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The (*a*, *b*)-Temperature Index of *H*-Naphtalenic Nanotubes

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Abstract, Recently, some temperature indices of a graph were introduced and studied. In this paper, we introduce the (*a, b*)-temperature index of a graph. Also we compute the (*a, b*)-temperature index for *H*-Naphtalenic nanotubes and compute some other temperature indices for some other particular values of *a* and *b* for *H*-Naphtalenic nanotubes.

Keywords: Connectivity temperature index, *F*-temperature index, (*a, b*)-temperature index, nanotube

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*35

1. Introduction

A molecular graph is a simple graph, representing the carbon atom skeleton of an organic molecule of the hydrocarbon. Therefore the vertices of a molecular graph represent the carbon atoms and its edges the carbon-carbon bonds. Chemical Graph Theory is a branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. Several graph indices have found some applications in Chemistry, especially in QSPR/QSAR research [1, 2, 3].

Throughout this paper, we consider simple graphs which are finite, connected, undirected graphs without loops and multiple edges. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. For term and concept not given here, we refer [4].

In [5], Fajtlowicz defined the temperature of a vertex u of a graph G as

$$T(u)=\frac{d_G(u)}{n-d_G(u)}, \text{ where } |V(G)| = n.$$

The second hyper temperature index and general second temperature index of a graph were introduced by Kulli in [6] and they are defined as

$$HT_2(G)=\sum_{uv\in E(G)}\left[T(u)T(v)\right]^2,$$

$$T_2^a(G)=\sum_{uv\in E(G)}\left[T(u)T(v)\right]^a,$$

where a is a real number.

Also in the same paper [6], Kulli introduced the product connectivity temperature index, reciprocal product connectivity temperature index, F-temperature index of a graph and they are defined as

$$PT(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{T(u)T(v)}},$$
$$RPT(G)=\sum_{uv\in E(G)}\sqrt{T(u)T(v)},$$
$$FT(G)=\sum_{uv\in E(G)}\left[T(u)^2+T(v)^2\right].$$

We introduce the symmetric division temperature index of a graph, defined as

$$SDT(G)=\sum_{uv\in E(G)}\left(\frac{T(u)}{T(v)}+\frac{T(v)}{T(u)}\right).$$

We now introduce the first and second Gourava temperature indices of a graph G, defined as

$$GT_1(G)=\sum_{uv\in E(G)}\left[T(u)+T(v)+T(u)T(v)\right].$$
$$GT_2(G)=\sum_{uv\in E(G)}\left[T(u)+T(v)\right]T(u)T(v).$$

The general temperature index was introduced by Kulli in [6] and this index is defined as

$$T_a(G)=\sum_{uv\in E(G)}\left[T(u)^a+T(v)^a\right],$$

where a is a real number.

Motivated by the work on degree based temperature indices, we define the (a, b)-temperature index of a graph G as

$$T_{a,b}(G)=\sum_{uv\in E(G)}\left[T(u)^a\,T(v)^b+T(u)^b\,T(v)^a\right],$$

where a, b are real numbers.

Recently, some temperature indices were introduced and studied such as multiplicative first and second temperature indices [7], general vertex temperature index [8], multiplicative (a, b)-temperature index [9]. Recently, some new topological indices were studied in [10, 11, 12, 13, 14, 15, 16, 17, 18, 19].

In this paper, we compute the (a, b)-temperature index and some other temperature indices for particular values of a and b for H-Naphtalenic nanotubes. For more information about this nanotube, see [20].

2. Observations

We observe the following observations between the (a, b)-temperature index with some other temperature indices.

(1) $HT_2(G)=\frac{1}{2}T_{2,2}(G).$ (2) $T_2^a(G)=\frac{1}{2}T_{a,a}(G).$

(3) $PT(G)=\frac{1}{2}T_{-\frac{1}{2},-\frac{1}{2}}(G).$ (4) $RPT(G)=\frac{1}{2}T_{\frac{1}{2},\frac{1}{2}}(G).$

(5) $FT(G)=T_{2,0}(G).$ (6) $SDT(G)=T_{1,-1}(G).$

(7) $GT_2(G)=T_{2,1}(G).$ (8) $T_a(G)=T_{a,0}(G).$

3. Results for H-Naphtalenic nanotubes

In this section we consider a family of *H*-Naphtalenic nanotubes. This nanotube is a trivalent decoration having a sequence of C_6, C_6, C_4, C_6, C_6, C_4, … in the first row and a sequence of C_6, C_8, C_6, C_8, … in other row. This nanotube is denoted by $NHPX[m, n]$, where m is the number of pair of hexagons in first row and n is the number of alternative hexagons in a column as shown in Figure 1.

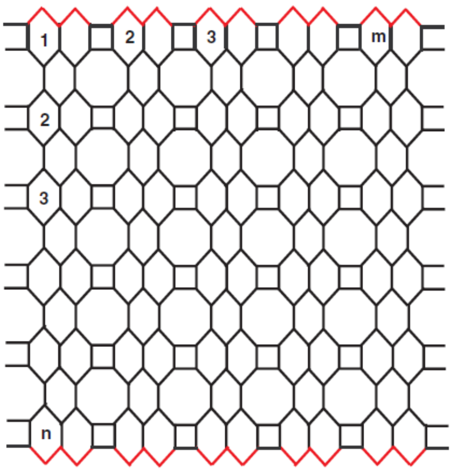

Figure 1:

Let G be a graph of a nanotube $NHPX$ $[m, n]$. By calculation, G has $10mn$ vertices and $15mn - 2m$ edges. We obtain that G has two types of edges based on the degree of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$ $|E_1| = 8m.$

$E_2 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$ $|E_2| = 15mn - 10m$.

Thus in G, there are two types of edges based on the temperature of end vertices of each edge as given in Table 1.

$T(u), T(v)\backslash uv \in E(G)$	$\left(\frac{2}{10mn-2}, \frac{3}{10mn-3}\right)$	$\left(\frac{3}{10mn-3}, \frac{3}{10mn-3}\right)$
Number of edges	$8m$	$15mn - 10m$

Table 1: Edge partition of G

Theorem 1. The (a, b)-temperature index of a nanotube $NHP[m, n]$ is

$$T_{a,b}\left(NHPX\left[m,n\right]\right)=8m\left[\left(\frac{2}{10mn-2}\right)^{a}\left(\frac{3}{10mn-3}\right)^{b}+\left(\frac{2}{10mn-2}\right)^{b}\left(\frac{3}{10mn-3}\right)^{a}\right]$$
$$+2\left(15mn-10m\right)\left(\frac{3}{10mn-3}\right)^{a+b} \qquad (1)$$

Proof: By definition and by Table 1, we deduce

$$T_{a,b}\left(NHPX\left[m,n\right]\right)=\sum_{uv\in E(G)}\left[T(u)^{a}\,T(v)^{b}+T(u)^{b}\,T(v)^{a}\right]$$
$$=8m\left[\left(\frac{2}{10mn-2}\right)^{a}\left(\frac{3}{10mn-3}\right)^{b}+\left(\frac{2}{10mn-2}\right)^{b}\left(\frac{3}{10mn-3}\right)^{a}\right]$$
$$+\left(15mn-10m\right)\left[\left(\frac{3}{10mn-3}\right)^{a}\left(\frac{3}{10mn-3}\right)^{b}+\left(\frac{3}{10mn-3}\right)^{b}\left(\frac{3}{10mn-3}\right)^{a}\right]$$
$$=8m\left[\left(\frac{2}{10mn-2}\right)^{a}\left(\frac{3}{10mn-3}\right)^{b}+\left(\frac{2}{10mn-2}\right)^{b}\left(\frac{3}{10mn-3}\right)^{a}\right]$$
$$+2\left(15mn-10m\right)\left(\frac{3}{10mn-3}\right)^{a+b}$$

We obtain the following results from Theorem 1.

Corollary 1.1. The second hyper temperature index of a nanotube *NHPX*[*m, n*] is

$$HT_{2}\left(NHPX\left[m,n\right]\right)=\frac{1}{2}T_{2,2}\left(NHPX\left[m,n\right]\right)$$
$$=8m\left[\frac{6}{(10mn-2)(10mn-3)}\right]^{2}+\left(15mn-10m\right)\left[\frac{3}{10mn-3}\right]^{4}.$$

Corollary 1.2. The general second temperature index of a nanotube *NHPX* [*m, n*] is

$$T_{2}^{a}\left(NHPX\left[m,n\right]\right)=\frac{1}{2}T_{a,a}\left(NHPX\left[m,n\right]\right)$$
$$=8m\left[\frac{6}{(10mn-2)(10mn-3)}\right]^{a}+\left(15mn-10m\right)\left[\frac{3}{10mn-3}\right]^{2a}.$$

Corollary 1.3. The product connectivity temperature index of a nanotube *NHPX*[*m, n*] is

$$PT\left(NHPX\left[m,n\right]\right)=\frac{1}{2}T_{-\frac{1}{2},-\frac{1}{2}}\left(NHPX\left[m,n\right]\right)$$
$$=\frac{8}{\sqrt{6}}m\sqrt{(10mn-2)(10mn-3)}+\frac{1}{3}(15mn-10m)(10mn-3).$$

Corollary 1.4. The reciprocal product connectivity temperature index of a nanotube *NHPX* [*m, n*] is

$$RPT\left(NHPX\left[m,n\right]\right)=\frac{1}{2}T_{\frac{1}{2},\frac{1}{2}}\left(NHPX\left[m,n\right]\right)$$

$$=\frac{8\sqrt{6}m}{\sqrt{(10mn-2)(10mn-3)}}+\frac{3(15mn-10m)}{10mn-3}.$$

Corollary 1.5. The *F*-temperature index of a nanotube *NHPX* [*m, n*] is

$$FT\left(NHPX\left[m,n\right]\right)=T_{2,0}\left(NHPX\left[m,n\right]\right)$$

$$=\frac{270}{(10mn-3)^2}mn+\left[\frac{32}{(10mn-2)^2}-\frac{108}{(10mn-3)^2}\right]m.$$

Corollary 1.6. The symmetric division temperature index of a nanotube *NHPX* [*m, n*] is

$$SDT\left(NHPX\left[m,n\right]\right)=T_{1,-1}\left(NHPX\left[m,n\right]\right)$$

$$=30mn+\left[\frac{4\left(1300m^2n^2-600mn+72\right)}{3(10mn-2)(10mn-3)}-20\right]m.$$

Corollary 1.7. The second Gourava temperature index of a nanotube *NHPX* [*m, n*] is

$$GT_2\left(NHPX\left[m,n\right]\right)=T_{2,1}\left(NHPX\left[m,n\right]\right)$$

$$=\frac{48m}{(10mn-2)(10mn-3)}\left[\frac{2}{10mn-2}+\frac{3}{10mn-3}\right]$$

$$+(30mn-20m)\left(\frac{3}{10mn-3}\right)^3.$$

Corollary 1.8. The general temperature index of a nanotube *NHPX* [*m, n*] is

$$T_a\left(NHPX\left[m,n\right]\right)=T_{a,0}\left(NHPX\left[m,n\right]\right)$$

$$=8m\left[\left(\frac{2}{10mn-2}\right)^a+\left(\frac{3}{10mn-3}\right)^a\right]+2(15mn-10m)\left(\frac{3}{10mn-3}\right)^a.$$

Theorem 2. The first Gourava temperature index of a nanotube *NHPX* [*m, n*] is

$$GT_2\left(NHPX\left[m,n\right]\right)=\left[\frac{50mn-6}{(10mn-2)(10mn-3)}\right]8m+\left[\frac{6mn-9}{(10mn-3)^2}\right](15mn-10m).$$

Proof: By definition and by using Table 1, we derive

$$T_{a,b}\left(NHPX\left[m,n\right]\right)=\sum_{uv\in E(G)}\left[T(u)+T(v)+T(u)T(v)\right]$$

$$=\left[\frac{2}{10mn-2}+\frac{3}{10mn-3}+\left(\frac{2}{10mn-2}\right)\left(\frac{3}{10mn-3}\right)\right]8m$$

$$+\left[\frac{3}{10mn-3}+\frac{3}{10mn-3}+\left(\frac{3}{10mn-3}\right)\left(\frac{3}{10mn-3}\right)\right](15mn-10m)$$

$$=\left[\frac{50mn-6}{(10mn-2)(10mn-3)}\right]8m+\left[\frac{6mn-9}{(10mn-3)^2}\right](15mn-10m).$$

4. Conclusion

In this paper, the (*a*, *b*)-temperature index and some other temperature indices for particular values of *a* and *b* for *H*-Naptalenic nanotubes are determined.

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