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A Study of $CNC_7[n]$ Carbon Nanocone by M-Eccentric Connectivity Polynomial

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Abstract: The Eccentric Connectivity Polynomial of a molecular graph, G, is defined as ECP(G,x) = $\sum_{u\in V(G)} \deg_G(u) x^{ecc(u)}$, where *ecc(u)* is defined as the length of a maximal path connecting *u* to another vertex of *G*. The m-eccentric connectivity polynomial of a molecular graph, G, is defined as MECP(G,x) = $\sum_{u\in V(G)} n_G(u) x^{ecc(u)}$. In this paper, the M-Eccentric Connectivity Polynomial of One–Heptagonal Carbon Nanocone is computed.

Key words: Eccentric connectivity polynomial, M-Eccentric connectivity polynomial, One–Heptagonal carbon nanocone.

INTRODUCTION

In recent years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. One pentagonal carbon nanocone originally discovered by Ge and Sattler in 1994 (Ge, Sattler, 1994). These are constructed from a graphene sheet by removing a 60° wedge and joining the edges produces a cone with a single pentagonal defect at the apex. If a 120° wedge is considered then a cone with a single square defect at the apex is obtained. The case of 240° wedge yields a single triangle defect at the apex (Nelson, 1987) . In figure 1, one can see two types of One-Heptagonal Carbon Nanocone (top and side view, respectively).

Topological indices are graph invariants and are used for Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR), (Dobrynin, 1999).

Many topological indices have been defined and several applications of them have been found in physical, chemical and pharmaceutical models and other properties of molecules. A topological index of a molecular graph *G* is a numeric quantity related to *G*. The oldest nontrivial topological index is the Wiener index which was introduced by Harold Wiener (Dobrynin ,2002). John Platt was the only person who immediately realized the importance of the Wiener's pioneering work and wrote papers analyzing and interpreting the physical meaning of the Wiener index. The name of topological index was introduced by Hosoya (Hosoya, 1971) .

Now some algebraic definitions are recalled that will be used in the paper. Let *G* be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by *V(G)* and *E(G),* respectively. The vertices in *G* are connected by an edge if there exists an edge $uv\in E(G)$ connecting the vertices *u* and *v* in *G* so that $u,v\in V(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The number of vertices and edges in a graph will be defined by $|V(G)|$ and $|E(G)|$ respectively. In graph theory, a path of length *n* in a graph is a sequence of $n + 1$ vertices such that from each of its vertices there is an edge to the next vertex in the sequence. For two vertices *x* and *y* of G, $d_G(x,y)$ denotes the length of a minimal path connecting *x* and *y*. A graph G is called connected, if there is a path connecting vertices *x* and *y* of *G*, for every $x, y \in V(G)$. Suppose *X* is a set, X_i, $1 \le i \le m$, are subsets of *X* and $F = \{X_i\}_{1\le i\le m}$ is a family of subsets of *X*. If X_i's are non-empty, $X = \bigcup_{i=1}^{m} X_i$ and $X_i \bigcap X_j = \Phi$ *(empty)*, for $i \neq j$ then *F* is called a partition of *X*. If *G* is not connected then *G* can be partitioned into some connected subgraphs, which is called components of *G*.

The eccentric connectivity index of the molecular graph *G*, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan (Sharma, 1997). It is defined as $\xi^c(G) = \sum_{u\in V(G)} \deg_G(u).ecc(u)$ where $deg_G(u)$ denotes the degree of the vertex *u* in *G* and $ecc(u)= Max\{d(x,u) \mid x \in V(G)\}$. The radius and diameter of *G* are defined as the minimum and maximum eccentricity among vertices of *G*, respectively(Ashrafi, A.R, 2010),(Ashrafi, A.R, 2009). Define the eccentric connectivity polynomial of a graph *G*, *ECP(G,x),* as *ECP(G,x)*= $\sum_{u\in V(G)} \deg_G(u) x^{ecc(u)}$ (Ashrafi, 2010). Then the eccentric connectivity index is the first derivative of *ECP(G, x)* evaluated at $x = 1$.

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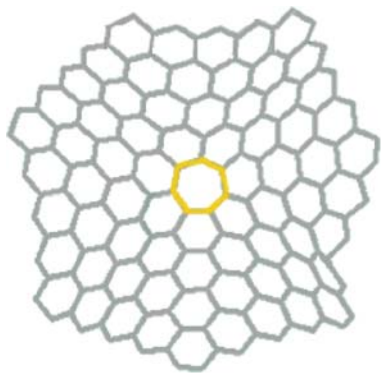
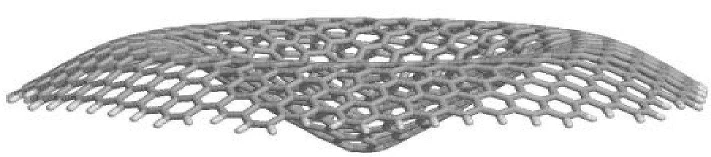
For example, if C_n denotes the cycle graph on n vertices, then, for every $v \in V(C_n)$, deg(v)=2 and ecc(v)= $\frac{n}{2}$ when n is even and ecc(v)=$\frac{n-1}{2}$ when n is odd. Hance:

$$ECP(C_n, x) = \begin{cases} 2nx^{\frac{n}{2}} & n \ is \ even \\ 2nx^{\frac{n-1}{2}} & n \ is \ odd \end{cases} \text{ and } \xi(C_n) = \begin{cases} n^2 & n \ is \ even \\ n(n-1) & n \ is \ odd \end{cases}.$$



(a)



(b)

Fig. 1: (a), (b): The One- Heptagonal Carbon Nanocone.

The Heptagonal ring is yellow

Main Results and Discussion:

In this section we calculate the eccentric connectivity index and polynomial of One–Heptagonal Carbon Nanocone by use an algebraic method. In continue a Matlab program is presented which is useful for computing the EC index and EC polynomial of a nanocone. We apply this program to compute of the molecular graph of nanocone $CNC_7[n]$, when $1 \le n$, see Fig.1. In this way the One–Heptagonal carbon nanocone are divided into several parts of the same. Calculations are done for a section and then generalized to the total carbon. Thus we determine maximum and minimum eccentric connectivity for every section of One–Heptagonal Carbon Nanocone with respect Fig.2. And finally the vertices set with same eccentric is determine, Fig.3.

Lemma 1. The number of vertices and edges in a molecular graph $CNC_7[n]$ is given by:

$|V(CNC_7[n])|=7(1+1+2+2+3+3+\ldots+(n-1)+(n-1)+n)=7n^2$ and

$|E(CNC_7[n])|=7(1+4+7+10+\ldots+(3n-5)+(3n-2))=\frac{7}{2}(3n^2-n)$.

Lemma 2. Max ecc(u)= 4n-1 and Min ecc(u)= 2n+1 for $u \in V(CNC_7[n])$

Proof. Suppose u is a vertex of the central heptagon of $CNC_7[n]$. Then from Fig. 2, one can see that there exists a vertex v of degree 2 such that d(u,v) =2n and there exists another vertex w of degree 2 such that d(u,w) =2n+1. Therefore, the shortest path with maximum length is connecting two vertices of degree 2 in $CNC_7[n]$. Then this poof is complete. ■

Theorem 3. The Eccentric Connectivity polynomial of One–Heptagonal Carbon Nanocone is computed as follows:

ECP(CNC$_7$[n],x)=$\frac{14nx^{4n}}{x}+\frac{21(1+x)x^{4n}}{x}\sum_{i=1}^{n-1}\frac{n-i}{x^{2i}}$

Proof. Suppose Q[n]= CNC$_7$[n]. With respect to figure 2, Q[n]=$\bigcup_{i=1}^{7}T_i$, where $\{T_i\}_{1\le i\le 7}$ is a partition of the molecular graph Q[n]. With respect to figure 3, we have maximum eccentric connectivity for *n* numbers of vertices type 1. Also , *n-1* numbers of vertices type 2 with eccentric equals to 4n-2, *n-1* numbers of vertices type 3 with eccentric equals to 4n-3, and so it continues until we have one vertex of type 2n-2 with eccentric 2n+2 and one vertex of type 2n-1 with minimum eccentric 2n+1. Also it is easy to check that, deg(u)=2 for vertices with maximum eccentric and deg(u)=3 for other vertices of T_i . See table 1 for vertices of T_i .

Table 1: Types of T_i Vertices

Vertices	No.	Ecc.	Degree	Vertices	No.	Ecc	Degree
Vertices Type 1	n	4n-1	2	Vertices Type 7	n-3	4n-7	3
Vertices Type 2	n-1	4n-2	3	…	…	…	…
Vertices Type 3	n-1	4n-3	3	Vertices Type 2n-4	2	2n+4	3
Vertices Type 4	n-2	4n-4	3	Vertices Type 2n-3	2	2n+3	3
Vertices Type 5	n-2	4n-5	3	Vertices Type 2n-2	1	2n+2	3
Vertices Type 6	n-3	4n-6	3	Vertices Type 2n-1	1	2n+1	3

Thus implies that

ECP(T_i ,x)= $\sum_{u\in V(T_i)}\deg_G(u)x^{ecc(u)}$

$$=2nx^{4n-1}+3(n-1)x^{4n-2}+3(n-1)x^{4n-3}+3(n-2)x^{4n-4}+3(n-2)x^{4n-5}$$

$$+\ldots+3\times 2x^{2n+4}+3\times 2x^{2n+3}+3x^{2n+2}+3x^{2n+1}$$

$$=2nx^{4n-1}+3(n-1)(1+x)x^{4n-3}+3(n-2)(1+x)x^{4n-5}+\ldots+3\times 2(1+x)x^{2n+3}$$

$$+3(1+x)x^{2n+1}$$

$$=2nx^{4n-1}+3(1+x)\sum_{i=1}^{n-1}(n-i)x^{4n-2i-1}$$

Therefore

ECP(Q[n],x)= $\sum_{u\in V(Q[n])}\deg_G(u)x^{ecc(u)}$ =7 ECP(T_i ,x)=7 $\sum_{u\in V(T_i)}\deg_G(u)x^{ecc(u)}$

$$=\frac{14nx^{4n}}{x}+\frac{21(1+x)x^{4n}}{x}\sum_{i=1}^{n-1}\frac{n-i}{x^{2i}}\ .\blacksquare$$

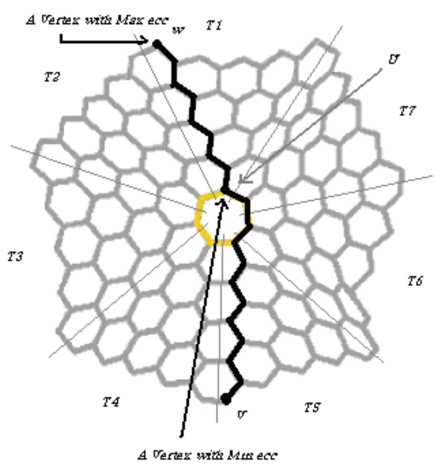


Fig. 2: A maximum and minimum path for computing ecc(u) in CNC$_7$[5] Carbon Nanocone.

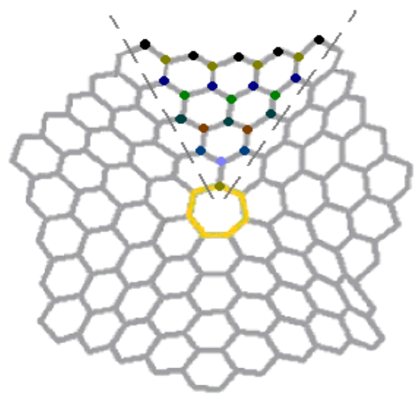


Fig. 3: The set of vertices with same ecc(u) in $CNC_7[5]$ Carbon Nanocone.

Theorem 4. The Eccentric Connectivity index of One–Heptagonal Carbon Nanocone is computed as follows:

$$\xi^c(CNC_7[n]) = \frac{7}{2}n(20n^2 - 11n + 3)$$

Proof. From the definitions, we'll have $\xi^c(CNC_7[n]) = \frac{\partial\left(ECP(CNC_7[n],x) \right)}{\partial x}\Big|_{x=1}$. So:

$$\xi^c(CNC_7[n]) = 14n(4n-2) + 21\sum_{i=1}^{n-1} 2(n-i)(4n-2-2i) + 21\sum_{i=1}^{n-1}(n-i)$$

$$= 14n(4n-2) + 42\left(4n^2(n-1) - 2n(n-1) + (2-2n)\sum_{i=1}^{n-1} i + \sum_{i=1}^{n-1} i^2 \right) + \frac{21}{2}n(n-1)$$

$$= 14n(4n-2) + 7n(n-1)(10n-8) + \frac{21}{2}n(n-1).$$

Therefore $\xi^c(CNC_7[n]) = \frac{7}{2}n(20n^2 - 11n + 3)$ .Then the Theorem is proved. ■

Theorem 5. The Modified Eccentric Connectivity polynomial of One–Heptagonal Carbon Nanocone is computed as follows:

ECP($CNC_7[n]$,x)= $= (6n-2)x^{4n-1} + 3(1+x)\sum_{i=1}^{n-1}(n-i)x^{4n-2i-1}$

Proof. Suppose Q[n]= $CNC_7[n]$. With respect to figure 2, Q[n]= $\bigcup_{i=1}^{7} T_i$, where $\{T_i\}_{1\leq i\leq 7}$ is a partition of the molecular graph Q[n]. By ues theorem 3 and theorem 4 we have:

MECP(T_i,x)= $\sum_{u\in V(T_i)} n_G(u)x^{ecc(u)}$

$$= (6n-2)x^{4n-1} + 7(n-1)x^{4n-2} + 9(n-1)x^{4n-3} + 9(n-2)x^{4n-4} + 9(n-2)x^{4n-5}$$

$$+ \ldots + 9\times 2x^{2n+4} + 9\times 2x^{2n+3} + 9x^{2n+2} + 9x^{2n+1}$$

$$= (6n-2)x^{4n-1} + 9(n-1)(1+x)x^{4n-3} + 9(n-2)(1+x)x^{4n-5} + \ldots + 9\times 2(1+x)x^{2n+3}$$

$$+ 9(1+x)x^{2n+1}$$

$$= (6n-2)x^{4n-1} + 3(1+x)\sum_{i=1}^{n-1}(n-i)x^{4n-2i-1}$$

Therefore

MECP(Q[n],x)= $\sum_{u\in V(Q[n])} n_G(u)x^{ecc(u)}$ =7 ECP(T_i,x)=7 $\sum_{u\in V(T_i)} n_G(u)x^{ecc(u)}$

$$= (6n-2)x^{4n-1} + 3(1+x)\sum_{i=1}^{n-1}(n-i)x^{4n-2i-1}$$

Then the Theorem is proved.

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