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On the topological index of one - Heptagonal Carbon nanocones

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ABSTRACT

A topological index is a real number related to a molecular graph. It must be a structural in variant, that is, it preserves by every graph automorphism. This number has very close affiliation with actual quantity such as potential, spot welding and the other chemical structures properties. The Wiener index is the first topological index has used in chemistry. Let G be a connected graph with vertexes and edges sets $V(G)$ and $E(G)$, respectively. We denote the distance between two arbitrary vertices x and y from G by $d(x,y)$ and it is defined as the number of edge in the minimal path connecting the vertices x and y. A molecular graph is a simple graph such that its vertices correspond to atoms and edges to the bonds. In this paper we compute the edge eccentric connectivity and edge modified eccentric connectivity topological indices and their polynomials, also we compute the atom - bond indices of types 1 and 4 for one - heptagonal carbon nanocones.

KEYWORDS: : Topological index , Carbon nanocone, molecular graph , atom - bond , edge eccentric connectivity and edge modified eccentric connectivity , indices polynomials.

1 INTRODUCTION

The study of molecular structures via graph theory is considered as chemical graph theory or molecular topology. This theory provides a valuable tools for a chemist successes. There into, topological index is defined well grounded on vertices distance in molecular graph. Using topological indices in chemistry and biology first began by Wiener to compute boiling point and he also used of Wiener index to predict molar bulk, thermo isomoisasion and thermo vaporization in his paper [9],[10]. The researches on carbon nanocones almost started when nano tubular was discovered in 1991 by scientist called Ball [11]. The numerous applications of this molecular graph in new technologies have prompted many studies, recourse [4],[5],[6],[8] and [12] . In paper [12] Padmakar - Ivan and edge Szeged indices of one-heptagonal nanocones and some index on nano tube were investigated. In this paper, we compute as edge eccentric an edge modified eccentric indices and their polynomial of one heptagonal carbon nanocones. It should be mentioned that nano cones are shown as $\mathrm{CNC}_m[n]$, where a cyclic graph C_m is

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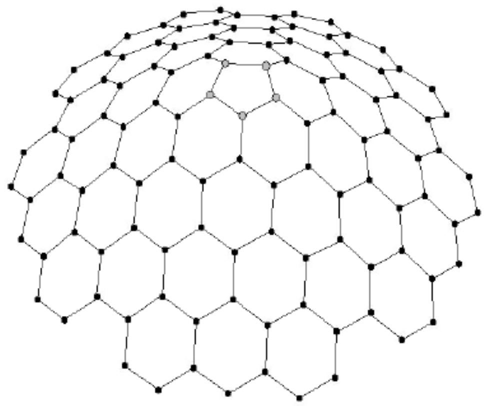
in the top or central nucleus of cone and n, number of hexagon which are connected to each C_m edge of nanocones. We should be careful that is always $n \geq 2$ and $3 \leq m \leq 7$.



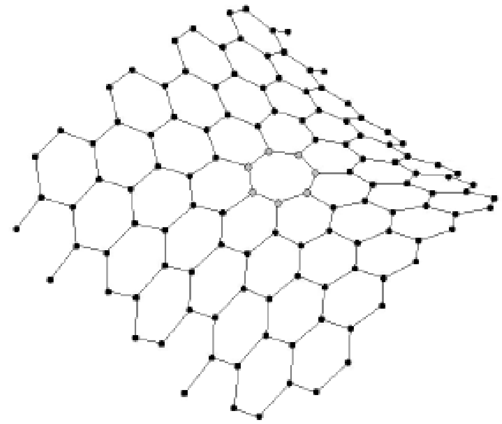


Figure 2. one - heptagonal nanocones **Figure 1. one - pentagonal nanocones**

Definition 1.1. Let G be a graph and $f = uv \in E(G)$. Then degree of f define $\deg_G(f) = \deg_G(u) + \deg_G(v) - 2$, [7].

Definition 1.2. Let $G = (V, E)$ be a graph and $f_1 = u_1v_1$ and $f_2 = u_2v_2$ is two edges in $E(G)$. Then distance between two edges f_1 and f_2 of G is denoted by $d_G(f_1, f_2)$ and it is define $d_G(f_1, f_2) = \min\{d_G(u_1,u_2), d_G(u_1,v_2), d_G(v_1,u_2), d_G(v_1,v_2)\}$, and especially distance between edge $f = uv$ from vertex x is tantamount distances minimal of two vertexes u and v of vertex x.

Definition 1.3. Let $G = (V, E)$ be a graph, then eccentric connectivity of f in $E(G)$ is denoted by $ecc_G(f)$ and it is defined $ecc_G(f) = \max\{d_G(f, e) / e \in E(G)\}$.

Definition 1.4. Let $G = (V, E)$ be a graph and $u \in V(G)$. We define $S_u = \sum_{v \in N_G(u)} d_v$ where

$N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$.

2 EDGE ECCENTRIC, EDGE MODIFIED ECCENTRIC POLYNOMIALS AND THEIR INDEX

This section we compute the edge eccentric and edge modified eccentric topological indices and their polynomials on one - heptagonal carbon nanocones (i.e $CNC_7[n]$). We consider easier $C_7[n] =: CNC_7[n]$. As we said before the graph $C_7[n]$ consist a cyclic graph of C_7 is in the central nucleus of cone and n number of hexagon which are connected to each C_7 edge of nanocones. For example Figure (3) is 2 - dimensional lattice of $C_7[3]$. Also this shape shows the minimal and maximal paths for computing edge eccentric connectivity in $C_7[3]$.

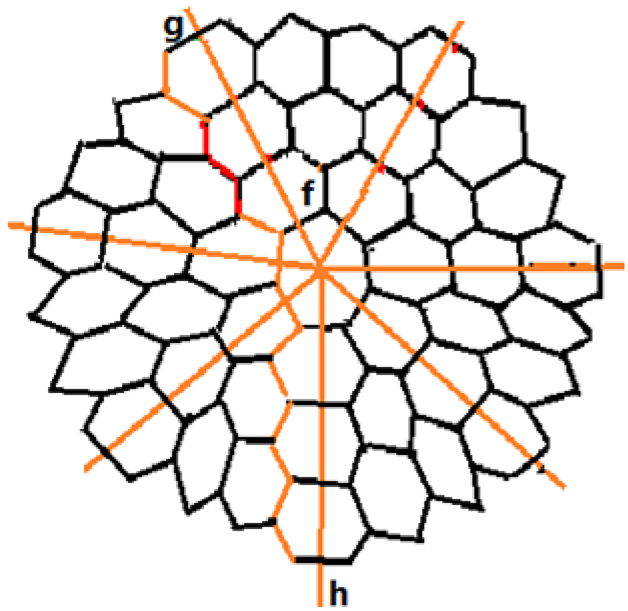


Figure 3 . The 2 - Dimensional Lattice of $C_7[3]$

We compute minimal and maximal edge eccentric for graph of $C_7[3]$ in after lemma.

Lemma 2-1. For every edge f in $E(C_7[n])$, we have,

$$Max(ecc(f)) = 4n+2 \ , \ Min(ecc(f)) = 2n+2.$$

Proof . Suppose f is one edge of C_7 in $C_7[n]$. Then as in Figure 3 there exist an edge of degree two such as g so that $d(f,g)=2n$ and also there exists another edge h of degree two such that $d(f,h)=2n+2$. Therefore the shortest path with maximum length is connecting two edges of degree 2 in $C_7[n]$, meantime long of path is $4n+2$. The proof is completed.□

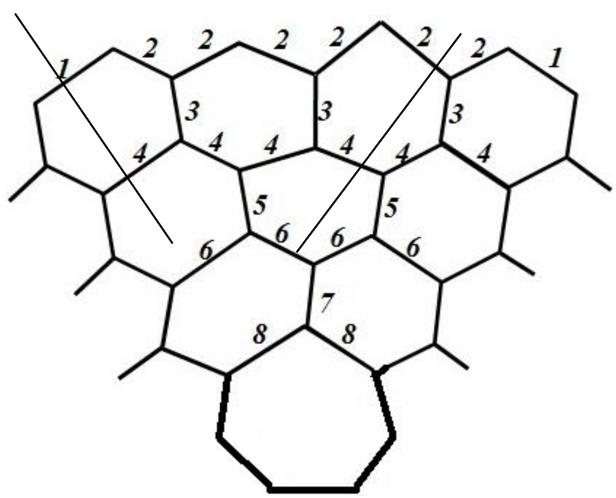


Figure 4. shows types edge with edge eccentric connectivity in T_1 of $C_7[3]$.

Theorem 2-2. The edge eccentric connectivity polynomial and it's index for $C_7[n]$ is given by the following formulas.

$$ECP_e(C_7[n],x)=\sum_{f\in E(C_7[n])}\deg(f)x^{ecc(f)}$$

$$=(14+42n)x^{4n+2}+\sum_{k=0}^{n-1}4(7n-7k)x^{4n-(2k-1)}+\sum_{k=1}^{n}4(14n-(14k-7))x^{4n-2(k-1)}.$$

$$\xi_e^c(C_7[n])=\frac{d}{dx}\left(ECP_e(C_7[n],x)\right)_{x=1}.$$

Proof. For computing of $ecc(f)$ there are $2n+2$ type edges in $C_7[n]$.

Refer to Figures (3) , (4) and Table (1) we can assume that $C_7[n]=\bigcup_{i=1}^{7}T_i$, where $\{T_i\}_{1\le i\le 7}$ is a partition of the molecular graph $C_7[n]$. Hence practically that, the maximum edge eccentric is equal $4n+2$ for edges of Type 1 and Type 2 with numbers 7 and $14n$ respectively. Also the numbers $7n$ edges of Type 3 with edge eccentric equal $4n+1$, the numbers $14n-7$ edges of Type 4 with edge eccentric equal $4n$ and so it continues until we have seven edges of Type $2n+1$ with edge eccentric equal $2n+3$ and seven edges of Type $2n+2$ with minimum edge eccentric equal $2n+2$. Also by Table 1, it is clear that there are seven edges of Type one with degree 2 and $14n$ edges of Type 2 with degree 3 and remaining edges are of degree 4.

Table 1. Types of T_i edges for compute $\deg(f)$ in $C_7[n]$

Types of Edges	Num	Ecc	Deg
1	7	$4n+2$	2
2	$14n$	$4n+2$	3
3	$7n$	$4n+1$	4
4	$14n-7$	$4n$	4
5	$7n-7$	$4n-1$	4
6	$14n-21$	$4n-2$	4
7	$7n-14$	$4n-3$	4
8	$14n-35$	$4n-4$	4
...	...	....	...
$2n-1$	14	$2n+5$	4
$2n$	21	$2n+4$	4
$2n+1$	7	$2n+3$	4

$2n+2$	7	$2n+2$	4

Therefore, we have:

$$ECP_e\left(C_7[n],x\right)=\sum_{f\in E(C_7[n])}\deg(f)x^{ecc(f)}=2\times7\times x^{4n+2}+3\times14n\times x^{4n+2}$$

$$+\sum_{k=0}^{n-1}4\left(7n-7k\right)x^{4n-(2k-1)}+\sum_{k=1}^{n}4\left(14n-\left(14k-7\right)\right)x^{4n-2(k-1)}.$$

$$\Rightarrow ECP_e\left(C_7[n],x\right)=\left(14+42n\right)x^{4n+2}+\sum_{k=0}^{n-1}4\left(7n-7k\right)x^{4n-(2k-1)}+\sum_{k=1}^{n}4\left(14n-\left(14k-7\right)\right)x^{4n-2(k-1)}.$$

As a result, the edge eccentric connectivity index is the first derivative of this polynomial for $x=1$. Then this theorem is proved. □

We compute edge modified eccentric connectivity index and it's polynomial for molecular graph of $C_7[n]$ in next theorem. Also S_f, that is, sum degrees of neighbors of edge f.

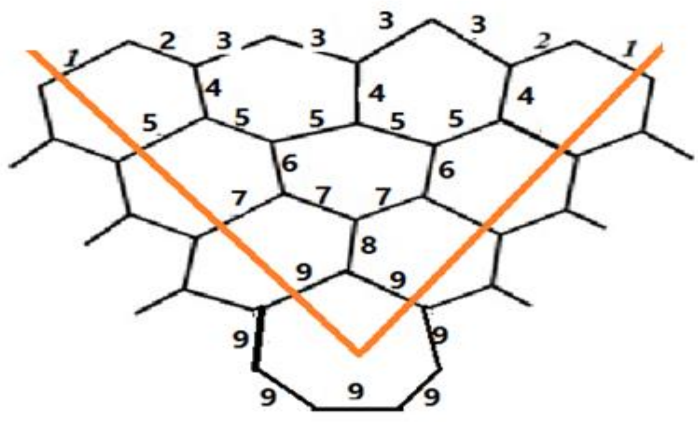


Figure 5. The 2 - Dimensional Lattice of edges set with edge eccentric connectivity for compute of S_f in T_1 of $C_7[3]$.

Theorem 2-3. The edge modified eccentric connectivity polynomial and it's index for $C_7[n]$, is given by formulas.

$$\Lambda_e\left(C_7[n],x\right)=\sum_{f\in E\left(C_7[n]\right)}S_f\,.x^{ecc(f)}==(140n+28)x^{4n+2}+98n\times x^{4n+1}$$

$$+\sum_{k=0}^{n-1}16(14n-7(2k+1))x^{4n-2k}+\sum_{k=1}^{n-1}14\left(7n-7k\right)x^{4n-(2k-1)}.$$

And $\Lambda_e\left(C_7[n]\right)=\frac{d}{dx}\left(\Lambda_e\left(C_7[n],x\right)\right)_{x=1}.$

Proof. We know for computing of S_f exists 2n+3 Type edge in $C_7[n]$. Refer to Figure 5 and Table 2, practically that edges of Types $1,2$ and 3 with are maximum edge eccentric equal $4n+2$ such that their numbers are 7, 14 and $14\mathrm{n}-14$ respectively. Also the numbers $7\mathrm{n}$ edges of Type 4 with edge eccentric equal $4\mathrm{n}+1$, the numbers $14\mathrm{n}-7$ edges of Type 5 with edge eccentric equal $4\mathrm{n}$, and numbers $7\mathrm{n}-7$ edges of Type 6 with edge eccentric equal $4\mathrm{n}-1$. So it continues until seven edges of Type $2\mathrm{n}+2$ in which edge eccentric equal $2\mathrm{n}+3$ and seven edges of Type $2\mathrm{n}+3$ with minimum edge eccentric equal $2\mathrm{n}+2$. Again refer to Table 2 there are 7 edges of Type 1 with $S_f=6$, 14 edges of Type 2 with $S_f=9$, the $14\mathrm{n}-14$ edges of Type 3 with $S_f=10$ and $7\mathrm{n}$ edges of Type 4 with $S_f=14$, and remaining edges are with $S_f=16$.

Table 2 . Types of T_i edges for compute of S_f in $C_7[n]$

Types of Edges	Num	Ecc	S_f
1	7	$4n+2$	6
2	14	$4n+2$	9
3	$14n-14$	$4n+2$	10
4	$7n$	$4n+1$	14
5	$14n-7$	$4n$	16
6	$7n-7$	$4n-1$	16
7	$14n-21$	$4n-2$	16
8	$7n-14$	$4n-3$	16
9	$14n-35$	$4n-4$	16
...	...	....	...
$2n$	14	$2n+5$	16
$2n+1$	21	$2n+4$	16
$2n+2$	7	$2n+3$	16
$2n+3$	7	$2n+2$	16

Therefore, we have :

$$\Lambda_e\left(\mathrm{C}_7[n],x\right)=\sum_{f\in E\left(C_7[n]\right)} S_f\,.x^{ecc(f)}=7\times 6\times x^{4n+2}+14\times 9\times x^{4n+2}$$

$$+(14n-14)\times 10\times x^{4n+2}+7n\times 14\times x^{4n+1}+\sum_{k=0}^{n-1}16\left(14n-7(2k+1)\right)x^{4n-2k}+\sum_{k=1}^{n-1}14\left(7n-7k\right)x^{4n-(2k-1)}$$

$$=\left(140n+28\right)x^{4n+2}+98n\times x^{4n+1}+\sum_{k=0}^{n-1}16\left(14n-7(2k+1)\right)x^{4n-2k}+\sum_{k=1}^{n-1}14\left(7n-7k\right)x^{4n-(2k-1)}\ .$$

As a result, the edge modified eccentric connectivity index is the first derivative of this polynomial for x=1. Then this theorem is proved. □

3 ATOM - BOND INDEX

In this section we compute atom - bond index by Table 1 and Figure 4 and also Fourth atom - bond index by Table 2 and Figure 5.

Theorem 3-1. The atom - bond index for $C_7[n]$, is given following formula.

$$ABC(C_7[n]) = 7n^2 + (7\sqrt{2} + \frac{7}{3})n + \frac{7\sqrt{2}}{2}.$$

Proof. Refer to Figure 3 there are $2n+2$ Type edges in $C_7[n]$ and in n^{th} stratum of it's exist 7 edges of type one and for every edge $e = uv$ in this stratum is $d_u = d_v = 2$. Also there are $14n$ edges of type two, such that for every edge $e = uv$ of this kind is $d_u = 2$, $d_v = 3$. And remain edges in other stratums this graph are $d_u = d_v = 3$. Hence by Table 1 corps edges of Type $1, 2, 3, 4, 5, \ldots, 2n, 2n+1$ and $2n+2$ is $7, 14n, 7n, 14n-7, 7n-7, \ldots, 21, 7$ and 7 respectively. Thus, it implies that :

$$ABC(C_7[n]) = \sum_{uv \in E(C_7[n])} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}} = 7\sqrt{\frac{2+2-2}{2\times 2}} + 14n\sqrt{\frac{2+3-2}{2\times 3}} +$$
$$\sqrt{\frac{3+3-2}{3\times 3}}\sum_{k=1}^{n} 14n - (14k-7) + \sqrt{\frac{3+3-2}{3.3}}\sum_{k=1}^{n} 7n - 7(k-1) = 7n^2 + (7\sqrt{2} + \frac{7}{3})n + \frac{7\sqrt{2}}{2}.$$

Then this theorem is proved. □

Theorem 3-2. 4^{th} Atom - bond index on $C_7[n]$, is given by the following formula:

$$ABC_4(C_7[n]) = \frac{14n^2}{3} + \frac{3582374052830603}{562949953421312}n - \frac{\sqrt{462}}{3} + \frac{4601356991849869}{562949953421312}.$$

Proof. Let f be a edge of $E(C_7[n])$. By Table 2 and Figure 2, for compute of S_f there are $2n+3$ kinds of edge in $C_7[n]$. In n^{th} stratum of it exist 7 edges of Type 1 that for every edge $f = uv$ of this type is $S_u = S_v = 5$. There are 14 edges of type two that for every edge $f = uv$ of this type is $S_u = 5$, $S_v = 7$ and there are $14n-4$ edges of Type 3 that for every edge $f = uv$ of this type is $S_u = 7$, $S_v = 6$. And also there are $7n$ edges of Type 4 that between stratum $(n-1)$ and stratum n, for every edge $f = uv$ of this type is $S_u = 7$, $S_v = 9$. For the remain edges analogue $f = uv$ in other deferent stratums of this graph we have $S_u = S_v = 9$. Hence refer to Table 2, corps edges of Type $1, 2, 3, 4, 5, 6, 7, 8, \ldots, 2n, 2n+1, 2n+2$ and $2n+3$ is $7, 14, 14n-14, 7n, 14n-7, 7n-7, 14n-21, 7n-14, \ldots, 14, 21, 7$ and 7 respectively. Accordingly we have :

$$ABC_4(C_7[n]) = \sum_{uv \in E(C_7[n])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} = 7\sqrt{\frac{5+5-2}{5\times 5}} + 14\sqrt{\frac{5+7-2}{5\times 7}} + (14n-14)\sqrt{\frac{6+7-2}{6\times 7}}$$
$$+7n\sqrt{\frac{7+9-2}{7\times 9}} + \sqrt{\frac{9+9-2}{9\times 9}}\sum_{k=1}^{n}(14n - 7(2k-1)) + \sqrt{\frac{9+9-2}{9\times 9}}\sum_{k=1}^{n-1}(7n - 7k).$$

Hence $ABC_4\left(C_7[n]\right)=\frac{14n^2}{3}+\frac{3582374052830603}{562949953421312}n-\frac{\sqrt{462}}{3}+\frac{4601356991849869}{562949953421312}$.

Then this theorem is proved.

Conclusion.

At first in this paper characterized Max and Min edge eccentric for $C_7[n]$. Also by some Figures and Tables, we computed the edge eccentric and edge modified eccentric connectivity topological indices and their polynomials for molecular graph of $C_7[n]$. In last part we computed Atom - bond index and type four of Atom - bond index for molecular graph of $C_7[n]$ by Table 5.

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