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Research Article

Investigation of Dendrimer Structures by Means of K-Banhatti Invariants

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Dendrimers are highly branched macromolecules. The structural chemistry of dendrimers could be shaped by their topological invariants to target the particular design with appropriate properties to bring the drugs to mark a carrier vehicle. This study is about some new topological indices of dendrimer generations. Here, we calculate K Banhatti indices for five generations of dendrimers. Precisely speaking, we computed the 1st K Banhatti redefined Zagreb index, 2nd K Banhatti redefined Zagreb indices, and 3rd K Banhatti redefined Zagreb index for the dendrimers $D_i(p)$ for $i = 1, 2, 3, 4, 5$.

1. Introduction

Dendrimers are highly structured, polymeric branching molecules. Similar dendrimer names include arborol and cascade molecules. In general, dendrimers are about the same in context and generally take on a three-dimensional circular morphology. The word dendron is also used interchangeably.

The term dendrimers mean an artificially generated nanomolecular structure which is highly useful in drug delivery [1, 2]. Commonly, there are three types of dendrimers: (a) central core dendrimer, (b) interior surface dendrimer, and (c) outer surface dendrimers [3]. Due to their different molecular nanoshapes, organic science and dendrimes act as a solubilizing agent in different reactions [4]. For detailed applications of dendrimers, we recommend the readers [5, 6]. The structure of the dendrimer is well known and there are three main components of the dendrimer architecture;

(i) Initiator core
(ii) Interior layer
(iii) Terminal functionalities

Due to their molecular architecture, dendrimers display some undoubtedly enhanced physical and chemical properties when correlated with a conventional liner polymer [2, 7]. The rare architectural layout of dendrimer, branching intensity, multivalency, globular, and well-defined molecular weight implies that dendrimers are rare and excellent nanocarriers in medical utilization such as drug delivery, gene transfection, tumor therapy, etc. The dendrimer architecture is shown in Figure 1.

Consider a graph G with vertex set V and the edge set E. For a vertex v, the degree is denoted by d_v which is the number of vertices at distance one from v. The distance between two vertices is the length of the shortest path between them.

By a topological index, we mean a number associated with the graph that is unique up to graph isomorphism and that helps us to determine the hidden properties based on the symmetric structure of the graph [8–10]. Numerous methods are present in history to check the quality of a *topological index*. There are two main clashes of topological

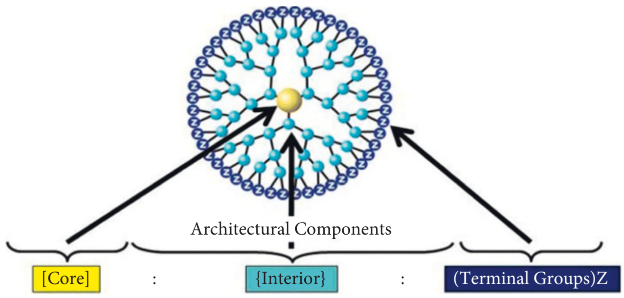

Figure 1: Dendrimer architecture.

indices; first one is the degree-based topological indices and the second class is known as distance-based topological indices [11–13]. The study of topological index begun with the work of Wiener [14] in the year 1947 when he introduced the very first topological index while computing the boiling points of alkane which is today known as the Wiener index. The Wiener index is a distance-based topological index. In 1975, the very first degree-based topological index was introduced by Randić in [15] which is today known as the Randić index. After Randić index, many degree-based indices are introduced and studied by the researchers [16, 17]. All the introduced topological indices give some information about the concerned chemical structure [13]. For example, the redefined Zagreb indices are helpful to compute π-electronic energy of chemical structures [18].

Continuing the work on topological indices, two variants of K Banhatti indices were put forward by Kulli in [19].

$$B_1(G) = \sum_{ue}\left[d_G(u) + d_G(e)\right],$$
$$B_2(G) = \sum_{ue}\left[d_G(u) \times d_G(e)\right]. \tag{1}$$

For other variants of K Banhatti indices, we recommend [20].

Motivated by the work of Kulli [19], in this paper, we introduced the K Banhatti redefined Zagreb indices as follows:

$$KBR_1(G) = \sum_{ue}\frac{d_u + d_e}{d_u \times d_e},$$
$$KBR_2(G) = \sum_{ue}\frac{d_u \times d_e}{d_u + d_e}, \tag{2}$$
$$KBR_3(G) = \sum_{ue}\left(d_u + d_e\right)\left(d_u \times d_e\right).$$

In this report, we introduced a new class of topological indices for dendrimer generations. We calculated K Banhatti indices for five generations of dendrimers. Precisely speaking,

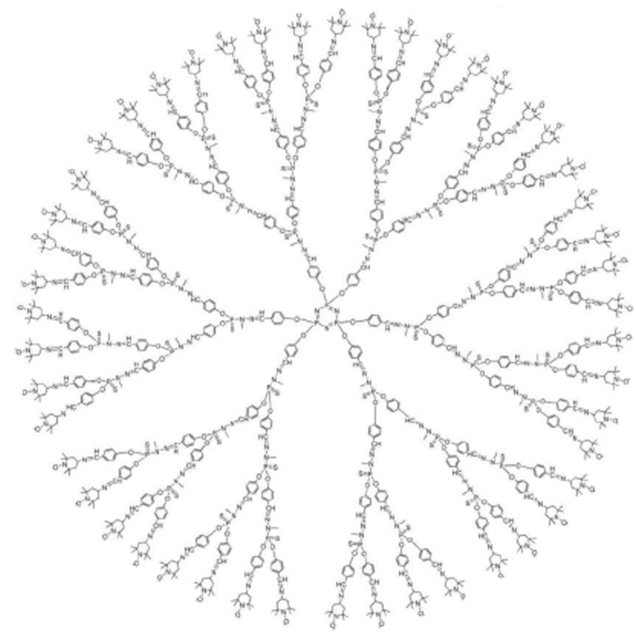

Figure 2: $D_1(p)$ for $m = p$.

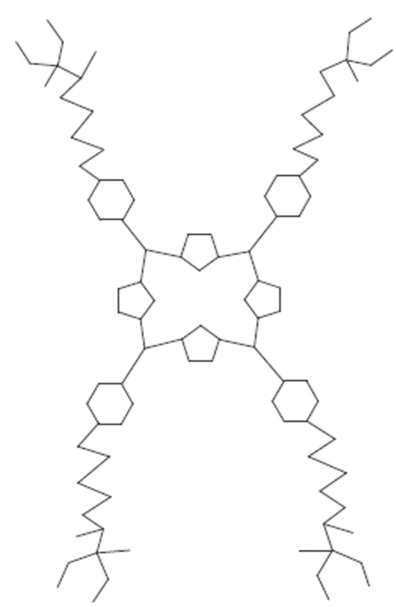

Figure 3: $D_2(p)$ for $p = 1$.

we computed 1st K Banhatti redefined Zagreb index, 2nd K Banhatti redefined Zagreb indices, and 3rd K Banhatti redefined Zagreb index for $D_{1i}(p)$, where $i = 1, 2, 3, 4, 5$.

2. Main Results

In this section, we will discuss molecular graphs of five generations of dendrimers and calculate K Banhatti indices for abovementioned dendrimers; molecular graphs of these five generations can be found in Figures 2–6.

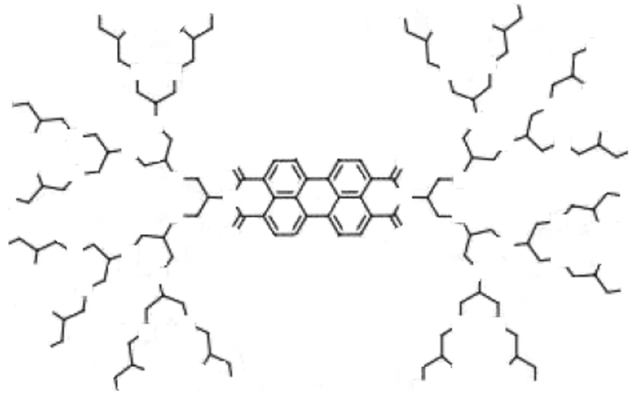

Figure 4: $D_2(p)$ for $p = 1$.

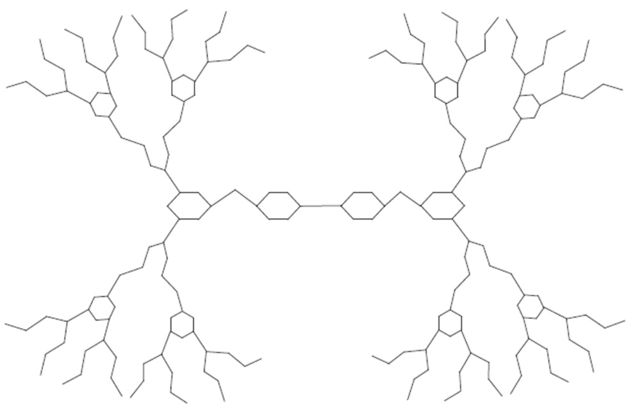

Figure 5: $D_4(p)$ for $p = 2$.

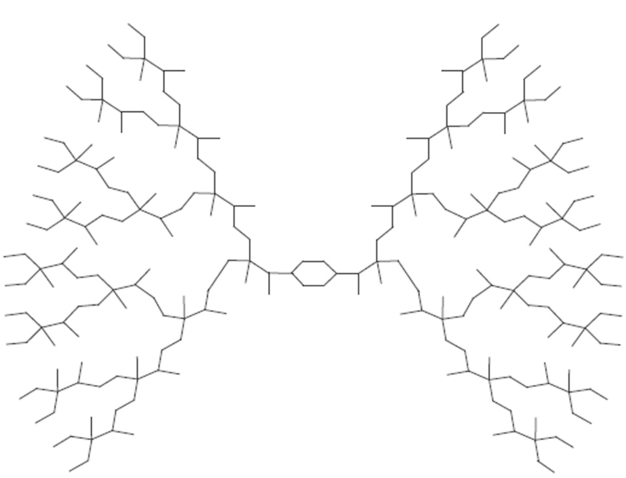

Figure 6: $D_5(p)$ for $m = p$.

2.1. Phosphorus-Containing Dendrimers. The first generation of dendrimers we studied in this paper is phosphorus-containing dendrimers [2]. The graph of this generation is denoted by $D_1(p)$ where the number of stages is represented by p, see Figure 2.

Table 1: Partition of the edges of $D_1(p)$.

(d_u, d_v)	d_e	Frequency
(1, 3)	2	$6(2^p - 1)$
(1, 4)	3	$6(5 \times 2^p - 1)$
(2, 2)	2	$18(2^{p+1} - 1)$
(2, 3)	3	$6(2^{p+4} - 7)$
(2, 4)	4	$(3 \times 2^{p+3})$
(3, 4)	5	$6(3 \times 2^p - 1)$

By observing Figure 2, we can give the following remarks.

Remark 1. The graph $D_1(p)$ of phosphorus-containing dendrimers has $9(11 \times 2^{p+1} - 8)$ vertices and $6(9 \times 2^{p+2} - 13)$ edges.

Remark 2. The set of vertex of the graph $D_1(p)$ can be divided in to four different classes with respect to the degrees. The number of vertices of degree one are $42 \times 2^p - 12$, the number of vertices of degree two are $96 \times 2^p - 39$, the number of vertices of degree three $42 \times 2^p - 18$, and the number of vertices of degree four are $18 \times 2^p - 3$.

Remark 3. The edge set of the graph $D_1(p)$ can also be divided into different classes with respect to the degrees of the end vertices of edges and this division is given in Table 1.

Now, we are ready to present the first main result of this paper.

Theorem 1. *The KBR_1, KBR_2, and KBR_3 indices for $D_1(p)$ are as follows:*

(i) $KBR_1(D_1(p)) = (293/5).2^p - (366/5) + 18.2^{p+1} + 5.2^{p+4} + (9/4).2^{p+3}$,

(ii) $KBR_2(D_1(p)) = (241/4).2^p - (1763/20) + 18.2^{p+1} + (36/5).2^{p+4} + 4.2^{p+3}$,

(iii) $KBR_3(D_1(p)) = 2556.2^p - 2376 + 288.2^{p+1} + 180.2^{p+4} + 144.2^{p+3}$.

Proof

$$KBR_1(D_1) = \sum_{ue} \frac{d_u + d_e}{d_u \times d_e}$$

$$= \left(\frac{1+2}{1\times 2}\right)(6\times 2^p - 6) + \left(\frac{1+3}{1\times 3}\right)(30\times 2^p - 6)$$

$$+ \left(\frac{2+2}{2\times 2}\right)\left(18\times 2^{p+1} - 18\right)$$

$$+ \left(\frac{2+3}{2\times 3}\right)\left(6\times 2^{p+4} - 42\right)$$

$$+ \left(\frac{2+4}{2\times 4}\right)\left(3\times 2^{p+3}\right) + \left(\frac{3+4}{3\times 4}\right)(18\times 2^p - 6)$$

$$= \frac{293}{5}.2^p - \frac{366}{5} + 18.2^{p+1} + 5.2^{p+4} + \frac{9}{4}.2^{p+3},$$

$$KBR_2(D_1) = \sum_{ue} \frac{d_u \times d_e}{d_u + d_e}$$

$$= \left(\frac{1\times 2}{1+2}\right)(6\times 2^p - 6) + \left(\frac{1\times 3}{1+3}\right)(30\times 2^p - 6)$$

$$+ \left(\frac{2\times 2}{2+2}\right)\left(18\times 2^{p+1} - 18\right)$$

$$+ \left(\frac{2\times 3}{2+3}\right)\left(6\times 2^{p+4} - 42\right)$$

$$+ \left(\frac{2\times 4}{2+4}\right)\left(3\times 2^{p+3}\right) + \left(\frac{3\times 4}{3+4}\right)(18\times 2^p - 6)$$

$$= \frac{241}{4}.2^p - \frac{1763}{20} + 18.2^{p+1} + \frac{36}{5}.2^{p+4} + 4.2^{p+3},$$

$$KBR_3(D_1) = \sum_{ue} (d_u \times d_e)(d_u + d_e)$$

$$= (1\times 2)(1+2)(6\times 2^p - 6)$$

$$+ (1\times 3)(1+3)(30\times 2^p - 6)$$

$$+ (2\times 2)(2+2)\left(18\times 2^{p+1} - 18\right)$$

$$+ (2\times 3)(2+3)\left(6\times 2^{p+4} - 42\right)$$

$$+ (2\times 4)(2+4)\left(3\times 2^{p+3}\right)$$

$$+ (3\times 4)(3+4)(18\times 2^p - 6)$$

$$= 2556.2^p - 2376 + 288.2^{p+1}$$

$$+ 180.2^{p+4} + 144.2^{p+3}. \quad (3)$$

□

Table 2: Partition of the edges of $D_2(p)$.

(d_u, d_v)	d_e	Frequency
$(1,2)$	1	4×2^p
$(1,3)$	2	$4\times 2^p - 4$
$(1,4)$	3	$4\times 2^p - 4$
$(2,2)$	2	$4\times 2^p + 20$
$(2,3)$	3	$4\times 2^p + 32$
$(2,4)$	4	$8\times 2^p - 8$
$(3,3)$	4	12
$(3,4)$	5	$4\times 2^p - 4$

Table 3: Partition of the edges of $D_3(p)$.

(d_u, d_v)	d_e	Frequency
$(1,2)$	1	2^{p+1}
$(1,3)$	2	$4(2^{p-1} + 1)$
$(2,2)$	2	$3\times 2^{p+1} + 1$
$(2,3)$	3	$20\times 2^{p-1}$
$(3,3)$	4	22

2.2. Porphyrin-Cored Dendrimer. Now, we study the porphyrin-cored dendrimer. The graph of porphyrin-cored dendrimer is denoted by $D_2(p)$ [2], see Figure 3.

By observing Figure 3, we can give the following remarks:

Remark 4. The graph of porphyrin-cored dendrimer $D_2(p)$ has $4(2^{p+3} + 9)$ vertices and $4(2^{p+3} + 11)$ edges.

Remark 5. The vertex set of porphyrin-cored dendrimer $D_2(p)$ can be divided into the four classes with respect to the degrees. The number of vertices of degree one is $12\times 2^p - 8$, the number of vertices of degree two is $12\times 2^p + 32$, the number of vertices of degree three are $4\times 2^p + 16$, and the number of vertices of degree is $4\times 2^p - 4$.

Remark 6. The edge set of porphyrin-cored dendrimer $D_2(p)$ can also be divided into different classes based on the degree of end vertices and this division is presented in Table 2.

Theorem 2. *For the porphyrin-cored dendrimer $D_2(p)$, we have the following:*

(i) $KBR_1(D_2(p)) = (487/15).2^p + (548/15)$
(ii) $KBR_2(D_2(p)) = (1109/30).2^p + (11089/210)$
(iii) $KBR_3(D_2(p)) = 1128.2^p + 1352$

Proof

$$\begin{aligned}
KBR_1(D_2) &= \sum_{ue} \frac{d_u + d_e}{d_u \times d_e} \\
&= \left(\frac{1+1}{1\times 1}\right)(4\times 2^p) + \left(\frac{1+2}{1\times 2}\right)(4\times 2^p - 4) \\
&\quad + \left(\frac{1+3}{1\times 3}\right)(4\times 2^p - 4) + \left(\frac{2+2}{2\times 2}\right)(4\times 2^p + 20) \\
&\quad + \left(\frac{2+3}{2\times 3}\right)(4\times 2^p + 32) + \left(\frac{2+4}{2\times 4}\right)(8\times 2^p - 8) \\
&\quad + \left(\frac{3+4}{3\times 4}\right)(12) + \left(\frac{3+5}{3\times 5}\right)(4\times 2^p - 4) \\
&= \frac{487}{15}.2^p + \frac{548}{15}, \\
KBR_2(D_2) &= \sum_{ue} \frac{d_u \times d_e}{d_u + d_e} \\
&= \left(\frac{1\times 1}{1+1}\right)(4\times 2^p) + \left(\frac{1\times 2}{1+2}\right)(4\times 2^p - 4) \\
&\quad + \left(\frac{1\times 3}{1+3}\right)(4\times 2^p - 4) + \left(\frac{2\times 2}{2+2}\right)(4\times 2^p + 20) \\
&\quad + \left(\frac{2\times 3}{2+3}\right)(4\times 2^p + 32) + \left(\frac{2\times 4}{2+4}\right)(8\times 2^p - 8) \\
&\quad + \left(\frac{3\times 4}{3+4}\right)(12) + \left(\frac{3\times 5}{3+5}\right)(4\times 2^p - 4) \\
&= \frac{1109}{30}.2^p + \frac{11089}{210}, \\
KBR_3(D_2) &= \sum_{ue} (d_u \times d_e)(d_u + d_e) \\
&= (1\times 1)(1+1)(4\times 2^p) + (1\times 2)(1+2)(4\times 2^p - 4) \\
&\quad + (1\times 3)(1+3)(4\times 2^p - 4) \\
&\quad + (2\times 2)(2+2)(4\times 2^p + 20) \\
&\quad + (2\times 3)(2+3)(4\times 2^p + 32) \\
&\quad + (2\times 4)(2+4)(8\times 2^p - 8) \\
&\quad + (3\times 4)(3+4)(12) + (3\times 5)(3+5)(4\times 2^p - 4) \\
&= 1128.2^p + 1352.
\end{aligned} \tag{4}$$

□

2.3. PDI-Cored Dendrimers. The graph of PDI-cored dendrimers is denoted by $D_3(p)$ [2], see Figure 4.

By observing Figure 4, we can give the following remarks:

Remark 7. The graph of PDI-cored dendrimers $D_3(p)$ has $20 \times 2^p + 20$ vertices and $20 \times 2^{2p} + 20$ edges.

Remark 8. The vertex set of the graph of PDI-cored dendrimers $D_3(p)$ can be divided into different classes with respect to the degree of vertices. The number of vertices of degree one is $2 \times 2^{p+1} + 4$, the number of vertices of degree two is $6 \times 2^{p+1}$, and the number of vertices of degree three is $2 \times 2^{p+1} + 16$.

Remark 9. The edge set of the graph of PDI-cored dendrimers $D_3(p)$ can also be divided into different classes with respect to the degree of the end vertices and this division is presented in Table 3.

Theorem 3. *The KBR_1, KBR_2, and KBR_3 indices for $D_3(p)$ are as follows:*

(i) $KBR_1(D_3(p)) = 5.2^{p+1} + (68/3).2^{p-1} + (119/6)$

(ii) $KBR_2(D_3(p)) = 5.2^{p+1} + (80/3).2^{p-1} + (869/21)$

(iii) $KBR_3(D_3(p)) = 50.2^{p+1} + 624.2^{p-1} + 1888$

Proof

$$\begin{aligned}
KBR_1(D_3) &= \sum_{ue} \frac{d_u + d_e}{d_u \times d_e} \\
&= \left(\frac{1+1}{1\times 1}\right)(2^{p+1}) + \left(\frac{1+2}{1\times 2}\right)(4\times 2^{p-1} + 4) + \left(\frac{3+3}{3\times 3}\right)(22) \\
&\quad + \left(\frac{2+2}{2\times 2}\right)(3\times 2^{p+1} + 1) + \left(\frac{2+3}{2\times 3}\right)(20\times 2^{p-1}) \\
&= 5.2^{p+1} + \frac{68}{3}.2^{p-1} + \frac{119}{6}, \\
KBR_2(D_3) &= \sum_{ue} \frac{d_u \times d_e}{d_u + d_e} \\
&= \left(\frac{1\times 1}{1+1}\right)(2^{p+1}) + \left(\frac{1\times 2}{1+2}\right)(4\times 2^{p-1} + 4) + \left(\frac{3\times 3}{3+3}\right)(22) \\
&\quad + \left(\frac{2\times 2}{2+2}\right)(3\times 2^{p+1} + 1) + \left(\frac{2\times 3}{2+3}\right)(20\times 2^{p-1}) \\
&= 5.2^{p+1} + \frac{80}{3}.2^{p-1} + \frac{869}{21}, \\
KBR_3(D_3) &= \sum_{ue} (d_u \times d_e)(d_u + d_e) \\
&= (1\times 1)(1+1)(2^{p+1}) \\
&\quad + (1\times 2)(1+2)(4\times 2^{p-1} + 4) \\
&\quad + (3\times 3)(3+3)(22) \\
&\quad + (2\times 2)(2+2)(3\times 2^{p+1} + 1) \\
&\quad + (2\times 3)(2+3)(20\times 2^{p-1}) \\
&= 50.2^{p+1} + 624.2^{p-1} + 1888.
\end{aligned} \tag{5}$$

□

2.4. Triazine-Based Dendrimer. The graph of triazine-based dendrimers is denoted by $D_4(p)$ [2], see Figure 5.

By observing Figure 5, we can give the following remarks:

Remark 10. The graph of the triazine-based dendrimer $D_4(p)$ has $(2(5 \times 2^{2p+2} + 1)/3)$ vertices and $7 \times 2^{2p+1} + 1$ edges.

Remark 11. The vertices of the graph of triazine-based dendrimer $D_4(p)$ is divided into three classes. The number of vertices of degree one is 2^{2p+1}, the number of vertices of degree two is $2^{2p+1} + (7 \times 4^{p+1}/6) + (4^{p+1}/3)$, and the number of vertices of degree three is $4 + (5 \times 4^{p+1}/6) - (10/3)$.

Remark 12. The edges of the graph of triazine-based dendrimer $D_4(p)$ can also be divided into different classes and this division is presented in Table 4.

Theorem 4. *The KBR_1, KBR_2, and KBR_3 indices for $D_4(p)$ are as follows:*

(i) $KBR_1(D_4(p)) = 2.2^{p+1} + (85/9).2^{2p} + (25/36) + (7/18).2^{2p+1}$

(ii) $KBR_2(D_4(p)) = 2.2^{p+1} + (182/15).2^{2p} + (136/105) + (8/7).2^{2p+1}$

(iii) $KBR_3(D_4(p)) = 2.2^{p+1} + (820/3).2^{2p} + (92/3) + 56.2^{2p+1}$

Proof

$$KBR_1(D_4) = \sum_{ue} \frac{d_u + d_e}{d_u \times d_e}$$
$$= \left(\frac{1+2}{1\times 2}\right)\left(2^{p+1}\right) + \left(\frac{2+2}{2\times 2}\right)\left(\frac{2\left(5\times 2^{2p}-2\right)}{3}\right)$$
$$= +\left(\frac{2+3}{2\times 3}\right)\left(\frac{2\left(11\times 2^{2p}+4\right)}{3}\right) + \left(\frac{3+4}{3\times 4}\right)\left(\frac{2\times 2^{2p+1}-1}{3}\right)$$
$$= 2.2^{p+1} + \frac{85}{9}.2^{2p} + \frac{25}{36} + \frac{7}{18}.2^{2p+1},$$
$$KBR_2(D_4) = \sum_{ue} \frac{d_u \times d_e}{d_u + d_e}$$
$$= \left(\frac{1\times 2}{1+2}\right)\left(2^{p+1}\right) + \left(\frac{2\times 2}{2+2}\right)\left(\frac{2\left(5\times 2^{2p}-2\right)}{3}\right)$$
$$+\left(\frac{2\times 3}{2+3}\right)\left(\frac{2\left(11\times 2^{2p}+4\right)}{3}\right) + \left(\frac{3\times 4}{3+4}\right)\left(\frac{2\times 2^{2p+1}-1}{3}\right)$$
$$= 2.2^{p+1} + \frac{182}{15}.2^{2p} + \frac{136}{105} + \frac{8}{7}.2^{2p+1},$$
$$KBR_3(D_4) = \sum_{ue} (d_u \times d_e)(d_u + d_e)$$
$$= (1\times 2)(1+2)\left(2^{p+1}\right) + (2\times 2)(2+2)\left(\frac{2\left(5\times 2^{2p}-2\right)}{3}\right)$$
$$+ (2\times 3)(2+3)\left(\frac{2\left(11\times 2^{2p}+4\right)}{3}\right)$$
$$+ (3\times 4)(3+4)\left(\frac{2\times 2^{2p+1}-1}{3}\right)$$
$$= 2.2^{p+1} + \frac{820}{3}.2^{2p} + \frac{92}{3} + 56.2^{2p+1}. \quad (6)$$

□

Table 4: Partition of the edges of $D_4(p)$.

(d_u, d_v)	d_e	Frequency
$(1, 2)$	1	2^{p+1}
$(2, 2)$	2	$(2(5 \times 2^{2p} - 2)/3)$
$(2, 3)$	3	$(2(11 \times 2^{2p} + 4)/3)$
$(3, 3)$	4	$(2 \times 2^{2p+1} - 1/3)$

Table 5: Partition of the edges of $D_5(p)$.

(d_u, d_v)	d_e	Frequency
$(1, 2)$	1	2^{p+1}
$(2, 3)$	3	2^{p+1}
$(1, 3)$	2	$2(2^p - 1)$
$(1, 4)$	3	$2(2^p - 1)$
$(2, 2)$	2	$2(2^p - 1)$
$(3, 4)$	5	$2(2^p - 1)$
$(3, 3)$	4	2
$(2, 4)$	4	$2^{p+2} - 4$

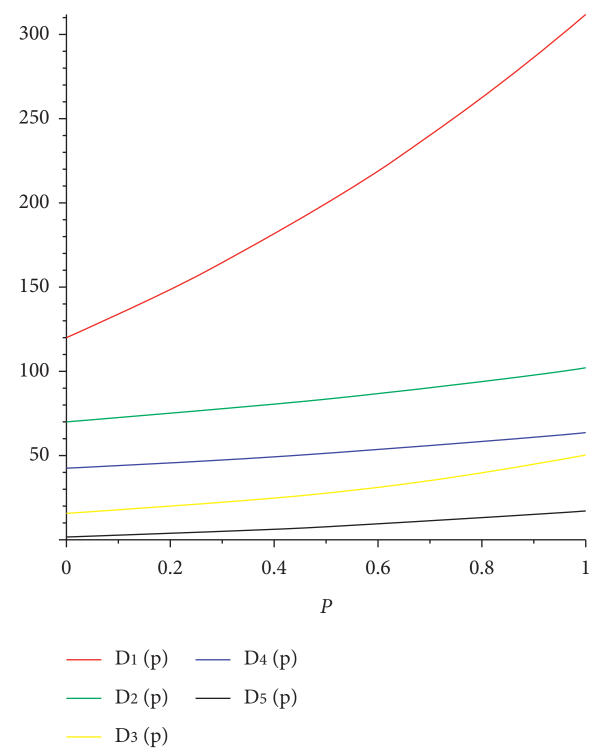

Figure 7: Comparison of KBR_1 for $D_i(p)$, where $i = 1, 2, 3, 4, 5$.

2.5. Aliphatic Polyamide Dendrimers. The graph of aliphatic polyamide dendrimers is denoted by $D_5(p)$ [2], see Figure 6.

By observing Figure 6, we can give the following remarks:

Remark 13. The vertices of the graph of aliphatic polyamide dendrimers $D_5(p)$ can be divided into classes. The number of vertices of degree one is $4(3 \times 2^{p-1} - 1)$, the number of vertices of degree two is $4(3 \times 2^{p-1} - 1)$, and the number of vertices of degree three is $2^{p+1}2(2^p - 1)$.

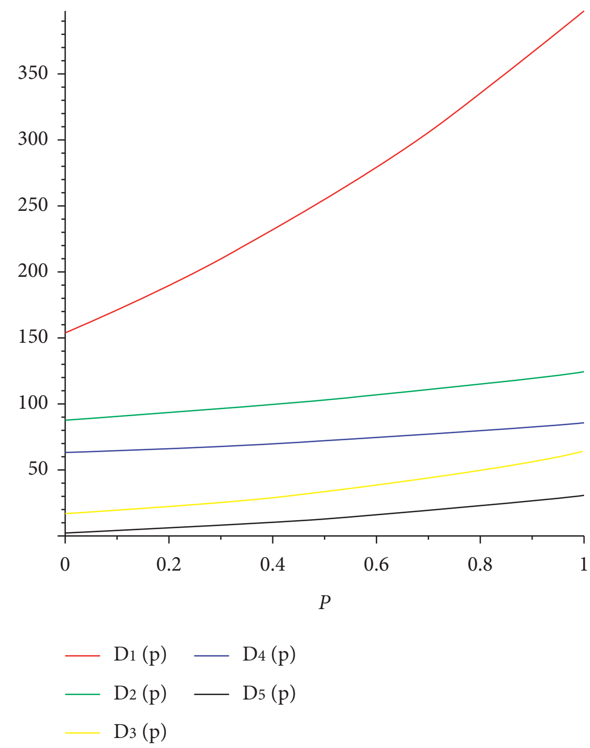

FIGURE 8: Comparison of KBR_1 for $D_i(p)$, where $i = 1, 2, 3, 4, 5$.

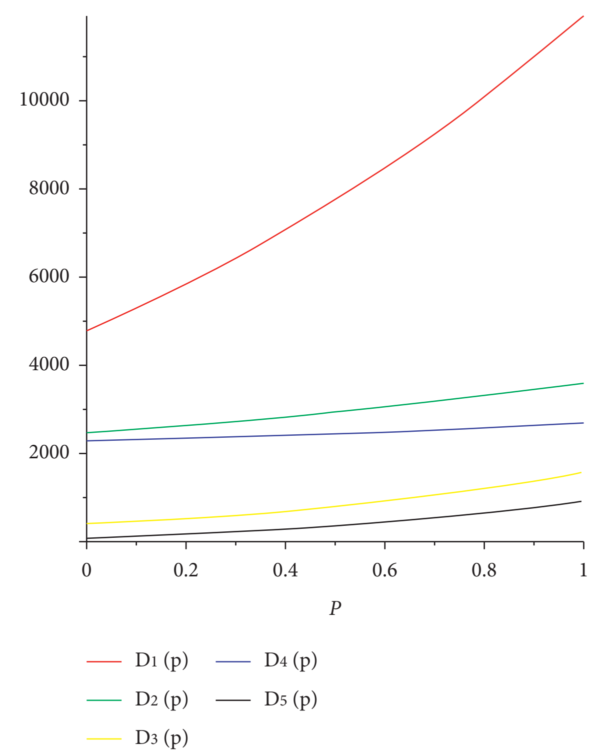

FIGURE 9: Comparison of KBR_1 for $D_i(p)$, where $i = 1, 2, 3, 4, 5$.

Remark 14. The edges of the graph of aliphatic polyamide dendrimers $D_5(p)$ can also be divided into classes and this division is given in Table 5.

Theorem 5. *The KBR_1, KBR_2, and KBR_3 indices for $D_5(p)$ are as follows:*

(i) $KBR_1(D_5(p)) = (4/3).2^{p+1} + (106/15).2^p - (89/10) + (3/4).2^{2p+2}$

(ii) $KBR_2(D_5(p)) = (16/5).2^{p+1} + (82/8).2^p - (1021/84) + (4/3).2^{2p+2}$

(iii) $KBR_3(D_5(p)) = 32.2^{p+1} + 308.2^p - 332 + 48.2^{2p+2}$

Proof

$$\begin{aligned}
KBR_1(D_5) &= \sum_{ue} \frac{d_u + d_e}{d_u \times d_e} \\
&\quad + \left(\frac{1+3}{1\times 3}\right)(2\times 2^p - 2) \\
&\quad + \left(\frac{1+4}{1\times 4}\right)(2\times 2^p - 2) + \left(\frac{3+3}{3\times 3}\right) d2 \\
&\quad + \left(\frac{3+5}{3\times 5}\right)(2\times 2^p - 2) + \left(\frac{2+4}{2\times 4}\right)\left(2^{p+2} - 4\right) \\
&= \frac{4}{3}.2^{p+1} + \frac{106}{15}.2^p - \frac{89}{10} + \frac{3}{4}.2^{2p+2}, \\
KBR_2(D_5) &= \sum_{ue} \frac{d_u \times d_e}{d_u + d_e} \\
&\quad + \left(\frac{1\times 3}{1+3}\right)(2\times 2^p - 2) \\
&\quad + \left(\frac{1\times 4}{1+4}\right)(2\times 2^p - 2) + \left(\frac{3\times 3}{3+3}\right)(2) \\
&\quad + \left(\frac{3\times 5}{3+5}\right)(2\times 2^p - 2) + \left(\frac{2\times 4}{2+4}\right)\left(2^{p+2} - 4\right) \\
&= \frac{16}{5}.2^{p+1} + \frac{82}{8}.2^p - \frac{1021}{84} + \frac{4}{3}.2^{2p+2}, \\
KBR_3(D_5) &= \sum_{ue} (d_u \times d_e)(d_u + d_e) \\
&= (1\times 2)(1+2)\left(2^{p+1}\right) + (2\times 3)(2+3)\left(2^{p+1}\right) \\
&\quad + (1\times 2)(1+2)(2\times 2^p - 2) \\
&\quad + (1\times 3)(1+3)(2\times 2^p - 2) \\
&\quad + (1\times 4)(1+4)(2\times 2^p - 2) \\
&\quad + (3\times 5)(3+5)(2\times 2^p - 2) \\
&\quad + (3\times 3)(3+3)(2) \\
&\quad + (2\times 4)(2+4)\left(2^{m+2} - 4\right) \\
&= 32.2^{p+1} + 308.2^p - 332 + 48.2^{2p+2}.
\end{aligned} \tag{7}$$

□

3. Graphical Representation

4. Concluding Remarks

The topological index is very helpful in biology, material science, informatics, arithmetic, etc. The most valuable use of a topological index is in QSPR and QSAR. By mean of the topological index, we can assign a number to the graph of a dendrimer and this number help us to determine the hidden information in the symmetric structure of dendrimer. This paper introduced and computed K Banhatti redefined Zagreb indices, i.e., 1st K Banhatti redefined Zagreb index, 2nd K Banhatti redefined Zagreb indices, and 3rd K Banhatti redefined Zagreb index for the dendrimers $D_i(p)$, where $i = 1, 2, 3, 4, 5$. Figures 7, 8, and 9 show the graphical behavior of computed results of $D_i(p)$, where $i = 1, 2, 3, 4, 5$.

5. Future Directions

It will be interesting to compute the different versions of graph energies of understudied dendrimers. It will also be interesting to define the corresponding energies for the presented topological indices.

Data Availability

All data required in this research are included within this paper.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

Cheng-Gang Huo analyzed the work, approved the results, and arranged the funding for this paper. Fozia Azhar proved the results. Abaid ur Rehman Virk proposed the problem and supervised this work. Tarig Ismaeel wrote the final version of this paper and sketched the correct graphs presented in this paper.

References

[1] P. S. Ranjini, V. Lokesha, and A. Usha, "Relation between phenylene and hexagonal squeeze using harmonic index," *International Journal of Graph Theory*, vol. 1, no. 4, pp. 116–121, 2013.

[2] S. Amin, A. U. Rehman Virk, M. A. Rehman, and N. A. Shah, "Analysis of dendrimer generation by sombor indices," *Journal of Chemistry*, vol. 202111 pages, 2021.

[3] B. K. Nanjwade, H. M. Bechra, G. K. Derkar, F. V. Manvi, and V. K. Nanjwade, "Dendrimers: emerging polymers for drug-delivery systems," *European Journal of Pharmaceutical Sciences*, vol. 38, no. 3, pp. 185–196, 2009.

[4] D. Astruc, E. Boisselier, and C. Ornelas, "Dendrimers designed for functions: from physical, photophysical, and supramolecular properties to applications in sensing, catalysis, molecular electronics, photonics, and nanomedicine," *Chemical Reviews*, vol. 110, no. 4, pp. 1857–1959, 2010.

[5] R. K. Tekade, T. Dutta, V. Gajbhiye, and N. K. Jain, "Exploring dendrimer towards dual drug delivery: pH responsive simultaneous drug-release kinetics," *Journal of Microencapsulation*, vol. 26, no. 4, pp. 287–296, 2009.

[6] F. M. Brückler, T. Doslic, A. Graovac, and I. Gutman, "On a class of distance-based molecular structure descriptors," *Chemical Physics Letters*, vol. 503, no. 4-6, pp. 336–338, 2011.

[7] H. Gonzalez-Diaz, S. Vilar, L. Santana, and E. Uriarte, "Medicinal chemistry and bioinformatics-current trends in drugs discovery with networks topological indices," *Current Topics in Medicinal Chemistry*, vol. 7, no. 10, pp. 1015–1029, 2007.

[8] H. Hosoya, K. Hosoi, and I. Gutman, "A topological index for the totalp-electron energy," *Theoretica Chimica Acta*, vol. 38, no. 1, pp. 37–47, 1975.

[9] M. Ajmal, W. Nazeer, M. Munir, S. M. Kang, and C. Y. Jung, "The M-polynomials and topological indices of generalized prism network," *International Journal of Mathematical Analysis*, vol. 11, no. 6, pp. 293–303, 2017.

[10] M. Munir, W. Nazeer, Z. Shahzadi, and S. Kang, "Some invariants of circulant graphs," *Symmetry*, vol. 8, no. 11, p. 134, 2016.

[11] A. U. R. Virk, M. A. Rehman, and W. Nazeer, "New definition of atomic bond connectivity index to overcome deficiency of structure sensitivity and abruptness in existing definition," *Scientific Inquiry and Review*, vol. 3, no. 4, pp. 1–20, 2019.

[12] A. R. Virk, "Multiplicative shingali and kanabour indices for bismuth tri-iodide," *Journal of Prime Research in Mathematics*, vol. 16, no. 2, pp. 80–88, 2020.

[13] Y. C. Kwun, A. U. R. Virk, W. Nazeer, M. A. Rehman, and S. M. Kang, "On the multiplicative degree-based topological indices of silicon-carbon Si2C3-I [*p*, *q*] and Si2C3-II [*p*, *q*]," *Symmetry*, vol. 10, no. 8, p. 320, 2018.

[14] H. Wiener, "Structural determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.

[15] M. Randic, "Characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, no. 23, pp. 6609–6615, 1975.

[16] A. U. R. Virk, M. N. Jhangeer, and M. A. Rehman, "Reverse zagreb and reverse hyper-zagreb indices for silicon carbide Si2C3I [*r*, *s*] and Si2C3II [*r*, *s*]," *Engineering and Applied Science Letters*, vol. 1, no. 2, pp. 37–50, 2018.

[17] Z. Shao, A. u. R. Virk, M. S. Javed, M. A. Rehman, and M. R. Farahani, "Degree based graph invariants for the molecular graph of bismuth tri-iodide," *English Applied Science Letter*, vol. 2, no. 1, pp. 01–11, 2019.

[18] S. Noreen and A. Mahmood, "Zagreb polynomials and redefined zagreb indices for the line graph of carbon nanocones," *Open Journal of Mathematical Analysis*, vol. 2, no. 1, pp. 66–73, 2018.

[19] V. R. Kulli, "On banhatti-sombor indices," *International Journal of Applied Chemistry*, vol. 8, no. 1, pp. 21–25, 2021.

[20] V. R. Kulli, "K Banhatti polynomials of remdesivir, chloroquine and hydroxychloroquine: research advances for the prevention and treatment of COVID-19," *SSRG International Journal of Applied Chemistry*, vol. 7, no. 2, pp. 48–55, 2020.