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Computation of Some Temperature Indices of HC_5C_7 [*p*, *q*] Nanotubes

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Abstract. In Chemical Science, the connectivity indices are used in the analysis of drug molecular structures which are helpful for chemical scientists, medical scientists and pharmaceutical scientists to find out the chemical and biological characteristics of drugs. In this study, we introduce the first and second hyper temperature indices, sum connectivity temperature index, product connectivity temperature index, reciprocal product connectivity temperature index, general first and second temperature indices, F-temperature index, general temperature index of a molecular graph. Furthermore, we determine these newly defined temperature indices for $HC_5C_7[p, q]$ nanotubes.

Keywords: Hyper temperature indices, sum connectivity temperature index, product connectivity temperature index, *F*-temperature index, nanotube.

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*12, 05*C*35

1. Introduction

In this paper, we consider only finite, simple, connected graphs. Let *G* be such a graph with vertex set *V*(*G*) and edge set *E*(*G*). The degree $d_G(v)$ of a vertex *v* is the number of vertices adjacent to v. For undefined concepts and notations, we refer [1].

A molecular graph is a graph whose vertices correspond to the atoms and the edges to the bonds. Studying molecular graphs is a constant focus in Chemical Graph Theory; an effort to better understand molecular structure. Several graph indices have found some applications in Chemistry, especially in QSPR/QSAR study [2, 3, 4].

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

$$T(v) = \frac{d_G(v)}{n - d_G(v)},$$

where *n* is the number of vertices of *G*.

Motivated by the work on degree based topological indices, we define some temperature indices as follows:

We introduce first and second hyper temperature indices of a graph *G*, defined as

$$HT_1(G) = \sum_{uv \in E(G)} [T(u) + T(v)]^2, \qquad HT_2(G) = \sum_{uv \in E(G)} [T(u)T(v)]^2.$$

We introduce the sum connectivity temperature index of a graph G and it is defined as

$$ST(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{T(u)+T(v)}}.$$

We propose the product connectivity temperature index of a graph G, defined as

$$PT(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{T(u)T(v)}}.$$

The reciprocal product connectivity temperature index of a graph G is defined as

$$RPT(G)=\sum_{uv\in E(G)}\sqrt{T(u)T(v)}.$$

The arithmetic-geometric temperature index of a graph G is defined as

$$AGT(G)=\sum_{uv\in E(G)}\frac{T(u)+T(v)}{2\sqrt{T(u)T(v)}}.$$

The general first and second temperature indices of a graph G are defined as

$$T_1^a(G)=\sum_{uv\in E(G)}\left[T(u)+T(v)\right]^a,\ \ T_2^a(G)=\sum_{uv\in E(G)}\left[T(u)T(v)\right]^a,$$

where a is a real number.

We introduce the following temperature indices as follows:

The F-temperature index of a graph G is defined as

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

The general temperature index of a graph G is defined as

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

Recently, some new temperature indices were studied in [6, 7, 8] and also some new connectivity indices were studied, for example, in [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22,23, 24,25,26,27,28]. In this paper, some newly defined temperature indices of $HC_5C_7[p, q]$ nanotubes are computed.

2. Results for HC_5C_7 [p, q] nanotubes

We consider HC_5C_7 [p, q] nanotubes in which p is the number of heptagons in the first row and q rows of pentagons repeated alternately. The 2-D lattice of HC_5C_7[8, 4] nanotube is shown in Figure 1.

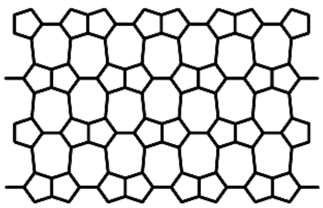

Figure 1: 2-D lattice of HC_5C_7 [8, 4] nanotube

Let G be a graph of a nanotube $HC_5C_7[p, q]$. By calculation, G has $4pq$ vertices and $6pq - p$ edges. In G, there are two types of edges based on the temperature of the vertices of each edge as given in Table 1.

$T(u), T(v) \backslash uv \in E(G)$	$\left(\frac{2}{4pq-2}, \frac{3}{4pq-3}\right)$	$\left(\frac{3}{4pq-3}, \frac{3}{4pq-3}\right)$
Number of edges	$4p$	$6pq - 5p$

Table 1: Edge partition of G

Theorem 1. The general first temperature index of a nanotube $HC_5C_7[p, q]$ is

$$T_1^a\left(HC_5C_7\,[p,q]\right) = 4p\left[\frac{20pq-12}{(4pq-2)(4pq-3)}\right]^a + (6pq-5p)\left(\frac{6}{4pq-3}\right)^a. \quad (1)$$

Proof: Let $G = HC_5C_7\,[p, q]$. By definition, we have

$$T_1^a(G) = \sum_{uv\in E(G)} \left[T(u)+T(v)\right]^a.$$

Thus by using Table 1, we deduce

$$T_1^a\left(HC_5C_7\,[p,q]\right) = 4p\left(\frac{2}{4pq-2}+\frac{3}{4pq-3}\right)^a + (6pq-5p)\left(\frac{3}{4pq-3}+\frac{3}{4pq-3}\right)^a$$

$$= 4p\left[\frac{20pq-12}{(4pq-2)(4pq-3)}\right]^a + (6pq-5p)\left(\frac{6}{4pq-3}\right)^a.$$

From Theorem 1, we deduce the following results.

Corollary 1.1. The first hyper temperature index of a nanotube $HC_5C_7\,[p, q]$ is

$$HT_1\left(HC_5C_7\,[p,q]\right) = 4p\left[\frac{20pq-12}{(4pq-2)(4pq-3)}\right]^2 + (6pq-5p)\left(\frac{6}{4pq-3}\right)^2$$

Corollary 1.2. The sum connectivity temperature index of a nanotube $HC_5C_7\,[p, q]$ is

$$ST\left(HC_5C_7\,[p,q]\right) = 4p\left[\frac{20pq-12}{(4pq-2)(4pq-3)}\right]^{-\frac{1}{2}} + (6pq-5p)\left(\frac{6}{4pq-3}\right)^{-\frac{1}{2}}$$

Proof: Put $a = 2, -½$ in equation (1), we obtain the desired results.

Theorem 2. The general second temperature index of a nanotube $HC_5C_7\,[p, q]$ is

$$T_2^a\left(HC_5C_7\,[p,q]\right) = 4p\left[\frac{6}{(4pq-2)(4pq-3)}\right]^a + (6pq-5p)\left(\frac{3}{4pq-3}\right)^{2a}. \quad (2)$$

Proof: Let $G = HC_5C_7\,[p, q]$. By definition, we have

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

Thus by using Table 1, we derive

$$T_2^a\left(HC_5C_7[p,q]\right)=4p\left(\frac{2}{4pq-2}\times\frac{3}{4pq-3}\right)^a+(6pq-5p)\left(\frac{3}{4pq-3}\times\frac{3}{4pq-3}\right)^a$$
$$=4p\left[\frac{6}{(4pq-2)(4pq-3)}\right]^a+(6pq-5p)\left(\frac{3}{4pq-3}\right)^{2a}.$$

We establish the following results from Theorem 2.

Corollary 2.1. The second hyper temperature index of a nanotube $HC_5C_7[p, q]$ is

$$HT_2\left(HC_5C_7[p,q]\right)=4p\left[\frac{6}{(4pq-2)(4pq-3)}\right]^2+(6pq-5p)\left(\frac{3}{4pq-3}\right)^4.$$

Corollary 2.2. The product connectivity temperature index of a nanotube $HC_5C_7[p,q]$ is

$$PT\left(HC_5C_7[p,q]\right)=\frac{4}{\sqrt{6}}p\sqrt{(4pq-2)(4pq-3)}+\frac{1}{3}(6pq-5p)(4pq-3).$$

Corollary 2.3. The reciprocal product connectivity temperature index of a nanotube $HC_5C_7[p, q]$ is

$$RPT\left(HC_5C_7[p,q]\right)=\frac{4\sqrt{6}p}{\sqrt{(4pq-2)(4pq-3)}}+\frac{3(6pq-5p)}{4pq-3}.$$

Proof: Put a = 2, - ½ , ½ in equation (2), we get the desired results.

Theorem 3. The arithmetic-geometric temperature index of a nanotube $HC_5C_7[p, q]$ is given by

$$AGT\left(HC_5C_7[p,q]\right)=\frac{2p(20pq-12)}{\sqrt{6(4pq-2)(4pq-3)}}+6pq-5p.$$

Proof: Let $G = HC_5C_7[p, q]$. By definition, we have

$$AGT(G)=\sum_{uv\in E(G)}\frac{T(u)+T(v)}{2\sqrt{T(u)T(v)}}.$$

Thus by using Table 1, we deduce

$$AGT\left(HC_5C_7[p,q]\right)=4p\left[\left(\frac{2}{4pq-2}+\frac{3}{4pq-3}\right)\div\left(2\sqrt{\frac{2}{4pq-2}\times\frac{3}{4pq-3}}\right)\right]$$
$$+(6pq-5p)\left[\left(\frac{3}{4pq-3}+\frac{3}{4pq-3}\right)\div 2\sqrt{\frac{3}{4pq-3}\times\frac{3}{4pq-3}}\right]$$
$$=\frac{2p(20pq-12)}{\sqrt{6(4pq-2)(4pq-3)}}+6pq-5p.$$

Theorem 4. The general temperature index of a nanotube $HC_5C_7[p, q]$ is given by

$$T_a\left(HC_5C_7[p,q]\right)=4p\left[\left(\frac{2}{4pq-2}\right)^a+\left(\frac{3}{4pq-3}\right)^a\right]+2(6pq-5p)\left(\frac{3}{4pq-3}\right)^a \quad (3)$$

Proof: Let $G = HC_5C_7[p, q]$. By definition, we have

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

Hence by using Table 1, we derive

$$T_a\left(HC_5C_7[p,q]\right)=4p\left[\left(\frac{2}{4pq-2}\right)^a+\left(\frac{3}{4pq-3}\right)^a\right]$$

$$+(6pq-5p)\left[\left(\frac{3}{4pq-3}\right)^a+\left(\frac{3}{4pq-3}\right)^a\right]$$

$$=4p\left[\left(\frac{2}{4pq-2}\right)^a+\left(\frac{3}{4pq-3}\right)^a\right]+2(6pq-5p)\left(\frac{3}{4pq-3}\right)^a.$$

We obtain the following result from Theorem 4.

Corollary 4.1. The F-temperature index of a nanotube $HC_5C_7[p, q]$ is

$$FT\left(HC_5C_7[p,q]\right)=pq\frac{108}{(4pq-3)^2}+p\left[\frac{16}{(4pq-2)^2}-\frac{54}{(4pq-3)^2}\right].$$

Proof: Put $a = 2$ in equation (3), we get the desired result.

5. Conclusion

In this study, the expressions for the first and second hyper temperature indices, sum connectivity temperature index, product connectivity temperature index, arithmetic-geometric temperature index, F-temperature index, general first and second temperature indices of $HC_5C_7[p,q]$ nanotubes have been computed.

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