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On Molecular Topological Properties of Dendrimers

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Abstract. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. In QSAR/QSPR study, physico-chemical properties and topological indices such as Randić, atom-bond connectivity (ABC) and geometric-arithmetic (GA) index are used to predict the bioactivity of different chemical compounds. Graph theory has found a considerable use in this area of research.

In this paper, we study the degree based molecular topological indices like ABC_4 and GA_5 for certain families of dendrimers. We derive the analytical closed formulae for these classes of dendrimers.

Keywords:*Atom-bond connectivity* (ABC) *index, geometric-arithmetic* (GA) *index,* ABC_4 *index,* GA_5 *index, dendrimer*

1 Introduction and preliminary results

Graph theory has provided chemists and pharmaceuticals with a variety of useful tools, such as topological descriptors. Molecules and molecular compounds are often modeled via a molecular graph. A molecular graph is just a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds between the atoms. *Cheminformatics* is relatively a new subject which is a combination of chemistry, mathematics and information science. It studies Quantitative structure-activity (QSAR) and Quantitave structure-property (QSPR) relationships that are used to predict the biological activities and properties of different chemical compounds. In the QSAR/QSPR study, physico-chemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb indices and ABC index are used to predict bioactivity of different chemical compounds.

A graph can be recognized by a numeric number, a polynomial, a drawing, a sequence of numbers or by a matrix. A *topological index* is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. There are some major classes of topological indices such as distance based topological indices, degree-based topological indices and counting related polynomials and indices of graphs. Among these classes degree-based topological indices are of great importance and play a vital role in chemical graph theory and particularly in chemistry. In more precise way, a topological index $Top(G)$ of a graph G, is a number with the property that for every graph H isomorphic to G, we have $Top(H) = Top(G)$. The concept of topological indices came from the work done by Wiener[1] while he was working on boiling point of paraffin. He named this index as *path number*. Later on, the path number was renamed as *Wiener index*[2] and the whole theory of topological indices started.

In this article, G is considered to be a *molecular network* with vertex set $V(G)$ and edge set $E(G)$, deg(u) is the degree of vertex $u \in V(G)$ and $S_u = \sum_{v \in N_G(u)} \deg(v)$ where $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$. The notations used in this article are mainly taken from the books[3,4].

Let G be a connected graph. Then the *Wiener index* of G is defined as

$$W(G) = \frac{1}{2} \sum_{(u,v)} d(u,v) \tag{1}$$

where (u, v) is any ordered pair of vertices in G and $d(u, v)$ is $u - v$ geodesic.

The very first and oldest degree-based topological index is *Randić* index[5] denoted by $R_{-\frac{1}{2}}(G)$ and was introduced by Milan Randić and was defined as follows:

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg(u)deg(v)}} \tag{2}$$

The *general Randić index* $R_\alpha(G)$ is the sum of $(\text{deg(u)deg(v)})^\alpha$ over all edges $e = uv \in E(G)$ defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} (deg(u)deg(v))^\alpha \quad \text{for} \quad \alpha = 1, \frac{1}{2}, -1, -\frac{1}{2} \tag{3}$$

An important topological index introduced by Ivan Gutman and Trinajstić is the *Zagreb* index denoted by $M_1(G)$ and is defined as

$$M_1(G) = \sum_{uv \in E(G)} (deg(u) + deg(v)) \tag{4}$$

One of the well-known degree-based topological index is *atom-bond connectivity* (ABC) index introduced by Estrada *et al.*[6] and defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{deg(u) + deg(v) - 2}{deg(u)deg(v)}} \tag{5}$$

Another well-known degree-based connectivity topological descriptor is *geometric-arithmetic* (GA) index which was introduced by Vukičević *et al.*[7] and was defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{deg(u)deg(v)}}{deg(u) + deg(v)} \tag{6}$$

The ABC, GA, ABC_4 and GA_5 indices can be computed if we are able to find the suitable edge partition of these interconnection chemical networks based on sum of the degrees of end vertices of each edge in these chemical networks. The fourth version of ABC index was introduced by Ghorbani *et al.*[8] and was defined as

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \tag{7}$$

Recently, the fifth version of GA index was proposed by Graovac *et al.*[9] and was defined as follows

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

Dendrimers are constructed by hyper-branchad macromolecules, with a fully tailored architecture. They can be arranged, in a composed manner, either by convergent or divergent form. Dendrimers have got a huge range of applications in all branches of chemistry, especially in host guest reaction and self-assembly procedures.Their applications in nanoscience, biology and chemistry are infinite. Currently, the topological indices of some families of dendrimers have been studied[10−23]. In this article, we compute the ABC_4 and GA_5 indices for certain infinite families of dendrimers nanostars.

2 The ABC_4 and GA_5 indices of the dendrimer $D_1[n]$

In this section, we consider a molecular graph $G(n) = D_1[n]$, where n denotes the step of growth in this type of dendrimer of generation $1-3$. The dendrimer of first kind of generation $1-3$ with 4 growth stages, $D_1[4]$ is shown in Fig. 1. Note that $D_1[n]$ is constructed by 2^n hexagons at each step. Define s_{ij} to be the number of edges joining a vertex of degree i with vertex of degree j. Let represent a vertex of degree i with i-vertex, and an edge relating a j-vertex with k-vertex by (j,k)-edge. By an easy calculation, we have $V(D_1[n]) = 2^{n+4} - 9$ and $E(D_1[n]) = 18 \times 2^n - 11$ see [10].

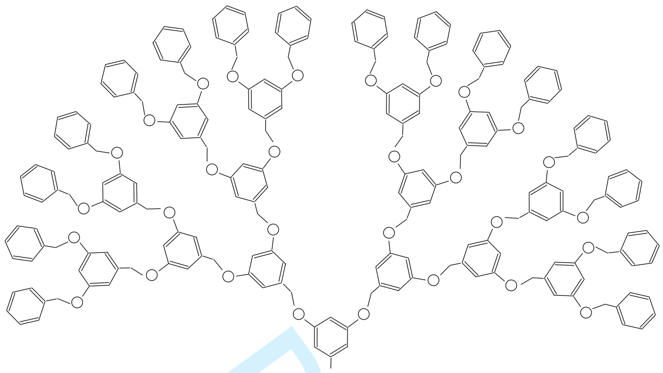

Fig. 1. The first kind of dendrimer of generation $1-3$ with 4 growth stages

(S_u, S_v) where $uv\epsilon E(G)$	Number of edges
$(5,3)$	1
$(6,6)$	$6 \times 2^n - 8$
$(5,5)$	2^n
$(4,4)$	$4 \times 2^n - 4$
$(5,4)$	$4 \times 2^n - 4$
$(5,6)$	$3 \times 2^n + 4$

Table 1. Edge partition of dendrimer $D_1[n]$ based on degree sum of neighbors of end vertices of each edge.

Theorem 2.1 *Let $n \in N$, then ABC_4 index for $D_1[n]$ is calculated as*

$$ABC_4(D_1[n]) = \left(\sqrt{10} + \sqrt{6} + \frac{2\sqrt{2}}{5} + 2\sqrt{\frac{7}{5}} + 3\sqrt{\frac{3}{10}}\right)2^n - \left(8 + \sqrt{6} + 2\sqrt{\frac{7}{5}} - 4\sqrt{\frac{3}{10}} - \sqrt{\frac{2}{5}}\right).$$

Proof. The graph $D_1[n]$ has the edge partition of the form $(5,3), (6,6), (5,5), (4,4), (5,4)$ *and* $(5,6)$. We compute the ABC_4 index of $D_1[n]$ through the information given in Table 1. Since we have

$$ABC_4(D_1[n]) = \sum_{uv\in E(D_1[n])} \sqrt{\frac{S_u+S_v-2}{S_uS_v}}.$$

This implies that

$$ABC_4\left(D_1\left[n\right]\right) = (1)\sqrt{\tfrac{5+3-2}{5\times3}}+(6\times2^n-8)\sqrt{\tfrac{6+6-2}{6\times6}}+(2^n)\sqrt{\tfrac{5+5-2}{5\times5}}+(4\times2^n-4)\sqrt{\tfrac{4+4-2}{4\times4}}+(4\times2^n-4)\sqrt{\tfrac{5+4-2}{5\times4}}$$

$$+\left(3\times2^n+4\right)\sqrt{\tfrac{5+6-2}{5\times6}}.$$

Which can be reduced to

$$ABC_4\left(D_1\left[n\right]\right) = \left(\sqrt{10}+\sqrt{6}+\tfrac{2\sqrt{2}}{5}+2\sqrt{\tfrac{7}{5}}+3\sqrt{\tfrac{3}{10}}\right)2^n-\left(8+\sqrt{6}+2\sqrt{\tfrac{7}{5}}-4\sqrt{\tfrac{3}{10}}-\sqrt{\tfrac{2}{5}}\right).$$

□

In the next theorem, we have computed the fifth version of geometric arithmetic index (GA_5) of the graph $D_1[n]$.

Theorem 2.2 *Consider the graph $D_1\left[n\right]$, then its GA_5 index is calculated as*

$$GA_5\left(D_1\left[n\right]\right) = \left(11+\tfrac{16\sqrt{5}}{9}+\tfrac{6\sqrt{30}}{11}\right)2^n-2\left(3+\tfrac{\sqrt{5}}{9}+\tfrac{\sqrt{15}}{8}+\tfrac{2\sqrt{30}}{11}\right)$$

Proof. By using edge partition given in Table 1, the GA_5 index of $D_1\left[n\right]$ can be computed easily. Since we have

$$GA_5(D_1\left[n\right]) = \sum_{uv\in E(D_1[n])}\tfrac{2\sqrt{S_uS_v}}{S_u+S_v}.$$

This implies that

$$GA_5\left(D_1\left[n\right]\right) = (1)\tfrac{2\sqrt{5\times3}}{5+3}+(6\times2^n-8)\tfrac{2\sqrt{6\times6}}{6+6}+(2^n)\tfrac{2\sqrt{5\times5}}{5+5}+(4\times2^n-4)\tfrac{2\sqrt{4\times4}}{4+4}+(4\times2^n-4)\tfrac{2\sqrt{5\times4}}{5+4}$$

$$+\left(3\times2^n+4\right)\tfrac{2\sqrt{5\times6}}{5+6}.$$

After an easy simplification, we get the following

$$GA_5\left(D_1\left[n\right]\right) = \left(11+\tfrac{16\sqrt{5}}{9}+\tfrac{6\sqrt{30}}{11}\right)2^n-2\left(3+\tfrac{\sqrt{5}}{9}+\tfrac{\sqrt{15}}{8}+\tfrac{2\sqrt{30}}{11}\right).$$

□

3 The ABC_4 and GA_5 indices of dendrimers $D_3[n]$

In this section, we study the molecular topological properties of another type of molecular graph denoted by $G(n) = D_3[n]$, where $n \geq 1$. The third kind of dendrimers denoted by $D_3[n]$ of generation $1-3$ with 3 growth stages is shown in Fig. 2. It is important to note that the graph of $D_3[n]$ contain $48 \times 2^n - 24$ edges. In the next two theorems we compute the ABC_4 and GA_5 indices of the graph $D_3[n]$.

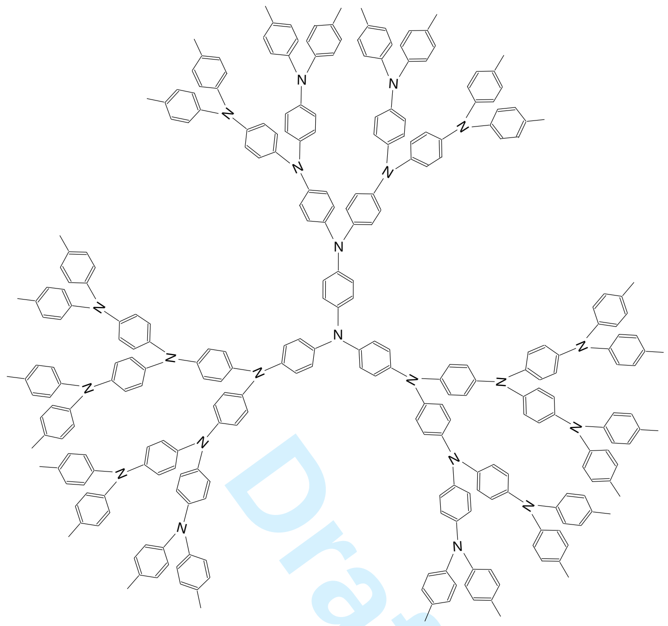

Fig. 2. The third kind of dendrimer $D_3[n]$ of generation $1-3$ with 3 growth stages

(S_u, S_v) where $uv\epsilon E(G)$	Number of Edges
$(5,3)$	3×2^n
$(5,5)$	$18 \times 2^n - 6$
$(5,7)$	$18 \times 2^n - 12$
$(7,9)$	$9 \times 2^n - 6$

Table 2. Edge partition for the graph of $D_3[n]$ based on degree sum of neighbors of end vertices of each edge.

Theorem 3.1 *For $n \geq 1$, the ABC_4 index of $D_3[n]$ is*

$$ABC_4(D_3[n]) = 3\left(\sqrt{\tfrac{6}{15}} + 6\sqrt{\tfrac{10}{35}} + 3\sqrt{\tfrac{14}{63}} + \tfrac{12\sqrt{2}}{5}\right)2^n - 6\left(2\sqrt{\tfrac{10}{35}} + \sqrt{\tfrac{14}{63}} + \tfrac{2\sqrt{2}}{5}\right).$$

Proof. For the molecular graph denoted by $D_3[n]$, we have the edges of the form $(5,3), (5,5), (5,7)$ and $(7,9)$. We use the values given in Table 2 to calculate the formula for $ABC_4(D_3[n])$. We have

$$ABC_4\left(D_3\left[n\right]\right) = \sum_{uv\in E(D_3[n])} \sqrt{\tfrac{S_u+S_v-2}{S_uS_v}}$$

$$= 3\times 2^n\sqrt{\tfrac{5+3-2}{5\times 3}} + (18\times 2^n-6)\sqrt{\tfrac{5+5-2}{5\times 5}} + (18\times 2^n-12)\sqrt{\tfrac{5+7-2}{5\times 7}} + (9\times 2^n-6)\sqrt{\tfrac{7+9-2}{7\times 9}}.$$

After an easy simplification, we have

$$ABC_4(D_3\left[n\right]) = 3\left(\sqrt{\tfrac{6}{15}} + 6\sqrt{\tfrac{10}{35}} + 3\sqrt{\tfrac{14}{63}} + \tfrac{12\sqrt{2}}{5}\right)2^n - 6\left(2\sqrt{\tfrac{10}{35}} + \sqrt{\tfrac{14}{63}} + \tfrac{2\sqrt{2}}{5}\right).$$

□

Theorem 3.2 *Let $n\geq 1$. Then GA_5 index of $D_3\left[n\right]$ is computed by the following formula.*

$$GA_5\left(D_3\left[n\right]\right) = 3\left(\tfrac{\sqrt{15}}{4} + \tfrac{3\sqrt{63}}{8} + \sqrt{35} + 6\right)2^n - 6\left(\tfrac{2\sqrt{35}}{6} + \tfrac{\sqrt{63}}{8} + 1\right).$$

Proof. By using the edge partition given in Table 2, we calculate the GA_5 index of dendrimer $D_3\left[n\right]$ as follows

$$GA_5\left(D_3\left[n\right]\right) = \sum_{uv\in E(D_3[n])} \tfrac{2\sqrt{S_uS_v}}{S_u+S_v}$$

$$= 3\times 2^n\tfrac{2\sqrt{5\times 3}}{5+3} + (18\times 2^n-6)\tfrac{2\sqrt{5\times 5}}{5+5} + (18\times 2^n-12)\tfrac{2\sqrt{5\times 7}}{5+7} + (9\times 2^n-6)\tfrac{2\sqrt{7\times 9}}{7+9}.$$

After an easy simplification, we have

$$GA_5\left(D_3\left[n\right]\right) = 3\left(\tfrac{\sqrt{15}}{4} + \tfrac{3\sqrt{63}}{8} + \sqrt{35} + 6\right)2^n - 6\left(\tfrac{2\sqrt{35}}{6} + \tfrac{\sqrt{63}}{8} + 1\right).$$

□

4 The ABC, GA, ABC_4 and GA_5 indices of the tetrathiafulvalene dendrimers

In this section, we compute the ABC, GA, ABC_4 and GA_5 indices of the class of dendrimers known as tetrathiafulvalene dendrimer [12] with core unit. By construction of dendrimer generations G_n has grown n stages. We denote simply this graph by $TD_2[n]$. Fig. 3 shows the generations G_2 has grown 2 stages. We shall now determine the ABC and GA indices of the graph of dendrimer denoted by $TD_2\left[n\right]$ of tetrathiafulvalene dendrimer of generation G_n with n growth stages. By using the edge partition given in Table 3, we can compute the ABC and GA indices of tetrahiafulvalene dendrimer.

Theorem 4.1 *Let $n\geq 0$. Then ABC index of tetrahiafulvalene dendrimer is given by*

$$ABC\left(TD_2\left[n\right]\right) = \left(\tfrac{23}{\sqrt{2}} + \tfrac{7}{\sqrt{2}} + \sqrt{\tfrac{2}{3}} + \sqrt{2} + 2\right)2^{n+2} - 2\left(\tfrac{28}{\sqrt{2}} + \tfrac{8}{\sqrt{2}} + 2\sqrt{\tfrac{2}{3}} + \sqrt{2} + 3\right).$$

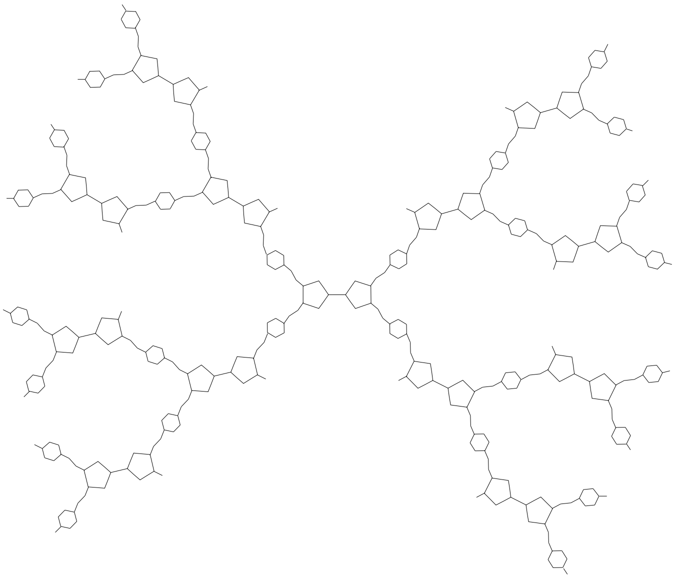

Fig. 3. Tetrathiafulvalene dendrimer of generations G_n has grown 2 stages; $TD_2[n]$.

(d_u, d_v) where $uv\epsilon E(G)$	Number of Edges
$(3,3)$	$12(2^n-1)+3$
$(2,2)$	$14(2^{n+1}-1)-2$
$(2,3)$	$92(2^n-1)+36$
$(2,1)$	$4(2^{n+1}-1)$
$(1,3)$	$4(2^n-1)$

Table 3. Edge partition of the graph $TD_2[n]$ which depend on the degree of vertices having unit distance from each edge.

Proof. The graph denoted by $TD_2[n]$ has the edges of the form $(3,3),(2,2),(2,3),(2,1)$ and $(1,3)$. Since

$$ABC(TD_2[n]) = \sum_{uv\in E(TD_2[n])} \sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$

$$= (92\times 2^n-56)\sqrt{\frac{2+3-2}{2\times 3}}+(28\times 2^n-16)\sqrt{\frac{2+2-2}{2\times 2}}+(12\times 2^n-9)\sqrt{\frac{3+3-2}{3\times 3}}+(8\times 2^n-4)\sqrt{\frac{1+2-2}{1\times 2}}$$

$$+(4\times 2^n-4)\sqrt{\frac{1+3-2}{1\times 3}}.$$

After an easy simplification, we get

$$ABC(TD_2[n]) = \left(\frac{23}{\sqrt{2}}+\frac{7}{\sqrt{2}}+\sqrt{\frac{2}{3}}+\sqrt{2}+2\right)2^{n+2}-2\left(\frac{28}{\sqrt{2}}+\frac{8}{\sqrt{2}}+2\sqrt{\frac{2}{3}}+\sqrt{2}+3\right).$$

□

Theorem 4.2 *Consider the tetrahiafulvalene dendrimer $TD_2[n]$, then we have*

$$GA(TD_2[n]) = \left(\frac{23\sqrt{6}}{5}+\frac{4\sqrt{2}}{3}+\frac{\sqrt{3}}{2}+10\right)2^{n+2}-\left(\frac{112\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}+\frac{4\sqrt{3}}{2}+25\right).$$

Proof. By using the edge partition given in Table 3, we have

$$GA(TD_2[n]) = \sum_{uv\in E(TD_2[n])} \frac{2\sqrt{d_ud_v}}{d_u+d_v}$$

$$= (92\times 2^n - 56)\frac{2\sqrt{2\times3}}{2+3} + (28\times 2^n - 16)\frac{2\sqrt{2\times2}}{2+2} + (12\times 2^n - 9)\frac{2\sqrt{3\times3}}{3+3} + (8\times 2^n - 4)\frac{2\sqrt{1\times2}}{1+2}$$

$$+ (4\times 2^n - 4)\frac{2\sqrt{1\times3}}{1+3}.$$

After an easy simplification, we get

$$GA(TD_2[n]) = \left(\frac{23\sqrt6}{5} + \frac{4\sqrt2}{3} + \frac{\sqrt3}{2} + 10\right)2^{n+2} - \left(\frac{112\sqrt6}{5} + \frac{8\sqrt2}{3} + \frac{4\sqrt3}{2} + 25\right).$$

□

Now we compute the ABC_4 and GA_5 indices of tetrahiafulvalene dendrimer, denoted by $TD_2[n]$.

(S_u, S_v) where $uv \in E(G)$	Number of Edges
$(7,7)$	$8(2^n-1)+3$
$(6,7)$	$32(2^n-1)+8$
$(5,7)$	$12(2^n-1)+4$
$(5,5)$	$28(2^n-1)+12$
$(5,6)$	$44(2^n-1)+20$
$(6,4)$	$8(2^n-1)+4$
$(2,4)$	$8(2^n-1)+4$
$(3,6)$	$2\times2^n-2$
$(6,6)$	$2\times2^n-2$

Table 4. Edge partition of the graph $TD_2[n]$ which depend on the degree sum of vertices having unit distance from each edge.

Theorem 4.3 *Let $n \in \mathbb{N}$. Then ABC_4 index of tetrahiafulvalene dendrimer, $TD_2[n]$ is given by*

$$ABC_4(TD_2[n]) = \left(\frac{8\sqrt3}{7} + 16\sqrt{\frac{11}{42}} + 6\sqrt{\frac{10}{35}} + \frac{66}{\sqrt{30}} + \frac{28\sqrt2}{5} + \frac{\sqrt2}{3} + \frac{\sqrt7}{3\sqrt2} + 2\sqrt2\right)2^{n+2}$$

$$-2\left(\frac{5\sqrt3}{7} + 12\sqrt{\frac{11}{42}} + 4\sqrt{\frac{10}{35}} + \frac{36}{\sqrt{30}} + \frac{8\sqrt2}{3} + \frac{\sqrt2}{3} + \frac{\sqrt7}{3\sqrt2} + \sqrt2\right).$$

Proof. The graph $TD_2[n]$ have the edges of the form $(7,7), (7,6), (7,5), (5,6), (5,5), (6,4), (2,4)$ and $(6,6), (3,6)$. Since we have

$$ABC_4(TD_2[n]) = \sum_{uv\epsilon E(TD_2[n])} \sqrt{\frac{S_u+S_v-2}{S_uS_v}}$$

$$= (8\times 2^n - 5)\sqrt{\frac{7+7-2}{7\times7}} + (32\times 2^n - 24)\sqrt{\frac{7+6-2}{7\times6}} + (12\times 2^n - 8)\sqrt{\frac{7+5-2}{7\times5}} + (44\times 2^n - 24)\sqrt{\frac{5+6-2}{5\times6}}$$

$+(28\times 2^n-16)\sqrt{\frac{5+5-2}{5\times 5}}+(8\times 2^n-4)\sqrt{\frac{6+4-2}{6\times 4}}+(8\times 2^n-4)\sqrt{\frac{2+4-2}{2\times 4}}+(2\times 2^n-2)\sqrt{\frac{6+6-2}{6\times 6}}+$ $(2\times 2^n-2)\sqrt{\frac{3+6-2}{3\times 6}}$.

After simplification, we get

$$ABC_4\left(TD_2\left[n\right]\right)=\left(\frac{8\sqrt{3}}{7}+16\sqrt{\frac{11}{42}}+6\sqrt{\frac{10}{35}}+\frac{66}{\sqrt{30}}+\frac{28\sqrt{2}}{5}+\frac{\sqrt{2}}{3}+\frac{\sqrt{7}}{3\sqrt{2}}+2\sqrt{2}\right)2^{n+2}$$

$$-2\left(\frac{5\sqrt{3}}{7}+12\sqrt{\frac{11}{42}}+4\sqrt{\frac{10}{35}}+\frac{36}{\sqrt{30}}+\frac{8\sqrt{2}}{3}+\frac{\sqrt{2}}{3}+\frac{\sqrt{7}}{3\sqrt{2}}+\sqrt{2}\right).$$

□

Theorem 4.4 *Let $n\in\mathbb{N}$. Then GA_5 index of $TD_2\left[n\right]$ is given by*

$$GA_5\left(TD_2\left[n\right]\right)=\left(\frac{32\sqrt{42}}{13}+\frac{44\sqrt{30}}{11}+\frac{8\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}+\frac{2\sqrt{2}}{3}+\sqrt{35}+19\right)2^{n+1}$$

$$-\left(\frac{48\sqrt{42}}{13}+\frac{8\sqrt{35}}{6}+\frac{48\sqrt{30}}{11}+\frac{8\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}+\frac{4\sqrt{2}}{3}+23\right).$$

Proof. The formula for GA_5 index of the graph of tetrahiafulvalene dendrimer can be reduced in the following form

$$GA_5\left(TD_2\left[n\right]\right)=\sum_{uv\in E(TD_2[n])}\frac{2\sqrt{S_uS_v}}{S_u+S_v}$$

$$=(8\times 2^n-5)\frac{2\sqrt{7\times 7}}{7+7}+(32\times 2^n-24)\frac{2\sqrt{7\times 6}}{7+6}+(12\times 2^n-8)\frac{\sqrt{7\times 5}}{7+5}+(44\times 2^n-24)\frac{2\sqrt{5\times 6}}{5+6}$$

$$+(28\times 2^n-16)\frac{2\sqrt{5\times 5}}{5+5}+(8\times 2^n-4)\frac{2\sqrt{6\times 4}}{6+4}+(8\times 2^n-4)\frac{2\sqrt{2\times 4}}{2+4}+(2\times 2^n-2)\frac{2\sqrt{6\times 6}}{6+6}$$

$$+(2\times 2^n-2)\frac{2\sqrt{3\times 6}}{3+6}.$$

After simplification, we get

$$GA_5\left(TD_2\left[n\right]\right)=\left(\frac{32\sqrt{42}}{13}+\frac{44\sqrt{30}}{11}+\frac{8\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}+\frac{2\sqrt{2}}{3}+\sqrt{35}+19\right)2^{n+1}$$

$$-\left(\frac{48\sqrt{42}}{13}+\frac{8\sqrt{35}}{6}+\frac{48\sqrt{30}}{11}+\frac{8\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}+\frac{4\sqrt{2}}{3}+23\right).$$

□

5 Conclusion

In this paper, some degree-based topological indices for certain infinite classes of dendrimers were studied for the first time and analytical closed formulas for these dendrimers were determined which will help the people working in network science to understand and explore the underlying topologies of these chemical networks.

In future, we are interested to design some new architectures/networks and then study their topological indices which will be quite helpful to understand their underlying topologies.

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Figure Captions

Fig. 1. The first kind of dendrimer of generation $1-3$ with 4 growth stages

Fig. 2. The third kind of dendrimer $D_3[n]$ of generation $1-3$ with 3 growth stages

Fig. 3. Tetrathiafulvalene dendrimer of generations G_n has grown 2 stages; $TD_2[n]$.