ECCENTRIC INDICES OF CRYSTAL CUBIC CARBON STRUCTURE

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***Abstract*— Chemical graph theory helps to understand the structural properties of a molecular graph. The molecular graphs are the graphs that consists of atoms called vertices and the covalent bond between them called edges. The eccentricity ϵ_u of vertex u in a connected graph G, is the distance between u and a vertex farthermost from u. In this article, we study the modified eccentric connectivity index $\xi_c(G)$, Ediz eccentric connectivity index ${}^E\xi^c(G)$, Augmented Eccentric Connectivity index ${}^A\xi^c(G)$, superaugmented eccentric connectivity index-1, index-2, index-3 and modified eccentric connectivity polynomial $\xi_c(G,x)$ of $CCC(n)$ of crystal structure of cubic carbon for n-levels.**

***Keywords*— Eccentricity indices, Crystal Cubic Carbon.**

I. INTRODUCTION

There are certain chemical compounds that are useful for the survival of living things. Carbon, oxygen, hydrogen and nitrogen are the main elements that helps in the production of cells in the living things. Carbon is an essential element for human life. It is useful in the formation of proteins, carbohydrates and nucleic acids. It is vital for the growth of plants in the form of carbon dioxide. The carbon atoms can bond together in various ways, called allotropes of carbon. The well known forms are graphite and diamond. Recently, many new forms have been discovered including nanotubes, buckminsterfullerene and sheets, crystal cubic structure, etc. The applications of different allotropes of carbon are discussed in detail in Pierson (2012), Vajtai (2013). In molecular graph, the vertices speaks to the carbon molecules and the edges speaks to the carbon-carbon bonds.

Consider $G(V,E)$ to be a basic simple graph, where V and E speak to the arrangement of vertices and the arrangement of edges. The quantity of components in V is known as the order of the graph G and the quantity of components in E is known as the size of the graph G. The quantity of vertices neighboring the vertex $v \in V$ is known as the degree of v and is signified as d_v. If no vertices in $u-v$ walk are rehashed then it is called $u-v$ path in graph G. The length of a path is the quantity of edges in it. The distance $d(u,v)$ from vertex u to vertex v is the length of a most limited $u-v$ path in a graph G where $u,v \in V$. In a connected graph G; the eccentricity ϵ_u of vertex u is the distance amongst u and a vertex most distant from u in G.

The properties of a graph can be perceived by a numeric number, a polynomial, a grouping of numbers or a network. A topological index (molecular structure descriptor) is a numerical estimate related with synthetic constitution for relationship of chemical structure with different physical properties, compound reactivity or organic action. There are some significant classes of topological indices, for example, distance based topological indices, eccentricity based topological indices, degree based topological indices and counting related polynomials and indices of graphs.

The first topological index is Wiener index which was proposed in 1947 when Harold Wiener (1947) was working on the boiling point of paraffin. It was the first topological index which depends upon the concept of distance between two vertices in graph. Wiener called it the path number. But after that it was renamed as Wiener index and it is denoted by W. The theory of topological indices started from Wiener index. Wiener described the path number as the sum of the number of bonds between all pair of atoms (Wiener, 1947), and is defined as follows:

$$W(G) = \frac{1}{2}\sum_{(u,v)} d(u,v),$$

where (u,v) is any arbitrary pair of vertices in G and $d(u,v)$ is $u-v$ the length of shortest path between u and v. A novel highly discriminating topological descriptor, namely Eccentric-connectivity index, for structure-property and structure-activity studies of molecular structures was proposed by Sharma *et al.* (1997) defined as.

$$\xi(G) = \sum_{u\in V(G)} d_u \epsilon_u. \quad (1)$$

In the study of fullerenes by MEC polynomials, Ashrafi and Ghorbani (2010) introduced modified eccentric connectivity index $\xi_c(G)$ and is defined as

$$\xi_c(G) = \sum_{v\in V(G)} (S_v \epsilon_v), \quad (2)$$

where $S_v = \sum_{u\in N(v)} d_u$ that is where S_v is the sum of degrees of all vertices adjacent to vertex v.

Recently Ediz (2010), defined Ediz eccentric connectivity index of G which is characterized as

$${}^E\xi^c(G) = \sum_{v\in V(G)} \left(\frac{S_v}{\epsilon_v}\right), \quad (3)$$

On the other hand, Augmented Eccentric Connectivity index ${}^A\xi(G)$ was introduced by Dǒslic and Saheli (2011), and is defined as summation of the quotients of the product of adjacent vertex degrees and eccentricity of the concerned vertex and expressed as follows;

$${}^A\xi(G) = \sum_{v\in V(G)} \left(\frac{M_v}{\epsilon_v}\right), \quad (4)$$

where $M_v = \prod_{u \in N(v)} d_u$ that is denotes the product of degrees of all neighbors of vertex v of G.

Dureja Anil and Madan (2007) introduced the superaugmented eccentric connectivity index-1, index-2 and index-3 denoted by ${}^{SA}\xi_1^c$, ${}^{SA}\xi_2^c$ and ${}^{SA}\xi_3^c$. These are defined as

$$ {}^{SA}\xi_1^c(G) = \sum_{v \in V(G)} \frac{M_v}{(\epsilon_v)^2}, \tag{5}$$

$$ {}^{SA}\xi_2^c(G) = \sum_{v \in V(G)} \frac{M_v}{(\epsilon_v)^3}, \tag{6}$$

$$ {}^{SA}\xi_3^c(G) = \sum_{v \in V(G)} \frac{M_v}{(\epsilon_v)^4}, \tag{7}$$

The *Eccentric connectivity polynomial* is the polynomial version of the eccentric-connectivity index which was proposed by Alaeiyan *et al.* (2011). They define the Eccentric connectivity polynomial of a graph G as

$$ECP(G, x) = \sum_{v \in V(G)} d_u x^{\epsilon_u}, \tag{8}$$

where value of x is greater than 1. The relationship between eccentric connectivity polynomial and eccentric-connectivity index is given by

$$\xi(G) = \xi(G, 1),$$

where $\xi(G, 1)$ is the first derivative of $ECP(G, x)$ (Bindusree *et al.*, 2015). Similar to other topological polynomials, the modified eccentric connectivity polynomial of a graph was introduced in De *et al.* (2014) and is defined as:

$$\xi_c(G, x) = \sum_{v \in V(G)} S_u x^{\epsilon_u}, \tag{9}$$

so that the modifed eccentric connectivity index is the first derivative of this polynomial for $x = 1$. For more information and properties of eccentricity based topological index, see Asadpour and Safikhani (2013), De *et al.* (2012), Gupta *et al.* (2002) and Huo *et al.* (2017).

II. ECCENTRIC INDICES OF CRYSTAL STRUCTURE OF CUBIC CARBON

The structure of crystal cubic carbon (or crystal structure of cubic carbon) consist of cubes and its degree based topological indices study was discussed in Baig *et al.* (2017). The molecular graph of crystal cubic carbon $CCC(n)$ for first level is depicted in Fig. 1. For second level, new cubes are attached at every end vertex of degree 3 of first level. Similarly, this procedure is repeated to get the next level and so on. The cardinality of vertices and edges in $CCC(n)$ are given below respectively.

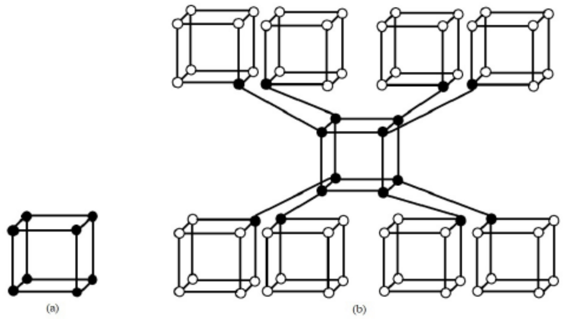

Figure 1: Crystal Structure Cubic Carbon (a) $CCC(1)$. (b) $CCC(2)$.

$$|V(CCC(n)| = 2\{24\sum_{r=3}^{n}(2^3-1)^{r-3} + 31(2^3-1)^{n-2} + 2\sum_{r=0}^{n-2}(2^3-1)^r + 3\}$$

$$|E(CCC(n)| = 4\{24\sum_{r=3}^{n}(2^3-1)^{r-3} + 24(2^3-1)^{n-2} + 2\sum_{r=0}^{n-2}(2^3-1)^r + 3\}.$$

Let Q_k be the set of all cubic free vertices in $CCC(k)$ at the k-th level with $2 \le k \le n$, where we say that a vertex is cubic free if its degree is 3 at the k-th level. Let $v \in Q_k$, be an arbitrary element, in $(k+1)$-th level, we partition the new coming vertices in four sets. The number of new vertices at every $(k+1)$-th level is $448(2^3-1)^{k-3}$. The partition of these vertices is given as follows: B_1^k is the set of vertices at distance 1 from any $v \in Q_k$ with number of such vertices is $56(2^3-1)^{k-3}$, B_2^k is the set of vertices at distance 2 from $v \in Q_k$ with cardinality $|B_2^k| = 168(2^3-1)^{k-3}$, B_3^k is the set of vertices at distance 3 from $v \in Q_k$ with cardinality $|B_3^k| = 168(2^3-1)^{k-3}$ and B_4^k is the set of vertices at distance 4 from $v \in Q_k$ with cardinality $|B_4^k| = 56(2^3-1)^{k-3}$. Also we denote by B the set of vertices of $CCC(1)$ that is the initial vertices in each k-th level, so cardinality $|B| = 8$. This partition is also described in Table 1.

In Table 2 we gave the partition of all the vertices of $CCC(n)$, for $n \ge 3$, based on degree sum, eccentricity and the membership to the sets B_1, B_2, B_3 and B_4.

Table 1: Vertex partition of new coming vertices at $(k+1)$-th level, $k \ge 2$.

Set	number of vertices	Distance from any $v \in Q_k$
B_1^k	$56(2^3-1)^{k-3}$	1
B_2^k	$168(2^3-1)^{k-3}$	2
B_3^k	$168(2^3-1)^{k-3}$	3
B_4^k	$56(2^3-1)^{k-3}$	4

Table 2: Vertex partition of $CCC(n)$ based on degree sum and eccentricity of each vertex.

Representative	d_v	S_v	Eccentricity ϵ_v	frequency	Range
$v \in B$	4	16	$3+4(n+k-2)$	8	$k=1$, for all $n \ge 2$
$v \in B_1^k$	4	16	$4(n+k-2)$	$56(2^3-1)^{k-3}$	$2 \le k \le n-1$
$v \in B_1^k$	4	13	$4(n+k-2)$	$56(2^3-1)^{k-3}$	$k=n$
$v \in B_2^k$	4	16	$4(n+k)-7$	$168(2^3-1)^{k-3}$	$2 \le k \le n-1$
$v \in B_2^k$	3	10	$8n-7$	$168(2^3-1)^{k-3}$	$k=n$
$v \in B_3^k$	4	16	$4(n+k)-6$	$168(2^3-1)^{k-3}$	$2 \le k \le n-1$
$v \in B_3^k$	3	9	$8n-6$	$168(2^3-1)^{k-3}$	$k=n$
$v \in B_4^k$	4	16	$4(n+k)-5$	$56(2^3-1)^{k-3}$	$2 \le k \le n-1$
$v \in B_4^k$	3	9	$8n-5$	$56(2^3-1)^{k-3}$	$k=n$

Table 3: Vertex partition of $CCC(n)$ based on degree product and eccentricity of each vertex.

Representative	d_v	M_v	Eccentricity ϵ_v	frequency	Range
$v \in B$	4	256	$3+4(n+k-2)$	8	$k=1$, for all $n \geq 2$
$v \in B_1^k$	4	256	$4(n+k-2)$	$56(2^3-1)^{k-3}$	$2 \leq k \leq n-1$
$v \in B_1^k$	4	108	$4(n+k-2)$	$56(2^3-1)^{k-3}$	$k=n$
$v \in B_2^k$	4	256	$4(n+k)-7$	$168(2^3-1)^{k-3}$	$2 \leq k \leq n-1$
$v \in B_2^k$	3	36	$8n-7$	$168(2^3-1)^{k-3}$	$k=n$
$v \in B_3^k$	4	256	$4(n+k)-6$	$168(2^3-1)^{k-3}$	$2 \leq k \leq n-1$
$v \in B_3^k$	3	27	$8n-6$	$168(2^3-1)^{k-3}$	$k=n$
$v \in B_4^k$	4	256	$4(n+k)-5$	$56(2^3-1)^{k-3}$	$2 \leq k \leq n-1$
$v \in B_4^k$	3	27	$8n-5$	$56(2^3-1)^{k-3}$	$k=n$

In the coming Theorems, we have computed modified eccentric connectivity index $\xi_c(G)$, Ediz eccentric connectivity index ${}^E\xi^c(G)$, Augmented Eccentric Connectivity index ${}^A\xi(G)$, superaugmented eccentric connectivity index-1, index-2 and index-3 of $CCC(n)$.

Theorem 1. Consider the graph $G \cong CCC(n)$ with $n \geq 2$, then its modified eccentric connectivity index $\xi_c(G)$ is equal to

$$\xi_c(G) = \frac{3712}{9} - \frac{512\,n}{3} + \frac{4096n}{147}7^n - \frac{17152}{441}7^n + 2912(2\,n-2)7^{n-3} + 1680\,(8\,n-7)7^{n-3} + 1512\,(8\,n-6)7^{n-3} + 504\,(8\,n-5)7^{n-3}.$$

Proof: Let $G \cong CCC(n)$ be the crystal structure of cubic carbon. The vertex partition of $CCC(n)$ based on degrees sum of vertices and eccentricities with their frequencies is given in Table 2. Then by using Table 2 the modified eccentric connectivity index $\xi_c(G)$ can be calculated as follows:

$$\xi_c(G) = \sum_{v\in V(G)}(S_v\epsilon_v) = 16 \times 8\big(3+4(n-1)\big) + \sum_{k=2}^{n-1} 16 \times 56(2^3-1)^{k-3}\big(4(n+k-2)\big) + 13 \times 56(2^3-1)^{n-3}4(2n-2) + \sum_{k=2}^{n-1}(16 \times 168)(2^3-1)^{k-3}(4(n+k)-7) + 10 \times 168(2^3-1)^{n-3}(8n-7) + \sum_{k=2}^{n-1}(16 \times 168)(2^3-1)^{k-3}(4(n+k)-6) + 9 \times 168(2^3-1)^{n-3}(8n-6) =.$$
$$\frac{3712}{9} - \frac{512\,n}{3} + \frac{4096n}{147}7^n - \frac{17152}{441}7^n + 2912(2\,n-2)7^{n-3} + 1680\,(8\,n-7)7^{n-3} + 1512\,(8\,n-6)7^{n-3} + 504\,(8\,n-5)7^{n-3}.$$

□

Theorem 2. Consider the graph $G \cong CCC(n)$ with $n \geq 2$, then its Ediz eccentric connectivity index ${}^E\xi^c(G)$ is equal to

$${}^E\xi^c(G) = \frac{128}{3+4(n-1)} + \frac{728 \times 7^{n-3}}{4(2n-2)} + \frac{1680\times 7^{n-3}}{8n-7} + \frac{1512\times 7^{n-3}}{8n-6} + \frac{504\times 7^{n-3}}{8n-5} + \sum_{k=2}^{n-1}\frac{896 \times 7^{k-3}}{4(n+k-2)} + \sum_{k=2}^{n-1}\frac{2688 \times 7^{k-3}}{4(n+k)-7} + \sum_{k=2}^{n-1}\frac{2688 \times 7^{k-3}}{4(n+k)-6} + \sum_{k=2}^{n-1}\frac{896 \times 7^{k-3}}{4(n+k)-5}.$$

Proof: Let $G \cong CCC(n)$ be the crystal structure of cubic carbon. The vertex partition of $CCC(n)$ based on degrees sum of vertices and eccentricities with their frequencies is given in Table 2. Then by using Table 2 the Ediz eccentric connectivity index ${}^E\xi^c(G)$ is calculated as follows:

$${}^E\xi^c(G) = \sum_{v\in V(G)}\left(\frac{S_v}{\epsilon_v}\right) = 8\frac{16}{3+4(n-1)} + \sum_{k=2}^{n-1} 56(2^3-1)^{k-3}\frac{16}{4(n+k-2)} + 56(2^3-1)^{n-3}\frac{13}{4(2n-2)} + \sum_{k=2}^{n-1} 168(2^3-1)^{k-3}\frac{16}{4(n+k)-7} + 168(2^3-1)^{n-3}\frac{10}{(8n-7)} + \sum_{k=2}^{n-1} 168(2^3-1)^{k-3}\frac{16}{4(n+k)-6} + 168(2^3-1)^{n-3}\frac{9}{(8n-6)} + \sum_{k=2}^{n-1} 56(2^3-1)^{k-3}\frac{16}{4(n+k)-5} + 56(2^3-1)^{n-3}\frac{9}{(8n-5)}.$$

After, some easy computations, we get the stated result.

□

In Table 3 we gave the partition of all the vertices of $CCC(n)$, for $n \geq 3$, based on degree product, eccentricity and the membership to the sets B_1, B_2, B_3 and B_4.

Theorem 3. Consider the graph $G \cong CCC(n)$ with $n \geq 3$, then its Augmented Eccentric Connectivity index ${}^A\xi(G)$ is equal to

$${}^A\xi(G) = \frac{2048}{3+4(n-1)} + \frac{6048 \times 7^{n-3}}{4(2n-2)} + \frac{6048\times 7^{n-3}}{8n-7} + \frac{4536\times 7^{n-3}}{8n-6} + \frac{1512\times 7^{n-3}}{8n-5} + \sum_{k=2}^{n-1}\frac{14336 \times 7^{k-3}}{4(n+k-2)} + \sum_{k=2}^{n-1}\frac{43008 \times 7^{k-3}}{4(n+k)-7} + \sum_{k=2}^{n-1}\frac{43008 \times 7^{k-3}}{4(n+k)-6} + \sum_{k=2}^{n-1}\frac{14336 \times 7^{k-3}}{4(n+k)-5}.$$

Proof: Let $G \cong CCC(n)$ be the crystal structure of cubic carbon. The vertex partition of $CCC(n)$ based on degrees of vertices and eccentricities with their frequencies is given in Table 3. Then by using Table 3 the Augmented Eccentric Connectivity index ${}^A\xi(G)$ is calculated as follows:

$${}^A\xi^c(G) = \sum_{v\in V(G)}\left(\frac{M_v}{\epsilon_v}\right) = 8\frac{256}{3+4(n-1)} + \sum_{k=2}^{n-1} 56(2^3-1)^{k-3}\frac{256}{4(n+k-2)} + 56(2^3-1)^{n-3}\frac{108}{4(2n-2)} + \sum_{k=2}^{n-1} 168(2^3-1)^{k-3}\frac{256}{4(n+k)-7} + 168(2^3-1)^{n-3}\frac{36}{(8n-7)} + \sum_{k=2}^{n-1} 168(2^3-1)^{k-3}\frac{256}{4(n+k)-6} + 168(2^3-1)^{n-3}\frac{37}{(8n-6)} + \sum_{k=2}^{n-1} 56(2^3-1)^{k-3}\frac{256}{4(n+k)-5} + 56(2^3-1)^{n-3}\frac{27}{(8n-5)}.$$

After, some easy computations, we get the stated result.

□

Using Table 3 and Eqs. (5-7) the following corollaries gives superaugmented eccentric connectivity index-1, index-2 and index-3 denoted by $S^{SA}\xi_1^c$, ${}^{SA}\xi_2^c$ and ${}^{SA}\xi_3^c$.

Corollary 1. Consider the graph $G \cong CCC(n)$ with $n \geq 3$, then its superaugmented eccentric connectivity index-1 $S^{SA}\xi_1^c$ is equal to

$$S^{SA}\xi_1^c = \frac{2048}{(3+4(n-1))^2} + \frac{6048 \times 7^{n-3}}{(4(2n-2))^2} + \frac{6048\times 7^{n-3}}{(8n-7)^2} +$$

$$\frac{4536\times7^{n-3}}{(8n-6)^2}+\frac{1512\times7^{n-3}}{(8n-5)^2}+\sum_{k=2}^{n-1}\frac{14336\times7^{k-3}}{(4(n+k-2))^2}+\sum_{k=2}^{n-1}\frac{43008\times7^{k-3}}{(4(n+k)-7)^2}+\sum_{k=2}^{n-1}\frac{43008\times7^{k-3}}{(4(n+k)-6)^2}+\sum_{k=2}^{n-1}\frac{14336\times7^{k-3}}{(4(n+k)-5)^2}$$

Corollary 2. Consider the graph $G \cong CCC(n)$ with $n \geq 3$, then its superaugmented eccentric connectivity index-1 $S^{SA}\xi_2^c$ is equal to

$$S^{SA}\xi_2^c=\frac{2048}{(3+4(n-1))^3}+\frac{6048\times7^{n-3}}{(4(2n-2))^3}+\frac{6048\times7^{n-3}}{(8n-7)^3}+\frac{4536\times7^{n-3}}{(8n-6)^3}+\frac{1512\times7^{n-3}}{(8n-5)^3}+\sum_{k=2}^{n-1}\frac{14336\times7^{k-3}}{(4(n+k-2))^3}+\sum_{k=2}^{n-1}\frac{43008\times7^{k-3}}{(4(n+k)-7)^3}+\sum_{k=2}^{n-1}\frac{43008\times7^{k-3}}{(4(n+k)-6)^3}+\sum_{k=2}^{n-1}\frac{14336\times7^{k-3}}{(4(n+k)-5)^3}$$

Corollary 3. Consider the graph $G \cong CCC(n)$ with $n \geq 3$, then its superaugmented eccentric connectivity index-1 $S^{SA}\xi_3^c$ is equal to

$$S^{SA}\xi_3^c=\frac{2048}{(3+4(n-1))^4}+\frac{6048\times7^{n-3}}{(4(2n-2))^4}+\frac{6048\times7^{n-3}}{(8n-7)^4}+\frac{4536\times7^{n-3}}{(8n-6)^4}+\frac{1512\times7^{n-3}}{(8n-5)^4}+\sum_{k=2}^{n-1}\frac{14336\times7^{k-3}}{(4(n+k-2))^4}+\sum_{k=2}^{n-1}\frac{43008\times7^{k-3}}{(4(n+k)-7)^4}+\sum_{k=2}^{n-1}\frac{43008\times7^{k-3}}{(4(n+k)-6)^4}+\sum_{k=2}^{n-1}\frac{14336\times7^{k-3}}{(4(n+k)-5)^4}$$

III. ECCENTRIC POLYNOMIAL OF CRYSTAL STRUCTURE OF CUBIC CARBON

In this section we shall compute the modified eccentric connectivity polynomial Crystal Structure of Cubic Carbon.

Theorem 4. Consider the graph graph $G \cong CCC(n)$ with $n \geq 3$, then its modified eccentric connectivity polynomial $\xi_c(G,x)$ is equal to

$$\xi_c(G,x)=\frac{1}{343x^4-49}\Big((728x^4-104)7^n x^{4(2n-2)}+(43904x^4-6272)x^{-2+4n}+(1680x^4-240)7^n x^{8n-7}+(1512x^4-216)7^n x^{8n-6}+(504x^4-72)7^n x^{8n-5}+128x^{4n-5}7^n(x^4)^n+128x^{4n-8}7^n(x^4)^n+384x^{4n-7}7^n(x^4)^n+384x^{4n-6}7^n(x^4)^n-18816x^{4n+1}-18816x^{4n+2}-6272x^{4n+3}-6272x^{4n}\Big).$$

Proof: Let $G \cong CCC(n)$ be the crystal structure of cubic carbon. The vertex partition of $CCC(n)$ based on degrees sum of vertices and eccentricities with their frequencies is given in Table 2. Then by using Table 2 the modified eccentric connectivity polynomial $\xi_c(G,x)$ can be calculated as follows:

$$\xi_c(G,x)=\sum_{v\in V(G)}S_v x^{\epsilon_v}=16\times8x^{(3+4(n-1))}+\sum_{k=2}^{n-1}(16\times56)(2^3-1)^{k-3}x^{(4(n+k-2))}+(13\times56)(2^3-1)^{n-3}x^{(4(2n-2))}+\sum_{k=2}^{n-1}(16\times168)(2^3-1)^{k-3}x^{(4(n+k)-7)}+(10\times168)(2^3-1)^{n-3}x^{(8n-7)}+\sum_{k=2}^{n-1}(16\times168)(2^3-1)^{k-3}x^{(4(n+k)-6)}+(9\times168)(2^3-1)^{n-3}x^{(8n-6)}+\sum_{k=2}^{n-1}(16\times56)(2^3-1)^{k-3}x^{(4(n+k)-5)}+(9\times56)(2^3-1)^{n-3}x^{(8n-5)}=\frac{1}{343x^4-49}\Big((728x^4-104)7^n x^{4(2n-2)}+(43904x^4-6272)x^{-2+4n}+(1680x^4-240)7^n x^{8n-7}+(1512x^4-216)7^n x^{8n-6}+(504x^4-72)7^n x^{8n-5}+128x^{4n-5}7^n(x^4)^n+128x^{4n-8}7^n(x^4)^n+384x^{4n-7}7^n(x^4)^n+384x^{4n-6}7^n(x^4)^n-18816x^{4n+1}-18816x^{4n+2}-6272x^{4n+3}-6272x^{4n}\Big).$$

□

IV. COMPARISON

In this section we shall add a Table 4 and a Fig. 2 which shows the comparison of all the computed eccentric indices.

V. CONCLUSION

As an effective modeling, analysis and computational tool, graph theory is widely used in chemical mathematics to deal with various chemistry problems. Graph can express the molecule structure, where atom can be denoted as vertex and connect element can be regraded as edge. In our article, we mainly study the chemistry features of chemical structures in term of eccentricity based indices computations that help to predict many physico-chemical properties of the chemical compound under study. In this regard we have computed the eccentric based topological indices of carbon cubic structure of n-layers. Namely we have computed and gave a numerical comparison table of modified eccentric connectivity index $\xi_c(G)$, Ediz eccentric connectivity index ${}^E\xi^c(G)$, Augmented Eccentric Connectivity index ${}^A\xi^c(G)$, super-augmented eccentric connectivity index-1, index-2 and index-3 of $CCC(n)$.

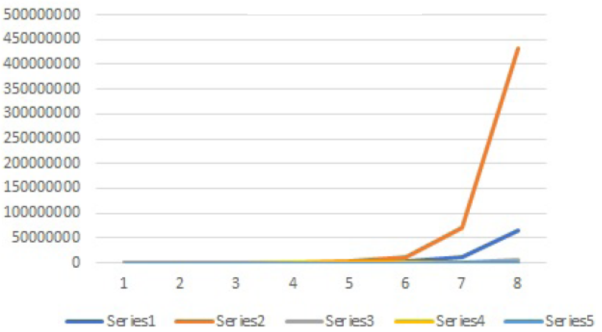

Figure 2: Graphical Comparison of computed indices from Table 4.

Table 4: Comparison of the $\xi_c(G)$, ${}^E\xi^c(G)$, ${}^A\xi^c(G)$, $S^{SA}\xi_1^c$, ${}^{SA}\xi_2^c$ and ${}^{SA}\xi_3^c$ of $G \cong CCC(n)$.

n	$\xi_c(G)$	${}^E\xi^c(G)$	${}^A\xi^c(G)$	$S^{SA}\xi_1^c$	${}^{SA}\xi_2^c$	${}^{SA}\xi_3^c$
3	92232	342.65	2470.2	170.69	12.072	0.87
4	960696	1621.6	11489	515.05	23.5	1.1
5	8.93×10^6	8532.2	59507	1957.5	65.036	2.1855
6	7.79×10^7	47824	330110	8573.8	224.04	5.9
7	6.5×10^8	279180	1.9137×10^6	41088	885.67	19.2
8	5.33×10^9	1.6762×10^6	1.1433×10^7	209300	3841.9	70.7
9	4.26×10^{10}	1.0272×10^7	6.9814×10^7	1.1141×10^6	17814	285.5
10	3.36×10^{11}	6.3947×10^7	4.3338×10^8	6.1304×10^6	86853	1232.5

REFERENCES

Alaeiyan, M., Mojarad, R. and Asadpour, J. (2011). "A new method for computing eccentric connectivity polynomial of an infinite family of linear polycene parallelogram benzenod," *Optoelectronics and Advanced Materials-Rapid Communications*, **5**, 761-770.

Ashra, A.R. and Ghorbani, M. (2010). "A study of fullerenes by MEC polynomials," *Electronic Materials Letters*, **6**, 87-90.

Asadpour, J. and Safikhani, L. (2013). "Study of $CNC_7[n]$ Carbon Nanocone by M-Eccentric Connectivity Polynomial," *Australian Journal of Basic and Applied Sciences*, **7**, 883-887.

Baig, A.Q., Imran, M., Khalid, W. and Naeem, M. (2017). "Molecular description of carbon graphite and crystal cubic carbon structures," *Can. J. Chem*., **95**, 674-686.

Bindusree, A.R., Lokesha, V. and Ranjini, P.S. (2015). "Eccentric connectivity index and polynomial of some graphs," *British Journal of Mathematics and Computer Science*, **6**, 457-463.

De, N., Nayeem, S.M.A. and Pal, A. (2012). "Total eccentricity index of the generalized index and polynomial of thorn graph," *Applied Mathematics*, **3**, 931-934.

De, N., Pal, A. and Nayeem, S.M.A. (2014). "Modified Eccentric Connectivity of Generalized Thorn Graphs," *International Journal of Computational Mathematics*, **2014**, 436140.

Doslic, T. and Saheli, M. (2011). "Augmented eccentric-connectivity index," *Miskolc Mathematical Notes,* **12,** 149-157.

Dureja Anil, H. and Madan, K. (2007). "Superaugmented eccentric connectivity indices: new-generation highly discriminating topological descriptors for QSAR/QSPR modeling," *Medicinal Chemistry Research*, **16**, 331-341.

Ediz, S. (2010). "Computing Ediz eccentric connectivity index of an infinite class of nanostar dendrimers," *Optoelectron. Adv. Mater. Rapid Commun*., **4**, 1847-1848.

Gupta, S., Singh, M. and Madan, A.K. (2002). "Application of Graph Theory: Relationship of Eccentric Connectivity Index and Wiener's Index with Anti-inflammatory Activity," *J. Math. Anal. Appl*., **266**, 259-268.

Huo, Y., Lio, J.B., Baig, A.Q., Sajjad, W. and Farahani, M.H. (2017). "Connective Eccentric Index of NA_m^n Nanotube," *Journal of Computational and Theoretical Nanoscience*, **14**, 1832-1836.

Pierson, H.O. (2012). *Handbook of Carbon, Graphite, Diamonds and Fullerenes: Processing, Properties and Applications*, NOYES Publications, Park Ridge, New Jersey, U.S.A.

Sharma, V., Goswami, R. and Madan, A.K. (1997). "Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies," *J. Chem. Inf. Comput. Sci*., **37**, 273-282.

Vajtai, R.(2013). *Springer Handbook of Nanomaterials*, Springer Science & Business Media, 2013.

Wiener, H. (1947). "Structural determination of paraffin boiling points," *J. Am. Chem. Soc.,* **69**, 17-20.

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