

Research Article

On Topological Indices of Fractal and Cayley Tree Type Dendrimers

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The topological descriptors are the numerical invariants associated with a chemical graph and are helpful in predicting their bioactivity and physiochemical properties. These descriptors are studied and used in mathematical chemistry, medicines, and drugs designs and in other areas of applied sciences. In this paper, we study the two chemical trees, namely, the fractal tree and Cayley tree. We also compute their topological indices based on degree concept. These indices include atom bond connectivity index, geometric arithmetic index and their fourth and fifth versions, Sanskruti index, augmented Zagreb index, first and second Zagreb indices, and general Randić index for $\alpha = \{-1, 1, 1/2, -1/2\}$. Furthermore, we give closed analytical results of these indices for fractal trees and Cayley trees.

1. Introduction

Graph theory provides a gateway for chemists and scientist to focus on the topological descriptors of molecular graphs. Molecular compounds can be modeled by using graph theoretic method. These topological descriptors provide a better way to understand and to predict the properties and bioactivities of compounds. Molecular graph is the illustration of a chemical compound or complex structure in which nodes correspond to atoms and edges correspond to chemical bond or physical link between two nodes/vertices. In the QSAR/QSPR study, the topological indices, mainly the Wiener index, Randić index, Zagreb indices, and GA and ABC index, are used to predict the chemical and physical properties and bioactivities of different compounds and structures.

The graph G can be represented by a numerical number, an eigen value, polynomial, and topological index, etc., which represents the structure of a graph. A topological index is a numerical value which indicates some useful information about the chemical compound or structure. It is

the arithmetic invariants of a molecular graph and is fruitful and vital to correlate with physiochemical properties and bioactivities of molecular compound/network/dendrimer. Recently, many researchers have found topological descriptor vital for the study of structural properties of molecular graph or network or chemical tree. An acyclic connected graph is called a tree graph. The degree 3 or greater of every vertex of tree is called branching point of tree. A chemical tree is a connected acyclic graph having maximum degree 4. We provide now some literature review of molecular descriptors of molecular graphs/networks, which motivate us to work in this field. The alkanes are the example of chemical trees and the series of saturated hydrocarbons, including methane, ethane, and propane. Motivated by the chemical importance of molecular descriptors of chemical compounds and structures, a lot of research has been done by researchers. The caterpillar trees represent the structure of benzenoid hydrocarbon molecules. The first and second Zagreb index of star-like trees and sun-like graphs and also caterpillar trees containing the hydrocarbons specially ethane, propane, and butane is studied and computed in [1]. The computation

of topological indices of degree based for the line graphs of Banana tree graph and Firecracker graph is investigated in [2]. The chemical applications of topological descriptors related to acyclic organic molecules are mentioned in detail in [3–9].

The dendrimers consist of highly branched organic macromolecules with successive generations/iterations of branch units surrounding a central core. There are different types of dendrimers that are discovered so far. These have a wide range of applications in the field of chemistry, nanoscience, biology, etc. The topological indices of famous dendrimers is recently investigated in [10, 11] and the references therein. For instance, the bond incident degree (*BID*) indices of nanostructures and polyomino chains are computed in [12, 13]. The edge version of geometric arithmetic index of polyomino chains of 8 cycles and arbitrary carbon nanocones is computed by [14]. Certain topological indices of honeycomb derived networks are computed in [15]. With the rapid increase of development in medicine manufacturing organizations and industries, a large number of drug products are produced each year. In order to determine the chemical properties of these drugs we focus on theoretical examination of topological indices. Smart polymer family is widely used in anticancer drugs and its some topological indices are computed in [16]. The computation of topological indices and their properties of certain networks, carbon graphite, crystal cubic carbon, copper oxide, and nanotubes are discussed in [17–22]. The Sanskruti index $S(G)$ of line graphs of subdivision graphs of 2D-lattice, nanotube, nanotorus of $TUC_4C_8[p, q]$ and polycyclic aromatic hydrocarbons PAH_k is investigated in [23, 24].

There are certain types of topological indices that depend on eccentric based, degree based, and distance based indices, etc. In this article, we compute degree based topological indices only.

$$R_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u \times d_v}}. \quad (1)$$

Bollobás et al. [25] and Amic et al. [26] introduced the general Randić index independently. The properties and useful results of general Randić are referred to in [27–29]. It is defined as follows:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u \times d_v)^\alpha, \quad (2)$$

where $\alpha \in \mathbb{R}$.

The atom bond connectivity index is of vital importance and used in the study of heat formation of alkanes. It is introduced by Estrada et al. [30] and is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}}, \quad (3)$$

where d_u is the degree of vertex u .

In 1972, the first Zagreb index was introduced by [31]. Later on, the second Zagreb index was introduced by [32]. Both, the first and the second, Zagreb indexes are defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v). \quad (4)$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

Furtula et al. [33] proposed the modified version of *ABC* index, which is called augmented Zagreb index. It is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u \times d_v}{d_u + d_v - 2} \right)^3. \quad (5)$$

The geometric arithmetic index *GA* of a graph G is introduced by Vukičević et al. [34] and is defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u \times d_v}}{d_u + d_v}. \quad (6)$$

The fourth version of atom bond connectivity index ABC_4 of a graph G is introduced by Ghorbani et al. [35] and is defined as

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

where $S_u = \sum_{uv \in E(G)} d_v$ and $S_v = \sum_{uv \in E(G)} d_u$.

The fifth version of geometric arithmetic index GA_5 of a graph G is introduced by Graovac et al. [36] and is defined as

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

The Sanskruti index $S(G)$ of a molecular graph G is introduced by S. M. Hosamani [24] in 2016. It is defined as

$$S(G) = \sum_{uv \in E(G)} \left(\frac{S_u \times S_v}{S_u + S_v - 2} \right)^3. \quad (9)$$

Moreover the paper is organized as follows.

We compute additive topological indices based on degree concept of graph for the fractal and Cayley tree dendrimers. We compute the atom bond connectivity *ABC*, geometric arithmetic *GA*, general Randić $\alpha = \{-1, 1, 1/2, -1/2\}$ only, first and second Zagreb, augmented Zagreb, GA_5 , ABC_4 , and Sanskruti indices for fractal tree. Also, we compute the atom bond connectivity *ABC*, geometric arithmetic *GA*, general Randić $\alpha = \{-1, 1, 1/2, -1/2\}$ only, augmented Zagreb, GA_5 , ABC_4 , and Sanskruti index. Furthermore, we compute close formulas of these indices for the fractal and Cayley tree dendrimers.

2. Applications of Topological Indices

The first and second Zagreb indices were found to be helpful for calculation of the aggregate π -electron energy of

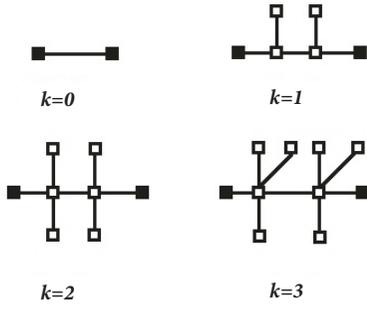


FIGURE 1: Construction model for next generations of the fractal trees.

the particles inside particular rough articulations [37]. The Randic index is a topological descriptor related to a great deal of synthetic qualities of atoms and was discovered parallel to processing the boiling point and Kovats constants of the particles. The particle bond network (ABC) index connects to the security of direct alkanes and stretched alkanes and is used to process the strain vitality of cycloalkanes [38, 39]. In terms of physicoconcoction properties, the GA index has prescient control superior to the prescient energy of the Randic connectivity index [40]. These are among the graph invariants proposed for the estimation of skeletons of stretching of carbon atoms [41]. The Sanskruti index $S(G)$ shows good correlation with entropy of an octane isomers.

2.1. Fractal Tree Dendrimer. The word fractal comes from the Latin word meaning "to break". Fractals are geometric patterns in which every smaller part of the structure is similar to the whole. There are countless examples of fractals like sierpinski triangle, von koch curve, broccoli, ferns, lotus white flower, etc. In this paper, the proposed fractal tree dendrimers are considered F_p where $p \geq 0$ is the iterations. If $p = 0$, then F_0 is an edge connecting two vertices. F_p is obtained from F_{p-1} by using two steps on each existing edge in F_{p-1} . The first step is to create a path of three links with the two same end points. The second step is to create k new vertices for each of the two middle vertices in the path. After that, attach them to the middle vertices.

Figure 1 depicts structure for different values of k . The fractal trees F_3 and F_4 for $k = 2$ and $k = 3$ are depicted in Figures 2(a) and 2(b), respectively.

Firstly, we compute above-mentioned topological indices for fractal tree dendrimer by using edge partition technique and graph theoretic methods. In F_p , the pendent vertices are $42pk - 28k + 14p - 8$, the 4 degree vertices are $7p - 5$, and the $k + 2$ degree vertices are $42p - 28$. The edge set of F_p is divided into three partitions based on the degree of end vertices. The first edge partition consists of $42pk - 28k + 14p - 8$ edges uv , where $d_u = 1$ and $d_v = k + 2$. The second edge partition consists of $28p - 20$ edges uv , where $d_u = 4$ and $d_v = k + 2$. The third edge partition consists of $21p - 14$ edges uv , where $d_u = d_v = k + 2$. The cardinality of vertices and edges in F_p is $42pk - 28k + 63p - 41$ and $42pk - 28k + 63p - 42$, respectively. The

TABLE 1: Edge partition of F_p based on degrees of end vertices of each edge.

(d_u, d_v)	Frequency
$(1, k + 2)$	$42pk - 28k + 14p - 8$
$(4, k + 2)$	$28p - 20$
$(k + 2, k + 2)$	$21p - 14$

tabular representation of edge partition technique is depicted in Table 1.

Theorem 1. Consider the fractal tree dendrimer F_p with $p, k \geq 2$. Its atom bond connectivity index is as follows:

$$\begin{aligned}
 ABC(F_p) = & \frac{1}{k+2} \left((42pk\sqrt{(k+1)(k+2)} \right. \\
 & - 28k\sqrt{(k+1)(k+2)}) + 7p(2\sqrt{(k+1)(k+2)} \\
 & + 2\sqrt{(k+2)(k+4)} + 3\sqrt{2(k+1)}) \\
 & - 2(4\sqrt{(k+1)(k+2)} + 5\sqrt{(k+4)(k+2)} \\
 & \left. + 7\sqrt{2(k+1)}) \right)
 \end{aligned} \tag{10}$$

Proof. Let fractal tree dendrimer F_p be a tree graph for p iterations. The atom bond connectivity index of F_p can be computed by using Table 1 in the following formula.

$$\begin{aligned}
 ABC(F_p) = & \sum_{uv \in E(F_p)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} \\
 ABC(F_p) = & (42pk - 28k + 14p - 8) \sqrt{\frac{1 + k + 2 - 2}{(1 \times k + 2)}} \\
 & + (28p - 20) \sqrt{\frac{4 + k + 2 - 2}{(4 \times k + 2)}} \\
 & + (21p - 14) \sqrt{\frac{k + 2 + k + 2 - 2}{(k + 2 \times k + 2)}}
 \end{aligned} \tag{11}$$

After simplification of the above form, we get our required result of (10). \square

Theorem 2. Consider the fractal tree dendrimer F_p with $p, k \geq 2$. Its geometric arithmetic index is as follows:

$$\begin{aligned}
 GA(F_p) = & 21p - 14 + \sqrt{k+2} \left(\frac{84pk}{k+3} - \frac{56k}{k+3} \right. \\
 & \left. + \frac{28p}{k+3} + \frac{112p}{k+6} - \frac{16}{k+3} - \frac{80}{k+6} \right)
 \end{aligned} \tag{12}$$

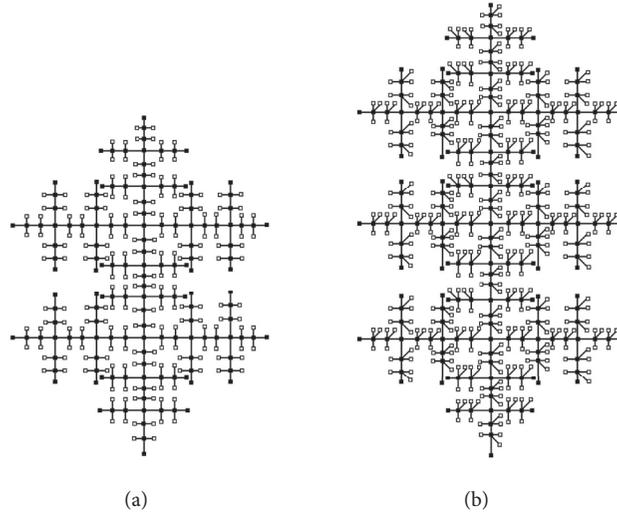


FIGURE 2: (a)The representation of fractal tree F_3 for $k = 2$ is illustrated. (b) The representation of fractal tree F_4 for $k = 3$ is illustrated.

Proof. Let fractal tree dendrimers F_p be a chemical tree graph for p iterations. The geometric arithmetic index of F_p can be computed by using Table 1 in the following formula:

$$GA(F_p) = \sum_{uv \in E(F_p)} \frac{2\sqrt{d_u \times d_v}}{d_u + d_v}.$$

$$GA(F_p) = (42pk - 28k + 14p - 8) \frac{2\sqrt{(1 \times k + 2)}}{1 + k + 2}$$

$$+ (28p - 20) \frac{2\sqrt{(4 \times k + 2)}}{4 + k + 2}$$

$$+ (21p - 14) \frac{2\sqrt{(k + 2 \times k + 2)}}{k + 2 + k + 2}$$
(13)

After simplification of the above form, we got our required versions of (12). □

Theorem 3. Consider the fractal tree dendrimer F_p with $p, k \geq 2$. Its first and second Zagreb index are as follows:

$$M_1(F_p) = 42k^2p + 210pk - 28k^2 - 140k + 294p$$

$$- 200$$
(14)

and

$$M_2(F_p) = 63k^2p + 294pk - 42k^2 - 200k + 336p$$

$$- 232.$$
(15)

Proof. Let fractal tree dendrimer F_p be a tree graph for p iterations. The first and second Zagreb index of F_p can be computed by using Table 1. First we compute first Zagreb index of F_p .

$$M_1(F_p) = \sum_{uv \in E(F_p)} (d_u + d_v).$$

$$M_1(F_p) = (42pk - 28k + 14p - 8)(1 + k + 2)$$

$$+ (28p - 20)(4 + k + 2)$$

$$+ (21p - 14)(k + 2 + k + 2)$$

$$M_1(F_p) = 42k^2p + 210pk - 28k^2 - 140k + 294p$$

$$- 200$$
(16)

The second Zagreb index of F_p can be computed by using the following formula:

$$M_2(F_p) = \sum_{uv \in E(G)} (d_u \times d_v).$$

$$M_2(F_p) = (42pk - 28k + 14p - 8)(1 \times k + 2)$$

$$+ (28p - 20)(4 \times k + 2)$$

$$+ (21p - 14)(k + 2 \times k + 2)$$

$$M_2(F_p) = 63k^2p + 294pk - 42k^2 - 200k + 336p$$

$$- 232$$
(17)

□

Theorem 4. Consider the fractal tree dendrimer F_p with $p, k \geq 2$. Its general Randić index is as follows:

$$R_\alpha(F_p) = \begin{cases} 63k^2p + 294pk - 42k^2 - 200k + 336p - 232, & \text{if } \alpha = 1, \\ \frac{42k^2p + 105pk - 28k^2 - 69k + 63p - 40}{(k+2)^2}, & \text{if } \alpha = -1, \\ 21pk - 14k + 42p - 28 + \sqrt{k+2}(|E| + 7p - 6), & \text{if } \alpha = \frac{1}{2}, \\ \frac{42pk - 28k + 28p - 18}{\sqrt{k+2}} + \frac{21p - 14}{k+2}, & \text{if } \alpha = -\frac{1}{2}. \end{cases} \tag{18}$$

Proof. Let fractal tree dendrimer F_p be a tree graph for p iterations. The general Randić index R_α of F_p can be computed by using Table 1. For $\alpha = 1$, the general Randić index takes the following form:

$$R_1(F_p) = \sum_{uv \in E(F_p)} (d_u \times d_v)$$

$$R_1(F_p) = (42pk - 28k + 14p - 8)(1 \times k + 2) + (28p - 20)(4 \times k + 2) + (21p - 14)(k + 2 \times k + 2) \tag{19}$$

$$R_1(F_p) = 63k^2p + 294pk - 42k^2 - 200k + 336p - 232$$

For $\alpha = -1$, the formula of general Randić index takes the following form:

$$R_{-1}(F_p) = \sum_{uv \in E(F_p)} \frac{1}{(d_u \times d_v)}$$

$$R_{-1}(F_p) = (42pk - 28k + 14p - 8) \frac{1}{1 \times k + 2} + (28p - 20) \frac{1}{4 \times k + 2} + (21p - 14) \frac{1}{k + 2 \times k + 2} \tag{20}$$

$$R_{-1}(F_p) = \frac{42k^2p + 105pk - 28k^2 - 69k + 63p - 40}{(k+2)^2}$$

For $\alpha = 1/2$, the formula of general Randić index takes the following form:

$$R_{1/2}(F_p) = \sum_{uv \in E(F_p)} \sqrt{(d_u \times d_v)}$$

$$R_{1/2}(F_p) = (42pk - 28k + 14p - 8) \sqrt{1 \times k + 2} + (28p - 20) \sqrt{4 \times k + 2} + (21p - 14) \sqrt{k + 2 \times k + 2}$$

$$R_{1/2}(F_p) = 21pk - 14k + 42p - 28 + \sqrt{k+2}(|E| + 7p - 6) \tag{21}$$

For $\alpha = -1/2$, the formula of general Randić index takes the following form:

$$R_{-1/2}(F_p) = \sum_{uv \in E(F_p)} \frac{1}{\sqrt{(d_u \times d_v)}}$$

$$R_{-1/2}(F_p) = (42pk - 28k + 14p - 8) \frac{1}{\sqrt{1 \times k + 2}} + (28p - 20) \frac{1}{\sqrt{4 \times k + 2}} + (21p - 14) \frac{1}{\sqrt{k + 2 \times k + 2}} \tag{22}$$

$$R_{-1/2}(F_p) = \frac{42pk - 28k + 28p - 18}{\sqrt{k+2}} + \frac{21p - 14}{k+2}.$$

□

Theorem 5. Consider the fractal tree dendrimer F_p with $p, k \geq 2$. Its augmented Zagreb index is as follows:

$$AZI(F_p) = (21pk^3 - 14k^3 + 126pk^2 - 84k^2 + 588pk - 392k + 280p - 176) \left(\frac{(k+2)}{2(k+1)} \right)^3 + 256(7p-5) \left(\frac{(k+2)}{(k+4)} \right)^3 \tag{23}$$

Proof. Let fractal tree dendrimer F_p be a tree graph for p iterations. The augmented Zagreb index of F_p can be computed by using Table 1 in the following formula.

TABLE 2: Edge partition of F_p based on degree sum of end vertices of each edge.

(S_u, S_v)	frequency
$(k+2, 2k+3)$	$(14p-8)(k+1)$
$(k+2, 2k+6)$	$28pk-20k$
$(2k+3, 2k+6)$	$14p-8$
$(2k+6, 2k+6)$	$7p-6$
$(2k+6, 4k+8)$	$28p-20$

$$AZI(F_p) = \sum_{uv \in E(F_p)} \left(\frac{d_u \times d_v}{d_u + d_v - 2} \right)^3.$$

$$AZI(F_p)$$

$$= (42pk - 28k + 14p - 8) \left(\frac{(1) \times (k+2)}{1 + k + 2 - 2} \right)^3 \quad (24)$$

$$+ (28p - 20) \left(\frac{(4) \times (k+2)}{4 + k + 2 - 2} \right)^3$$

$$+ (21p - 14) \left(\frac{(k+2) \times (k+2)}{k + 2 + k + 2 - 2} \right)^3$$

After simplification of the above form, we got (23). \square

Table 2 shows the edge partition of fractal tree dendrimer F_p based on the sum of degrees of end vertices of each edge. This table is used in computing the fourth atom bond connectivity and fifth geometric arithmetic index.

Theorem 6. Consider the fractal tree dendrimer F_p with $p, k \geq 2$. Its fourth atom bond connectivity index is as follows:

$$ABC_4(F_p)$$

$$= \frac{(7p-6)(\sqrt{4k+10})}{2k+6}$$

$$+ \frac{14p-8}{\sqrt{2k+3}} \left(\frac{\sqrt{3}(k+1)^{3/2}}{\sqrt{k+2}} + \sqrt{\frac{4k+7}{2k+6}} \right) \quad (25)$$

$$+ (1+2^{3/2}k) \frac{\sqrt{3}(14p-10)}{\sqrt{k+3}}$$

Proof. Let fractal tree dendrimer F_p be a tree graph for p iterations. The fourth atom bond connectivity index of F_p can be computed by using Table 2 in the following formula:

$$ABC_4(F_p) = \sum_{uv \in E(F_p)} \sqrt{\frac{S_u + S_v - 2}{S_u \times S_v}}$$

$$ABC_4(F_p)$$

$$= ((14p-8)(k+1)) \sqrt{\frac{k+2+2k+3-2}{(k+2) \times (2k+3)}}$$

$$+ (28pk-20k) \sqrt{\frac{k+2+2k+6-2}{(k+2) \times (2k+6)}}$$

$$+ (14p-8) \sqrt{\frac{2k+3+2k+6-2}{(2k+3) \times (2k+6)}}$$

$$+ (7p-6) \sqrt{\frac{2k+6+2k+6-2}{(2k+6) \times (2k+6)}}$$

$$+ (28p-20) \sqrt{\frac{2k+6+4k+8-2}{(2k+6) \times (4k+8)}}$$

$$(26)$$

After simplification of the above form, we got (25). \square

Theorem 7. Consider the fractal tree dendrimer F_p with $p, k \geq 2$. Its fifth geometric arithmetic index is as follows:

$$GA_5(F_p)$$

$$= (7p-6)$$

$$+ (7p-5) \left(\frac{8(3k+4)\sqrt{(2k+6)}(k+2)^{3/2}}{(3k+7)(3k+8)} \right) \quad (27)$$

$$+ 4(7p-4) \sqrt{(2k+3)} \left(\frac{\sqrt{k+2}}{3k+5} + \frac{\sqrt{2k+6}}{4k+9} \right)$$

Proof. Let fractal tree dendrimer F_p be a tree graph for p iterations. The fifth geometric arithmetic index of F_p can be computed by using Table 2 in the following formula:

$$GA_5(F_p) = \sum_{uv \in E(F_p)} \frac{2\sqrt{S_u \times S_v}}{S_u + S_v}.$$

$$GA_5(F_p)$$

$$= ((14p-8)(k+1)) \frac{2\sqrt{(k+2) \times (2k+3)}}{k+2+2k+3}$$

$$+ (28pk-20k) \frac{2\sqrt{(k+2) \times (2k+6)}}{k+2+2k+6} \quad (28)$$

$$+ (14p-8) \frac{2\sqrt{(2k+3) \times (2k+6)}}{2k+3+2k+6}$$

$$+ (7p-6) \frac{2\sqrt{(2k+6) \times (2k+6)}}{2k+6+2k+6}$$

$$+ (28p-20) \frac{2\sqrt{(2k+6) \times (4k+8)}}{2k+6+4k+8}$$

After simplification of the above form, we got our result of (27). \square

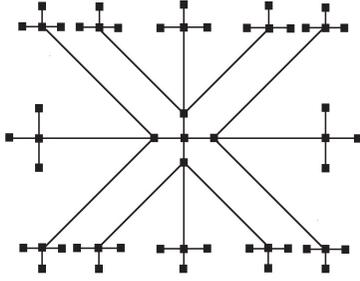


FIGURE 3: The representation of Cayley tree $C_{4,3}$ is illustrated.

Theorem 8. Consider the fractal tree dendrimer F_p with $p, k \geq 2$. Its Sanskruti index is as follows:

$$\begin{aligned}
 S(F_p) &= \frac{1}{(27(5+2k)^3(-7+4k)^3)} (110592(3+k)^3 \\
 &\cdot (-7+4k)^3(27+27k+98k^2+k^3)(-6+7p) \\
 &+ 2(5+2k)^3(24524+k^2(17112-22596p) \\
 &- 33313p+128k^4(-5+7p)+8k^3(-328+497p) \\
 &+ k(-49442+71260p)) \\
 &+ \frac{(14p-8)((k+2)(2k+3))^3}{27(k+1)^2}
 \end{aligned} \tag{29}$$

Proof. Let fractal tree dendrimer F_p be a tree graph for p iterations. The Sanskruti index of F_p can be computed by using Table 2 in the following formula:

$$\begin{aligned}
 S(F_p) &= \sum_{uv \in E(F_p)} \left(\frac{S_u \times S_v}{S_u + S_v - 2} \right)^3 \\
 S(F_p) &= ((14p-8)(k+1)) \left(\frac{(k+2) \times (2k+3)}{k+2+2k+3-2} \right)^3 \\
 &+ (28pk-20k) \left(\frac{(k+2) \times (2k+6)}{k+2+2k+6-2} \right)^3 \\
 &+ (14p-8) \left(\frac{(2k+3) \times (2k+6)}{2k+3+2k+6-2} \right)^3 \\
 &+ (7p-6) \left(\frac{(2k+6) \times (2k+6)}{2k+6+2k+6-2} \right)^3 \\
 &+ (28p-20) \left(\frac{(2k+6) \times (4k+8)}{2k+6+4k+8-2} \right)^3
 \end{aligned} \tag{30}$$

After simplification of the above form, we got (29). □

3. Cayley Tree Dendrimer

The Cayley tree is a kind of dendrimers, also called Bethe lattice. The construction procedure of Cayley tree $C_{s,t}$ ($s \geq$

TABLE 3: Edge partition of $C_{s,t}$ based on degrees of end vertices of each edge.

(d_u, v_v)	Frequency
$(1, s)$	$s(s-1)^{t-1}$
(s, s)	$s \sum_{i=1}^t (s-1)^{i-1} - s(s-1)^{t-1}$

3, $t \geq 0$) consists of t iterations. s is the number of nodes at first iteration. $C_{s,0}$, for $t = 0$, consist of only a central vertex. For $t = 1$, $C_{s,1}$ is obtained by creating s nodes and attaching them to the central vertex by an edge. For $t > 1$, the Cayley tree $C_{s,t}$ is obtained from $C_{s,t-1}$ by creating $s - 1$ nodes and attaching them to each of the pendent vertices of $C_{s,t-1}$. The Cayley tree network $C_{4,3}$ is depicted in Figure 3.

In $C_{s,t}$, the pendent vertices are $s(s-1)^{n-1}$ and the s degree vertices are $2 \sum_{i=1}^t (s-1)^{i-1} - (s-1)^{n-1}$. The edge set of $C_{s,t}$ is divided into two partitions based on the degree of end vertices. The first edge partition consists of $s(s-1)^{n-1}$ edges uv , where $d_u = 1$ and $d_v = s$. The second edge partition consists of $s \sum_{i=1}^t (s-1)^{i-1} - s(s-1)^{t-1}$ edges uv , where $d_u = d_v = s$. The cardinality of vertices and edges in $C_{s,t}$ is $2 \sum_{i=1}^t (s-1)^{i-1} + (s-1)^t$ and $s \sum_{i=1}^t (s-1)^{i-1}$, respectively. The tabular representation of edge partition technique is depicted in Table 3.

Theorem 9. Consider the Cayley tree dendrimer $C_{s,t}$ with $s, t \geq 3$. Its atom bond connectivity index is as follows:

$$\begin{aligned}
 ABC(C_{s,t}) &= \sqrt{s}(s-1)^{t-1/2} \\
 &+ \sqrt{2(s-1)} \left(\sum_{i=1}^t (s-1)^{i-1} - (s-1)^{t-1} \right)
 \end{aligned} \tag{31}$$

Proof. Let Cayley tree dendrimer $C_{s,t}$ be a tree graph for t iterations. The atom bond connectivity index of $C_{s,t}$ can be computed by using Table 3 in the following formula:

$$\begin{aligned}
 ABC(C_{s,t}) &= \sum_{uv \in E(C_{s,t})} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} \\
 ABC(C_{s,t}) &= (s(s-1)^{t-1}) \sqrt{\frac{1+s-2}{(1 \times s)}} \\
 &+ \left(s \sum_{i=1}^t (s-1)^{i-1} - s(s-1)^{t-1} \right) \sqrt{\frac{s+s-2}{(s \times s)}}
 \end{aligned} \tag{32}$$

After simplification of the above form, we got (31). □

Theorem 10. Consider the Cayley tree dendrimer $C_{s,t}$ with $s, t \geq 3$. Its geometric arithmetic index is as follows:

$$GA(C_{s,t}) = \frac{s(s-1)^{t-1}(2\sqrt{s}-s-1) + s(s+1)\sum_{i=1}^t (s-1)^{i-1}}{s+1} \quad (33)$$

Proof. Let Cayley tree dendrimer $C_{s,t}$ be a tree graph for t iterations. The geometric arithmetic index of $C_{s,t}$ can be computed by using Table 3 in the following formula:

$$GA(C_{s,t}) = \sum_{uv \in E(C_{s,t})} \frac{2\sqrt{d_u \times d_v}}{d_u + d_v} \quad (34)$$

$$GA(C_{s,t}) = (s(s-1)^{t-1}) \frac{2\sqrt{(1 \times s)}}{1+s} + \left(s \sum_{i=1}^t (s-1)^{i-1} - s(s-1)^{t-1} \right) \frac{2\sqrt{(s \times s)}}{s+s}$$

After simplification of the above form, we got (33). □

Theorem 11. Consider the Cayley tree dendrimer $C_{s,t}$ with $s, t \geq 3$. Its general Randić index is as follows:

$$R_\alpha C_{s,t} = \begin{cases} s^3 \sum_{i=1}^t (s-1)^{i-1} - s^2 (s-1)^t, & \text{if } \alpha = 1, \\ \frac{1}{s} \left((s-1)^t + \sum_{i=1}^t (s-1)^{i-1} \right), & \text{if } \alpha = -1, \\ s^2 \sum_{i=1}^t (s-1)^{i-1} + s(s-1)^{t-1} (\sqrt{s}-s), & \text{if } \alpha = \frac{1}{2}, \\ \sum_{i=1}^t (s-1)^{i-1} - (s-1)^{t-1} (1-\sqrt{s}), & \text{if } \alpha = -\frac{1}{2}. \end{cases} \quad (35)$$

Proof. Let Cayley tree dendrimer $C_{s,t}$ be a tree graph for t iterations. The general Randić index R_α of $C_{s,t}$ can be computed by using Table 3. For $\alpha = 1$, the general Randić index takes the following form:

$$R_1(C_{s,t}) = \sum_{uv \in E(C_{s,t})} (d_u \times d_v) \quad (36)$$

$$R_1(C_{s,t}) = (s(s-1)^{t-1})(1 \times s) + \left(s \sum_{i=1}^t (s-1)^{i-1} - s(s-1)^{t-1} \right) (s \times s) + s^3 \sum_{i=1}^t (s-1)^{i-1} - s^2 (s-1)^t$$

For $\alpha = -1$, the formula of general Randić index takes the following form:

$$R_{-1}(C_{s,t}) = \sum_{uv \in E(C_{s,t})} \frac{1}{(d_u \times d_v)} \quad (37)$$

$$R_{-1}(C_{s,t}) = (s(s-1)^{t-1}) \frac{1}{(1 \times s)} + \left(s \sum_{i=1}^t (s-1)^{i-1} - s(s-1)^{t-1} \right) \frac{1}{(s \times s)}$$

$$R_{-1}(C_{s,t}) = \frac{1}{s} \left((s-1)^t + \sum_{i=1}^t (s-1)^{i-1} \right)$$

For $\alpha = 1/2$, the formula of general Randić index takes the following form:

$$R_{1/2}(C_{s,t}) = \sum_{uv \in E(C_{s,t})} \sqrt{(d_u \times d_v)} \quad (38)$$

$$R_{1/2}(C_{s,t}) = (s(s-1)^{t-1}) \sqrt{(1 \times s)} + \left(s \sum_{i=1}^t (s-1)^{i-1} - s(s-1)^{t-1} \right) \sqrt{(s \times s)}$$

$$R_{1/2}(C_{s,t}) = s^2 \sum_{i=1}^t (s-1)^{i-1} + s(s-1)^{t-1} (\sqrt{s}-s)$$

For $\alpha = -1/2$, the formula of general Randić index takes the following form:

$$R_{-1/2}(C_{s,t}) = \sum_{uv \in E(C_{s,t})} \frac{1}{\sqrt{(d_u \times d_v)}} \quad (39)$$

$$R_{-1/2}(C_{s,t}) = (s(s-1)^{t-1}) \frac{1}{\sqrt{(1 \times s)}} + \left(s \sum_{i=1}^t (s-1)^{i-1} - s(s-1)^{t-1} \right) \frac{1}{\sqrt{(s \times s)}}$$

$$R_{-1/2}(C_{s,t}) = \sum_{i=1}^t (s-1)^{i-1} - (s-1)^{t-1} (1-\sqrt{s}).$$

□

Theorem 12. Consider the Cayley tree dendrimer $C_{s,t}$ with $s, t \geq 3$. Its augmented Zagreb index is as follows:

$$AZI(C_{s,t}) = \frac{s^4}{8} \left((8-s^3)(s-1)^{t-4} + \frac{s^3}{(s-1)^3} \sum_{i=1}^t (s-1)^{i-1} \right) \quad (40)$$

TABLE 4: Edge partition of $C_{s,t}$ based on degree sum of end vertices of each edge.

(S_u, S_v)	frequency
$(s, 2s - 1)$	$s(s - 1)^{t-1}$
$(2s - 1, s^2)$	$s(s - 1)^{t-2}$
(s^2, s^2)	$s \sum_{i=1}^t (s - 1)^{i-1} - s^2 (s - 1)^{t-2}$

Proof. Let Cayley tree dendrimer $C_{s,t}$ be a tree graph for t iterations. The augmented Zagreb index of $C_{s,t}$ can be computed by using Table 3 in the following formula:

$$\begin{aligned}
 AZI(C_{s,t}) &= \sum_{uv \in E(C_{s,t})} \left(\frac{d_u \times d_v}{d_u + d_v - 2} \right)^3 \\
 AZI(C_{s,t}) &= (s(s - 1)^{t-1}) \left(\frac{(1) \times (s)}{1 + s - 2} \right)^3 \\
 &\quad + \left(s \sum_{i=1}^t (s - 1)^{i-1} - s^2 (s - 1)^{t-1} \right) \left(\frac{(s) \times (s)}{s + s - 2} \right)^3
 \end{aligned} \tag{41}$$

After simplification of the above form, we got (40). \square

Table 4 shows the edge partition of Cayley tree dendrimer $C_{s,t}$ based on the sum of degrees of end vertices of each edge. This table is used in computing the fourth atom bond connectivity and fifth geometric arithmetic index.

Theorem 13. Consider the Cayley tree dendrimer $C_{s,t}$ with $s, t \geq 3$. Its fourth atom bond connectivity index is as follows:

$$\begin{aligned}
 ABC_4(C_{s,t}) &= (s - 1)^{t-3/2} \left(\sqrt{\frac{(s + 3)}{(2s - 1)}} - \sqrt{2(s + 1)} \right) \\
 &\quad + s(s - 1)^{t-1/2} \sqrt{\frac{3}{s(2s - 1)}} \\
 &\quad + \frac{\sqrt{2(s^2 - 1)}}{s} \sum_{i=1}^t (s - 1)^{i-1}
 \end{aligned} \tag{42}$$

Proof. Let Cayley tree dendrimer $C_{s,t}$ be a tree graph for t iterations. The fourth atom bond connectivity index of $C_{s,t}$ can be computed by using Table 4 in the following formula:

$$\begin{aligned}
 ABC_4(C_{s,t}) &= \sum_{uv \in E(C_{s,t})} \sqrt{\frac{S_u + S_v - 2}{S_u \times S_v}} \\
 ABC_4(C_{s,t}) &= (s(s - 1)^{t-1}) \sqrt{\frac{s + 2s - 1 - 2}{(s) \times (2s - 1)}}
 \end{aligned}$$

$$\begin{aligned}
 &+ (s(s - 1)^{t-2}) \sqrt{\frac{2s - 1 + s^2 - 2}{(2s - 1) \times (s^2)}} \\
 &+ \left(s \sum_{i=1}^t (s - 1)^{i-1} - s^2 (s - 1)^{t-2} \right) \sqrt{\frac{s^2 + s^2 - 2}{(s^2) \times (s^2)}}
 \end{aligned} \tag{43}$$

After simplification of the above form, we got (42). \square

Theorem 14. Consider the Cayley tree dendrimer $C_{s,t}$ with $s, t \geq 3$. Its fifth geometric arithmetic index is as follows:

$$\begin{aligned}
 GA_5(C_{s,t}) &= s(s - 1)^{t-1} \\
 &\cdot \left(\frac{2\sqrt{s(2s - 1)}}{3s - 1} - \frac{s}{s - 1} + \frac{2s\sqrt{2s - 1}}{(s - 1)(s^2 + 2s - 1)} \right) \\
 &+ s \sum_{i=1}^t (s - 1)^{i-1}
 \end{aligned} \tag{44}$$

Proof. Let Cayley tree dendrimer $C_{s,t}$ be a tree graph for t iterations. The fifth geometric arithmetic index of $C_{s,t}$ can be computed by using Table 4 in the following formula:

$$\begin{aligned}
 GA_5(C_{s,t}) &= \sum_{uv \in E(C_{s,t})} \frac{2\sqrt{S_u \times S_v}}{S_u + S_v} \\
 GA_5(C_{s,t}) &= (s(s - 1)^{t-1}) \frac{2\sqrt{(s) \times (2s - 1)}}{(s + 2s - 1)} \\
 &\quad + (s(s - 1)^{t-2}) \frac{2\sqrt{(2s - 1) \times (s^2)}}{(2s - 1 + s^2)} \\
 &\quad + \left(s \sum_{i=1}^t (s - 1)^{i-1} - s^2 (s - 1)^{t-2} \right) \frac{2\sqrt{(s^2) \times (s^2)}}{(s^2 + s^2)}
 \end{aligned} \tag{45}$$

After simplification of the above form, we got (44). \square

Theorem 15. Consider the Cayley tree dendrimer $C_{s,t}$ with $s, t \geq 3$. Its Sanskruti index is as follows:

$$\begin{aligned}
 S(C_{s,t}) &= s^4 (s - 1)^{t-4} \left(\frac{(2s - 1)^3}{27} + \frac{(s(2s - 1))^3}{(s - 1)(s + 3)^3} \right. \\
 &\quad \left. - \frac{s^{10}}{(2(s + 1))^3 (s - 1)} \right) + \frac{s^{13}}{(2(s^2 - 1))^3} \sum_{i=1}^t (s - 1)^{i-1}
 \end{aligned} \tag{46}$$

Proof. Let Cayley tree dendrimer $C_{s,t}$ be a tree graph for t iterations. The Sanskruti index of $C_{s,t}$ can be computed by using Table 4 in the following formula:

$$\begin{aligned}
 S(C_{s,t}) &= \sum_{uv \in E(C_{s,t})} \left(\frac{S_u \times S_v}{S_u + S_v - 2} \right)^3 \\
 S(C_{s,t}) &= (s(s-1)^{t-1}) \left(\frac{(s) \times (2s-1)}{s+2s-1-2} \right)^3 \\
 &+ (s(s-1)^{t-2}) \left(\frac{(2s-1) \times (s^2)}{2s-1+s^2-2} \right)^3 \\
 &+ \left(s \sum_{i=1}^t (s-1)^{i-1} - s^2 (s-1)^{t-2} \right) \left(\frac{(s^2) \times (s^2)}{s^2 + s^2 - 2} \right)^3
 \end{aligned} \tag{47}$$

After simplification of the above form, we got (46). \square

4. Conclusion

In this paper, we have computed some degree based topological indices for fractal tree and Cayley tree dendrimers. We have computed the atom bond connectivity ABC , geometric arithmetic GA , general Randić, first and second Zagreb, augmented Zagreb, GA_5 , ABC_4 , and Sanskruti indices for fractal tree. Also, we have computed the atom bond connectivity ABC , geometric arithmetic GA , general Randić, augmented Zagreb, GA_5 , ABC_4 , and Sanskruti index. Furthermore, we have computed closed results of above-mentioned indices for both fractal and Cayley tree dendrimers.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

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