

Temperature indices of V-Phenylenic nanostructures and Porous Graphene

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Abstract

Topological descriptors are numerical values that are based on the underlying structure of a chemical compound. Chemical graph theory actively utilizes topological indices, particularly in Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Property Relationship (QSPR) research. In this paper, we presented generalized temperature indices of V-Phenylenic Nanotubes, V-Phenylenic Nanotorus and Porous Graphene.

Keywords: Temperature index, V-Phenylenic nanotubes and nanotorus, Porous Graphene

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1. Introduction

Graph theory is a mathematical discipline that deals with the study of graphs, which are mathematical structures consisting of vertices (also called nodes) connected by edges. In recent years, graph theory has found numerous applications in various fields, including chemistry, computer science, biology, and social networks. One important aspect of graph theory is the characterization and quantification of graph properties through topological indices (*cf.* [16]-[19]). Topological indices are numerical parameters associated with graphs that provide valuable information about their structural and chemical properties. These indices capture specific structural features of graphs and are widely used in different branches of science and engineering and many indices have some applications in chemistry, especially in QSPR/QSAR studies (*cf.* [8, 11], [13]-[15], [22, 25, 26]).




For a simple graph \mathcal{G} , we denote the vertex set

$$\mathcal{V}(\mathcal{G}) = \{x_1, x_2, x_3, \dots, x_n\}$$

and the edge set by

$$\mathcal{E}(\mathcal{G}) = \{\epsilon_1, \epsilon_2, \epsilon_3, \dots, \epsilon_n\}.$$

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The degree of a vertex $x \in \mathcal{V}(\mathcal{G})$ is denoted by d_x .

In [3], Fajtlowicz defined the temperature of a vertex x , it is defined as

$$\psi(x) = \frac{d_x}{n - d_x},$$

where n is the number of vertices of \mathcal{G} .

In [12], Kulli defined the temperature indices as follows:

The general first temperature index,

$$\psi_1(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y)]^\alpha.$$

The first hyper temperature index,

$$HT_1(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y)]^2.$$

The sum connectivity temperature index,

$$ST(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y)]^{-\frac{1}{2}}.$$

Let \times denote the classical multiplication.

Then, the general second temperature index,

$$\psi_2(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) \times \psi(y)]^\alpha.$$

The second hyper temperature index,

$$HT_2(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) \times \psi(y)]^2.$$

The product connectivity index,

$$PT(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) \times \psi(y)]^{-\frac{1}{2}}.$$

The reciprocal product connectivity index,

$$RPT(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) \times \psi(y)]^{\frac{1}{2}}.$$

The general temperature index,

$$\psi_\alpha(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x)^\alpha + \psi(y)^\alpha].$$

The F-temperature index,

$$FT(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x)^2 + \psi(y)^2].$$

Lokesha et al. [20] introduced VL-temperature index

$$VLTI(\mathcal{G}) = \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y) + \psi(x)\psi(y)].$$

Farahani et al. [6] studied the second Hyper-Zagreb index of molecular graphs V-Phenylenic Nanotubes and V-Phenylenic Nanotorus. Motivated from this studies, we formulated the results of various temperature indices of V-Phenylenic Nanotubes, V-Phenylenic Nanotorus and Porous Graphene.

1.1. Preliminaries

V-Phenylenic Nanotubes $[VPHX[q, p](\forall p, q \in \mathbb{N} - \{1\})]$ and V-Phenylenic Nanotorus $[VPHY[m, n](\forall m, n \in \mathbb{N} - \{1\})]$ are two types of Nanostructures whose architectures are made up of cycles with distinct compounds of lengths of four, six, and eight. A square net embedded on the toroidal surface can be used to build the innovative Phenylenic and Naphthylenic lattices that are suggested (cf. [1], [4]-[7], [10, 21]).

1.2. Methodology

We obtained the results by using analytical method, edge partition method, graph theoretical method, degree sum method. Also we used MATLAB and MAPLE 2015 for graphical representations.

2. Main results

2.1. V-Phenylenic Nanotubes $VPHX[q, p](\forall p, q \in \mathbb{N} - \{1\})$

Let \mathcal{G} be the molecular graph of V-Phenylenic Nanotubes $VPHX[q, p](\forall p, q \in \mathbb{N} - \{1\})$, in which first row and column represent the number of hexagons by integer numbers q and p .

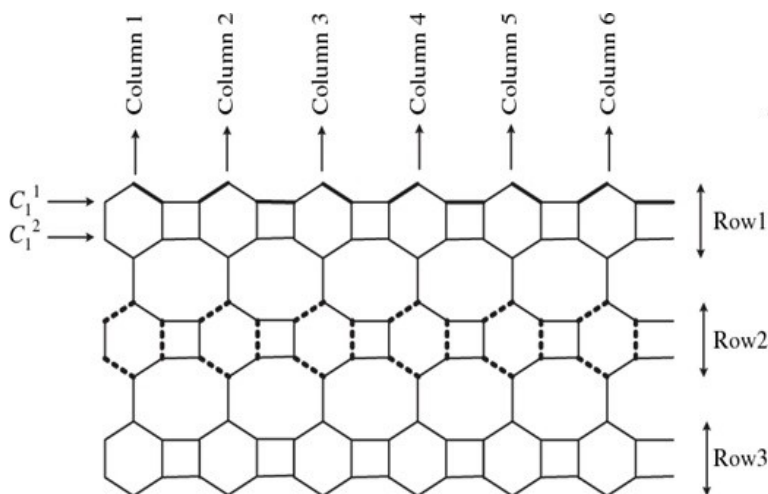


Figure 1. V-Phenylenic Nanotubes $VPHX[q, p]$

From general structure of this V-Phenylenic Nanotube, we can observe that $6pq$ number of atoms or vertices and $9pq - q$ number of bonds or edges of \mathcal{G} .

$$\begin{aligned} \text{i.e., } |V(VPHX[q, p])| &= 6pq, \quad \forall p, q \in \mathbb{N} - \{1\}, \\ |E(VPHX[q, p])| &= 9pq - q. \end{aligned}$$

Edge partition of V-Phenylenic Nanotube is given below

$$\mathcal{E}_{2,3} = 4q \quad \text{and} \quad \mathcal{E}_{3,3} = 9pq - 5q.$$

Here the vertices with degree sequences are 2 and 3. If $d_x = 2$, temperature of the vertex x is

$$\psi(x) = \frac{d_x}{n - d_x} = \frac{2}{6pq - 2} = \frac{1}{3pq - 1}.$$

If $d_x = 3$, temperature of the vertex x is

$$\psi(x) = \frac{d_x}{n - d_x} = \frac{3}{6pq - 3} = \frac{1}{2pq - 1}.$$

Theorem 2.1. The general first temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by

$$\psi_1^\alpha(\mathcal{G}) = 4q \left[\frac{5pq - 2}{(3pq - 1)(2pq - 1)} \right]^\alpha + (9pq - 5q) \left(\frac{2}{2pq - 1} \right)^\alpha. \tag{2.1}$$

Proof. From the edge partition of $VPHX[q, p]$, the general first temperature index,

$$\begin{aligned} \psi_1^\alpha(\mathcal{G}) &= \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y)]^\alpha \\ &= \mathcal{E}_{2,3} [\psi(x) + \psi(y)]^\alpha + \mathcal{E}_{3,3} [\psi(x) + \psi(y)]^\alpha \\ &= 4q \left[d \frac{1}{3pq - 1} + \frac{1}{2pq - 1} \right]^\alpha + (9pq - 5q) \left[\frac{2}{2pq - 1} \right]^\alpha \end{aligned}$$

which gives the assertion of theorem. □

Corollary 2.2. The first hyper temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by

$$HT_1(\mathcal{G}) = 4q \left[\frac{5pq - 2}{(3pq - 1)(2pq - 1)} \right]^2 + (9pq - 5q) \left(\frac{2}{2pq - 1} \right)^2.$$

Corollary 2.3. The sum connectivity temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by

$$ST(\mathcal{G}) = 4q \left[\frac{5pq - 2}{(3pq - 1)(2pq - 1)} \right]^{-\frac{1}{2}} + (9pq - 5q) \left(\frac{2}{2pq - 1} \right)^{-\frac{1}{2}}.$$

Proof. In equation (2.1), put $\alpha = 2, -\frac{1}{2}$, we obtain the Corollary 2.2 and Corollary 2.3 respectively. □

Theorem 2.4. The general second temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by

$$\psi_2^\alpha(\mathcal{G}) = 4q \left[\frac{1}{(3pq - 1)(2q - 1)} \right]^\alpha + (9pq - 5q) \left(\frac{1}{2pq - 1} \right)^\alpha. \tag{2.2}$$

Proof. From the edge partition of $VPHX[q, p]$, the general second temperature index,

$$\begin{aligned} \psi_2^\alpha(\mathcal{G}) &= \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x)\psi(y)]^\alpha \\ &= \mathcal{E}_{2,3} [\psi(x)\psi(y)]^\alpha + \mathcal{E}_{3,3} [\psi(x)\psi(y)]^\alpha \end{aligned}$$

which gives the assertion of theorem. □

Corollary 2.5. The second hyper temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by

$$HT_2(\mathcal{G}) = 4q \left[\frac{1}{(3pq - 1)(2pq - 1)} \right]^2 + (9pq - 5q) \left(\frac{1}{2pq - 1} \right)^2.$$

Corollary 2.6. The product connectivity temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by

$$PT(\mathcal{G}) = 4q \sqrt{(3pq - 1)(2pq - 1)} + (9pq - 5q) \sqrt{(2pq - 1)}.$$

Corollary 2.7. The reciprocal product connectivity temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by

$$RPT(\mathcal{G}) = \frac{4q}{\sqrt{(3pq - 1)(2pq - 1)}} + \frac{(9pq - 5q)}{\sqrt{(2pq - 1)}}.$$

Proof. In equation (2.2), put $\alpha = 2, -\frac{1}{2}, \frac{1}{2}$, we obtain the Corollary 2.5, Corollary 2.6 and Corollary 2.7 respectively. □

Theorem 2.8. *The general temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by*

$$\psi_\alpha(\mathcal{G}) = 4q \left[\frac{1}{(3pq - 1)^\alpha} + \frac{1}{(2q - 1)^\alpha} \right] + (9pq - 5q) \left(\frac{2}{(2pq - 1)^\alpha} \right). \tag{2.3}$$

Proof. From the edge partition of $VPHX[q, p]$, the general temperature index,

$$\begin{aligned} \psi_\alpha(\mathcal{G}) &= \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x)^\alpha + \psi(y)^\alpha] \\ &= \mathcal{E}_{2,3} [\psi(x)^\alpha + \psi(y)^\alpha] + \mathcal{E}_{3,3} [\psi(x)^\alpha + \psi(y)^\alpha] \\ &= 4q \left[\left(\frac{1}{3pq - 1} \right)^\alpha + \left(\frac{1}{2pq - 1} \right)^\alpha \right] + (9pq - 5q) \left[\left(\frac{1}{2pq - 1} \right)^\alpha + \left(\frac{1}{2pq - 1} \right)^\alpha \right] \end{aligned}$$

which gives the assertion of theorem. □

By replacing $\alpha = 2$ in equation (2.3), we get the following result.

Corollary 2.9. *The F-temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by*

$$FT(\mathcal{G}) = 4q \left[\frac{1}{(3pq - 1)^2} + \frac{1}{(2q - 1)^2} \right] + (9pq - 5q) \left(\frac{2}{(2pq - 1)^2} \right).$$

Theorem 2.10. *VL-temperature index of V-Phenylenic Nanotubes $VPHX[q, p]$ is given by*

$$VLTI(\mathcal{G}) = 2q \left[\frac{5pq - 1}{(3pq - 1)(2pq - 1)} \right] + \frac{(9pq - 5q)}{2} \left[\frac{4pq - 1}{(2pq - 1)^2} \right]. \tag{2.4}$$

Proof. From the edge partition of $VPHX[q, p]$, the VL-temperature index,

$$\begin{aligned} VLTI(\mathcal{G}) &= \frac{1}{2} \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x) + \psi(y) + \psi(x)\psi(y)] \\ &= \mathcal{E}_{2,3} [\psi(x) + \psi(y) + \psi(x)\psi(y)] + \mathcal{E}_{3,3} [\psi(x) + \psi(y) + \psi(x)\psi(y)] \\ &= 2q \left[\frac{1}{3pq - 1} + \frac{1}{2pq - 1} + \frac{1}{3pq - 1} \times \frac{1}{2pq - 1} \right] + \frac{(9pq - 5q)}{2} \left[\frac{2}{2pq - 1} + \frac{1}{(2pq - 1)^2} \right] \end{aligned}$$

which gives the assertion of theorem. □

2.2. V-Phenylenic Nanotorus $VPHY[m, n](\forall m, n \in \mathbb{N} - \{1\})$

Let \mathcal{H} be the molecular graph of V-Phenylenic Nanotorus $VPHY[m, n]$, in which first row and column represent the number of hexagons by integer number m and n .

The number of atoms or vertices of $VPHY[m, n] = 6mn$.

The number of bonds or edges of $VPHY[m, n] = 9mn$.

Edge partition of V-Phenylenic Nanotorus is $\mathcal{E}_{3,3} = 9mn$.

Here all the vertices are of degree 3. If $d_x = 3$, temperature of the vertex x is

$$\psi(x) = \frac{d_x}{n - d_x} = \frac{3}{6mn - 3} = \frac{1}{2mn - 1}.$$

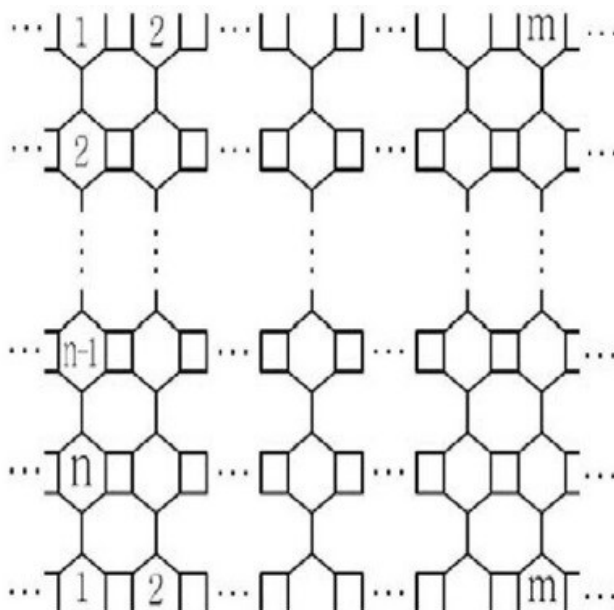


Figure 2. V-Phenylenic Nanotorus $VPHY[m, n]$

Theorem 2.11. *The general first temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$\psi_1^\alpha(\mathcal{H}) = 9mn \left[\frac{2}{(2mn - 1)} \right]^\alpha. \tag{2.5}$$

Proof. From the edge partition of $VPHY[m, n]$, the general first temperature index,

$$\begin{aligned} \psi_1^\alpha(\mathcal{H}) &= \sum_{x,y \in \mathcal{E}(\mathcal{H})} [\psi(x) + \psi(y)]^\alpha \\ &= \mathcal{E}_{3,3} [\psi(x) + \psi(y)]^\alpha \\ &= 9mn \left[\frac{1}{2mn - 1} + \frac{1}{2mn - 1} \right]^\alpha \end{aligned}$$

which gives the assertion of theorem. □

Corollary 2.12. *The first hyper temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$HT_1(\mathcal{H}) = 9mn \left[\frac{2}{(2mn - 1)} \right]^2.$$

Corollary 2.13. *The sum connectivity temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$ST(\mathcal{H}) = \frac{9}{\sqrt{2}} mn \sqrt{(2mn - 1)}.$$

Proof. In equation (2.5), put $\alpha = 2, -\frac{1}{2}$, we obtain the Corollary 2.12 and Corollary 2.13 respectively. □

Theorem 2.14. *The general second temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$\psi_2^\alpha(\mathcal{H}) = 9mn \left[\frac{1}{(2mn - 1)} \right]^{2\alpha}. \tag{2.6}$$

Proof. From the edge partition of $VPHY[m, n]$, the general second temperature index,

$$\begin{aligned} \psi_2^\alpha(\mathcal{H}) &= \sum_{x,y \in \mathcal{E}(\mathcal{H})} [\psi(x)\psi(y)]^\alpha \\ &= \mathcal{E}_{3,3} [\psi(x)\psi(y)]^\alpha \\ &= 9mn \left[\frac{1}{(2mn-1)(2mn-1)} \right]^\alpha \end{aligned}$$

which gives the assertion of theorem. □

Corollary 2.15. *The second hyper temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$HT_2(\mathcal{H}) = 9mn \left[\frac{1}{(2mn-1)} \right]^4.$$

Corollary 2.16. *The product connectivity temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$PT(\mathcal{H}) = 9mn(2mn-1).$$

Corollary 2.17. *The reciprocal product connectivity temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$RPT(\mathcal{H}) = \frac{9mn}{2mn-1}.$$

Proof. In equation (2.6), put $\alpha = 2, -\frac{1}{2}, \frac{1}{2}$, we obtain the Corollary 2.15, Corollary 2.16 and Corollary 2.17 respectively. □

Theorem 2.18. *The general temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$\psi_\alpha(\mathcal{H}) = 18mn \left[\frac{1}{(2mn-1)} \right]^\alpha. \tag{2.7}$$

Proof. From the edge partition of $VPHY[m, n]$, the general temperature index,

$$\begin{aligned} \psi_\alpha(\mathcal{H}) &= \sum_{x,y \in \mathcal{E}(\mathcal{G})} [\psi(x)^\alpha + \psi(y)^\alpha] \\ &= \mathcal{E}_{3,3} [\psi(x)^\alpha + \psi(y)^\alpha] \\ &= 9mn \left[\left(\frac{1}{2mn-1} \right)^\alpha + \left(\frac{1}{2mn-1} \right)^\alpha \right] \end{aligned}$$

which gives the assertion of theorem. □

Corollary 2.19. *The F-temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$FT(\mathcal{H}) = 18mn \left[\frac{1}{(2mn-1)} \right]^2.$$

By replacing $\alpha = 2$ in equation (2.7), we get the result.

Theorem 2.20. *The VL-temperature index of V-Phenylenic Nanotorus $VPHY[m, n]$ is given by*

$$VLTl(\mathcal{H}) = \frac{9mn}{2} \left[\frac{4mn-1}{(2mn-1)^2} \right]. \tag{2.8}$$

Proof. From the edge partition of $VPHY[m, n]$, the VL -temperature index,

$$\begin{aligned} VLTl(\mathcal{H}) &= \sum_{x,y \in \mathcal{E}(\mathcal{H})} [\psi(x) + \psi(y) + \psi(x)\psi(y)] \\ &= \mathcal{E}_{3,3} [\psi(x) + \psi(y) + \psi(x)\psi(y)] \\ &= \frac{9mn}{2} \left[\frac{1}{2mn-1} + \frac{1}{2mn-1} + \frac{1}{2mn-1} \times \frac{1}{2mn-1} \right] \end{aligned}$$

which gives the assertion of theorem. □

2.3. Porous Graphene $\mathcal{P}[s, t]$

Theoretical and practical investigations in Chemistry are being drawn to the significant and fascinating substance known as Graphene. Because of its unique properties and applications, Graphene is helpful in the field of material science. Nanopores in the plane of Porous Graphene, a material similar to Graphene. Because there are nanopores in the Graphene plane, Porous Graphene exhibits unique features. As a result, Porous Graphene has uses in the separation of gases, hydrogen storage, DNA sequencing, biosensors, diagnostics, and DNA sensors that are useful in the use of sensors and super capacitors (cf. [2, 9, 27]). Figure 3 depicts the structure of Porous Graphene. Additionally, the six hexagon structure is connected linearly row-wise and column-wise by edges between two carbon atoms. The structure consists of six hexagons.

The molecular graph of Porous Graphene $G = \mathcal{P}[4, 4]$, a six-carbon grid with four rows and four columns in the plane, is shown in Figure 3. In general, if there are s and t , respectively, rows and columns (cf. [23, 24]).

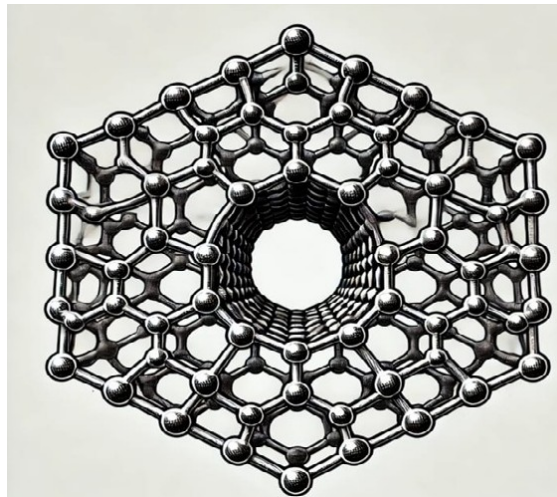


Figure 3. Porous Graphene $\mathcal{P}[4, 4]$

Let $\mathcal{P}[s, t]$ be the molecular graph of Porous Graphene with $12st + 12s + 12t$ vertices and $15st + 14s + 14t - 1$ edges.

Edge partition of Porous Graphene is given below

$$\begin{aligned} \mathcal{E}_{2,2} &= 4s + 4t + 4, \\ \mathcal{E}_{2,3} &= 12st + 8s + 8t - 4, \\ \mathcal{E}_{3,3} &= 3st + 2s + 2t - 1. \end{aligned}$$

Here the vertices with degree sequences are 2 and 3. If $d_x = 2$, temperature of the vertex x is

$$\psi(x) = \frac{d_x}{n - d_x} = \frac{2}{12st + 12s + 12t - 2}.$$

If $d_x = 3$, temperature of the vertex x is

$$\psi(x) = \frac{d_x}{n - d_x} = \frac{3}{12st + 12s + 12t - 3}.$$

Theorem 2.21. *The general first temperature index of Porous Graphene $\mathcal{P}(s, t)$ is given by*

$$\begin{aligned} \psi_1^\alpha(\mathcal{P}) &= (4s + 4t + 4) \left[\frac{4}{12st + 12s + 12t - 2} \right]^\alpha \\ &+ (12st + 8s + 8t - 4) \left[\frac{12(5st + 5s + 5t - 1)}{(12st + 12s + 12t - 2)(12st + 12s + 12t - 3)} \right]^\alpha \\ &+ (3st + 2s + 2t - 1) \left[\frac{6}{12st + 12s + 12t - 3} \right]^\alpha. \end{aligned} \tag{2.9}$$

Proof. From the edge partition of \mathcal{P} , the general first temperature index,

$$\begin{aligned} \psi_1^\alpha(\mathcal{P}) &= \sum_{x,y \in \mathcal{E}(\mathcal{P})} [\psi(x) + \psi(y)]^\alpha \\ &= \mathcal{E}_{2,2} [\psi(x) + \psi(y)]^\alpha + \mathcal{E}_{2,3} [\psi(x) + \psi(y)]^\alpha + \mathcal{E}_{3,3} [\psi(x) + \psi(y)]^\alpha \\ &= (4s + 4t + 4) \left[\frac{2}{12st + 12s + 12t - 2} + \frac{2}{12st + 12s + 12t - 2} \right]^\alpha \\ &+ (12st + 8s + 8t - 4) \left[\frac{2}{(12st + 12s + 12t - 2)} + \frac{3}{(12st + 12s + 12t - 3)} \right]^\alpha \\ &+ (3st + 2s + 2t - 1) \left[\frac{3}{12st + 12s + 12t - 3} + \frac{3}{12st + 12s + 12t - 3} \right]^\alpha \end{aligned}$$

which gives the assertion of theorem. □

Corollary 2.22. *The first hyper temperature index of Porous Graphene $\mathcal{P}(s, t)$ is given by*

$$\begin{aligned} HT_1(\mathcal{P}) &= (4s + 4t + 4) \left[\frac{4}{12st + 12s + 12t - 2} \right]^2 \\ &+ (12st + 8s + 8t - 4) \left[\frac{12(5st + 5s + 5t - 1)}{(12st + 12s + 12t - 2)(12st + 12s + 12t - 3)} \right]^2 \\ &+ (3st + 2s + 2t - 1) \left[\frac{6}{12st + 12s + 12t - 3} \right]^2. \end{aligned}$$

Corollary 2.23. *The sum connectivity temperature index of Porous Graphene $\mathcal{P}(s, t)$ is given by*

$$\begin{aligned} ST(\mathcal{P}) &= (4s + 4t + 4) \left[\frac{4}{12st + 12s + 12t - 2} \right]^{-\frac{1}{2}} \\ &+ (12st + 8s + 8t - 4) \left[\frac{12(5st + 5s + 5t - 1)}{(12st + 12s + 12t - 2)(12st + 12s + 12t - 3)} \right]^{-\frac{1}{2}} \\ &+ (3st + 2s + 2t - 1) \left[\frac{6}{12st + 12s + 12t - 3} \right]^{-\frac{1}{2}}. \end{aligned}$$

Proof. In equation (2.9), put $\alpha = 2, -\frac{1}{2}$, we obtain the Corollary 2.22 and Corollary 2.23 respectively. □

Theorem 2.24. The general second temperature index of Porous Graphene $\mathcal{P}(s, t)$ is given by

$$\begin{aligned} \psi_2^\alpha(\mathcal{P}) &= (4s + 4t + 4) \left[\frac{1}{6st + 6s + 6t - 1} \right]^{2\alpha} \\ &\quad + (12st + 8s + 8t - 4) \left[\frac{1}{(6st + 6s + 6t - 1)(4st + 4s + 4t - 1)} \right]^\alpha \\ &\quad + (3st + 2s + 2t - 1) \left[\frac{1}{4st + 4s + 4t - 1} \right]^{2\alpha}. \end{aligned} \tag{2.10}$$

Proof. From the edge partition of \mathcal{P} , the general first temperature index,

$$\begin{aligned} \psi_2(\mathcal{P}) &= \sum_{x,y \in \mathcal{E}(\mathcal{P})} [\psi(x) \times \psi(y)]^\alpha \\ &= \mathcal{E}_{2,2} [\psi(x) \times \psi(y)]^\alpha + \mathcal{E}_{2,3} [\psi(x) \times \psi(y)]^\alpha + \mathcal{E}_{3,3} [\psi(x) \times \psi(y)]^\alpha. \\ &= (4s + 4t + 4) \left[\frac{2}{12st + 12s + 12t - 2} \times \frac{2}{12st + 12s + 12t - 2} \right]^\alpha \\ &\quad + (12st + 8s + 8t - 4) \left[\frac{2}{(12st + 12s + 12t - 2)} \times \frac{2}{(12st + 12s + 12t - 3)} \right]^\alpha \\ &\quad + (3st + 2s + 2t - 1) \left[\frac{3}{12st + 12s + 12t - 3} \times \frac{3}{12st + 12s + 12t - 3} \right]^\alpha \end{aligned}$$

which gives the assertion of theorem. □

Corollary 2.25. The second hyper temperature index of Porous Graphene $\mathcal{P}[s, t]$ is given by

$$\begin{aligned} HT_2(\mathcal{P}) &= (4s + 4t + 4) \left[\frac{1}{6st + 6s + 6t - 1} \right]^4 \\ &\quad + (12st + 8s + 8t - 4) \left[\frac{1}{(6st + 6s + 6t - 1)(4st + 4s + 4t - 1)} \right]^2 \\ &\quad + (3st + 2s + 2t - 1) \left[\frac{1}{4st + 4s + 4t - 1} \right]^4. \end{aligned}$$

Corollary 2.26. The product connectivity temperature index of Porous Graphene $\mathcal{P}[s, t]$ is given by

$$\begin{aligned} PT(\mathcal{P}) &= (4s + 4t + 4)(6st + 6s + 6t - 1) \\ &\quad + (12st + 8s + 8t - 4) \sqrt{(6st + 6s + 6t - 1)(4st + 4s + 4t - 1)} \\ &\quad + (3st + 2s + 2t - 1)(4st + 4s + 4t - 1). \end{aligned}$$

Corollary 2.27. The reciprocal product connectivity temperature index of Porous Graphene $\mathcal{P}[s, t]$ is given by

$$\begin{aligned} RPT(\mathcal{P}) &= (4s + 4t + 4) \left[\frac{1}{6st + 6s + 6t - 1} \right] \\ &\quad + (12st + 8s + 8t - 4) \left[\frac{1}{\sqrt{(6st + 6s + 6t - 1)(4st + 4s + 4t - 1)}} \right] \\ &\quad + (3st + 2s + 2t - 1) \left[\frac{1}{4st + 4s + 4t - 1} \right]. \end{aligned}$$

Proof. In equation (2.10), put $\alpha = 2, -\frac{1}{2}, \frac{1}{2}$, we obtain the Corollary 2.25, Corollary 2.26 and Corollary 2.27 respectively. □

Theorem 2.28. The general temperature index of Porous Graphene $\mathcal{P}(s, t)$ is given by

$$\begin{aligned} \psi_\alpha(\mathcal{P}) &= (8s + 8t + 8) \left[\frac{1}{6st + 6s + 6t - 1} \right]^\alpha \\ &\quad + (12st + 8s + 8t - 4) \left(\left[\frac{1}{6st + 6s + 6t - 1} \right]^\alpha + \left[\frac{1}{4st + 4s + 4t - 1} \right]^\alpha \right) \\ &\quad + (6st + 4s + 4t - 2) \left[\frac{1}{4st + 4s + 4t - 1} \right]^\alpha. \end{aligned} \tag{2.11}$$

Proof. From the edge partition of \mathcal{P} , the general temperature index,

$$\begin{aligned} \psi_\alpha(\mathcal{P}) &= \sum_{x,y \in \mathcal{E}(\mathcal{P})} [\psi(x)^\alpha + \psi(y)^\alpha] \\ &= \mathcal{E}_{2,2} [\psi(x)^\alpha + \psi(y)^\alpha] + \mathcal{E}_{2,3} [\psi(x)^\alpha + \psi(y)^\alpha] + \mathcal{E}_{3,3} [\psi(x)^\alpha + \psi(y)^\alpha] \\ &= (4s + 4t + 4) \left[\left(\frac{2}{12st + 12s + 12t - 2} \right)^\alpha + \left(\frac{2}{12st + 12s + 12t - 2} \right)^\alpha \right] \\ &\quad + (12st + 8s + 8t - 4) \left[\left(\frac{2}{12st + 12s + 12t - 2} \right)^\alpha + \left(\frac{3}{12st + 12s + 12t - 3} \right)^\alpha \right] \\ &\quad + (3st + 2s + 2t - 1) \left[\left(\frac{3}{12st + 12s + 12t - 3} \right)^\alpha + \left(\frac{3}{12st + 12s + 12t - 3} \right)^\alpha \right] \\ &= 2(4s + 4t + 4) \left[\frac{2}{12st + 12s + 12t - 2} \right]^\alpha \\ &\quad + (12st + 8s + 8t - 4) \left[\left(\frac{2}{12st + 12s + 12t - 2} \right)^\alpha + \left(\frac{3}{12st + 12s + 12t - 3} \right)^\alpha \right] \\ &\quad + 2(3st + 2s + 2t - 1) \left[\frac{3}{12st + 12s + 12t - 3} \right]^\alpha \end{aligned}$$

which gives the assertion of theorem. □

Corollary 2.29. The F -temperature index of Porous Graphene $\mathcal{P}[s, t]$ is given by

$$\begin{aligned} FT(\mathcal{P}) &= (8s + 8t + 8) \left[\frac{1}{6st + 6s + 6t - 1} \right]^2 \\ &\quad + (12st + 8s + 8t - 4) \left(\left[\frac{1}{6st + 6s + 6t - 1} \right]^2 + \left[\frac{1}{4st + 4s + 4t - 1} \right]^2 \right) \\ &\quad + (6st + 4s + 4t - 2) \left[\frac{1}{4st + 4s + 4t - 1} \right]^2. \end{aligned}$$

Proof. In equation (2.11), put $\alpha = 2$, we obtain the Corollary 2.29. □

Theorem 2.30. The VL -temperature index of Porous Graphene $\mathcal{P}(s, t)$ is given by

$$\begin{aligned} VLTI(\mathcal{P}) &= (2s + 2t + 2) \left[\frac{12st + 12s + 12t - 1}{(6st + 6s + 6t - 1)^2} \right] \\ &\quad + (12st + 8s + 8t - 4) \left[\frac{(5st + 5s + 5t - 1)}{(6st + 6s + 6t - 1)(4st + 4s + 4t - 1)} \right] \end{aligned} \tag{2.12}$$

$$+ \frac{(3st + 2s + 2t - 1)}{2} \left[\frac{8st + 8s + 8t - 1}{(4st + 4s + 4t - 1)^2} \right]. \tag{2.13}$$

Proof. From the edge partition of \mathcal{P} , the VL-temperature index,

$$\begin{aligned}
 VLTI(\mathcal{P}) &= \sum_{x,y \in \mathcal{E}(\mathcal{P})} [\psi(x) + \psi(y) + \psi(x)\psi(y)] \\
 &= \mathcal{E}_{2,2} [\psi(x) + \psi(y) + \psi(x)\psi(y)] + \mathcal{E}_{2,3} [\psi(x) + \psi(y) + \psi(x) + \psi(y)] + \mathcal{E}_{3,3} [\psi(x) + \psi(y) + \psi(x)\psi(y)] \\
 &= \frac{(4s + 4t + 4)}{2} \left[\frac{2}{12st + 12s + 12t - 2} + \frac{2}{12st + 12s + 12t - 2} + \frac{4}{(12st + 12s + 12t - 2)^2} \right] \\
 &\quad + \frac{(12st + 8s + 8t - 4)}{2} \left[\frac{2}{(12st + 12s + 12t - 2)} + \frac{3}{(12st + 12s + 12t - 3)} \right. \\
 &\quad \left. + \frac{6}{(12st + 12s + 12t - 2)(12st + 12s + 12t - 3)} \right] \\
 &\quad + \frac{(3st + 2s + 2t - 1)}{2} \left[\frac{3}{12st + 12s + 12t - 3} + \frac{3}{12st + 12s + 12t - 3} + \frac{9}{(12st + 12s + 12t - 3)^2} \right]
 \end{aligned}$$

which gives the assertion of theorem. \square

3. Conclusion

Biological and chemical properties of molecular structures are essential for drug design in medical science. Topological indices are used for predicting these properties in QSAR/QSPR studies. We computed the temperature indices of molecular structure of V-Phenylenic Nanotubes $VPHX[q, p]$, V-Phenylenic Nanotorus $VPHY[m, n]$ and Porous Graphene $\mathcal{P}[s, t]$. This result will help us to predict many chemical and physical properties of nanotubes and graphene.

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