

# VALENCY BASED TOPOLOGICAL INDICES OF CARBON NANOCONES

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**ABSTRACT.** Topological indices are the global parameters defined for the simple graphs such that they give the same numerical value if the graphs are isomorphic. These numbers are of much importance because of their chemical importance, they correlate certain physico-chemical properties of certain organic compounds such hydrocarbons etc. A chemical graph is a graph which is created from some molecular structure by applying some graphical operations. Valency/degree is a local graph parameter, which is defined for every vertex as the number of connections with other vertices in a graph, just like for an atom in a molecule. Degree based topological indices play a vital role in QSAR/QSPR studies and correlate various physico-chemical properties of chemical compound. Carbon nanocones are conical structures which are allotropes of carbon having at least one dimension of the order one micrometer or smaller.

In this paper, valency based topological indices of carbon nanocones are strong-minded.

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## 1 INTRODUCTION

Mathematical chemistry is a branch of theoretical chemistry in which we discuss and predict the chemical structure by using mathematical tools and does not necessarily refer to the quantum mechanics. Chemical graph theory is a branch of mathematical chemistry in which we apply tools of graph theory to model the chemical phenomenon mathematically. This theory plays a prominent role in the fields of chemical sciences. A molecular/chemical graph is a simple finite graph in which vertices denote the atoms and edges denote the chemical bonds in underlying chemical structure. This is more important to say that the hydrogen atoms are often omitted in any molecular graph.

Nanobiotechnology is a rapidly advancing area of scientific and technological opportunity that applies the tools and processes of nanofabrication to build devices for studying biosystems. Chemical graph theory found a prominent place in this prestigious area of research. In the last few decades there is a lot of research which has been done in this field. This theory contributes a main role in the fields of chemical sciences. A molecular/chemical graph is a simple finite hydrogen depleted graph in which vertices denote the atoms and edges denote the chemical bonds in underlying chemical structure.

A nanostructure is an object of intermediate size between microscopic and molecular structures. It is product derived through engineering at molecular scale. Carbon nanocones are conical structures which are allotropes of carbon having at least one dimension of the order one micrometer or smaller.

A topological index is a function “Top” from  $\sum$  to the set of real numbers, where  $\sum$  is the set of finite simple graphs with the property that  $Top(G) = Top(H)$  if both  $G$  and  $H$  are isomorphic. Obviously, the number of edges and vertices of a graph are topological indices also. A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix which represents the whole graph, and these representations are aimed to be uniquely defined for that graph.

Throughout in this article,  $G$  is considered to be connected graph with vertex set  $V(G)$  and edge set  $E(G)$  and  $d_u$  is the degree of vertex  $u \in V(G)$ . The notations are standard and mainly taken from books [12, 21].

The very first and oldest degree based topological index is Randić index [20] denoted by  $\chi(H)$  and introduced by Milan Randić in 1975. The Randić index of graph  $G$  is defined as

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

The general Randić index was proposed by Bollobás and Erdős [5] and Amic et al. [3] independently, in 1998. Then it has been extensively studied by both mathematicians and theoretical chemists [13]. Many important mathematical properties have been established. For a survey of results, we refer to the new book by Li and Gutman [18].

The general Randić index  $R_\alpha(G)$  is the sum of  $(d_u d_v)^\alpha$  over all edges  $e = uv \in E(G)$  defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$$

Obviously  $R_{-\frac{1}{2}}(G)$  is the particular case of

$$R_\alpha(G) \text{ when } \alpha = -\frac{1}{2}.$$

An important topological index introduced about forty years ago by Ivan Gutman and Trinajstić is the Zagreb index or more precisely first zagreb index denoted by  $M_1(G)$  and was defined as the sum of degrees of end vertices of all edges of  $G$ .

The first zagreb index is defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

The second zagreb index is defined as

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$$

The reduced version of second zagreb index is defined [7] as follows:

$$RM_2(G) = \sum_{uv \in E(G)} (d_u - 1) \times (d_v - 1)$$

With motivation from the Randić  $c'$  index, a closely related variant of the Randić  $c'$  connectivity index called the sum-connectivity index was recently proposed by Zhou and Trinajstić  $c'$  [22] in 2009. The sum-connectivity index  $\chi(G)$  was defined as follows:

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

Another variant of the Randić  $c'$  index named the harmonic index which first appeared in [6]. For a graph  $G$ , the harmonic index  $H(G)$  is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$$

Harmonic index is extensively studied for unicyclic and bicyclic graphs in [11].

## 2 MOTIVATIONS, RESULTS AND DISCUSSION

In this paper, we study carbon nanocones having triangle and pentagon as their cores and having hexagonal layers on its conical surface. A type of pentagonal nanocone is shown in Fig. 1. It has a pentagon on its top which acts as its core and is encompassing the hexagonal layers on its conical surface. The study of physico-chemical properties of these carbon containing chemical compounds is a respected problem in nanotechnology and theoretical chemistry. The study of topological descriptors of these chemical compounds supports this phenomenon in a productive way. Because of importance of topological indices in these organic compounds, we intend to study them for two important classes of carbon nanocones. These results provide a basis to understand the topology of these chemical compounds.

Wiener index is one of the most studied topological index in the literature. Alipour et al. studied the Wiener index of one-heptagonal nanocone [1]. They gave the idea to compute this so-called index numerically. The vertex PI, Szeged and omega polynomials of carbon nanocones  $CNC_4[n]$  have been studied by Ghorbani et al. in [8]. For further study of topological indices of various nanostructures, networks and graphs see [2, 4, 9, 10, 14, 15, 16, 17, 19].

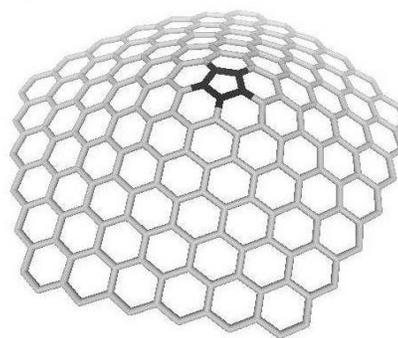


Figure 1: A type of pentagonal nanocone having a pentagon as its core.

### 2.1 RESULTS FOR $CNC_3[n]$ NANOCONE

In this section, we compute degree based topological indices of  $CNC_3[n]$  nanocones. A  $CNC_3[n]$  nanocones consists of a triangle as its core and encompassing the layers of hexagons on its conical surface. If there are  $n$  layers of hexagons on the conical surface around triangle, then we represent the graph of that nanocones as  $CNC_3[n]$  in which number  $n$  denotes the number of layers of hexagons and number in the subscript shows the sides of polygon which acts as the core of nanocones. The  $CNC_3[2]$  nanocone is shown in Fig. 2.

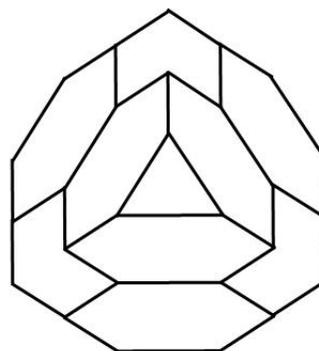


Figure 2: Graph of  $CNC_3[2]$  nanocone.

Following theorem presents the analytically closed formula of general Randić  $c'$  index  $R_\alpha(G)$  with  $\alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}$  for  $CNC_3[n]$  nanocone.

**Theorem 2.1.1.** Consider the  $CNC_3[n]$  nanocone, then its general Randić  $c'$  index is equal to

$$R_\alpha(CNC_3[n]) = \begin{cases} \frac{81}{2}n^2 + \frac{99}{2}n + 12, & \alpha = 1; \\ \frac{27}{2}n^2 + (6\sqrt{6} + \frac{9}{2})n + 6, & \alpha = \frac{1}{2}; \\ \frac{1}{2}n^2 + \frac{7}{6}n + \frac{3}{4}, & \alpha = -1; \\ \frac{3}{2}n^2 + (\sqrt{6} + \frac{1}{2})n + \frac{3}{2}, & \alpha = -\frac{1}{2}. \end{cases}$$

**Proof.** Consider  $H$  be the  $CNC_3[n]$  nanocone with defining parameter  $n$ . The number of vertices and edges in  $H$  are  $3(n+1)^2$  and  $\frac{9}{2}n^2 + \frac{15}{2}n + 3$  respectively. There are three types of edges in  $H$  based on degrees of end vertices of each edge. Table 1 shows such an edge partition of  $H$ .

**Table 1: Edge partition of  $CNC_3[n]$  nanocone based on degrees of end vertices of each edge. For  $\alpha = 1$**

$(d_u, d_v)$ where $uv \in E(G)$	Number of edges
(2,2)	3
(2,3)	$6n$
(3,3)	$\frac{9}{2}n^2 + \frac{3}{2}n$

Now we apply the formula of  $R_\alpha(G)$  for  $\alpha = 1$ .

$$R_1(G) = \sum_{uv \in E(G)} (d_u \times d_v)$$

By using edge partition given in table 1, we get a this expression in parameter  $n$ ,

$$R_1(H) = 3(2 \times 2) + 6n(2 \times 3) + (\frac{9}{2}n^2 + \frac{3}{2}n)(3 \times 3)$$

After simplifying, we get

$$R_1(H) = \frac{81}{2}n^2 + \frac{99}{2}n + 12$$

**For  $\alpha = \frac{1}{2}$**

We apply the formula of  $R_\alpha(G)$  for  $\alpha = \frac{1}{2}$ .

$$R_{\frac{1}{2}}(G) = \sum_{uv \in E(G)} \sqrt{d_u \times d_v}$$

By using edge partition given in table 1, we get this expression in parameter  $n$ ,

$$R_{\frac{1}{2}}(H) = 3\sqrt{2 \times 2} + 6n\sqrt{2 \times 3} + (\frac{9}{2}n^2 + \frac{3}{2}n)\sqrt{3 \times 3}$$

$$R_{\frac{1}{2}}(H) = \frac{27}{2}n^2 + (6\sqrt{6} + \frac{9}{2})n + 6$$

**For  $\alpha = -1$**

We apply the formula of  $R_\alpha(G)$  for  $\alpha = -1$ .

$$R_{-1}(G) = \sum_{uv \in E(G)} \frac{1}{(d_u \times d_v)}$$

$$R_{-1}(H) = 3(\frac{1}{2 \times 2}) + 6n(\frac{1}{2 \times 3}) + (\frac{9}{2}n^2 + \frac{3}{2}n)(\frac{1}{3 \times 3})$$

$$R_{-1}(H) = \frac{1}{2}n^2 + \frac{7}{6}n + \frac{3}{4}$$

**For  $\alpha = -\frac{1}{2}$**

We apply the formula of  $R_\alpha(G)$  for  $\alpha = -\frac{1}{2}$ .

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u \times d_v}}$$

$$R_{-\frac{1}{2}}(H) = 3(\frac{1}{\sqrt{2 \times 2}}) + 6n(\frac{1}{\sqrt{2 \times 3}}) + (\frac{9}{2}n^2 + \frac{3}{2}n)(\frac{1}{\sqrt{3 \times 3}})$$

$$R_{-\frac{1}{2}}(H) = \frac{3}{2}n^2 + (\sqrt{6} + \frac{1}{2})n + \frac{3}{2}$$

In the following theorem, we compute reduced second Zagreb index for this nanocone.

**Theorem 2.1.2.** For  $CNC_3[n]$  nanocone, the reduced second Zagreb index  $RM_2$  is equal to

$$RM_2(CNC_3[n]) = 18n^2 + 18n + 3$$

**Proof.** Let  $G$  be the  $CNC_3[n]$  nanocone. By using edge partition from table 1, we easily prove it. We know

$$RM_2(G) = \sum_{uv \in E(G)} (d_u - 1) + (d_v - 1)$$

$$RM_2(G) = 3((2-1) \times (2-1)) + 6n((2-1) \times (3-1)) + (\frac{9}{2}n^2 + \frac{3}{2}n)((3-1) \times (3-1))$$

By doing some calculation, we get our required result

$$RM_2(G) = 18n^2 + 18n + 3.$$

In the following theorem, we compute sum-connectivity index for this class of nanocones.

**Theorem 2.1.3.** For  $CNC_3[n]$  nanocone, the sum-connectivity index is equal to

$$X(CNC_3[n]) = \frac{3\sqrt{6}}{4}n^2 + (\frac{\sqrt{6}}{4} + \frac{6\sqrt{5}}{5})n + \frac{3}{2}$$

**Proof.** Let  $CNC_3[n]$  be the chemical graph of triangular

nanocones. By using edge partition from table 1, we easily prove it. We know

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

$$X(CNC_3[n]) = 3\left(\frac{1}{\sqrt{2+2}}\right) + 6n\left(\frac{1}{\sqrt{2+3}}\right) + \left(\frac{9}{2}n^2 + \frac{3}{2}n\right)\left(\frac{1}{\sqrt{3+3}}\right)$$

By doing some calculation, we get our required result

$$X(CNC_3[n]) = \frac{3\sqrt{6}}{4}n^2 + \left(\frac{\sqrt{6}}{4} + \frac{6\sqrt{5}}{5}\right)n + \frac{3}{2}$$

In the following theorem, we compute harmonic index for triangular nanocones  $CNC_3[n]$ .

**Theorem 2.1.4.** For  $CNC_3[n]$  nanocone, the harmonic index is equal to

$$H(CNC_3[n]) = \frac{3}{2}n^2 + \frac{29}{10}n + \frac{3}{2}$$

*Proof.* Let  $CNC_3[n]$  be the chemical graph of triangular nanocones. We prove it by using edge partition from table 1. We know

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$$

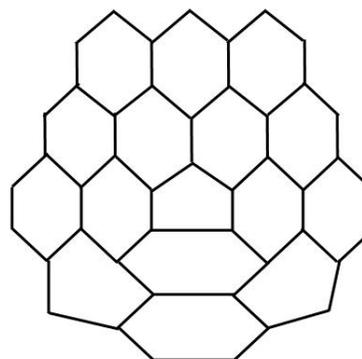
$$H(CNC_3[n]) = 3\left(\frac{2}{2+2}\right) + 6n\left(\frac{2}{2+3}\right) + \left(\frac{9}{2}n^2 + \frac{3}{2}n\right)\left(\frac{2}{3+3}\right)$$

By doing some calculation, we get our required result

$$H(CNC_3[n]) = \frac{3}{2}n^2 + \frac{29}{10}n + \frac{3}{2}$$

**2.2 Results for  $CNC_5[n]$  nanocone**

In this section, we determine valency based topological indices of  $CNC_5[n]$  nanocone. The vertex and edge cardinalities are  $|V(CNC_5[n])| = 5(n+1)^2$  and  $|E(CNC_5[n])| = \frac{15}{2}n^2 + \frac{25}{2}n + 5$ . This family of nanocones are often called *one pentagonal nanocones*, and word pentagonal used for pentagon as its core and like other families of nanocones there are hexagonal layers on its conical surface (Fig. 3).



**Figure 3:** Graph of one pentagonal nanocone  $CNC_5[n]$  with  $n = 2$ .

Following theorem presents the analytically closed formula of general Randi  $c'$  index  $R_\alpha(G)$  with  $\alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}$

for  $CNC_5[n]$  nanocone.

**Theorem 2.2.1.** Consider the  $CNC_5[n]$  nanocone, then its general Randi  $c'$  index is equal to

$$R_\alpha(CNC_5[n]) = \begin{cases} \frac{135}{2}n^2 + 65n + 20, & \alpha = 1; \\ \frac{45}{2}n^2 + (4\sqrt{6} + \frac{15}{2})n + 10, & \alpha = \frac{1}{2}; \\ \frac{5}{6}n^2 + \frac{35}{18}n + \frac{5}{4}, & \alpha = -1; \\ \frac{5}{2}n^2 + (\frac{5\sqrt{6}}{3} + \frac{5}{6})n + \frac{5}{2}, & \alpha = -\frac{1}{2}. \end{cases}$$

*Proof.* Consider the  $CNC_5[n]$  nanocone with defining parameter  $n$ . The number of vertices and edges in  $H$  are  $5(n+1)^2$  and  $\frac{15}{2}n^2 + \frac{25}{2}n + 5$  respectively. There are three types of edges in  $H$  based on degrees of end vertices of each edge. Table 2 shows such an edge partition of  $H$ .

**Table 2:** Edge partition of  $CNC_5[n]$  nanocone based on degrees of end vertices of each edge.

For $\alpha = 1$	
$(d_u, d_v)$ where $uv \in E(G)$	Number of edges
(2,2)	5
(2,3)	$10n$
(3,3)	$\frac{15}{2}n^2 + \frac{5}{2}n$

Now we apply the formula of  $R_\alpha(G)$  for  $\alpha = 1$ .

$$R_1(G) = \sum_{uv \in E(G)} (d_u \times d_v)$$

By using edge partition given in table 2, we get a this expression in parameter  $n$ ,

$$R_1(CNC_5[n]) = 5(2 \times 2) + 10n(2 \times 3) + (\frac{15}{2}n^2 + \frac{5}{2}n)(3 \times 3)$$

After simplifying, we get

$$R_1(CNC_5[n]) = \frac{135}{2}n^2 + 65n + 20$$

For  $\alpha = \frac{1}{2}$

We apply the formula of  $R_\alpha(G)$  for  $\alpha = \frac{1}{2}$ .

$$R_{\frac{1}{2}}(G) = \sum_{uv \in E(G)} \sqrt{d_u \times d_v}$$

By using edge partition given in table 1, we get this expression in parameter  $n$ ,

$$R_{\frac{1}{2}}(CNC_5[n]) = 5\sqrt{2 \times 2} + 10n\sqrt{2 \times 3} +$$

$$(\frac{15}{2}n^2 + \frac{5}{2}n)\sqrt{3 \times 3}$$

$$R_{\frac{1}{2}}(CNC_5[n]) = \frac{45}{2}n^2 + (4\sqrt{6} + \frac{15}{2})n + 10$$

For  $\alpha = -1$

We apply the formula of  $R_\alpha(G)$  for  $\alpha = -1$ .

$$R_{-1}(G) = \sum_{uv \in E(G)} \frac{1}{(d_u \times d_v)}$$

$$R_{-1}(CNC_5[n]) = 5(\frac{1}{2 \times 2}) + 10n(\frac{1}{2 \times 3}) +$$

$$(\frac{15}{2}n^2 + \frac{5}{2}n)(\frac{1}{3 \times 3})$$

$$R_{-1}(CNC_5[n]) = \frac{5}{6}n^2 + \frac{35}{18}n + \frac{5}{4}$$

For  $\alpha = -\frac{1}{2}$

We apply the formula of  $R_\alpha(G)$  for  $\alpha = -\frac{1}{2}$ .

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u \times d_v}}$$

$$R_{-\frac{1}{2}}(CNC_5[n]) = 5(\frac{1}{\sqrt{2 \times 2}}) + 10n(\frac{1}{\sqrt{2 \times 3}}) +$$

$$(\frac{15}{2}n^2 + \frac{5}{2}n)(\frac{1}{\sqrt{3 \times 3}})$$

$$R_{-\frac{1}{2}}(CNC_5[n]) = \frac{5}{2}n^2 + (\frac{5\sqrt{6}}{3} + \frac{5}{6})n + \frac{5}{2}.$$

In the following theorem, we compute reduced second Zagreb index for this nanocone.

**Theorem 2.2.2.** For  $CNC_5[n]$  nanocone, the reduced second Zagreb index  $RM_2$  is equal to

$$RM_2(CNC_5[n]) = 30n^2 + 30n + 5$$

*Proof.* Let  $G$  be the  $CNC_5[n]$  nanocone. We easily prove it by using edge partition in table 2. We know

$$RM_2(G) = \sum_{uv \in E(G)} (d_u - 1) + (d_v - 1)$$

$$RM_2(G) = 5((2-1) \times (2-1)) + 10n((2-1) \times (3-1)) + (\frac{15}{2}n^2 + \frac{5}{2}n)((3-1) \times (3-1))$$

By doing some calculation, we get our required result

$$RM_2(G) = 30n^2 + 30n + 5.$$

In the following theorem, we compute sum-connectivity index for this class of nanocones.

**Theorem 2.2.3.** For  $CNC_5[n]$  nanocone, the sum-connectivity index is equal to

$$X(CNC_5[n]) = \frac{5\sqrt{6}}{4}n^2 + (\frac{5\sqrt{6}}{12} + 2\sqrt{5})n + \frac{5}{2}$$

*Proof.* Let  $CNC_5[n]$  be the chemical graph of one-pentagonal nanocones. We prove it by using edge partition from table 2. We know

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

$$X(CNC_5[n]) = 5(\frac{1}{\sqrt{2+2}}) + 10n(\frac{1}{\sqrt{2+3}}) + (\frac{15}{2}n^2 + \frac{5}{2}n)(\frac{1}{\sqrt{3+3}})$$

By doing some calculation, we get our required result

$$X(CNC_5[n]) = \frac{5\sqrt{6}}{4}n^2 + (\frac{5\sqrt{6}}{12} + 2\sqrt{5})n + \frac{5}{2}.$$

In the following theorem, we compute harmonic index for one-pentagonal nanocones  $CNC_5[n]$ .

**Theorem 2.2.4.** For  $CNC_5[n]$  nanocone, the harmonic index is equal to

$$H(CNC_5[n]) = \frac{5}{2}n^2 + \frac{29}{6}n + \frac{5}{2}$$

*Proof.* Let  $CNC_5[n]$  be the chemical graph of one-pentagonal nanocones. We prove it by using edge partition from table 2. We know

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$$

$$H(CNC_5[n]) = 5\left(\frac{2}{2+2}\right) + 10n\left(\frac{2}{2+3}\right) + \left(\frac{15}{2}n^2 + \frac{5}{2}n\right)\left(\frac{2}{3+3}\right)$$

By doing some calculation, we get our required result

$$H(CNC_5[n]) = \frac{5}{2}n^2 + \frac{29}{6}n + \frac{5}{2}.$$

### 3 CONCLUDING REMARKS

Topological indices play a vital role in the study of physico-chemical properties of chemical compounds. Valency based topological indices have got a prominent place in this study due to prediction of various chemical properties such as stability, Kovat's constant, enthalpy etc. with high predictive power. To compute and study these topological indices for various nanostructures like nanotubes, nanostar dendrimers and nanocones is a respected problem in nanotechnology. In this study, we compute various valency based topological indices of two important classes of carbon nanocones. These results give valuable information regarding chemical properties of these nanocones. In future, we are interested to study topological description of these chemical graphs by studying their distance based topological indices.

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