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TEMPERATURE INDICES OF WELL KNOWN DENDRIMER NETWORKS

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Abstract. Chemical graph theory is a branch of graph theory. In this field, molecules are modeled using graph theory and a mathematical approach is obtained. Thus, predictions can be made about the physical, chemical and bioactivity properties of molecules. In this study, temperature indices depending on the vertex degree are considered. Temperature indices of Polyamidoamine (PAMAM) dendrimers, Porphyrin core dendrimers are obtained and the results are compared numerically using the MATLAB program.

1. Introduction

Graph theory is used to solve problems in daily life by expressing objects and the relationships between them with vertices and edges, respectively [1]. Due to the changing living conditions and increasing diseases, it is necessary to discover new chemicals and drugs quickly and inexpensively. With the help of graph indices in chemical graph theory, it has been possible to predict the physical, chemical and bioactivity properties of molecules [2].

Graph indices are the numerical values of chemical networks. Chemical networks are obtained by representing chemical structures with vertices and edges. The atoms of a chemical structure are represented by vertices and the relationships between the chemical structures are represented by edges. The numerical results obtained by using graph indices of chemical networks are used in programs such as SPSS to obtain equations. These equations are used to predict the properties of new chemical structures [2].

Throughout this article, let $\wedge$ be a graph with $V(\wedge), E(\wedge)$. The element numbers of the vertex (edge) set are defined by $|V(\wedge)|(|E(\wedge)|)$. The degree of a vertex υ is defined by d_υ [1].

Fajtlowicz [3] defined the temperature of a vertex υ as

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$$T_\upsilon = \frac{d_\upsilon}{|V(\wedge)| - d_\upsilon}. \tag{1.1}$$

With this motivation, Kulli [4] defined the general first and second temperature indices as follows:

$$GT_1^k(\wedge) = \sum_{\tau\upsilon \in E(\wedge)} \left(T_\tau + T_\upsilon\right)^k \tag{1.2}$$

$$GT_2^k(\wedge) = \sum_{\tau\upsilon \in E(\wedge)} \left(T_\tau T_\upsilon\right)^k. \tag{1.3}$$

Kansal et al. studied temperature indices for predict the physical properties of COVID-19 drugs [5]. Nabeel et al. found temperature indices of some nanotubes [6]. Khan et al. investigated various graph indices based temperate of silicates moleculas [7]. Kulli obtained results about temperatures indices of important nanostructures [8].

Dendrimers have a symmetric core and radially symmetric molecules. Therefore, dendrimer networks are similar to tree graphs. Dendrimers are often used in drug discovery due to their favorable chemical properties. Therefore, dendrimers are widely studied [9]. Zhao et al. studied irregularity indices of some dendrimers [10]. Hasani and Gods investigated M-polynomials of porphrin dendrimers [11]. Sarkar et al. studied generalized Zagreb indices of some reguler dendrimers [12]. Khalaf et al. calculated the degree based indices of four layered prophyrin core dendrimers [13].

In this study, the polyamidoamine and porphyrin core dendrimers are studied. The temperature indices of these dendrimer networks are obtained and the results are compared.

2. Preliminaries

In this section,informations about Polyamidoamine dendrimers and Porphyrin cored dendrimers are given.

PAMAM DENDRIMERS

Polyamidoamine (PAMAM) dendrimers have an ethylenediamine core, a repetitive branching amidoamine internal structure and a primary amine terminal surface [14]. Figure 1 shows the structure of the PAMAM [14]. Let $PAMAM[r]$ be molecular graph of the polyamidoamine (PAMAM) dendrimers. The PAMAM network have $|V(PAMAM[r])| = 12 \times 2^{r+2} - 23$ and $|E(PAMAM[r])| = 12 \times 2^{r+2} - 24$.

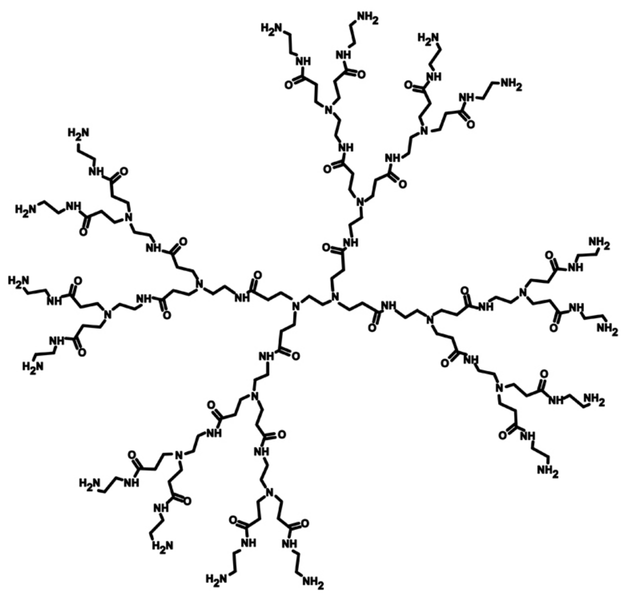

FIGURE 1. Chemical Structure of PAMAM.

PORPHYRIN CORED DENDRIMERS

Porphyrin cored dendrimers have a central core and at least 2 branches[15]. In this study, 3 porphyrin cored dendrimers will be examined.

Porphyrin Cored Dendrimers-2

Porphyrin cored dendrimers-2 have one central core and 4 branches. Figure 2 shows the structure of Porphyrin cored dendrimers-2 [15]. Let $PC2[n]$ be molecular graphs of porphyrin cored dendrimers-2. Then, $|V(PC2[n])| = 8 \times 2^n + 21$ and $|E(PC2[n])| = 8 \times 2^n + 28$ by calculated.

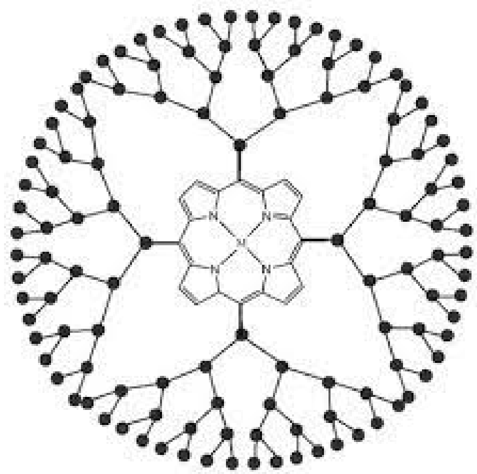

FIGURE 2. Structure of Porphyrin cored dendrimers-2 .

Porphyrin Cored Dendrimers-3

Porphyrin cored dendrimers-3 have one central core and 8 branches. Figure 3 shows the structure of Porphyrin cored dendrimers-3 [15]. Let $PC3[n]$ be molecular graphs of porphyrin cored dendrimers-3. Then, $|V(PC3[n])| = 16 \times 2^n + 17$ and $|E(PC3[n])| = 16 \times 2^n + 24$ by calculated.

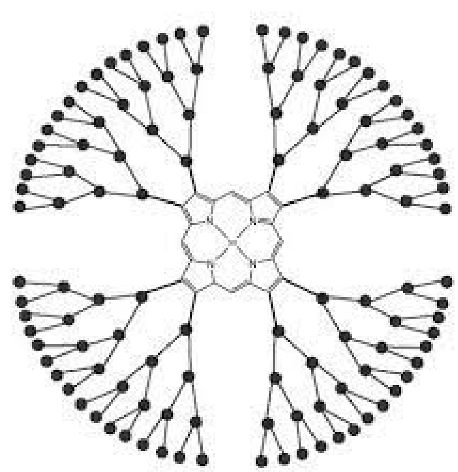

FIGURE 3. Structure of Porphyrin cored dendrimers-3 .

Porphyrin Cored Dendrimers-4

Porphyrin cored dendrimers-4 have a central core and 12 branches. Figure 4 shows the structure of Porphyrin cored dendrimers-4 [15]. Let $PC4[n]$ be molecular graphs of porphyrin cored dendrimers-4. Then,$|V(PC4[n])| = 24 \times 2^n + 13$ and $|E(PC3[n])| = 24 \times 2^n + 20$ by calculated.

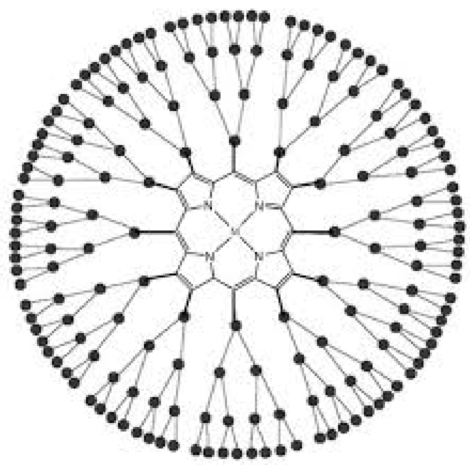

FIGURE 4. Structure of Porphyrin cored dendrimers-4 .

3. MAIN RESULTS

In this section, the values of the general first temperature and general second temperature indices of the dendrimer networks mentioned above are calculated. Numerical comparisons of the general first and second temperature indices of each dendrimer network introduced above are made using the MATLAB program.

Theorem 3.1. *i. Let the general first temperature index of $PAMAM[r]$ be $GT_1^k(PAMAM[r])$. Then*

$$\begin{aligned} GT_1^k(PAMAM[r]) &= (3 \times 2^r)\left(\frac{1}{12 \times 2^{r+2} - 24} + \frac{2}{12 \times 2^{r+2} - 25}\right)^k \\ &+ (6 \times 2^r - 3)\left(\frac{1}{12 \times 2^{r+2} - 24} + \frac{3}{12 \times 2^{r+2} - 26}\right)^k \\ &+ (18 \times 2^r - 9)\left(\frac{2}{12 \times 2^{r+2} - 25} + \frac{2}{12 \times 2^{r+2} - 25}\right)^k \\ &+ (21 \times 2^r - 12)\left(\frac{2}{12 \times 2^{r+2} - 25} + \frac{3}{12 \times 2^{r+2} - 26}\right)^k. \end{aligned}$$

ii. Let general second temperature index of $PAMAM[r]$ be $GT_2^k(PAMAM[r])$. Then,

$$\begin{aligned} GT_2^k(PAMAM[r]) &= (3 \times 2^r)\left(\frac{1}{12 \times 2^{r+2} - 24} \times \frac{2}{12 \times 2^{r+2} - 25}\right)^k \\ &+ (6 \times 2^r - 3)\left(\frac{1}{12 \times 2^{r+2} - 24} \times \frac{3}{12 \times 2^{r+2} - 26}\right)^k \\ &+ (18 \times 2^r - 9)\left(\frac{2}{12 \times 2^{r+2} - 25} \times \frac{2}{12 \times 2^{r+2} - 25}\right)^k \\ &+ (21 \times 2^r - 12)\left(\frac{2}{12 \times 2^{r+2} - 25} \times \frac{3}{12 \times 2^{r+2} - 26}\right)^k. \end{aligned}$$

Proof. The edge partitions of PAMAM dendrimer networks are shown Table 1.

TABLE 1. The edge partitions of PAMAM networks.

(d_τ, d_υ) **for** $E(PAMAM[r])$	$(T_\tau + T_\upsilon)$ **for** $E(PAMAM[r])$	**The number of edge**
(1,2)	$(\frac{1}{12\times2^{r+2}-24}, \frac{1}{12\times2^{r+2}-25})$	3×2^r
(1,3)	$(\frac{1}{12\times2^{r+2}-24}, \frac{1}{12\times2^{r+2}-26})$	$6 \times 2^r - 3$
(2,2)	$(\frac{2}{12\times2^{r+2}-25}, \frac{2}{12\times2^{r+2}-25})$	$18 \times 2^r - 9$
(2,3)	$(\frac{2}{12\times2^{r+2}-25}, \frac{3}{12\times2^{r+2}-26})$	$21 \times 2^r - 12$

Let E_{d_τ, d_υ} be (d_τ, d_υ) for $E(PAMAM[r])$. From Table 1, it is written:

$$TI(PAMAM[r]) = \sum_{\tau\upsilon \in E_{1,2}} W_{\tau\upsilon} + \sum_{\tau\upsilon \in E_{1,3}} W_{\tau\upsilon} + \sum_{\tau\upsilon \in E_{2,2}} W_{\tau\upsilon} + \sum_{\tau\upsilon \in E_{2,3}} W_{\tau\upsilon} \tag{3.1}$$

i. If $W_{\tau\upsilon} = (T_\tau + T_\upsilon)^k$ in Eq.(3.1), then

$$\begin{aligned} GT_1^k(PAMAM[r]) &= (3 \times 2^r)\left(\frac{1}{12 \times 2^{r+2} - 24} + \frac{2}{12 \times 2^{r+2} - 25}\right)^k \\ &+ (6 \times 2^r - 3)\left(\frac{1}{12 \times 2^{r+2} - 24} + \frac{3}{12 \times 2^{r+2} - 26}\right)^k \\ &+ (18 \times 2^r - 9)\left(\frac{2}{12 \times 2^{r+2} - 25} + \frac{2}{12 \times 2^{r+2} - 25}\right)^k \\ &+ (21 \times 2^r - 12)\left(\frac{2}{12 \times 2^{r+2} - 25} + \frac{3}{12 \times 2^{r+2} - 26}\right)^k. \end{aligned}$$

ii. If $W_{\tau\upsilon} = (T_\tau \times T_\upsilon)^k$ in Eq.(3.1), then

$$\begin{aligned} GT_2^k(PAMAM[r]) &= (3 \times 2^r)\left(\frac{1}{12 \times 2^{r+2} - 24} \times \frac{2}{12 \times 2^{r+2} - 25}\right)^k \\ &+ (6 \times 2^r - 3)\left(\frac{1}{12 \times 2^{r+2} - 24} \times \frac{3}{12 \times 2^{r+2} - 26}\right)^k \\ &+ (18 \times 2^r - 9)\left(\frac{2}{12 \times 2^{r+2} - 25} \times \frac{2}{12 \times 2^{r+2} - 25}\right)^k \\ &+ (21 \times 2^r - 12)\left(\frac{2}{12 \times 2^{r+2} - 25} \times \frac{3}{12 \times 2^{r+2} - 26}\right)^k. \end{aligned}$$

□

Figure 5 shows plots a) GT_1^k and b) GT_2^k of $PAMAM[r]$. These plots show that the general first temperature index of the $PAMAM[r]$ network grows faster than the general second temperature index.

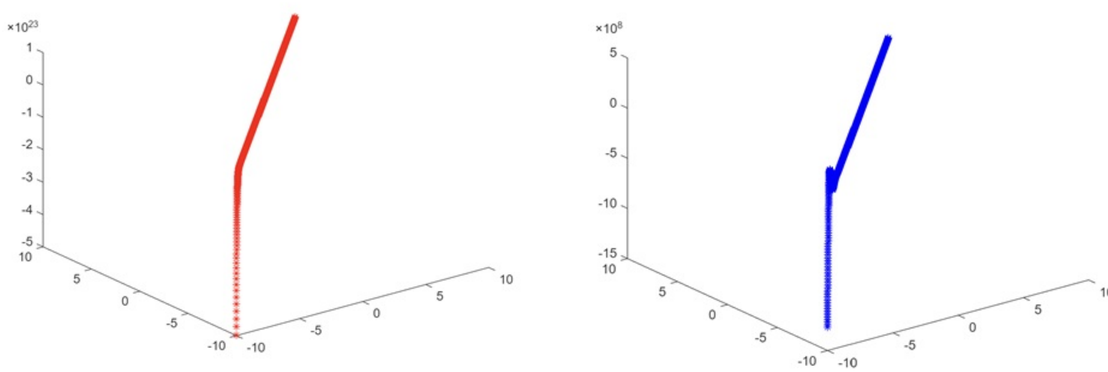

FIGURE 5. The plots of a) GT_1^k and b) GT_2^k of $PAMAM[r]$.

Theorem 3.2. *i.* $GT_1^k(PC2[n])$ *is equal to following equation:*

$$\begin{aligned} GT_1^k(PC2[n]) &= (4 \times 2^n)\left(\frac{1}{8 \times 2^n + 20} + \frac{3}{8 \times 2^n + 18}\right)^k \\ &+ 4\left(\frac{2}{8 \times 2^n + 19} + \frac{2}{8 \times 2^n + 19}\right)^k \\ &+ (4 \times 2^n + 12)\left(\frac{2}{8 \times 2^n + 19} + \frac{3}{8 \times 2^n + 18}\right)^k \\ &+ 4\left(\frac{3}{8 \times 2^n + 18} + \frac{4}{8 \times 2^n + 17}\right)^k. \end{aligned}$$

ii. $GT_2^k(PC2[n])$ *is equal to*

$$\begin{aligned} GT_2^k(PC2[n]) &= (4 \times 2^n) \left(\frac{1}{8 \times 2^n + 20} \times \frac{3}{8 \times 2^n + 18} \right)^k \\ &+ 4 \left(\frac{2}{8 \times 2^n + 19} \times \frac{2}{8 \times 2^n + 19} \right)^k \\ &+ (4 \times 2^n + 12) \left(\frac{2}{8 \times 2^n + 19} \times \frac{3}{8 \times 2^n + 18} \right)^k \\ &+ 4 \left(\frac{3}{8 \times 2^n + 18} \times \frac{4}{8 \times 2^n + 17} \right)^k. \end{aligned}$$

Proof. The edge partitons of $PC2[n]$ are shown in the following table (Table 2).

TABLE 2. The edge partitons of $PC2[n]$.

(d_τ, d_υ) **for** $E(PC2[n])$	$(T_\tau + T_\upsilon)$ **for** $E(PC2[n])$	**The number of edge**
(1,3)	$(\frac{1}{8\times2^n+20}, \frac{3}{8\times2^n+18})$	4×2^n
(2,2)	$(\frac{2}{8\times2^n+19}, \frac{2}{8\times2^n+19})$	4
(2,3)	$(\frac{2}{8\times2^n+19}, \frac{2}{8\times2^n+18})$	8
(3,3)	$(\frac{3}{8\times2^n+18}, \frac{3}{8\times2^n+18})$	$4 \times 2^n + 12$
(3,4)	$(\frac{3}{8\times2^n+18}, \frac{4}{8\times2^n+17})$	4

Using Table 2, it can be written:

(3.2)

$$TI(PC2[n]) = \sum_{\tau\upsilon \in E_{1,2}} W_{\tau\upsilon} + \sum_{\tau\upsilon \in E_{2,2}} W_{\tau\upsilon} + \sum_{\tau\upsilon \in E_{2,3}} W_{\tau\upsilon} + \sum_{\tau\upsilon \in E_{3,3}} W_{\tau\upsilon} + \sum_{\tau\upsilon \in E_{3,4}} W_{\tau\upsilon}$$

i. If $W_{\tau\upsilon} = (T_\tau + T_\upsilon)^k$ in Eq.(3.2), then

$$\begin{aligned} GT_1^k(PC2[n]) &= (4 \times 2^n) \left(\frac{1}{8 \times 2^n + 20} + \frac{3}{8 \times 2^n + 18} \right)^k \\ &+ 4 \left(\frac{2}{8 \times 2^n + 19} + \frac{2}{8 \times 2^n + 19} \right)^k \\ &+ 8 \left(\frac{2}{8 \times 2^n + 19} + \frac{2}{8 \times 2^n + 18} \right)^k \\ &+ (4 \times 2^n + 12) \left(\frac{3}{8 \times 2^n + 18} + \frac{3}{8 \times 2^n + 18} \right)^k \\ &+ 4 \left(\frac{3}{8 \times 2^n + 18} + \frac{4}{8 \times 2^n + 17} \right). \end{aligned}$$

ii. If $W_{\tau\upsilon} = (T_\tau \times T_\upsilon)^k$ in Eq.(3.2), then

$$\begin{aligned} GT_2^k(PC2[n]) &= (4\times 2^n)\left(\frac{1}{8\times 2^n+20}\times\frac{3}{8\times 2^n+18}\right)^k \\ &+ 4\left(\frac{2}{8\times 2^n+19}\times\frac{2}{8\times 2^n+19}\right)^k \\ &+ 8\left(\frac{2}{8\times 2^n+19}\times\frac{2}{8\times 2^n+18}\right)^k \\ &+ (4\times 2^n+12)\left(\frac{3}{8\times 2^n+18}\times\frac{3}{8\times 2^n+18}\right)^k \\ &+ 4\left(\frac{3}{8\times 2^n+18}\times\frac{4}{8\times 2^n+17}\right). \end{aligned}$$

□

Figure 6 shows plots a) GT_1^k and b) GT_2^k of $PC2[n]$. This plot gives $GT_1^k(PC2[n])$ growing faster than $GT_2^k(PC2[n])$.

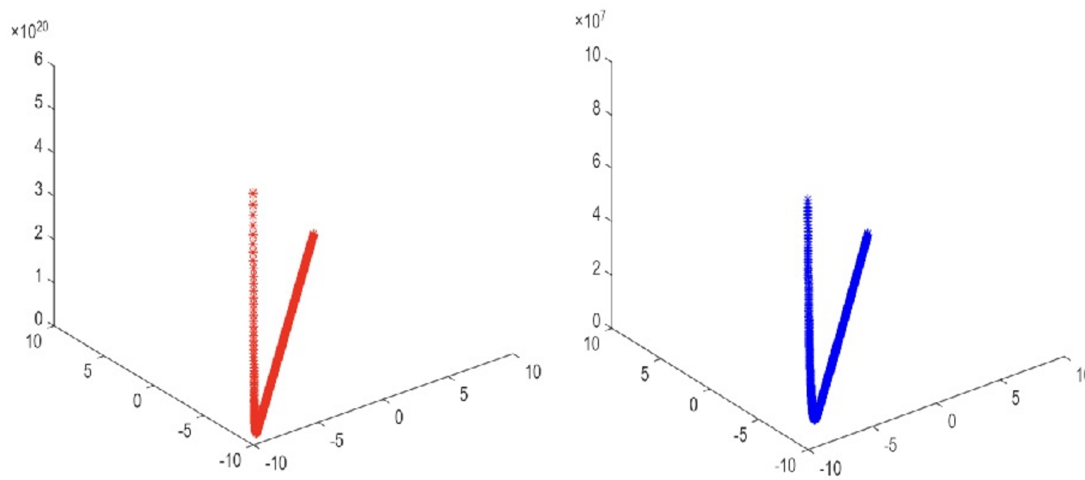

FIGURE 6. The plots of a) GT_1^k and b) GT_2^k of $PC2[n]$.

Theorem 3.3. *i.* $GT_1^k(PC3[n])$ *is*

$$\begin{aligned} GT_1^k(PC3[n]) &= 8\times 2^n\left(\frac{1}{16\times 2^n+16}+\frac{3}{16\times 2^n+14}\right)^k \\ &+ 8\left(\frac{2}{16\times 2^n+15}+\frac{3}{16\times 2^n+14}\right)^k \\ &+ (8\times 2^n+12)\left(\frac{3}{16\times 2^n+14}+\frac{3}{16\times 2^n+14}\right)^k \\ &+ 4\left(\frac{3}{16\times 2^n+14}+\frac{4}{16\times 2^n+13}\right)^k. \end{aligned}$$

ii. $GT_2^k(PC3[n])$ *is*

$$\begin{aligned} GT_2^k(PC3[n]) &= 8\times 2^n\left(\frac{1}{16\times 2^n+16}\times\frac{3}{16\times 2^n+14}\right)^k \\ &+ 8\left(\frac{2}{16\times 2^n+15}\times\frac{3}{16\times 2^n+14}\right)^k \\ &+ (8\times 2^n+12)\left(\frac{3}{16\times 2^n+14}\times\frac{3}{16\times 2^n+14}\right)^k \\ &+ 4\left(\frac{3}{16\times 2^n+14}\times\frac{4}{16\times 2^n+13}\right)^k. \end{aligned}$$

Proof. The edge partitions $PC3[n]$ are given in Table 3.

TABLE 3. The edge partitions of $PC3[n]$.

(d_τ, d_υ) **for** $E(PC3[n])$	$(T_\tau + T_\upsilon)$ **for** $E(PC3[n])$	**The number of edge**
(1,3)	$(\frac{1}{16\times2^n+16}, \frac{3}{16\times2^n+14})$	8×2^n
(2,3)	$(\frac{2}{16\times2^n+15}, \frac{3}{16\times2^n+14})$	8
(3,3)	$(\frac{3}{16\times2^n+14}, \frac{3}{16\times2^n+14})$	$8\times 2^n+12$
(3,4)	$(\frac{3}{16\times2^n+14}, \frac{4}{16\times2^n+13})$	4

From Table 3, the following equation can be written:

$$TI(PC3[n]) = \sum_{\tau\upsilon\in E_{1,3}} W_{\tau\upsilon} + \sum_{\tau\upsilon\in E_{2,3}} W_{\tau\upsilon} + \sum_{\tau\upsilon\in E_{3,3}} W_{\tau\upsilon} + \sum_{\tau\upsilon\in E_{3,4}} W_{\tau\upsilon} \quad (3.3)$$

i. If $W_{\tau\upsilon} = (T_\tau + T_\upsilon)^k$ in Eq.3.3, then the proof (i) is completed from Table .
ii. If $W_{\tau\upsilon} = (T_\tau \times T_\upsilon)^k$ in Eq.(3.3), then the proof (ii) is completed with some calculated from Table 3. □

The plots GT_1^k and GT_2^k of $PC3[n]$ are given below (see Figure 7). it is seen that GT_1^k index of $PC3[n]$ grows faster than GT_2^k index of $PC3[n]$ from Figure 7.

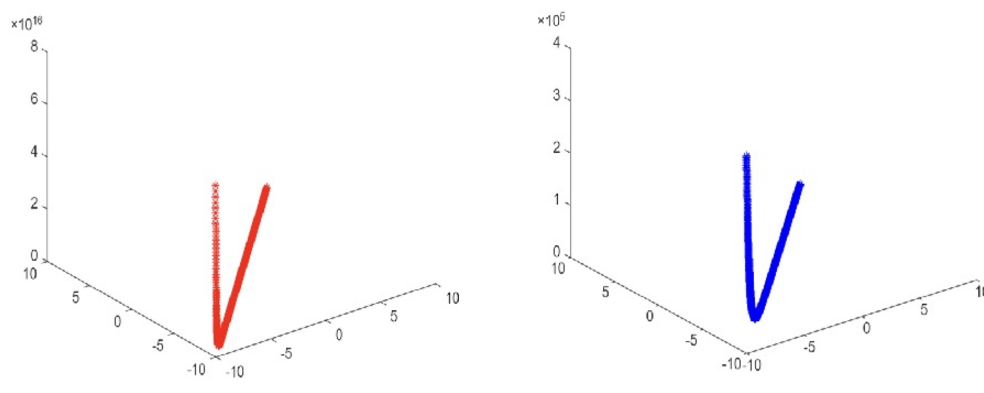

FIGURE 7. The plots of a) GT_1^k and b) GT_2^k of $PC3[n]$.

Theorem 3.4. *i. The general first temperature index of $PC4[n]$ is*

$$\begin{aligned} GT_1^k(PC4[n]) &= 12\times 2^n\left(\frac{1}{24\times 2^n+12}+\frac{3}{24\times 2^n+10}\right)^k \\ &+ 8\left(\frac{2}{24\times 2^n+11}+\frac{3}{24\times 2^n+10}\right)^k \\ &+ (8\times 2^n+12)\left(\frac{3}{24\times 2^n+10}+\frac{3}{24\times 2^n+10}\right)^k \\ &+ 4\left(\frac{3}{24\times 2^n+10}+\frac{4}{24\times 2^n+9}\right)^k. \end{aligned}$$

ii. $GT_2^k(PC4[n])$ *is*

$$\begin{aligned} GT_2^k(PC4[n]) &= 12\times 2^n\left(\frac{1}{24\times 2^n+12}\times\frac{3}{24\times 2^n+10}\right)^k \\ &+ 8\left(\frac{2}{24\times 2^n+11}\times\frac{3}{24\times 2^n+10}\right)^k \\ &+ (8\times 2^n+12)\left(\frac{3}{24\times 2^n+10}\times\frac{3}{24\times 2^n+10}\right)^k \\ &+ 4\left(\frac{3}{24\times 2^n+10}\times\frac{4}{24\times 2^n+9}\right)^k. \end{aligned}$$

Proof. The edge partitions $PC4[n]$ are given in Table 4.

TABLE 4. The edge partitions of $PC4[n]$.

(d_τ, d_υ) **for** $E(PC3[n])$	$(T_\tau + T_\upsilon)$ **for** $E(PC3[n])$	**The number of edge**
(1,3)	$(\frac{1}{24\times2^n+12}, \frac{3}{24\times2^n+10})$	12×2^n
(2,3)	$(\frac{2}{24\times2^n+11}, \frac{3}{24\times2^n+10})$	8
(3,3)	$(\frac{3}{24\times2^n+10}, \frac{3}{24\times2^n+10})$	$8\times 2^n+12$
(3,4)	$(\frac{3}{24\times2^n+10}, \frac{4}{24\times2^n+9})$	4

From Table 4, the following equation is written:

$$TI(PC4[n]) = \sum_{\tau\upsilon\in E_{1,3}} W_{\tau\upsilon} + \sum_{\tau\upsilon\in E_{2,3}} W_{\tau\upsilon} + \sum_{\tau\upsilon\in E_{3,3}} W_{\tau\upsilon} + \sum_{\tau\upsilon\in E_{3,4}} W_{\tau\upsilon} \tag{3.4}$$

i. If $W_{\tau\upsilon} = (T_\tau + T_\upsilon)^k$ in Eq.3.4, then the proof (i) is completed from Table .
ii. If $W_{\tau\upsilon} = (T_\tau \times T_\upsilon)^k$ in Eq.(3.4), then the proof (ii) is completed with some calculated from Table. □

Figure 8 shows plots a) GT_1^k and b) GT_2^k of $PC4[n]$. This plot shows that $GT_1^k(PC4[n])$ grows faster than $GT_2^k(PC4[n])$.

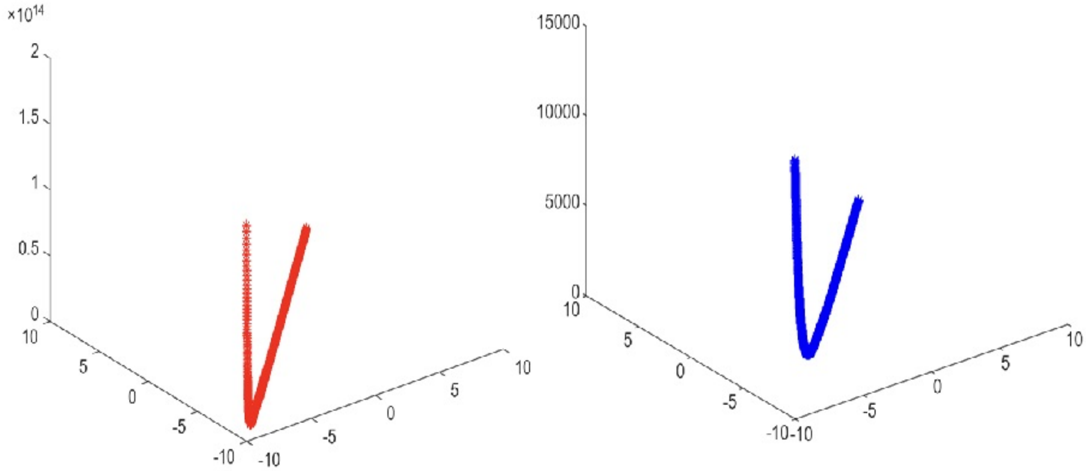

FIGURE 8. The plots of a) GT_1^k and b) GT_2^k of $PC4[n]$.

4. Conclusion

Since dendrimers are frequently used in drug discovery, dendrimer networks were considered in this study. Four important dendrimers were studied with temperature indices, which are among the graph indices that have attracted attention recently.

As a result, it was seen that the general first temperature index grew faster than the general second temperature index for PAMAM dendrimer and 3 porphyrin cored dendrimers. The results of this study will shed light on the field of chemical graph theory and fast and cost-effective drug discovery.

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The Declaration of Conflict of Interest/ Common Interest
The author(s) declared that no conflict of interest or common interest

The Declaration of Ethics Committee Approval
This study does not be necessary ethical committee permission or any special permission.

The Declaration of Research and Publication Ethics
The author(s) declared that they comply with the scientific, ethical, and citation rules of Journal of Universal Mathematics in all processes of the study and that they do not make any falsification on the data collected. Besides, the author(s)

declared that Journal of Universal Mathematics and its editorial board have no responsibility for any ethical violations that may be encountered and this study has not been evaluated in any academic publication environment other than Journal of Universal Mathematics.

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