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Some Topological Indices of Carbon Nanocones [CNC_k(n)] and Nanotori [$C_4C_6C_8(P, Q)$]

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Abstract— Chemical graph theory is a branch of graph theory which focuses on the topological indices of chemical molecular graphs, which correlate well with chemical properties of the chemical molecules. Topological indices play important role in mathematical chemistry especially in the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies. In this article, we compute the sum connectivity index, product connectivity index, geometric-arithmetic index and inverse sum indeg index for Carbon Nanocones [$CNC_k(n)$] and Nanotori [$C_4C_6C_8(p,q)$].

Keywords*— Sum connectivity index, Product connectivity index, Geometric-arithmetic index, Inverse sum indeg index, Carbon Nanocones [$CNC_k(n)$] and Nanotori [$C_4C_6C_8(p,q)$].*

I. INTRODUCTION

Let G be a simple connected graph with vertex set V and edge set E. In chemical graph theory the vertices and edges corresponds to the atoms and bonds of the molecular graph respectively. If e is an edge/bond of G, that connects the two vertices/atoms u and v, then we write $e = uv$ and say that the two vertices "u and v are adjacent" also the "vertex u and edge e are incident with each other, as v and e". For a vertex v, the number of edges incident to the vertex v is called the degree of vertex v, is denoted as d_v. For undefined terminologies we refer[1].

A number which is used to characterize some property of the graph of a molecule is called a topological index for that graph. There are numerous topological descriptors that have found applications in theoretical chemistry, especially in QSPR/QSAR research [2]. The oldest topological index introduced by Harold Wiener in 1947 is ordinary (vertex) version of Wiener index [3] which is the sum of all distance between vertices of a graph.

$$W(G) = \sum_{(u,v)\in V(G)} d(u,v) \qquad (1)$$

In [4], Zhou et al. introduced the sum connectivity index of a graph G, which is defined as,

$$X(G) = \sum_{(uv)\in E(G)} \frac{1}{\sqrt{(d_u + d_v)}} \qquad (2)$$

The product connectivity index or Randić index of a graph G was proposed by Randić in [5] and is defined as,

$$X(G) = \sum_{(uv)\in E(G)} \frac{1}{\sqrt{(d_u \times d_v)}} \qquad (3)$$

In [6], Vukičević et al. invented a new topological index i.e.,"geometric-arithmetic index" of a graph G, is denoted by $GA(G)$ and is defined by

$$GA(G) = \sum_{(uv)\in E(G)} \frac{2\sqrt{d_u \times d_v}}{\sqrt{(d_u + d_v)}} \qquad (4)$$

In [7], Vukičević and Gaśperov defined the inverse sum indeg index of graph G, is defined as

$$ISI(G) = \sum_{(uv)\in E(G)} \frac{d_u \times d_v}{(d_u + d_v)} \qquad (5)$$

Since 1968, Carbon Nanocones have been observed on the surface of naturally occurring graphite [8]. The walls of the Carbon Nanocones are usually curved and slightly regular to those Nanocones which are made in laboratory. Their bases are connected to the graphite and their length disparate between 1 to 40 micrometers.

Carbon Nanostructures have attained significant attention due to their potential use in many applications including biosensors, nano-electronic devices, chemical probes, gas sensors and energy storage [9]. Carbon Nanocones are one of the forms of carbon Nanostructures and these have been proposed as possible molecular gas storage devices. Recently, carbon Nanocones have attained increased scientific interest to their unique properties and promising uses in many novel applications such as energy and gas storage [10].

Carbon Nanotubes form an interesting class of carbon nanomaterials. There are three types of nanotubes: armchair, chiral and Zigzag structures. Carbon Nanotubes show remarkable mechanical properties. Experimental studies have shown that they belong to the stiffest and elastic known materials. Diudea was the first chemist who considered the problem of computing topological indices of nanostructures [11, 12, 13, 14].

II. RESULTS AND DISCUSSION

i. Priliminaries of Carbon Nanocones [$CNC_k(n)$]

In 1994, Ge and Sattler invented Carbon Nanocones [15] and are constructed from a graphene sheet by removing a 60° wedge and joining the edges produces a cone with single pentagonal defect at the apex. Removing additional wedges introduces more such defects and reduces the opening angle. A cone with pentagons has an opening angle of zero and is just a nanotube with one open end. We refer the references [16, 17, 18, 19] for some results on Carbon Nanocones.

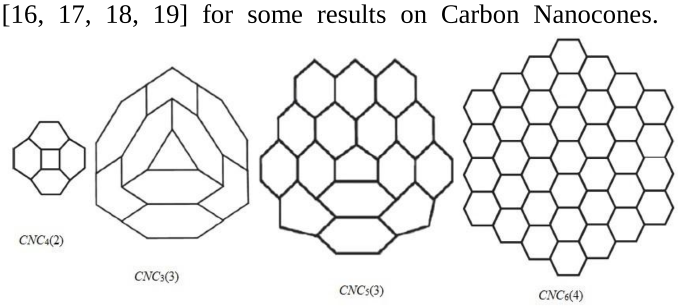

Figure 1: *Depicts growth of carbon Nanocones namely $CNC_4(2)$, $CNC_3(3)$, $CNC_5(3)$ and $CNC_6(4)$.*

∗ We need the following remarks to construct the results.

Remark A. [20] The graph $CNC_k(n)$ contains kn^2 vertices and $\frac{kn}{2}(3n-1)$ edges.

Remark B. The graph $CNC_k(n)$ have the vertices are of degree 2 and 3 (see fig. 1). We have taken edge partitions based on the degrees of the end vertices of each edge, which is as follows:

$$E_{22} = \{uv \in E(G)/d_u = 2, d_v = 2\} \Rightarrow |E_{22}| = k$$
$$E_{23} = \{uv \in E(G)/d_u = 2, d_v = 3\} \Rightarrow |E_{23}| = 2k(n-1)$$
$$E_{33} = \{uv \in E(G)/d_u = 3, d_v = 3\} \Rightarrow |E_{33}| = \frac{k}{2}(n-1)(3n-2)$$

ii. Results For The Carbon Nanocones [$CNC_k(n)$]

In this section, we compute sum connectivity index, Product connectivity index, geometric- arithmetic index and inverse sum indeg index for carbon Nanocones [$CNC_k(n)$].

Theorem 2.1. *Let $CNC_k(n)$ be the Carbon Nanocones $\forall k, n \in N$ and $k \geq 3$. Then the sum connectivity index of $CNC_k(n)$ is,*

$$X[CNC_k(n)] = k\left[\frac{1}{2} + (n-1)\left(\frac{2}{\sqrt{5}} + \frac{3n-2}{2\sqrt{6}}\right)\right]$$

Proof. Consider the graph carbon Nanocones $CNC_k(n)$, $\forall k, n \in N$ and $k \geq 3$. By **remark A**, the graph $CNC_k(n)$ contains kn^2 vertices and $\left[\frac{kn}{2}(3n-1)\right]$ edges.

Now to compute the sum connectivity index of $CNC_k(n)$ graph, we refer the **remark B**.

From equation (2),

$$X(CNC_k(n)) = \sum_{(uv)\in E(CNC_k(n))} \frac{1}{\sqrt{(d_u + d_v)}}$$
$$= k\left[\frac{1}{\sqrt{2+2}}\right] + 2k(n-1)\left[\frac{1}{\sqrt{2+3}}\right] + \frac{k}{2}(n-1)(3n-2)\left[\frac{1}{\sqrt{3+3}}\right]$$

On simplification we get,

$$X[CNC_k(n)] = k\left[\frac{1}{2} + (n-1)\left(\frac{2}{\sqrt{5}} + \frac{3n-2}{2\sqrt{6}}\right)\right].$$

Theorem 2.2. *Let $CNC_k(n)$ be the Carbon Nanocones $\forall k,n \in N$ and $k \geq 3$. Then the product connectivity index of $CNC_k(n)$ is,*

$$X[CNC_k(n)] = k\left[\frac{3n^2 - 5n + 5}{6} + \frac{2(n-1)}{\sqrt{6}}\right]$$

Proof. Consider the graph $CNC_k(n)$, $\forall k$, $n \in N$ and $k \geq 3$. Now we consider the **remark B**, to compute the product connectivity index or Randić index of $CNC_k(n)$ graph.
From equation (3),

$$X(CNC_k(n)) = \sum_{(uv)\in E(CNC_k(n))} \frac{1}{\sqrt{(d_u \times d_v)}}$$
$$= k\left[\frac{1}{\sqrt{2\times 2}}\right] + 2k(n-1)\left[\frac{1}{\sqrt{2\times 3}}\right] + \frac{k}{2}(n-1)(3n-2)\left[\frac{1}{\sqrt{3\times 3}}\right]$$

On simplification we get,

$$X[CNC_k(n)] = k\left[\frac{3n^2 - 5n + 5}{6} + \frac{2(n-1)}{\sqrt{6}}\right]$$

Theorem 2.3. *Let $CNC_k(n)$ be the Carbon Nanocones $\forall k$, $n \in N$ and $k \geq 3$. Then the geometric-arithmetic index of $CNC_k(n)$ is,*

$$GA[CNC_k(n)] = k\left[1 + (n-1)\left(\frac{4\sqrt{6}}{5} + \frac{3n-2}{2}\right)\right]$$

Proof. Consider the graph $CNC_k(n)$, $\forall k$, $n \in N$ and $k \geq 3$. Now to construct geometric-arithmetic index of $CNC_k(n)$, we consider the edge partition from **remark B**.
From equation (4),

$$GA(CNC_k(n)) = \sum_{(uv)\in E(CNC_k(n))} \frac{2\sqrt{d_u \times d_v}}{(d_u + d_v)}$$
$$= k\left[\frac{2\sqrt{2\times 2}}{2+2}\right] + \left[2k(n-1)\right]\left[\frac{2\sqrt{2\times 3}}{2+3}\right] + \left[\frac{k}{2}(n-1)(3n-2)\right]\left[\frac{2\sqrt{3\times 3}}{3+3}\right]$$

On simplification we get,

$$GA[CNC_k(n)] = k\left[1 + (n-1)\left(\frac{4\sqrt{6}}{5} + \frac{3n-2}{2}\right)\right]$$

.

Theorem 2.4. *Let $CNC_k(n)$ be the Carbon Nanocones $\forall k$, $n \in N$ and $k \geq 3$. Then the inverse sum indeg index of $CNC_k(n)$ is,*

$$ISI[CNC_k(n)] = k\left[\frac{45n^2 - 27n + 2}{20}\right]$$

.

Proof. Consider the graph $CNC_k(n)$, $\forall k$, $n \in N$ and $k \geq 3$. Now to compute the inverse sum indeg index of $CNC_k(n)$ graph, we consider the data from **remark B.**
From equation (5),

$$ISI(CNC_k(n)) = \sum_{(uv)\in E(CNC_k(n))} \frac{d_u \times d_v}{(d_u + d_v)}$$
$$= k\left[\frac{2\times 2}{2+2}\right] + \left[2k(n-1)\right]\left[\frac{2\times 3}{2+3}\right] + \left[\frac{k}{2}(n-1)(3n-2)\right]\left[\frac{3\times 3}{3+3}\right]$$

On simplification we get,

$$ISI[CNC_k(n)] = k\left[\frac{45n^2 - 27n + 2}{20}\right]$$

iii. Priliminaries of Nanotori [$C_4C_6C_8(p, q)$]

The Nanotori are obtained from a graphene sheet rolled into a carbon nanotube with the ends joined together to form a torus.

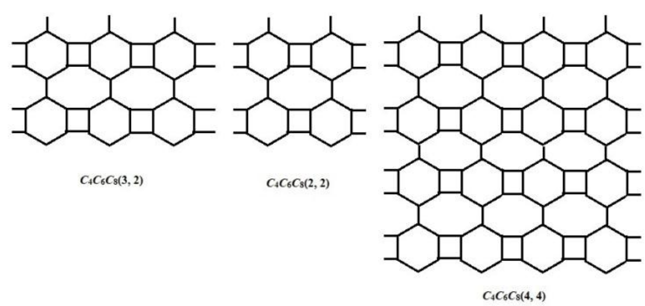

Figure 2: *Some examples of Nanotori namely $C_4C_6C_8(3, 2)$, $C_4C_6C_8(2, 2)$ and $C_4C_6C_8(4, 2)$.*

∗ *We need the below mentioned remark to construct the results.*

Remark C. The graph Nanotori [$C_4C_6C_8(p, q)$], with *p*-number of columns (which contains benzene rings) and *q*-

number of rows (which contains benzene rings), ∀*p*, *q* ∈ *N*. The graph $[C_4C_6C_8(p, q)]$ contains $(6pq + 4q + p)$ vertices and $(9pq + 2q)$ edges. The graph $[C_4C_6C_8(p, q)]$ have the vertices of degree 1, 2 and 3 (see fig. 2). We have taken edge partitions based on the degrees of the end vertices of each edge, which is as follows:

$$E_{13} = \{uv \in E(G) / d_u = 1, d_v = 3\} \Rightarrow |E_{13}| = 4q + p$$
$$E_{23} = \{uv \in E(G) / d_u = 2, d_v = 3\} \Rightarrow |E_{23}| = 2p$$
$$E_{33} = \{uv \in E(G) / d_u = 3, d_v = 3\} \Rightarrow |E_{33}| = 3p(3q-1) - 2q$$

iv. Results for Nanotori $[C_4C_6C_8(p, q)]$

In this section, we compute the four topological indices namely sum connectivity index, product connectivity index, geometric-arithmetic index and inverse sum indeg index for nanotori $[C_4C_6C_8(p, q)]$.

Theorem 2.5. *Let $[C_4C_6C_8(p, q)]$ be the Nanotori with p columns and q rows ∀p, q ∈ N. Then the sum connectivity index of $[C_4C_6C_8(p, q)]$ is,*

$$X[C_4C_6C_8(p,q)] = 3pq + \left[\frac{p(4-\sqrt{5})}{2\sqrt{5}}\right] + \frac{4q}{3}$$

Proof. Consider the graph Nanotori $[C_4C_6C_8(p, q)]$ with *p* columns and *q* rows ∀*p*, *q* ∈ *N*.
By **remark A,** we compute the sum connectivity index for graph $[C_4C_6C_8(p, q)]$.
From equation (2),

$$X(C_4C_6C_8(p,q)) = \sum_{(uv)\in E(C_4C_6C_8(p,q))} \frac{1}{\sqrt{(d_u + d_v)}}$$
$$= (p+4q)\left[\frac{1}{\sqrt{1+3}}\right] + [2p]\left[\frac{1}{\sqrt{2+3}}\right] + [3p(3q-1) - 2q]\left[\frac{1}{\sqrt{3+3}}\right]$$

On simplification we get,

$$X[C_4C_6C_8(p,q)] = 3pq + \left[\frac{p(4-\sqrt{5})}{2\sqrt{5}}\right] + \frac{4q}{3}.$$

Theorem 2.6. *Let $[C_4C_6C_8(p, q)]$ be the Nanotori with p columns and q rows ∀p, q ∈ N. Then the product connectivity index or Randić index of $[C_4C_6C_8(p, q)]$ is,*

$$X[C_4C_6C_8(p,q)] = 3pq + \left[\frac{p(\sqrt{2}-\sqrt{3}+1)}{\sqrt{3}}\right] + \left[\frac{q(12-2\sqrt{3}}{3\sqrt{3}}\right].$$

Proof. Consider the graph Nanotori $[C_4C_6C_8(p, q)]$ with *p* columns and *q* rows ∀*p*, *q* ∈ *N*. Now to compute the product connectivity index or Randić index for graph $[C_4C_6C_8(p, q)]$ Nanotori, we consider the **remark C.**
From equation (3),

$$X(C_4C_6C_8(p,q)) = \sum_{(uv)\in E(C_4C_6C_8(p,q))} \frac{1}{\sqrt{(d_u \times d_v)}}$$
$$= (p+4q)\left[\frac{1}{\sqrt{1\times 3}}\right] + [2p]\left[\frac{1}{\sqrt{2\times 3}}\right] + [3p(3q-1) - 2q]\left[\frac{1}{\sqrt{3\times 3}}\right]$$

On simplification we get,

$$X[C_4C_6C_8(p,q)] = 3pq + \left[\frac{p(\sqrt{2}-\sqrt{3}+1)}{\sqrt{3}}\right] + \left[\frac{q(12-2\sqrt{3}}{3\sqrt{3}}\right].$$

Theorem 2.7. *Let $[C_4C_6C_8(p, q)]$ be the Nanotori with p columns and q rows ∀p, q ∈ N. Then the geometric-arithmetic index of $[C_4C_6C_8(p, q)]$ is,*

$$GA[C_4C_6C_8(p,q)] = 9pq + p\left[\frac{5\sqrt{3}+12\sqrt{6}-30)}{10}\right] + 2q(\sqrt{3}-1).$$

Proof. Consider the graph Nanotori $[C_4C_6C_8(p, q)]$ with *p* columns and *q* rows ∀*p*, *q* ∈ *N*. Now we consider the remark C to compute the geometric-arithmetic index for graph $[C_4C_6C_8(p, q)]$.
From equation (4),

$$GA(C_4C_6C_8(p,q)) = \sum_{(uv)\in E(C_4C_6C_8(p,q))} \frac{2\sqrt{(d_u \times d_v)}}{(d_u + d_v)}$$
$$= (p+4q)\left[\frac{2\sqrt{1\times 3}}{(1+3)}\right] + [2p]\left[\frac{2\sqrt{2\times 3}}{(2+3)}\right] + [3p(3q-1) - 2q]\left[\frac{2\sqrt{3\times 3}}{(3+3)}\right]$$

On simplification we get,

$$GA[C_4C_6C_8(p,q)] = 9pq + p\left[\frac{5\sqrt{3}+12\sqrt{6}-30)}{10}\right] + 2q(\sqrt{3}-1).$$

Theorem 2.8. *Let $[C_4C_6C_8(p, q)]$ be the Nanotori with p columns and q rows ∀p, q ∈ N. Then the inverse sum indeg index of $[C_4C_6C_8(p, q)]$ is,*

$$ISI[C_4C_6C_8(p,q)] = \frac{p}{2}\left[\frac{153}{10} + 27q\right].$$

Proof. Consider the graph Nanotori $[C_4C_6C_8(p, q)]$ with *p* columns and *q* rows ∀*p*, *q* ∈ *N*. Now to compute the inverse

sum indeg index of graph $[C_4C_6C_8(p, q)]$ Nanotori, we consider the edge partition of graph from remark C.
From equation (5),

$$ISI(C_4C_6C_8(p,q)) = \sum_{(uv)\in E(C_4C_6C_8(p,q))} \frac{(d_u \times d_v)}{(d_u + d_v)}$$

$$= (p+4q)\left[\frac{1\times 3}{1+3}\right] + [2p]\left[\frac{2\times 3}{2+3}\right] + [3p(3q-1)-2q]\left[\frac{3\times 3}{3+3}\right]$$

On simplification we get,

$$ISI[C_4C_6C_8(p,q)] = \frac{p}{2}\left[\frac{153}{10} + 27q\right].\backslash$$

Conclusion and Future Scope

In this article we studied about Nanocones and Nanotories and also applied analytical methods to compute the topological indices namely Sum connectivity index, Product connectivity index, Geometric-arithmetic index and Inverse sum indeg index for these Nanocones and Nanotories. Hence Obtain the results. Nevertheless, there are some more topological indices were exist, one can apply and compute those indices for the above mentioned structures.

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