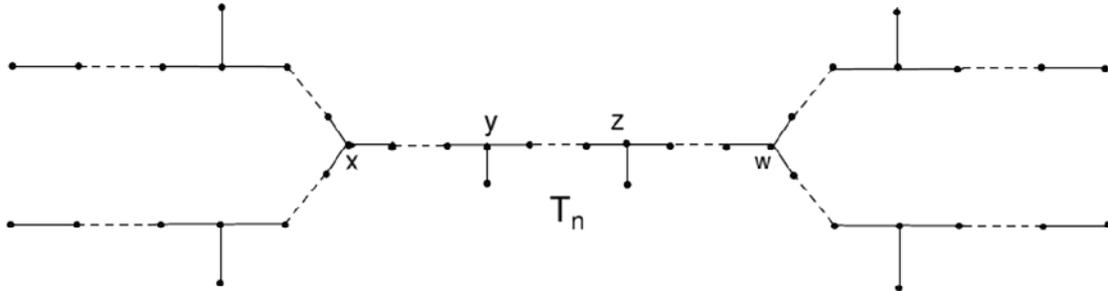


Fig. 6. Joining of T_{n_1} and T_{n_2} with T_n .

Let M denote a matching in $D[n]$ formed by the thick edges shown in Fig. 4. In the next theorem, we show that M represents a maximum matching in $D[n]$. Moreover, we give the size of this maximum matching.

Theorem 3.3 *The size of the maximum matching M in $D[n]$ is given by*

$$|M| = \begin{cases} 18 \times 2^t - 18 & \text{if } n = 2t \\ 11 \times 2^{t+1} - 18 & \text{if } n = 2t + 1, \end{cases}$$

where $t \geq 1$ is an integer.

Proof. Let $n = 2$. Then from Fig. 3, we see that there are two copies of a tree T_{17} each of which joined with one pendent vertex of $D[1]$. The tree T_{17} satisfies (i) and (ii) of observation 1. By Observation 1, the size of a maximum matching in T_{17} is $\left\lfloor \frac{17}{2} \right\rfloor - 1$. The size of maximum matching M in $D[2]$ is

$$\begin{aligned} |M| &= 2 \left(\left\lfloor \frac{17}{2} \right\rfloor - 1 \right) + 4 \\ &= 18 \\ &= 18 \times 2^1 - 18. \end{aligned} \tag{1}$$

Let $n = 3$. Then from Fig. 4, we note that there are two copies of a tree T_{25} each of which is joined with one pendent vertex of $D[1]$. The tree T_{25} satisfies (i) and (ii) of Observation 1. By Observation 1, the size of a maximum matching in T_{25} is $\left\lfloor \frac{25}{2} \right\rfloor - 1$. Thus, the size of maximum matching M in $D[3]$ is

$$\begin{aligned} |M| &= 2 \left(\left\lfloor \frac{25}{2} \right\rfloor - 1 \right) + 4 \\ &= 26 \\ &= 11 \times 2^{1+1} - 18. \end{aligned} \tag{2}$$

Let $n = 4$. Then from Fig. 3, we note that there are four copies of a tree T_{17} each of which is joined with one of pendent vertex of two copies of a tree T_{25} . The graph obtained after joining two copies of T_{17} with T_{25} satisfies the condition of Observation 2. Thus by Observation 2, the size of maximum matching in the join of two copies of T_{17} and T_{25} is $\left\lfloor \frac{25}{2} \right\rfloor + 2 \left\lfloor \frac{17}{2} \right\rfloor - 3$.

Thus the size of maximum matching M in $D[4]$ is

$$\begin{aligned} |M| &= 2 \left(\left\lfloor \frac{25}{2} \right\rfloor + 2 \left\lfloor \frac{17}{2} \right\rfloor - 3 \right) + 4 \\ &= 54 \\ &= 18 \times 2^2 - 18. \end{aligned} \tag{3}$$

Let $n = 5$. Then from Fig. 4, we observe that there are four copies of a tree T_{25} each of which is joined with one pendent vertex of two copies of a tree T_{25} . By similar arguments used to find the size of a maximum matching in $D[4]$, we conclude that the size of a maximum matching M in $D[5]$ is given by

$$\begin{aligned} |M| &= 2 \left(3 \left\lfloor \frac{25}{2} \right\rfloor - 3 \right) + 4 \\ &= 70 \\ &= 11 \times 2^{2+1} - 18. \end{aligned} \tag{4}$$

Since the growth of $D[n]$ is systematic, from (1) and

(3), we conclude that when $n = 2t$, $t = 1, 2, \dots$, the size of a maximum matching M in $D[n]$ is given by

$$|M| = 18 \times 2^t - 18.$$

From (2) and (4), we observe that when $n = 2t + 1$, where $t = 1, 2, \dots$, the size of a maximum matching M in $D[n]$ is given by:

$$|M| = 11 \times 2^{t+1} - 18.$$

This proves the required assertion.

From Theorem 3.3, we have the following result.

Corollary 3.4 The anti-Kekulé number of $D[n]$

for $n \geq 2$ is 0.

4. The nullity of hetrofunctional dendrimers $D[n]$

In this section, we calculate the nullity of the hetrofunctional dendrimers $D[n]$. Let M be the maximum matching in the graph $D[n]$ as shown in Fig. 3 and Fig. 4. The next lemma is useful in calculating the nullity of bipartite graphs.

Lemma 4.1 (Cvetkovic, Gutman [4]) If a bipartite graph G with $n \geq 1$ vertices does not contain any cycle of length $r \equiv 0 \pmod{4}$, then $\eta(G) = |V| - 2m$, 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 [5]) 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 computed as follows.

Lemma 4.3 (Cvetkovic, Gutman [5]) (i) The

eigenvalues of the path P_n are of the form $2 \cos\left(\frac{k\pi}{n+1}\right)$,

where $k = 1, \dots, n$. Thus,

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

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

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

The following lemma states that the sum of the nullities of components of a graph is equal to nullity of graph.

Next theorem gives the nullity of $D[n]$.

Lemma 4.4 (Gutman, Borovicanin [11]) Let

$G = \bigcup_{i=1}^t G_i$, where G_i , for each $i = 1, \dots, t$, are

connected components of G . Then $\eta(G) = \sum_{i=1}^t \eta(G_i)$.

Theorem 4.5 The nullity of $D[n]$ is given by

$$\eta(D[n]) = \begin{cases} 0 & \text{if } n = 1 \\ 4 \times 2^t - 2 & \text{if } n \geq 2, \end{cases}$$

where $t = \lfloor \frac{n}{2} \rfloor$.

Proof. Note that $D[1]$ is a bipartite graph and does not contain any cycle of length $r \equiv 0 \pmod{4}$. Also, the size of maximum matching in $D[1]$ is 5. Thus, Lemma 4.1 gives

$$\eta(D[1]) = 0$$

Now, let $n \geq 2$. Again $D[n]$ is a bipartite graph for each $n \geq 2$ and does not contain any cycle of length of $r \equiv 0 \pmod{4}$. By Theorem 3.3, the size of a maximum matching in $D[n]$ is $18 \times 2^t - 18$ when $n = 2t$ and $11 \times 2^{t+1} - 18$ when $n = 2t + 1$.

When $n = 2t$, Lemma 4.1 gives

$$\begin{aligned} \eta(D[n]) &= (16 \times 2^{t+1} + 8 \times 2^t - 38) - (18 \times 2^t - 18) \\ &= 4 \times 2^t - 2. \end{aligned}$$

When $n = 2t + 1$, Lemma 4.1 yields

$$\begin{aligned} \eta(D[n]) &= (24 \times 2^{t+1} - 38) - 2(11 \times 2^{t+1} - 18) \\ &= 4 \times 2^t - 2. \end{aligned}$$

This proves the assertion.

5. Some degree based topological indices of hetrofunctional dendrimers

This section deals with some degree based topological indices of the dendrimer $D[n]$. Let G be a simple connected graph with vertex set $V(G)$ and the edge set $E(G)$. The degree of vertex $v \in V(G)$ is denoted by d_v . Also, define $S_u = \sum_{v \in N_G(u)} d_v$, where $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$. Introduced by Estarada et al. [7], the atom bond connectivity index

(henceforth, *ABC – Index*) is defined by

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \quad (5)$$

Recently, Ghorbani et al. [9] introduced the fourth version of *ABC – Index* defined by

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}. \quad (6)$$

Another well-known connectivity topological descriptor is the geometric-arithmetic index (henceforth, *GA – index*), which was introduced by Vukićević and Furtula [16] and is defined by

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \quad (7)$$

Graovac et al. [10] proposed the fifth version of *GA – index*, which is defined by

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}. \quad (8)$$

With each edge uv , we associate two pairs (d_u, d_v) and (S_u, S_v) . The edge partition of the dendrimer $D[n]$ with respect to 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.

Table 1. (d_u, d_v) -type edge partition of $D[n]$, for $n \geq 3$ and $t = \lfloor \frac{n}{2} \rfloor$.

(d_u, d_v)	Number of edges
(1,2)	2^{t+1}
(2,3)	$\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)$
(2,2)	$2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=2}^t (2^i \times 4)$ if $n = 2t$
(2,2)	$2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=1}^t (2^{i+1} \times 4)$ if $n = 2t + 1$
(1,3)	$\sum_{i=1}^t 2^{i+1}$

Table 2. (S_u, S_v) -type edge partition of $D[n]$, for $n \geq 3$ and $t = \lfloor \frac{n}{2} \rfloor$.

(S_u, S_v)	Number of edges
(5,5)	$\sum_{i=0}^t 2^{i+1}$
(5,6)	$3 \times 2^{t+1} - 4$
(6,6)	$4 + \sum_{i=1}^t 2^{i+1}$
(5,3)	$\sum_{i=1}^t 2^{i+1}$
(5,4)	$3 \times 2^{t+1} - 8$
(4,4)	$\sum_{i=1}^t 2^{i+1} + \sum_{i=1}^{t-1} (4 \times 2^{i+1})$ if $n = 2t$
(4,4)	$\sum_{i=1}^t (5 \times 2^{i+1})$ if $n = 2t + 1$
(4,3)	2^{t+1}
(3,2)	2^{t+1}

5.1 Results for ABC and ABC₄ - Index

Now, we compute the *ABC* and *ABC₄*-indices of the dendrimer *D*[*n*] using the edge partition shown in Tables 1-2.

Theorem 5.1 *The atom-bond connectivity index of D*[*n*], for *n* = 2*t* + 1, where *t* ≥ 0 is given by

$$ABC(D[n]) = 22\sqrt{2} \times 2^t - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^t - \frac{4}{3}\sqrt{6}.$$

Proof. We use equation (5) and the edge partitions in Table 1.

For *n* = 1, we have

$$\begin{aligned} ABC(D[1]) &= \sum_{uv \in D(1)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= 2 \times \sqrt{\frac{1+2-2}{1 \times 2}} + 6 \times \sqrt{\frac{2+3-2}{2 \times 3}} + 2 \times \sqrt{\frac{2+2-2}{2 \times 2}} \\ &= 22\sqrt{2} \times 2^0 - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^0 - \frac{4}{3}\sqrt{6}. \end{aligned}$$

For *n* ≥ 3, we have

$$\begin{aligned} ABC(D[n]) &= \sum_{uv \in D(n)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= 2^{t+1} \times \sqrt{\frac{1+2-2}{1 \times 2}} + (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times \sqrt{\frac{2+3-2}{2 \times 3}} \\ &+ (2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=1}^t 2^{i+1} \times 4) \times \sqrt{\frac{2+2-2}{2 \times 2}} \\ &+ \sum_{i=1}^t 2^{i+1} \times \sqrt{\frac{1+3-2}{1 \times 3}} \end{aligned}$$

$$= 22\sqrt{2} \times 2^t - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^t - \frac{4}{3}\sqrt{6}.$$

This completes the proof.

Theorem 5.2 *The atom-bond connectivity index of D*[*n*], for *n* = 2*t*, where *t* ≥ 1 is given by

$$ABC(D[n]) = 18\sqrt{2} \times 2^t - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^t - \frac{4}{3}\sqrt{6}. \tag{9}$$

Proof. We use equation (5) and the edge partitions in Table-1.

For *n* = 2, we have

$$\begin{aligned} ABC(D[2]) &= \sum_{uv \in D(2)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= 4 \times \sqrt{\frac{1+2-2}{1 \times 2}} + 20 \times \sqrt{\frac{2+3-2}{2 \times 3}} + 14 \times \sqrt{\frac{2+2-2}{2 \times 2}} + 14 \times \sqrt{\frac{1+3-2}{1 \times 3}} \\ &= 19\sqrt{2} + \frac{4}{3}\sqrt{6} \\ &= 18\sqrt{2} \times 2^1 - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^1 - \frac{4}{3}\sqrt{6}. \end{aligned}$$

For *n* ≥ 4, we have

$$\begin{aligned} ABC(D[n]) &= \sum_{uv \in D(n)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= 2^{t+1} \times \sqrt{\frac{1+2-2}{1 \times 2}} + (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times \sqrt{\frac{2+3-2}{2 \times 3}} \\ &+ (2 + \sum_{i=2}^{t+1} 2^i \times 3 + \sum_{i=2}^t 2^i \times 4) \times \sqrt{\frac{2+2-2}{2 \times 2}} + \sum_{i=1}^t 2^{i+1} \times \sqrt{\frac{1+3-2}{1 \times 3}} \\ &= 18\sqrt{2} \times 2^t - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^t - \frac{4}{3}\sqrt{6}. \end{aligned}$$

This completes the proof.

Theorem 5.3 *The fourth atom-bond connectivity index of D*[*n*], for *n* = 2*t* + 1, where *t* ≥ 0 is given by

$$ABC_4(D[n]) = \begin{cases} \frac{9}{5}\sqrt{2} + \frac{2}{5}\sqrt{30} + \frac{2}{3}\sqrt{3} & \text{if } t = 0, \\ \frac{1}{15}(2^{\frac{2t+1}{2}} \times (9\sqrt{15} + 22\sqrt{5} + 75\sqrt{3} + 39) + 2^t \times (5\sqrt{15} - 9\sqrt{35}) - 6\sqrt{30} - 12\sqrt{10} - 12\sqrt{35}) - 5\sqrt{6} - \frac{4}{5}\sqrt{2}. & \text{if } t \geq 1. \end{cases}$$

Proof. When *n* = 1, the fourth atom-bond connectivity index of *D*[1] can be written as follows:

$$ABC_4(D[1]) = \sum_{uv \in E(D[n])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}$$

$$\begin{aligned} &= 2 \times \sqrt{\frac{5+5-2}{5 \times 5}} + 4 \times \sqrt{\frac{5+6-2}{5 \times 6}} + 2 \times \sqrt{\frac{6+4-2}{6 \times 4}} + 2 \times \sqrt{\frac{4+2-2}{4 \times 2}} \\ &= \frac{9}{5}\sqrt{2} + \frac{2}{5}\sqrt{30} + \frac{2}{3}\sqrt{3}. \end{aligned}$$

When *n* ≥ 3, using Table-2, the fourth atom-bond

connectivity index of $D[n]$ can be written as follows:

$$\begin{aligned}
 ABC_4(D[n]) &= \sum_{uv \in E(D[n])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\
 &= \sum_{i=0}^t 2^{i+1} \times \sqrt{\frac{5+5-2}{5 \times 5}} + (3 \times 2^{t+1} - 4) \times \sqrt{\frac{5+6-2}{5 \times 6}} + \\
 &\quad (4 + \sum_{i=1}^t 2^{i+1}) \times \sqrt{\frac{6+6-2}{6 \times 6}} + \sum_{i=1}^t 2^{i+1} \times \sqrt{\frac{5+3-2}{5 \times 3}} \\
 &\quad + (3 \times 2^{t+1} - 8) \times \sqrt{\frac{5+4-2}{5 \times 4}} + (\sum_{i=1}^t 5 \times 2^{i+1}) \times \sqrt{\frac{4+4-2}{4 \times 4}} \\
 &\quad + 2^{t+1} \times \sqrt{\frac{4+3-2}{4 \times 3}} + 2^{t+1} \times \sqrt{\frac{3+2-2}{3 \times 2}} \\
 &= \frac{1}{15} (2^{\frac{2t+1}{2}} \times (9\sqrt{15} + 22\sqrt{5} + 75\sqrt{3} + 39) + 2^t \times (5\sqrt{15} \\
 &\quad - 9\sqrt{35}) - 6\sqrt{30} - 12\sqrt{10} - 12\sqrt{35}) - 5\sqrt{6} - \frac{4}{5}\sqrt{2}.
 \end{aligned}$$

This completes the proof.

Theorem 5.4 The fourth atom-bond connectivity index of $D[n]$, for $n = 2t$, where $t \geq 1$ is given by

$$ABC_4(D[n]) = \begin{cases} \frac{22}{5}\sqrt{2} + \frac{4}{5}\sqrt{30} + \frac{32}{15}\sqrt{10} + \frac{2}{5}\sqrt{35} + \sqrt{6} + \frac{2}{3}\sqrt{15} & \text{if } t = 1, \\ \frac{1}{15} (2^{\frac{2t+1}{2}} \times (9\sqrt{15} + 22\sqrt{5} + 45\sqrt{3} + 39) + 2^t \times (5\sqrt{15} - 9\sqrt{35}) \\ - 6\sqrt{30} - 12\sqrt{10} - 12\sqrt{35}) - 5\sqrt{6} - \frac{4}{5}\sqrt{2}. & \text{if } t \geq 2. \end{cases}$$

Proof. When $n = 2$, the fourth atom-bond connectivity index of $D[2]$ can be written as follows:

$$\begin{aligned}
 ABC_4(D[2]) &= \sum_{uv \in E(D[2])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\
 &= 6 \times \sqrt{\frac{5+5-2}{5 \times 5}} + 8 \times \sqrt{\frac{5+6-2}{5 \times 6}} + 8 \times \sqrt{\frac{6+6-2}{6 \times 6}} + 4 \times \sqrt{\frac{5+3-2}{5 \times 3}} \\
 &\quad + 4 \times \sqrt{\frac{5+4-2}{5 \times 4}} + 4 \times \sqrt{\frac{4+4-2}{4 \times 4}} + 4 \times \sqrt{\frac{3+2-2}{3 \times 2}} + 4 \times \sqrt{\frac{4+3-2}{4 \times 3}} \\
 &= \frac{22}{5}\sqrt{2} + \frac{4}{5}\sqrt{30} + \frac{32}{15}\sqrt{10} + \frac{2}{5}\sqrt{35} + \sqrt{6} + \frac{2}{3}\sqrt{15}.
 \end{aligned}$$

When $n \geq 4$, using Table-2, the fourth atom-bond connectivity index of $D[n]$ can be written as follows:

$$ABC_4(D[n]) = \sum_{uv \in E(D[n])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}$$

5.2 Results for GA and GA₅ - Index

Now, we compute the GA and GA_5 -indices of the dendrimer $D[n]$ using the edge partitions shown in Tables 1-2.

$$\begin{aligned}
 &= \sum_{i=0}^t 2^{i+1} \times \sqrt{\frac{5+5-2}{5 \times 5}} + (3 \times 2^{t+1} - 4) \times \sqrt{\frac{5+6-2}{5 \times 6}} + (4 + \sum_{i=1}^t 2^{i+1}) \times \sqrt{\frac{6+6-2}{6 \times 6}} \\
 &\quad + \sum_{i=1}^t 2^{i+1} \times \sqrt{\frac{5+3-2}{5 \times 3}} + (3 \times 2^{t+1} - 8) \times \sqrt{\frac{5+4-2}{5 \times 4}} \\
 &\quad + (\sum_{i=1}^t 2^{i+1} + \sum_{i=1}^{t-1} (4 \times 2^{i+1})) \times \sqrt{\frac{4+4-2}{4 \times 4}} + 2^{t+1} \times \sqrt{\frac{4+3-2}{4 \times 3}} \\
 &\quad + 2^{t+1} \times \sqrt{\frac{3+2-2}{3 \times 2}} \\
 &= \frac{1}{15} (2^{\frac{2t+1}{2}} \times (9\sqrt{15} + 22\sqrt{5} + 45\sqrt{3} + 39) + 2^t \times (5\sqrt{15} \\
 &\quad - 9\sqrt{35}) - 6\sqrt{30} - 12\sqrt{10} - 12\sqrt{35}) - 5\sqrt{6} - \frac{4}{5}\sqrt{2}.
 \end{aligned}$$

The proof is complete.

Theorem 5.5 The geometric-arithmetic index of $D[n]$, for $n = 2t + 1$ where $t \geq 0$ is given by

$$GA(D[n]) = \begin{cases} \frac{4}{3}\sqrt{2} + \frac{12}{5}\sqrt{6} + 2 & \text{if } t = 0, \\ 2^{\frac{2t+1}{2}} \times (\frac{4}{3} + \frac{28}{5}\sqrt{3}) + 2^t \times (28 + 2\sqrt{3}) - \frac{16}{5}\sqrt{6} - 2\sqrt{3} - 26 & \text{if } t \geq 1. \end{cases}$$

Proof. When $n = 1$, the geometric-arithmetic index of $D[1]$ can be written as follows:

$$\begin{aligned} GA(D[1]) &= \sum_{uv \in D[1]} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= 2 \times \frac{2\sqrt{1 \times 2}}{1+2} + 6 \times \frac{2\sqrt{2 \times 3}}{2+3} + 2 \times \frac{2\sqrt{2 \times 2}}{2+2} \\ &= \frac{4}{3}\sqrt{2} + \frac{12}{5}\sqrt{6} + 2. \end{aligned}$$

When $n \geq 3$, using Table-1, the geometric-arithmetic index of $D[n]$ can be written as follows:

$$GA(D[n]) = \begin{cases} \frac{8}{3}\sqrt{2} + 8\sqrt{6} + 14 + 2\sqrt{3} & \text{if } t = 1, \\ 2^{\frac{2t+1}{2}} \times (\frac{4}{3} + \frac{28}{5}\sqrt{3}) + 2^t \times (20 + 2\sqrt{3}) - \frac{16}{5}\sqrt{6} - 2\sqrt{3} - 26 & \text{if } t \geq 2. \end{cases}$$

Proof. When $n = 2$, the geometric-arithmetic index of $D[2]$ can be written as follows:

$$\begin{aligned} GA(D[2]) &= \sum_{uv \in D[2]} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= 4 \times \frac{2\sqrt{1 \times 2}}{1+2} + 20 \times \frac{2\sqrt{2 \times 3}}{2+3} + 14 \times \frac{2\sqrt{2 \times 2}}{2+2} + 4 \times \frac{2\sqrt{1 \times 3}}{1+3} \\ &= \frac{8}{3}\sqrt{2} + 8\sqrt{6} + 14 + 2\sqrt{3}. \end{aligned}$$

When $n \geq 4$, using Table-1, the geometric-arithmetic index of $D[n]$ can be written as follows:

$$GA_5(D[n]) = \begin{cases} 2 + \frac{8}{11}\sqrt{30} + \frac{4}{5}\sqrt{6} + \frac{4}{3}\sqrt{2} & \text{if } t = 0, \\ 2^{\frac{2t+1}{2}} \times (\frac{12}{11}\sqrt{15} + \frac{4}{5}\sqrt{3}) + 2^t \times (28 + \sqrt{15} + \frac{8}{3}\sqrt{5} + \frac{8}{7}\sqrt{3}) - \frac{8}{11}\sqrt{30} - \frac{32}{9}\sqrt{5} - \sqrt{15} - 22 & \text{if } t \geq 1. \end{cases}$$

Proof. When $n = 1$, the fifth geometric-arithmetic index of $D[1]$ can be written as follows:

$$\begin{aligned} GA(D[n]) &= \sum_{uv \in D[n]} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= 2^{t+1} \times \frac{2\sqrt{1 \times 2}}{1+2} + (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times \frac{2\sqrt{2 \times 3}}{2+3} + \\ & (2 + \sum_{i=2}^{t+1} 2^i \times 3 + \sum_{i=1}^t 2^{i+1} \times 4) \times \frac{2\sqrt{2 \times 2}}{2+2} + \sum_{i=1}^t 2^{i+1} \times \frac{2\sqrt{1 \times 3}}{1+3} \\ &= 2^{\frac{2t+1}{2}} \times (\frac{4}{3} + \frac{28}{5}\sqrt{3}) + 2^t \times (28 + 2\sqrt{3}) - \frac{16}{5}\sqrt{6} - 2\sqrt{3} - 26. \end{aligned}$$

This completes the proof.

Theorem 5.6 The geometric-arithmetic index of $D[n]$, for $n = 2t$, where $t \geq 1$ is given by

$$\begin{aligned} GA(D[n]) &= \sum_{uv \in D[n]} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= 2^{t+1} \times \frac{2\sqrt{1 \times 2}}{1+2} + (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times \frac{2\sqrt{2 \times 3}}{2+3} + \\ & (2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=2}^t (2^i \times 4)) \times \frac{2\sqrt{2 \times 2}}{2+2} + (\sum_{i=1}^t 2^{i+1}) \frac{2\sqrt{1 \times 3}}{1+3} \\ &= 2^{\frac{2t+1}{2}} \times (\frac{4}{3} + \frac{28}{5}\sqrt{3}) + 2^t \times (20 + 2\sqrt{3}) - \frac{16}{5}\sqrt{6} - 2\sqrt{3} - 26, \end{aligned}$$

which is the required result.

Theorem 5.7 The fifth geometric-arithmetic index of $D[n]$, for $n = 2t + 1$, where $t \geq 0$ is given by

$$GA_5(D[1]) = \sum_{uv \in D[1]} \frac{2\sqrt{S_u S_v}}{S_u + S_v}$$

$$= 2 \times \frac{2\sqrt{5 \times 5}}{5+5} + 4 \times \frac{2\sqrt{5 \times 6}}{5+6} + 2 \times \frac{2\sqrt{6 \times 4}}{6+4} + 2 \times \frac{2\sqrt{4 \times 2}}{4+2}$$

$$= 2 + \frac{8}{11}\sqrt{30} + \frac{4}{5}\sqrt{6} + \frac{4}{3}\sqrt{2}.$$

When $n \geq 3$, using Table-2, the geometric-arithmetic index of $D[n]$ can be written as follows:

$$GA_5(D[n]) = \sum_{uv \in D[n]} \frac{2\sqrt{S_u S_v}}{S_u + S_v}$$

$$= \sum_{i=0}^t 2^{i+1} \times \frac{2\sqrt{5 \times 5}}{5+5} + (3 \times 2^{t+1} - 4) \times \frac{2\sqrt{5 \times 6}}{5+6} + (4 + \sum_{i=1}^t 2^{i+1}) \times \frac{2\sqrt{6 \times 6}}{6+6}$$

$$GA_5(D[n]) = \begin{cases} 18 + \frac{16}{11}\sqrt{30} + \sqrt{15} + \frac{16}{9}\sqrt{5} + \frac{8}{5}\sqrt{6} + \frac{16}{7}\sqrt{3} & \text{if } t = 1, \\ 2^{\frac{2t+1}{2}} \times (\frac{12}{11}\sqrt{15} + \frac{4}{5}\sqrt{3}) + 2^t \times (20 + \sqrt{15} + \frac{8}{3}\sqrt{5} + \frac{8}{7}\sqrt{3}) - \frac{8}{11}\sqrt{30} - \frac{32}{9}\sqrt{5} - \sqrt{15} - 22 & \text{if } t \geq 1. \end{cases}$$

Proof. When $n = 2$, the fifth geometric-arithmetic index of $D[2]$ can be written as follows:

$$GA_5(D[2]) = \sum_{uv \in D[2]} \frac{2\sqrt{S_u S_v}}{S_u + S_v}$$

$$= 6 \times \frac{2\sqrt{5 \times 5}}{5+5} + 8 \times \frac{2\sqrt{5 \times 6}}{5+6} + 8 \times \frac{2\sqrt{6 \times 6}}{6+6} + 4 \times \frac{2\sqrt{5 \times 3}}{5+3} + 4 \times \frac{2\sqrt{5 \times 4}}{5+4}$$

$$+ 4 \times \frac{2\sqrt{4 \times 4}}{4+4} + 4 \times \frac{2\sqrt{3 \times 2}}{3+2} + 4 \times \frac{2\sqrt{4 \times 3}}{4+3}$$

$$= 18 + \frac{16}{11}\sqrt{30} + \sqrt{15} + \frac{16}{9}\sqrt{5} + \frac{8}{5}\sqrt{6} + \frac{16}{7}\sqrt{3}.$$

When $n \geq 4$, using Table-2, the geometric-arithmetic index of $D[n]$ can be written as follows:

$$GA_5(D[n]) = \sum_{uv \in D[n]} \frac{2\sqrt{S_u S_v}}{S_u + S_v}$$

$$= (\sum_{i=0}^t 2^{i+1}) \times \frac{2\sqrt{5 \times 5}}{5+5} + (3 \times 2^{t+1} - 4) \times \frac{2\sqrt{5 \times 6}}{5+6} + (4 + \sum_{i=1}^t 2^{i+1}) \times \frac{2\sqrt{6 \times 6}}{6+6}$$

$$+ (\sum_{i=1}^t 2^{i+1}) \times \frac{2\sqrt{5 \times 3}}{5+3} + (3 \times 2^{t+1} - 8) \times \frac{2\sqrt{5 \times 4}}{5+4} +$$

$$(\sum_{i=1}^t 2^{i+1} + \sum_{i=1}^{t-1} 4 \times 2^{i+1}) \times \frac{2\sqrt{4 \times 4}}{4+4} + 2^{t+1} \times \frac{2\sqrt{4 \times 3}}{4+3} + 2^{t+1} \times \frac{2\sqrt{3 \times 2}}{3+2}$$

$$+ \sum_{i=1}^t 2^{i+1} \times \frac{2\sqrt{5 \times 3}}{5+3} + (3 \times 2^{t+1} - 8) \times \frac{2\sqrt{5 \times 4}}{5+4} + \sum_{i=1}^t 5 \times 2^{i+1} \times \frac{2\sqrt{4 \times 4}}{4+4}$$

$$+ (2^{t+1}) \times \frac{2\sqrt{4 \times 3}}{4+3} + (2^{t+1}) \times \frac{2\sqrt{3 \times 2}}{3+2}$$

$$= 2^{\frac{2t+1}{2}} \times (\frac{12}{11}\sqrt{15} + \frac{4}{5}\sqrt{3}) + 2^t \times (28 + \sqrt{15} + \frac{8}{3}\sqrt{5} + \frac{8}{7}\sqrt{3}) - \frac{8}{11}\sqrt{30}$$

$$- \frac{32}{9}\sqrt{5} - \sqrt{15} - 22.$$

This completes the proof.

Theorem 5.8 The fifth geometric-arithmetic index of $D[n]$, for $n = 2t$, where $t \geq 1$ is given by

$$= 2^{\frac{2t+1}{2}} \times (\frac{12}{11}\sqrt{15} + \frac{4}{5}\sqrt{3}) + 2^t \times (20 + \sqrt{15} + \frac{8}{3}\sqrt{5} + \frac{8}{7}\sqrt{3}) - \frac{8}{11}\sqrt{30}$$

$$- \frac{32}{9}\sqrt{5} - \sqrt{15} - 22.$$

This completes the proof.

6. Randić index

The very first and oldest degree based topological index is the Randić index, which was introduced by Milan Randić [14] in 1975. The Randić index of a graph $G = (V(G), E(G))$ is defined as

$$R_{\frac{1}{2}} = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}. \tag{10}$$

Later on, the general Randić index was introduced by Bollobas and Erdős [3] and Amic et al. [1] in 1988. The general Randić index of the graph is defined as

$$R_{\alpha}(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha}, \tag{11}$$

where $\alpha \in \{-1, -\frac{1}{2}, \frac{1}{2}, 1\}$.

Theorem 6.1 The Randić index is given by for $n = 2t + 1$, where $t \geq 0$ can be defined as

$$R_{\alpha}(D[n]) = \begin{cases} 106 \times 2^{t+1} - 164 & \text{if } \alpha = 1, \\ 2^{\frac{2t+1}{2}} \times (14\sqrt{3} + \sqrt{2}) + 2^t \times (4\sqrt{3} + 56) - 8\sqrt{6} - 4\sqrt{3} - 52 & \text{if } \alpha = \frac{1}{2}, \\ 2^{2t+1} \times \frac{35}{6} - \frac{55}{6} & \text{if } \alpha = -1, \\ 2^{\frac{2t+1}{2}} \times (1 + \frac{7}{\sqrt{3}}) + 2^t \times (14 + \frac{4}{\sqrt{3}}) - \frac{4}{3}\sqrt{6} - \frac{4}{3}\sqrt{3} - 13 & \text{if } \alpha = -\frac{1}{2}. \end{cases}$$

Proof. We use the Table-1 to prove the result.

When $\alpha = 1$: By using Table-1 and equation (11), we get:

$$\begin{aligned} R_1(D[n]) &= \sum_{uv \in E(D[n])} (d_u d_v)^1 \\ &= (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times (2 \times 3)^1 + (2 + \sum_{i=2}^{t+1} 2^i \times 3) \\ &+ \sum_{i=1}^t 2^{i+1} \times 4 \times (2 \times 2)^1 + (\sum_{i=1}^t 2^{i+1}) \times (1 \times 3)^1 \end{aligned}$$

$$= (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times (2 \times 3)^{\frac{1}{2}} + (2 + \sum_{i=2}^{t+1} (2^i \times 3)) + \sum_{i=1}^t (2^{i+1} \times 4) \times (2 \times 2)^{\frac{1}{2}}$$

$$+ (\sum_{i=1}^t 2^{i+1}) \times (1 \times 3)^{\frac{1}{2}} + 2^{t+1} \times (1 \times 2)^{\frac{1}{2}}$$

$$= 2^{\frac{2t+1}{2}} \times (14\sqrt{3} + \sqrt{2}) + 2^t \times (4\sqrt{3} + 56) - 8\sqrt{6} - 4\sqrt{3} - 52.$$

When $\alpha = -1$: By using Table-1 and equation (11), we

$$= (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times (2 \times 3)^{-1} + (2 + \sum_{i=2}^{t+1} (2^i \times 3)) + \sum_{i=1}^t (2^{i+1} \times 4) \times (2 \times 2)^{-1}$$

$$+ (\sum_{i=1}^t 2^{i+1}) \times (1 \times 3)^{-1} + 2^{t+1} \times (1 \times 2)^{-1}$$

$$= 2^{t+1} \times \frac{35}{6} - \frac{55}{6}.$$

When $\alpha = -\frac{1}{2}$: By using Table-1 and equation (11), we

$$= (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times (2 \times 3)^{-\frac{1}{2}} + (2 + \sum_{i=2}^{t+1} (2^i \times 3)) + \sum_{i=1}^t (2^{i+1} \times 4) \times (2 \times 2)^{-\frac{1}{2}}$$

$$+ (\sum_{i=1}^t 2^{i+1}) \times (1 \times 3)^{-\frac{1}{2}} + 2^{t+1} \times (1 \times 2)^{-\frac{1}{2}}$$

$$\begin{aligned} &+ 2^{t+1} \times (1 \times 2)^1 \\ &= 106 \times 2^{t+1} - 164. \end{aligned}$$

When $\alpha = \frac{1}{2}$: By using Table-1 and equation (11), we get:

$$R_{\frac{1}{2}}(D[n]) = \sum_{uv \in E(D[n])} (d_u d_v)^{\frac{1}{2}}$$

get:

$$R_{-1}(D[n]) = \sum_{uv \in E(D[n])} (d_u d_v)^{-1}$$

get:

$$R_{-\frac{1}{2}}(D[n]) = \sum_{uv \in E(D[n])} (d_u d_v)^{-\frac{1}{2}}$$

$$= 2^{\frac{2t+1}{2}} \times (1 + \frac{7}{\sqrt{3}}) + 2^t \times (14 + \frac{4}{\sqrt{3}}) - \frac{4}{3}\sqrt{6} - \frac{4}{3}\sqrt{3} - 13.$$

This completes the proof.

Theorem 6.2 The randic index of $D[n]$ for $n = 2t$,

where $t \geq 1$, can be defined as

$$R_\alpha(D[n]) = \begin{cases} 90 \times 2^{t+1} - 164 & \text{if } \alpha = 1, \\ 2^{\frac{2t+1}{2}} \times (14\sqrt{3} + \sqrt{2}) + 2^t \times (4\sqrt{3} + 40) - 8\sqrt{6} - 4\sqrt{3} - 52 & \text{if } \alpha = \frac{1}{2}, \\ 2^{2t+1} \times \frac{29}{6} - \frac{55}{6} & \text{if } \alpha = -1, \\ 2^{\frac{2t+1}{2}} \times (1 + \frac{7}{\sqrt{3}}) + 2^t \times (10 + \frac{4}{\sqrt{3}}) - \frac{4}{3}\sqrt{6} - \frac{4}{3}\sqrt{3} - 13 & \text{if } \alpha = -\frac{1}{2}. \end{cases}$$

Proof. We use the Table-1 to prove the results.

$$R_1(D[n]) = \sum_{uv \in E(D[n])} (d_u d_v)^1$$

When $\alpha = 1$: By using the edge partition in Table-1 and formula (11), we get:

$$\begin{aligned} &= (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times (2 \times 3)^1 + (2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=2}^t (2^i \times 4)) \times (2 \times 2)^1 \\ &+ (\sum_{i=1}^t 2^{i+1}) \times (1 \times 3)^1 + 2^{t+1} \times (1 \times 2)^1 \end{aligned}$$

formula (11), we get:

$$R_{\frac{1}{2}}(D[n]) = \sum_{uv \in E(D[n])} (d_u d_v)^{\frac{1}{2}}$$

$$= 90 \times 2^{t+1} - 164.$$

When $\alpha = \frac{1}{2}$: By using the edge partition in Table-1 and

$$\begin{aligned} &= (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times (2 \times 3)^{\frac{1}{2}} + (2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=2}^t (2^i \times 4)) \times (2 \times 2)^{\frac{1}{2}} \\ &+ (\sum_{i=1}^t 2^{i+1}) \times (1 \times 3)^{\frac{1}{2}} + 2^{t+1} \times (1 \times 2)^{\frac{1}{2}} \end{aligned}$$

formula (11), we get:

$$R_{-1}(D[n]) = \sum_{uv \in E(D[n])} (d_u d_v)^{-1}$$

$$= 2^{\frac{2t+1}{2}} \times (14\sqrt{3} + 2) + 2^t \times (4\sqrt{3} + 40) - 8\sqrt{6} - 4\sqrt{3} - 52.$$

When $\alpha = -1$: By using the edge partition in Table-1 and

$$\begin{aligned} &= (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times (2 \times 3)^{-1} + (2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=2}^t (2^i \times 4)) \times (2 \times 2)^{-1} \\ &+ (\sum_{i=1}^t 2^{i+1}) \times (1 \times 3)^{-1} + 2^{t+1} \times (1 \times 2)^{-1} \end{aligned}$$

$$R_{-\frac{1}{2}}(D[n]) = \sum_{uv \in E(D[n])} (d_u d_v)^{-\frac{1}{2}}$$

$$= 2^{t+1} \times \frac{29}{6} - \frac{55}{6}.$$

When $\alpha = -\frac{1}{2}$: By using the edge partition in Table-1 and formula (11), we get:

$$= (\sum_{i=1}^t 2^i + \sum_{i=0}^t (2^i \times 6)) \times (2 \times 3)^{-\frac{1}{2}} + (2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=2}^t (2^i \times 4)) \times (2 \times 2)^{-\frac{1}{2}}$$

$$\begin{aligned}
 & + \left(\sum_{i=1}^t 2^{i+1} \right) \times (1 \times 3)^{-\frac{1}{2}} + 2^{t+1} \times (1 \times 2)^{-\frac{1}{2}} \\
 & = 2^{\frac{2t+1}{2}} \times \left(1 + \frac{7}{\sqrt{3}} \right) + 2^t \times \left(10 + \frac{4}{\sqrt{3}} \right) - \frac{4}{3} \sqrt{6} - \frac{4}{3} \sqrt{3} - 13.
 \end{aligned}$$

This completes the proof.

7. Conclusion

We considered a class of hetrofunctional dendrimer and studied three types of topological descriptors for its underlying molecular graph. For the matching based topological indices, we studied number of perfect matchings, size of maximum matching and the anti-Kekulé number of the graph. For spectrum based topological indices, we computed nullity of the molecular graphs of these dendrimers. In the case of degree based topological indices, we calculated first and fourth version of atom-bond connectivity index, first and fifth versions of geometric-arithmetic index and the Randić of these hetrofunctional dendrimers.

Acknowledgements

The first author is thankful to the Higher Education Commission of Pakistan for supporting this research under the grant 20-3067/NRPU/R&D/HEC/12/831.

References

- [1] D. Amic, D. Beslo, B. Lucic, S. Nikolic, Trinajstić, *J. Chem. Inf. comput. Sci.* **38**, 819 (1998).
- [2] E. Bhuleier, W. Wehner, F. VÖgtle, *Synthesis*, **2**, 155 (1978).
- [3] B. Bollabás, P. Erdős, *Ars Combin*, **50**, 225 (1998).
- [4] D. Cvetkovic, I. Gutman, N. Trinajstić, *Croat. Chem. Acta*, **44**, 365 (1972).
- [5] D. Cvetkovic, I. Gutman, *Matematički Vesnik (Beograd)* **9**, 141 (1972).
- [6] L. Collatz, U. Sinogowitz, *Abh. Math. Sere. Univ. Hamburg*, **21**, 63 (1957).
- [7] E. Estrada, L. Torres, L. Rodriguez, I. Gutman, *Indian J. Chem.* **37(A)**, 849 (1998).
- [8] R. Farooq, N. Nazir, M. A. Malik, M. Arfan, *J. Optoelectron. Adv. Mater.* **17(11)** 1799 (2015).
- [9] M. Ghorbani, M. A. Hosseinzadeh, *Optoelectron. Adv. Mat.* **4**, 1419 (2010).
- [10] A. Graovac, M. Ghorbani, M. A. Hosseinzadeh, *J. Math. Nanosci.* **1**, 33 (2011).
- [11] I. Gutman, B. Borovicanin, *Zb. Rad. (Beogr.)* **22**, 137 (2011).
- [12] I. Gutman, O. Polansky, Springer-Verlag, Berlin, (1986).
- [13] B. K. Nanjwade, H. M. Bechara, G. K. Derkar, F. V. Manvi, V. K. Nanjwade, *European Journal of Pharmaceutical*, **38** (3), 185 (2009).
- [14] M. Randic, *J. Am. Chem. Soc.* **97(23)**, 6609 (1975).
- [15] M. Randic, *Chem. Rev.* **103**, 34 (2003).
- [16] D. Vukičević, B. Furtula, *J. Math. Chem.* **46**, 13 (2009).

*Corresponding author: alies.camp@gmail.com