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Degree Based Connectivity *F*-Indices of Nanotubes

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Abstract. The connectivity indices are helpful for medical scientists, chemical scientists to find out the chemical and biological characteristics of drugs. In this study, we compute the sum connectivity *F*-index, product connectivity *F*-index, atom bond connectivity *F*-index and geometric arithmetic *F*-index of certain nanotubes.

Keywords: connectivity *F*-indices, nanotube

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

1. Introduction

We consider only finite, simple connected graphs. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of edges incident to v. We refer to [1] for undefined term and notation. A topological index is a numerical parameter mathematically derived from the graph structure. The connectivity indices are used in the analysis of drug molecular structures in Chemical and Medical Sciences. Several topological indices have been considered in Chemistry and have found some applications, especially in QSPR/QSAR study, see [2, 3].

The first F-index [4] and second F-index [5] of a graph G are defined as

$$F_1(G) = \sum_{uv\in E(G)} \left[d_G(u)^2 + d_G(v)^2\right], \qquad F_2(G) = \sum_{uv\in E(G)} \left[d_G(u)^2 d_G(v)^2\right].$$

The sum connectivity F-index and product connectivity F-index were introduced by Kulli in [5] and defined as

$$SF(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)^2 + d_G(v)^2}} \tag{1}$$

$$PF(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)^2 d_G(v)^2}} \tag{2}$$

We now introduce the atom bond connectivity F-index and geometric arithmetic F-index of a graph G, defined as

$$ABCF(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_G(u)^2 + d_G(v)^2 - 2}{d_G(u)^2 d_G(v)^2}} \tag{3}$$

$$PF(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_G(u)^2 d_G(v)^2}}{d_G(u)^2+d_G(v)^2} \tag{4}$$

Recently, the reduced connectivity indices [6], product connectivity leap index and ABC leap index [7], atom bond connectivity index [9], multiplicative connectivity ve-degree indices [10], multiplicative connectivity Banhatti indices [11], multiplicative connectivity Revan indices [12], sum connectivity leap index [13], multiplicative atom bond connectivity index [14] were studied. In this paper, the sum connectivity *F*-Index, product connectivity *F*-index, atom bond connectivity *F*-Index and geometric arithmetic *F*-index of HC_5C_7 $[p, q]$ and $SC_5C_7[p, q]$ nanotubes are determined. For nanotubes, see [15].

2. HC_5C_7 $[p, q]$ Nanotubes

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

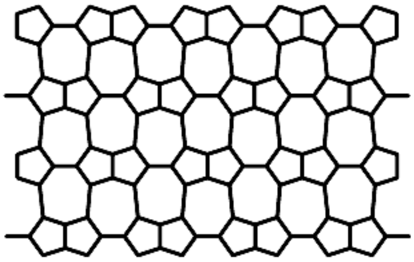

Figure 1: 2-dimensional lattice of nanotube HC_5C_7 [8, 4]

Let G be the graph of a nanotube $HC_5C_7[p, q]$. By algebraic method, we obtain that G has $4pq$ vertices and $6pq-p$ edges. The graph G has two types of edges based on the degree of end vertices of each edge as given in Table 1.

$d_G(u), d_G(v)\backslash uv \in E(G)$	(2, 3)	(3, 3)
Number of edges	$4p$	$6pq - 5p$

Table 1: Edge partition of $HC_5C_7[p, q]$

Theorem 1. The sum connectivity *F*-index of a nanotube $HC_5C_7[p, q]$ is

$$SF\left(HC_5C_7\left[p,q\right]\right)=\sqrt{2}pq+\left(\frac{4}{\sqrt{13}}-\frac{5}{\sqrt{18}}\right)p$$

Proof: Let G=$HC_5C_7[p, q]$. By using equation (1) and Table 1, we derive

$$SF\left(HC_5C_7\left[p,q\right]\right)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)^2+d_G(v)^2}}$$

$$=\left(\frac{1}{\sqrt{2^2+3^2}}\right)4p+\left(\frac{1}{\sqrt{3^2+3^2}}\right)(6pq-5p)$$

$$= \sqrt{2}\,pq + \left(\frac{4}{\sqrt{13}} - \frac{5}{\sqrt{18}}\right)p.$$

Theorem 2. The product connectivity *F*-index of a nanotube $HC_5C_7[p, q]$ is given by

$$PF\left(HC_5C_7[p,q]\right) = \frac{2}{3}pq + \frac{1}{9}p.$$

Proof: Let $G = HC_5C_7[p, q]$. From equation (2) and by using Table 1, we deduce

$$PF\left(HC_5C_7[p,q]\right) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)^2\, d_G(v)^2}}$$

$$= \left(\frac{1}{\sqrt{2^2 \times 3^2}}\right)4p + \left(\frac{1}{\sqrt{3^2 \times 3^2}}\right)(6pq - 5p)$$

$$= \frac{2}{3}pq + \frac{1}{9}p.$$

Theorem 3. The atom bond connectivity *F*-index of a nanotube $HC_5C_7[p, q]$ is

$$ABCF\left(HC_5C_7[p,q]\right) = \frac{8}{3}pq + \left(\frac{2\sqrt{11}}{3} - \frac{20}{9}\right)p$$

Proof: Let $G = HC_5C_7[p, q]$. By using equation (3) and Table 1, we obtain

$$ABCF\left(HC_5C_7[p,q]\right) = \sum_{uv\in E(G)} \sqrt{\frac{d_G(u)^2 + d_G(v)^2 - 2}{d_G(u)^2\, d_G(v)^2}}$$

$$= \left(\sqrt{\frac{2^2 + 3^2 - 2}{2^2 \times 3^2}}\right)4p + \left(\sqrt{\frac{3^2 + 3^2 - 2}{3^2 \times 3^2}}\right)(6pq - 5p)$$

$$= \frac{8}{3}pq + \left(\frac{2\sqrt{11}}{3} - \frac{20}{9}\right)p.$$

Theorem 4. The geometric-arithmetic *F*-index of a nanotube $HC_5C_7[p, q]$ is given by

$$GAF\left(HC_5C_7[p,q]\right) = 6pq - \frac{17}{13}p\,.$$

Proof: Let G be the graph of a nanotube $HC_5C_7[p, q]$. From equation (4) and by using Table 1, we have

$$GAF\left(HC_5C_7[p,q]\right) = \sum_{uv\in E(G)} \frac{2\sqrt{d_G(u)^2\, d_G(v)^2}}{d_G(u)^2 + d_G(v)^2}$$

$$= \left(\frac{2\sqrt{2^2 \times 3^2}}{2^2 + 3^2}\right)4p + \left(\frac{2\sqrt{3^2 \times 3^2}}{3^2 + 3^2}\right)(6pq - 5p)$$

$$= 6pq - \frac{17}{13}p.$$

3. *SC_5C_7[p, q]* Nanotubes

We consider $SC_5C_7[p, q]$ nanotubes in which p is the number of heptagons in the first row and q rows of vertices and edges are repeated alternately. The 2-*D* lattice a nanotube $SC_5C_7[p, q]$ is presented in Figure 2.

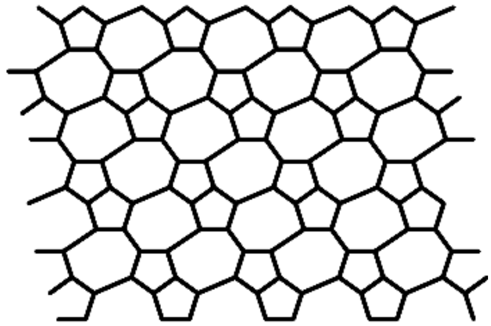

Figure 2: 2-dimensional lattice of nanotube SC_5C_7 [p, q]

Let G be the graph of a nanotube $SC_5C_7[p, q]$ with $6pq$-p edges. By algebraic method, we obtain that G has three types of edges based on the degree of the end vertices of each edge as given in Table 2.

$d_G(u)\ d_G(v)\backslash uv\in E(G)$	(2, 2)	(2, 3)	(3.3)
Number of edges	q	$6q$	$6pq - p - 7q$

Table 2: Edge partition of SC_5C_7 [pq]

Theorem 5. The sum connectivity F-index of a nanotube SC_5C_7 [p, q] is given by

$$SF\left(SC_5C_7[p,q]\right)=\sqrt{2}pq-\frac{1}{\sqrt{18}}p+\left(\frac{1}{\sqrt{8}}+\frac{6}{\sqrt{13}}-\frac{7}{\sqrt{18}}\right)q.$$

Proof: Let G be the graph of a nanotube SC_5C_7 [p, q]. From equation (1) and by using Table 2, we obtain

$$SF\left(SC_5C_7[p,q]\right)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)^2+d_G(v)^2}}$$

$$=\left(\frac{1}{\sqrt{2^2+2^2}}\right)q+\left(\frac{1}{\sqrt{2^2+3^2}}\right)6q+\left(\frac{1}{\sqrt{3^2+3^2}}\right)(6pq-p-7q)$$

$$=\sqrt{2}pq-\frac{1}{\sqrt{18}}p+\left(\frac{1}{\sqrt{8}}+\frac{6}{\sqrt{13}}-\frac{7}{\sqrt{18}}\right)q.$$

Theorem 6. The product connectivity F-index of $SC_5C_7[p, q]$ is

$$PF\left(SC_5C_7[p,q]\right)=\frac{2}{3}pq-\frac{1}{9}p+\frac{17}{36}q.$$

Proof: Let $G = SC_5C_7[p, q]$. By using equation (2) and Table 2, we derive

$$PF\left(SC_5C_7[p,q]\right)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)^2\, d_G(v)^2}}$$

$$=\left(\frac{1}{\sqrt{2^2\times 2^2}}\right)q+\left(\frac{1}{\sqrt{2^2\times 3^2}}\right)6q+\left(\frac{1}{\sqrt{3^2\times 3^2}}\right)(6pq-p-5q)$$
$$=\frac{2}{3}pq-\frac{1}{9}p+\frac{17}{36}q.$$

Theorem 7. The atom bond connectivity F-index of $SC_5C_7[p,q]$ is

$$ABCF\left(SC_5C_7[p,q]\right)=\frac{8}{3}pq-\frac{4}{9}p+\left(\frac{\sqrt{6}}{4}+\sqrt{11}-\frac{28}{9}\right)q.$$

Proof: Let G be the graph of a nanotube $SC_5C_7[p, q]$. By using equation (3) and Table 2, we obtain

$$ABCF\left(SC_5C_7[p,q]\right)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)^2+d_G(v)^2-2}{d_G(u)^2 d_G(v)^2}}$$
$$=\left(\sqrt{\frac{2^2+2^2-2}{2^2\times 2^2}}\right)q+\left(\sqrt{\frac{2^2+3^2-2}{2^2\times 3^2}}\right)6q+\left(\sqrt{\frac{3^2+3^2-2}{3^2\times 3^2}}\right)(6pq-p-7q)$$
$$=\frac{8}{3}pq-\frac{4}{9}p+\left(\frac{\sqrt{6}}{4}+\sqrt{11}-\frac{28}{9}\right)q.$$

Theorem 8. The geometric-arithmetic F-index of $SC_5C_7[p, q]$ is given by

$$GAF\left(SC_5C_7[p,q]\right)=6pq-p-\frac{66}{13}q.$$

Proof: Let $G = SC_5C_7\,[p, q]$. From equation (4) and by using Table 2, we have

$$GAF\left(SC_5C_7[p,q]\right)=\sum_{uv\in E(G)}\frac{2\sqrt{d_G(u)^2 d_G(v)^2}}{d_G(u)^2+d_G(v)^2}$$
$$=\left(\frac{2\sqrt{2^2\times 2^2}}{2^2+2^2}\right)p+\left(\frac{2\sqrt{2^2\times 3^2}}{2^2+3^2}\right)6q+\left(\frac{2\sqrt{3^2\times 3^2}}{3^2+3^2}\right)(6pq-p-7q)$$
$$=6pq-p-\frac{66}{13}q.$$

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