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Temperature Indices of PETAA and PETIM Dendrimer Structures

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Abstract
In mathematical chemistry, molecules' physical, chemical, and biological properties can be predicted. Topological indices are the numerical values of molecular graphs. Dendrimers have an important place in chemistry and drug discovery. In this paper, the temperature indices of PETAA and PETIM dendrimer structures are calculated.

Keywords: Graph Theory, Chemical graph, PETIM, PETAA, Temperature index
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1 Introduction

Chemical graph theory is a field of study of mathematical chemistry that combines chemical structure with graph theory, a branch of discrete mathematics. Topological indices are one of the subjects studied in chemical graph theory.

Let $\wp$ be a graph with $V(\wp)$ and $E(\wp)$. The degree of a vertex p is defined by d_p [1]. A molecular graph is the skeleton non-hydrogen of a molecular structure. It has the edges and the vertices which are represented the bonds and the atoms of a molecule, respectively. Topological indices (descriptors) are quantitative expressions of a chemical graph. Topological indices are used predict to bioactivity and physicochemical properties of molecules in structure-property/ structure-activity relationship (QSPR/QSAR) modeling. Therefore, they have an important role in drug discovery, chemistry, nanotechnology, and mathematics ([2], [3],[4]).

Harold Wiener made the first application using it to predict the physical properties of paraffin and defined the Wiener index in 1947 [5]. Temperature indices are the temperature of degree-based indices. Fajtlowicz introduced the temperature of a vertex p in 1988 [6] as

$$T_p = \frac{d_p}{|V(\wp)| - d_p}.$$

Table 1 shows the temperature indices which is introduced by Kulli [8]

Jahanbani et al. calculated temperature indices of some network [7]. Kulli defined some temprature indices and studied temprature of a nanostructure [8], [9]. Dendrimers have important a place in chemical graph theory (See detail [10], [11], [12]).

This study shows the temperature indices of propyletherimine and poly ethylene amide amine dendrimers.

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Table 1: The Temperature Indices.

Temperature Index	Formula
General First Temperature Index	$T_1^k(\wp) = \sum_{pq \in E(\wp)} (T_p + T_q)^k$
General Second Temperature Index	$T_2^k(\wp) = \sum_{pq \in E(\wp)} (T_p T_q)^k$

2 Main results

In this section, it is considered propyletherimine and poly ethylene amide amine dendrimers. It is calculated the temperature indices of propyletherimine and poly ethylene amide amine dendrimers

2.1 The porpyl ether imine dendrimers (PETIM)

The porpyl ether imine dendrimers (PETIM) have $|V(PETIM)| = 3 \times 2^{n+3} - 23$ and $|E(PETIM)| = 3 \times 2^{n+3} - 24$ by calculate and also see [13]. Figure 1 shows structure of PETIM.

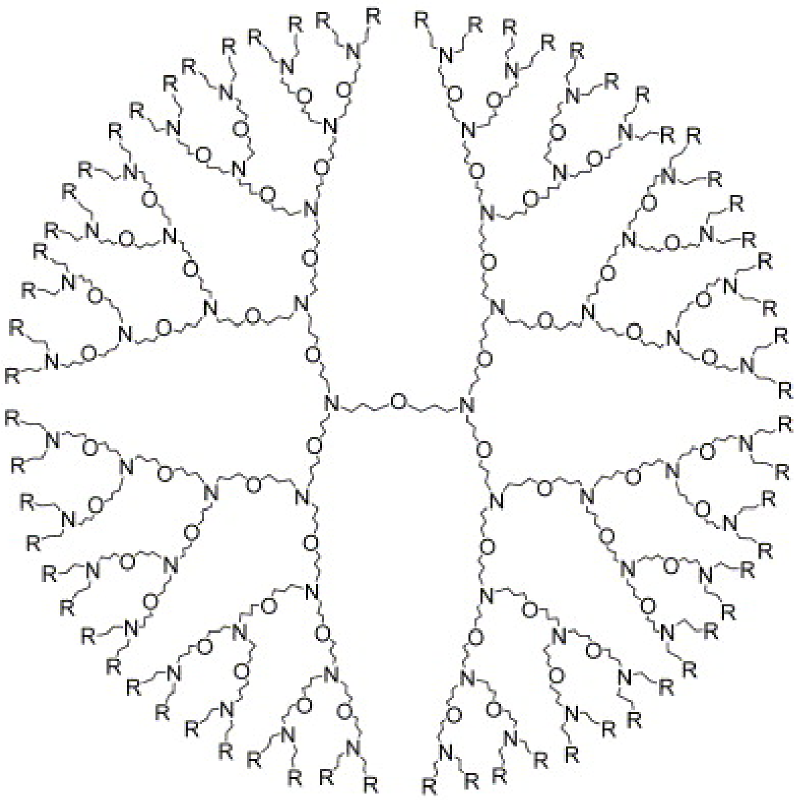

Figure 1: Structure of the porpyl ether imine dendrimers

Theorem 2.1. *Let $\wp$ be PETIM. Then*

i. General first temperature index of $\wp$ is

$$\begin{aligned} T_1^k(\wp) &= \frac{2^{n+1}}{3 \times 2^{n+3} - 25}\left((3 - \frac{1}{3 \times 2^{n+3} - 24})^k + 2^{2k+3} + 3 \times (5 + \frac{3}{2^{n+3} - 26})^k\right) \\ &- \frac{6}{2^{n+3} - 25})\left(3 \times 2^{2k} - (5 + \frac{3}{3 \times 2^{n+3} - 26})^k\right). \end{aligned}$$

ii. General second temperature index of $\wp$ *is*

$$\begin{aligned} T_2^k(\wp) &= \frac{2^{n+1+k}}{(3\times 2^{n+3}-25)^k}\left(\frac{1}{(3\times 2^{n+3}-24)^k}+\frac{2^{3+k}}{(3\times 2^{n+3}-25)^k}+\frac{2^k3^{k+1}}{3\times 2^{n+3}-26}\right)\\ &- 6(\frac{2}{3\times 2^{n+3}-25})^k\left(3\frac{2^k}{(3\times 2^{n+3}-25)^k}+\frac{3^k}{(3\times 2^{n+3}-26)^k}\right). \end{aligned}$$

Proof. Table 2 shows edge partitons of porpyl ether imine dendrimers. From Table 2, we can written

Table 2: The edge partitons of the porpyl ether imine dendrimers.

(d_p, d_q) for $E(\wp)$	(T_p, T_q) for $E(\wp)$	The number of edge
$(1,2)$	$(\frac{1}{3\times2^{n+3}-24}, \frac{2}{3\times2^{n+3}-25})$	2^{n+1}
$(2,2)$	$(\frac{2}{3\times2^{n+3}-25}, \frac{2}{3\times2^{n+3}-25})$	$2^{n+4}-18$
$(2,3)$	$(\frac{2}{3\times2^{n+3}-25}, \frac{3}{3\times2^{n+3}-26})$	$3\times 2^{n+1}-6$

$$TI(\wp) = \sum_{pq\in E_{1,2}}\pi_{pq}+\sum_{pq\in E_{2,2}}\pi_{pq}+\sum_{pq\in E_{2,3}}\pi_{pq} \qquad (1)$$

i. If $\pi_{pq} = (T_p + T_q)^k$ in Eq.(1), then we obtain the following equation

$$\begin{aligned} T_1^k(\wp) &= 2^{n+1}\times(\frac{1}{3\times 2^{n+3}-24}+\frac{2}{3\times 2^{n+3}-25})^k\\ &+ (16\times 2^n-18)\times(\frac{4}{3\times 2^{n+3}-25})^k\\ &+ (6\times 2^n-6)\times(\frac{2}{3\times 2^{n+3}-25}+\frac{3}{3\times 2^{n+3}-26})^k. \end{aligned}$$

The proof is completed by calculated .

ii. If $\pi_{pq} = (T_pT_q)^k$ in Eq.(1), then we obtain the following equation

$$\begin{aligned} T_2^k(\wp) &= 2^{n+1}\times(\frac{12}{3\times(2^{n+3}-24)(3\times 2^{n+3}-25)})^k\\ &+ (16\times 2^n-18)\times(\frac{4}{3\times 2^{n+3}-25})^{2k}\\ &+ (6\times 2^n-6)\times(\frac{6}{(3\times 2^{n+3}-25)(3\times 2^{n+3}-26)})^k. \end{aligned}$$

By some calculated, the proof is completed. □

Figure 2 shows plots a)T_1^k and b)T_2^k of PETIM.

2.2 The poly ethylene amido amine dendrimers

The poly ethylene amido amine (PETAA) have $|V(PETAA)| = 44\times2^n-18$ and $|E(PETAA)| = 44\times2^n-19$ by calculate. Figure 3 shows structure of PETAA.

Theorem 2.2. *Let* $\wp$ *be PETAA. Then*

i The general first temperature index of $\wp$ *is*

$$\begin{aligned} T_1^k(\wp) &= \frac{2^{n+2}}{(11\times 2^{n+2}-19)^k}\left((3+\frac{2}{11\times 2^{n+2}-20})^k+(4+\frac{6}{11\times 2^{n+2}-21})^k\right)\\ &- \frac{2^{k+1}}{(11\times 2^{n+2}-19)^k}(2+\frac{3}{11\times 2^{n+2}-21})^k\\ &+ \frac{1}{(11\times 2^{n+2}-20)^k}\left(2^{2k+3}(2^{n+1}-1)+(5+\frac{3}{11\times 2^{n+2}-21})^k(5\times 2^{n+2}-9)\right). \end{aligned}$$

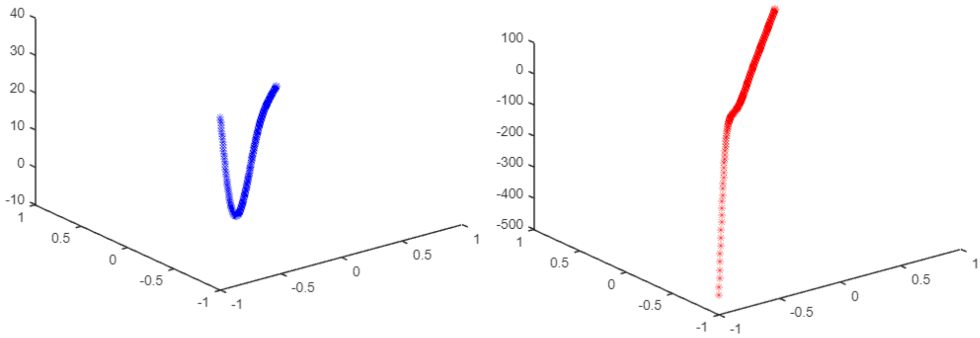

Figure 2: The plots of a)T_1^k, b)T_2^k of PETIM.

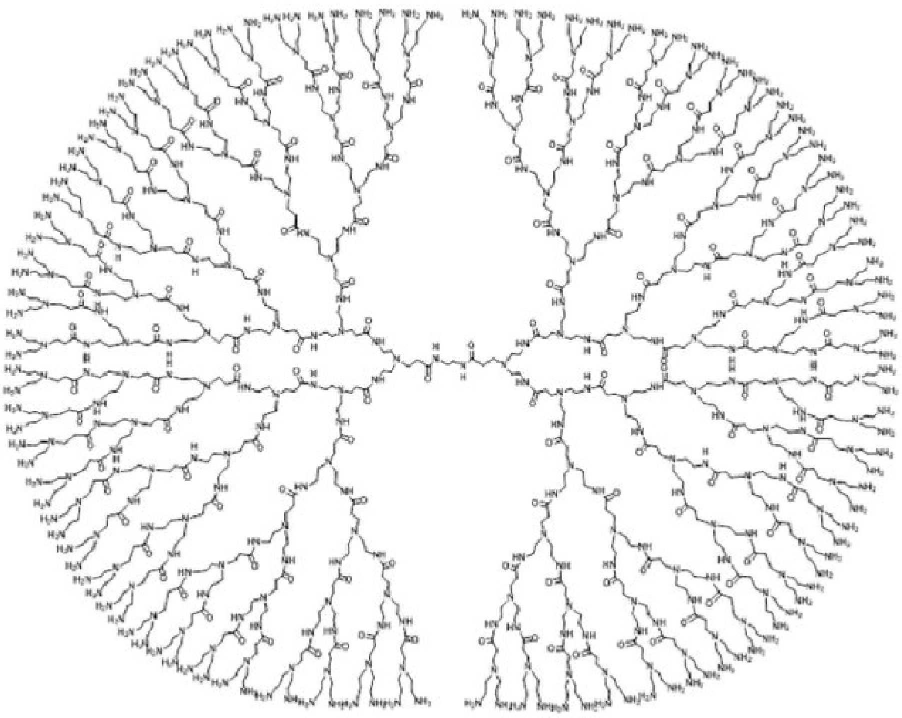

Figure 3: Structure of PETAA

ii. The general second temperature index of $\wp$ *is*

$$\begin{aligned} T_2^k(\wp) &= \frac{2^{n+2}}{(11\times 2^{n+2}-19)^k}\left(\frac{2^k}{(11\times 2^{n+2}-20)^k}+\frac{3^k}{(11\times 2^{n+2}-21)^k}\right) \\ &- \frac{2\times 3^k}{((11\times 2^{n+2}-20)^2-1)^k} \\ &+ \frac{2^k}{(11\times 2^{n+2}-20)^k}\left(\frac{2^{k+3}(2^{n+1}-1)}{(11\times 2^{n+2}-20)^k}+\frac{3^k}{(11\times 2^{n+2}-21)^k}(5\times 2^{n+2}-9)\right). \end{aligned}$$

Proof. Table 3 shows edge partitons of PETAA.

From Table 3, the following equation is obtained

$$\begin{aligned} TI(\wp) &= \sum_{pq\in E_{1,2}}\pi_{pq}+\sum_{pq\in E_{1,3}}\pi_{pq})+\sum_{pq\in E_{2,2}}\pi_{pq} \\ &+ \sum_{pq\in E_{2,3}}\pi_{pq} \end{aligned} \quad (2)$$

Table 3: The edge partitons of the poly ethylene amido amine dendrimer.

(d_p, d_q) for $E(\wp)$	(T_p, T_q) for $E(\wp)$	The number of edge
$(1,2)$	$(\frac{1}{44\times 2^n-19}, \frac{2}{44\times 2^n-20})$	4×2^n
$(1,3)$	$(\frac{1}{44\times 2^n-19}, \frac{3}{44\times 2^n-21})$	$4\times 2^n-2$
$(2,2)$	$(\frac{2}{44\times 2^n-20}, \frac{2}{44\times 2^n-20})$	$16\times 2^n-8$
$(2,3)$	$(\frac{2}{44\times 2^n-20}, \frac{3}{44\times 2^n-21})$	$20\times 2^n-9$

i If $\pi_{pq} = (T_p + T_q)^k$ in Eq.(2), then from Table 5 we have

$$\begin{aligned} T_1^k(\wp) &= (4\times 2^n)\times(\frac{1}{44\times 2^n-19}+\frac{2}{44\times 2^n-20})^k \\ &+ (4\times 2^n-2)\times(\frac{1}{44\times 2^n-19}+\frac{3}{44\times 2^n-21})^k \\ &+ (16\times 2^n-8)\times(\frac{2}{44\times 2^n-20}+\frac{2}{44\times 2^n-20})^k \\ &+ (20\times 2^n-9)\times(\frac{2}{44\times 2^n-20}+\frac{3}{44\times 2^n-21})^k \end{aligned}$$

ii. If $\pi_{pq} = (T_pT_q)^k$ in Eq.(2), then

$$\begin{aligned} T_2^k(\wp) &= (4\times 2^n)\times(\frac{1}{44\times 2^n-19}\times\frac{2}{44\times 2^n-20})^k \\ &+ (4\times 2^n-2)\times(\frac{1}{44\times 2^n-19}\times\frac{3}{44\times 2^n-21})^k \\ &+ (16\times 2^n-8)\times(\frac{2}{44\times 2^n-20}\times\frac{2}{44\times 2^n-20})^k \\ &+ (20\times 2^n-9)\times(\frac{2}{44\times 2^n-20}\times\frac{3}{44\times 2^n-21})^k. \end{aligned}$$

The proof is completed by calculated. □

Figure 4 shows plots a)T_1^k and b)T_2^k of PETAA.

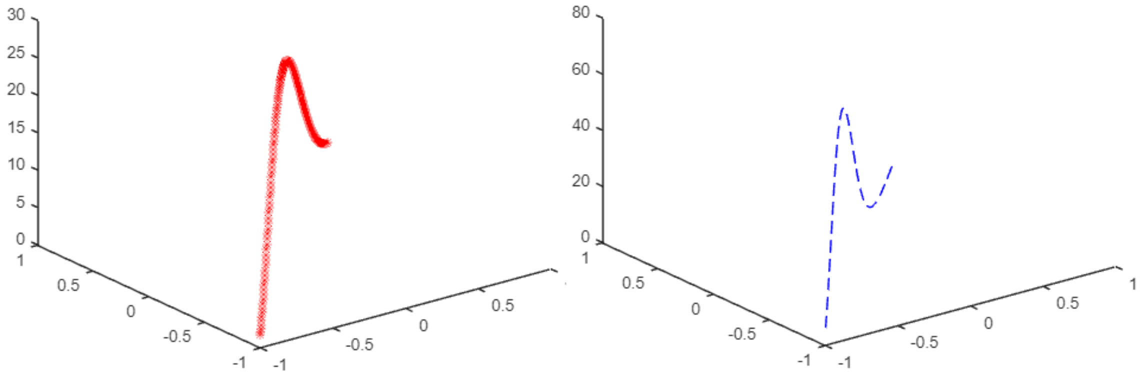

Figure 4: The plots of a)T_1^k, b)T_2^k of PETAA.

3 Conclusions

In this paper, the temperature indices are studied. PETIM and PETAA dendrimers structures are important for chemistry and drug discovery sciences. It is computed the temperature indices of these dendrimers. The results of this study can be used to predict the properties of molecules with these graph structures, saving money and time without experimenting in drug discovery, chemistry, and nanotechnology

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