



DEGREE-DISTANCE BASED TOPOLOGICAL INDICES OF PRECIOUS STONE CUBIC CARBON STRUCTURE

Mr. A. Aristatil¹, Mr. M.V. Suresh²

^{*1} Research Scholar, Department of Mathematics, SPIHER, Avadi, Chennai-54, India

² Assistant Professor, Department of Mathematics, SPIHER, Avadi, Chennai-54, India



Abstract:

Chemical diagram hypothesis fathoms the essential properties of a nuclear chart. The sub-nuclear outlines are the charts that are involved particles called vertices and the covalent bond between them are called edges. The unusualness ϵ_u of vertex u in a related diagram G , is the partition among u and a vertex farthestmost from u . In this article, we consider the valuable stone structure of cubic carbon and enrolled Eccentric-network list $\xi(G)$, Eccentric availability polynomial $ECP(G, x)$ and Connective Eccentric list $C\xi(G)$ of pearl structure of cubic carbon for n -levels.

Keywords: Degree; Capriciousness; Eccentric-Network Record $\Xi(G)$; Eccentric Availability Polynomial $ECP(G, X)$; Connective Eccentric List $C\xi(G)$; Precious Stone Cubic Carbon.

Cite This Article: Mr. A. Aristatil, and Mr. M.V. Suresh. (2019). "DEGREE-DISTANCE BASED TOPOLOGICAL INDICES OF PRECIOUS STONE CUBIC CARBON STRUCTURE." *International Journal of Engineering Technologies and Management Research*, 6(12), 101-110. DOI: <https://doi.org/10.29121/ijetmr.v6.i12.2019.491>.

1. Introduction

A part of logical science is Chemical chart theory, which identifies with the nontrivial usages of diagram speculation for dealing with the nuclear issues. Concoction chart hypothesis uses numerical invariants to restrict the structure of a molecule into a singular number which implies the vitality of particle, auxiliary segments, sub-nuclear extending and electronic structures. These diagram theoretic invariants are used to interface with physical recognitions found out by analyses. In synthetic chart theory should be seen not similarly as proportionate to various parts of hypothetical science yet in addition as comparing and basic for better understanding of the possibility of the compound structure.

There are certain manufactured strengthens that are significant for the survival of living things. Carbon, oxygen, hydrogen and nitrogen are the essential parts that assistant in the formation of cells in the living things. Carbon is a basic segment for human life. It is significant in the improvement of proteins, starches and nucleic acids. It is basic for the advancement of plants as carbon dioxide. The carbon particles can bond together in various ways, called allotropes of carbon. The eminent structures are graphite and valuable stone. Starting late, various new structures have been found including nano tubes, buckminsterfullerene and sheets, valuable stone cubic structure, etc. The usages of different allotropes of carbon.

A sub-atomic diagram is a straight forward chart addressing the carbon iota skeleton of a natural particle. In the atomic chart, the vertices address the carbon particles and the edges address the carbon-carbon bonds.

Consider $G(V, E)$ as a central fundamental chart, where V and E address the strategy of vertices and the approach of edges. The measure of parts in V is known as the solicitation of the outline G and the measure of sections in E is known as the degree of the graph G . The measure of vertices neighboring the vertex $v \in V$ is known as the degree of v and is meant as d_v . If no vertices in $u - v$ walk are emphasized, at that point it is called $u - v$ path in graph G . The length of a way is the measure of edges in it. The partition $d(u, v)$ from vertex u to vertex v is the length of a most obliged $u - v$ route in a diagram G where $u, v \in G$. In a related graph G , the unpredictability ε_u of vertex u is the partition among u and a vertex most expelled from u in G .

A diagram can be seen by a numeric number, a polynomial, a social occasion of numbers or a framework. A topological record (sub-atomic structure descriptor) is a numerical respect related with made constitution for relationship of substance structure with different physical properties, compound reactivity or characteristic action. There are some essential classes of topological documents, for example, separate-based topological records, eccentricity based topological records, degree-based topological records and counting related polynomials and arrangements of graphs.

The essential topological record is the Wiener list which was proposed in 1947 when Harold Wiener was tackling the limit of paraffin. It was the fundamental topological record which depended on the possibility of detachment between two vertices in a diagram. Wiener thought of it as the way number. Regardless, after that it was renamed as Wiener document and it is implied by W . The speculation of topological documents started from the Wiener record. Wiener depicted the route number as the aggregate of the amount of bonds between all blends of particles, and is characterized as seeks after:

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

Where (u, v) is any optional match of vertices in G and $d(u, v)$ is $u - v$ the length of most constrained path among u and v . The Eccentric-availability list

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

The Eccentric availability polynomial of a chart G as:

$$ECP(G, x) = \sum_{u \in V(G)} d_u \varepsilon_u \quad (2)$$

Where estimation of x is more prominent than 1. The connection between flighty network polynomial and offbeat availability record is given by

$$ECP(G, x) = \xi(G, 1), \tag{3}$$

Where $\xi(G, 1)$ is the key auxiliary of ECP (G, x) . Another fundamental Eccentricity based topological record is Connective Eccentric file $C^\xi(G)$. The Connective Eccentric file is described as:

$$C^\xi = \sum_{u \in V(G)} \frac{d_u}{\epsilon_u} \tag{4}$$

For more data and properties of Eccentricity based topological record.

2. Methods

To process our outcomes, we used a methodology for combinatorial selecting, a vertex partition technique, an edge apportionments, layout speculative instruments, predictable structures, a degree-checking strategy, and a degrees of neighbors system. Furthermore, we utilized MATLAB for wise estimations and confirmations. We likewise used Maple for plotting numerical outcomes.

3. Erratic Index of Crystal Structure of Cubic Carbon

The structure of valuable stone cubic carbon (or jewel structure of cubic carbon) is contained 3D squares. The nuclear outline of valuable stone cubic carbon OCC(n) for the principal level is depicted in Figure 1. For second level, new 3D shapes are joined at each end vertex of degree 3 of first level. The second degree of OCC(n) is depicted in Figure 2. Also, this technique is repeated to get the accompanying level and so on. The cardinality of vertices and edges in OCC(n) are given underneath independently.

$$|V(OCC(n))| = 2 \left\{ 24 \sum_{r=3}^n (2^3 - 1)^{r-3} + 31(2^3 - 1)^{n-2} + 2 \sum_{r=0}^{n-2} (2^3 - 1)^r + 3 \right\} \tag{5}$$

$$|B(OCC(n))| = 4 \left\{ 24 \sum_{r=3}^n (2^3 - 1)^{r-3} + 24(2^3 - 1)^{n-2} + 2 \sum_{r=0}^{n-2} (2^3 - 1)^r + 3 \right\} \tag{6}$$

Let Q_k be the arrangement of all cubic free vertices in OCC(k) at the k-th level with $k \geq 2$, where we state that a vertex is cubic free if its degree is 3 at the k-th level. Let $v \in Q_k$, be a self-assertive component, in $(k + 1)$ - th level, we parcel the new coming vertices in four sets. The quantity of new vertices at each $(k + 1)$ - th level is $448(2^3 - 1)^{k-3}$. The parcel of these vertices is given as pursues:

S_1^k is the arrangement of vertices at separation 1 from any $v \in Q_k$ with number of such vertices is $56(2^3 - 1)^{k-3}$, S_2^k is the arrangement of vertices at separation 2 from v with cardinality $|S_2^k| = 168(2^3 - 1)^{k-3}$, S_3^k is the arrangement of vertices at separation 3 from v with cardinality $|S_3^k| = 168(2^3 - 1)^{k-3}$ and S_4^k is the arrangement of vertices at separation 2 from v with cardinality

$|S_4^k| = 56(2^3 - 1)^{k-3}$.. What's more, we signify another set as S^k , which is the set of vertices of SCC(1) that is the underlying vertices in every k-th level, so cardinality $|S^k| = 8$.

This parcel is likewise depicted in Table 1.

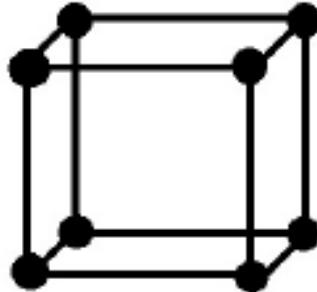


Figure 1: Stone Structure Cubic Carbon SCC (1)

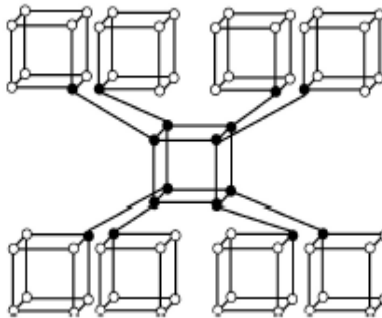


Figure 2: Stone Structure Cubic Carbon SCC (2)

Table 1: Vertex partition of new coming vertices at (k + 1) –th level.

Set	Number of Vertices	Distance from Arbitrary $v \in Q_k$
S_1	$56(2^3 - 1)^{k-3}$	1
S_2	$168(2^3 - 1)^{k-3}$	3
S_3	$168(2^3 - 1)^{k-3}$	3
S_4	$56(2^3 - 1)^{k-3}$	1

In Table 2 we give the partition of all the vertices of CCC(n) based on degree, eccentricity and the membership to the sets S_1, S_2, S_3 and S_4 .

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

Representative	Degree	Eccentricity	Frequency	Range
$v \in S^k$	4	$3 + 4(n-1)$	8	$2 \leq k \leq n$
$v \in S_1^k$	4	$4(n + k - 2)$	$56(2^3 - 1)^{k-3}$	$2 \leq k \leq n$
$v \in S_2^k$	4	$4(n + k) - 7$	$168(2^3 - 1)^{k-3}$	$2 \leq k \leq n-1$

$v\mathcal{E}_2^k$	3	$8n - 7$	$168(2^3 - 1)^{k-3}$	$k = n$
$v\mathcal{E}_3^k$	4	$4(n + k) - 6$	$168(2^3 - 1)^{k-3}$	$2 \leq k \leq n-1$
$v\mathcal{E}_3^k$	3	$8n - 6$	$168(2^3 - 1)^{k-3}$	$k = n$
$v\mathcal{E}_4^k$	4	$4(n + k) - 5$	$56(2^3 - 1)^{k-3}$	$2 \leq k \leq n-1$
$v\mathcal{E}_4^k$	3	$8n - 5$	$56(2^3 - 1)^{k-3}$	$k = n$

In the coming theorems, we have computed Eccentric – connectivity index $\xi(G)$, Eccentric connectivity polynomial $ECP(G,x)$ and Connective Eccentric index $C^\xi(G)$ for stone Structure of cubic carbon $SCC(n)$.

THEOREM 1: Consider the graph $G \cong SCC(n)$ with $n \geq 2$ then its Eccentric-connectivity index is equal to

$$\xi(G) = \frac{(2^6 \times 3 \times 7 \times 13n - 2^5 \times 503)7^n}{3^2 \times 7^2} - \frac{2^7}{3}n + \frac{2^5 \times 29}{3^2}$$

PROOF: Given
$$\xi(G) = \frac{(2^6 \times 3 \times 7 \times 13n - 2^5 \times 503)7^n}{3^2 \times 7^2} - \frac{2^7}{3}n + \frac{2^5 \times 29}{3^2} \tag{7}$$

Let $G \cong SCC(n)$ be the stone structure of cubic carbon. The vertex partition of $SCC(n)$ based on degrees of vertices and eccentricities with their frequencies is given in Table 2. Then by using Table 2 and equation (1), the Eccentric-connectivity index can be calculated as follows:

$$\begin{aligned} \xi(G) &= \sum_{u \in V(G)} d_u \varepsilon_u \\ \xi(G) &= 8(4(3 + 4(n - 1))) + 4X \sum_{k=2}^n 56(2^3 - 1)^{k-3} 4(n + k - 2) \\ &\quad + 4X \sum_{k=2}^{n-1} 168(2^3 - 1)^{k-3} (4(n + k) - 7) + 3X 168(2^3 - 1)^{n-3} (8n - 7) \\ &\quad + 4X \sum_{k=2}^{n-1} 168(2^3 - 1)^{k-3} (4(n + k) - 6) + 3X 168(2^3 - 1)^{n-3} (8n - 6) \\ &\quad + 4X \sum_{k=2}^{n-1} 56(2^3 - 1)^{k-3} (4(n + k) - 5) + 3X 56(2^3 - 1)^{n-3} (8n - 5) \end{aligned}$$

After, some easy computations, we get:

$$\xi(G) = \frac{(2^6 \times 3 \times 7 \times 13n - 2^5 \times 503)7^n}{3^2 \times 7^2} - \frac{2^7}{3}n + \frac{2^5 \times 29}{3^2} \tag{8}$$

The 3D – graphical representation of the Eccentric – connectivity index is depicted in Figure 3.

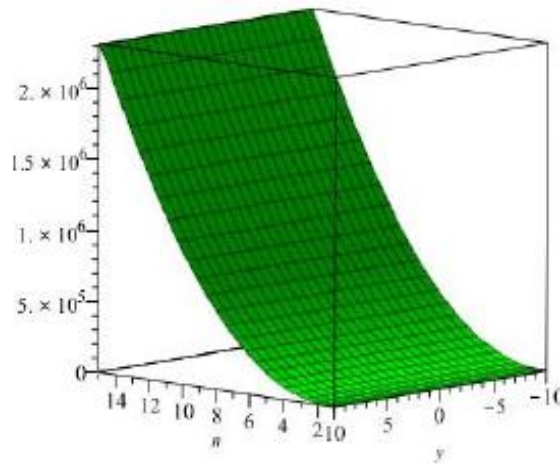


Figure 3: The graphical representation of the Eccentric – connectivity index

THEOREM 2: Consider the graph $G \cong SCC(n)$ with $n \geq 2$ then its Eccentric-connectivity polynomial is equal to

$$ECP(G, x) = 32x^{(4n-1)} + 168(7)^{n-3} x^{8n-5} + 504(7)^{n-3} x^{8n-6} + 504(7)^{n-3} x^{8n-7} + 224X \sum_{k=2}^n (7)^{k-3} x^{4(n+k-2)} + 672X \sum_{k=2}^{n-1} (7)^{k-3} x^{4(n+k)-7} + 672X \sum_{k=2}^{n-1} (7)^{k-3} x^{4(n+k)-6} + 224X \sum_{k=2}^{n-1} (7)^{k-3} x^{4(n+k)-5}$$

PROOF: Let $G \cong SCC(n)$ be the stone structure of cubic carbon. Then by using Table 2 and equation (2) the Eccentric connectivity polynomial is given by:

$$ECP(G, x) = \sum_{u \in V(G)} d_u x^{\epsilon_x}$$

$$ECP(G, x) = 8X 4x^{3+4(n-1)} + 4X \sum_{k=2}^n 56(2^3 - 1)^{k-3} x^{4(n+k-2)} + 4X \sum_{k=2}^{n-1} 168(2^3 - 1)^{k-3} x^{4(n+k)-7} + 3X 168(2^3 - 1)^{n-3} x^{8n-7} + 4X \sum_{k=2}^{n-1} 168(2^3 - 1)^{k-3} x^{4(n+k)-6} + 3X 168(2^3 - 1)^{n-3} x^{8n-6} + 4X \sum_{k=2}^{n-1} 56(2^3 - 1)^{k-3} x^{4(n+k)-5} + 3X 56(2^3 - 1)^{n-3} x^{8n-5}$$

After, an easy calculation, we get

$$\begin{aligned}
 ECP(G, x) = & 32x^{(4n-1)} + 168(7)^{n-3} x^{8n-5} + 504(7)^{n-3} x^{8n-6} + 504(7)^{n-3} x^{8n-7} \\
 & + 224X \sum_{k=2}^n (7)^{k-3} x^{4(n+k-2)} + 672X \sum_{k=2}^{n-1} (7)^{k-3} x^{4(n+k)-7} + 672X \sum_{k=2}^{n-1} (7)^{k-3} x^{4(n+k)-6} \\
 & + 224X \sum_{k=2}^{n-1} (7)^{k-3} x^{4(n+k)-5}
 \end{aligned}$$

The 3D – graphical representation of the Eccentric connectivity polynomial is depicted in

Figure 4.

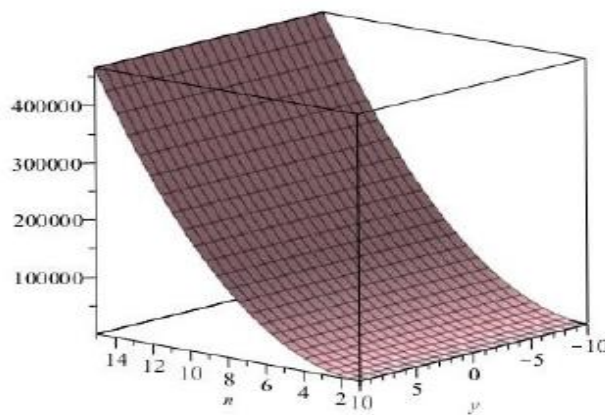


Figure 4: The graphical representation of the Eccentric connectivity polynomial.

THEOREM 1: Consider the graph $G \cong SCC(n)$ with $n \geq 2$ then its Connective Eccentric index is equal to

$$\begin{aligned}
 C^{\xi}(G) = & \frac{32}{(4n-1)} + \frac{727^n}{(392n-343)} + \frac{367^n}{(196n-147)} + \frac{247^n}{(392n-245)} + 224X \sum_{k=2}^n \frac{(7)^{k-3}}{4(n+k-2)} + 672X \sum_{k=2}^{n-1} \frac{(7)^{k-3}}{4(n+k)-7} \\
 & + 672X \sum_{k=2}^{n-1} \frac{(7)^{k-3}}{4(n+k)-6} + 224X \sum_{k=2}^n \frac{(7)^{k-3}}{4(n+k)-5}
 \end{aligned}$$

PROOF: Let $G \cong SCC(n)$ be the stone structure of cubic carbon. Then by using Table 2 and equation (4) the Connective Eccentric index is calculated as:

$$C^{\xi} = \sum_{u \in V(G)} \frac{d_u}{\epsilon_u}$$

$$C^\xi(G) = \frac{32}{3+4(n-1)} + 4X \sum_{k=2}^n \frac{56(2^3-1)^{n-3}}{4(n+k-2)} + 4X \sum_{k=2}^{n-1} \frac{168(2^3-1)^{n-3}}{4(n+k)-7}$$

$$+ 168(2^3-1)^{n-3} X \frac{3}{8n-7} + 4X \sum_{k=2}^{n-1} \frac{168(2^3-1)^{n-3}}{(4(n+k)-6)} + 168(2^3-1)^{n-3} X \frac{3}{8n-6}$$

$$+ 4X \sum_{k=2}^n \frac{56(2^3-1)^{n-3}}{4(n+k)-5} + 56(2^3-1)^{n-3} X \frac{3}{8n-5}$$

After an easy calculation, we get

$$C^\xi(G) = \frac{32}{(4n-1)} + \frac{727^n}{(392n-343)} + \frac{367^n}{(196n-147)} + \frac{247^n}{(392n-245)} + 224X \sum_{k=2}^n \frac{(7)^{k-3}}{4(n+k-2)} + 672X \sum_{k=2}^{n-1} \frac{(7)^{k-3}}{4(n+k)-7}$$

$$+ 672X \sum_{k=2}^{n-1} \frac{(7)^{k-3}}{(4(n+k)-6)} + 224X \sum_{k=2}^n \frac{(7)^{k-3}}{4(n+k)-5}$$

The 3D – graphical representation of the Connective Eccentric index is depicted in Figure 5.

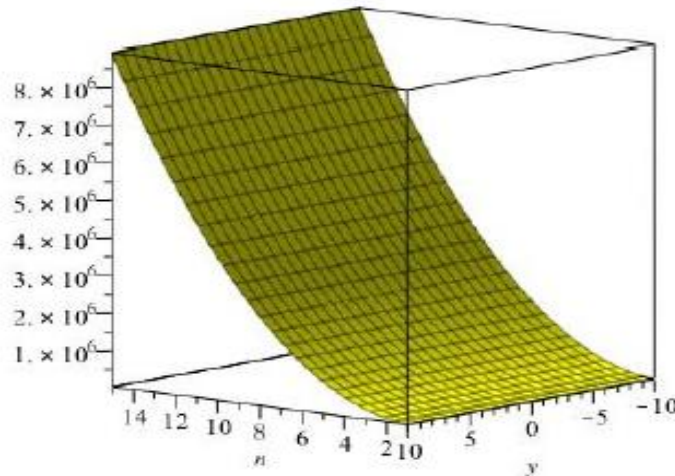


Figure 5: The graphical representation of the Connective Eccentric index.

4. Numerical and Graphical Comparison of Computed Indices

In this segment we will think about Eccentric-availability file, Eccentric network polynomial and Connective Eccentric file of SCC(n), both numerically and graphically. The Table 3 demonstrates a numerical correlation of the portrayed files and the polynomial. The graphical portrayal of the numerical examination is delineated in Figure 6.

Table 3: Comparison of the $\xi(G)$, $C^\xi(G)$ and ECP(G,x) of $G \cong SCC(n)$.

n	$\xi(G)$	$C^\xi(G)$	ECP(G,x) Approx.
2	5457.60	9352	32,038.4
3	533,337.60	538,880	3,224,281.6
4	4,183,459.20	31,716,640	242,651,430.4
5	30,899,311.808	2,065,600,096	1,612,928,748.80

6	22,891,814.30464	62,224,801,952	100,242,075,452.16
7	8,645,581,788.7936	7,559,088,080,480	5,974,731,403,050.24
8	541,359,817,758.7904	225,395,825,441,440	346,142,855,211,733.76
9	34,985,496,157,764.4224	7,144,399,013,120,096	196,480,917,540,735.5008
10	239,376,206,786,041.20768	401,075,576,608,315,552	10,983,346,993,039,897.4848

The next graph shows the graphical comparison of Eccentric – connectivity index, Eccentric connectivity polynomial and Connective Eccentric index of SCC(n).

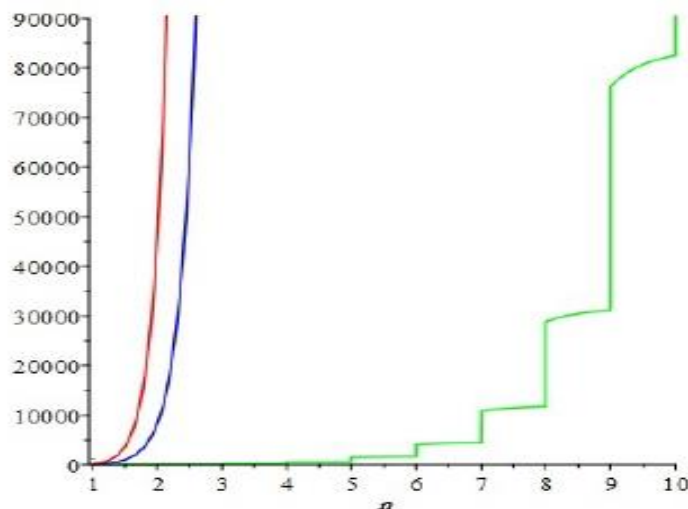


Figure 6: Graphical Comparison of indices of SCC(1), $\xi(G)$ is red, $C^\xi(G)$ is blue, and ECP(G,x) is given.

5. Conclusions

In this article, we have talked about the Eccentric Connectivity record, Eccentric availability polynomial and Connective Eccentric list. We consider the atomic chart of gem structure cubic carbon CCC(n) and we have registered Connective Eccentric list, Eccentric network polynomial and Connective Eccentric list of precious stone structure of cubic carbon SCC(n) compound diagrams for n-levels.

References

- [1] Randić, M. On characterization of molecular branching. J. Am. Chem. Soc. 1975, 97, 6609–6615. [CrossRef]
- [2] Gutman, I.; Trinajstić, N. Graph theory and molecular orbitals., Total p-electron energy of alternant hydrocarbons. Chem. Phys. Lett. 1972, 17, 535–538. [CrossRef]
- [3] Bonchev, D. Handbook of Graph Theory, Chemical Graph Theory; Virginia Commonwealth University: Richmond, VA, USA, 2013; Section 13.
- [4] Asadpour, J.; Safikhani, L. Study of CNC7[n] Carbon Nanocone by M-Eccentric Connectivity Polynomial. Aust. J. Basic Appl. Sci. 2013, 7, 883.
- [5] De, N.; Nayeem, S.M.A.; Pal, A. Total eccentricity index of the generalized index and polynomial of thorn graph. Appl. Math. 2012, 3, 931–934. [CrossRef]

- [6] Huo, Y.; Lio, J.B.; Baig, A.Q.; Sajjad, W.; Farahani, M.H. Connective Eccentric Index of NANm Nanotube. *J. Comput. Theor. Nanosci.* 2017, 14, 1832–1836. [CrossRef]
- [7] Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* 1947, 69, 17–20. [CrossRef][PubMed]
- [8] Sharma, V.; Goswami, R.; Madan, A.K. Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies. *J. Chem. Inf. Comput. Sci.* 1997, 37, 273–282. [CrossRef]
- [9] Alaeiyan, M.; Mojarad, R.; Asadpour, J. A new method for computing eccentric connectivity polynomial of an infinite family of linear polycene parallelogram benzenod. *Optoelectron. Adv. Mater. -Rapid Commun.* 2011,5, 761–770.
- [10] Bindusree, A.R.; Loksha, V.; Ranjini, P.S. Eccentric connectivity index and polynomial of some graphs. *Br. J.Math. Comput. Sci.* 2015, 6, 457–467. [CrossRef]
- [11] Gupta, S.; Singh, M.; Madan, A.K. Connective eccentricity index: a novel topological descriptor for predicting biological activity. *J. Mol. Graph Model* 2000, 18, 18–25. [CrossRef]
- [12] Gupta, S.; Singh, M.; Madan, A.K. Application of Graph Theory: Relationship of Eccentric Connectivity Index and Wiener's Index with Anti-inflammatory Activity. *J. Math. Anal. Appl.* 2002, 266, 259–268. [CrossRef]
- [13] Ramane, H.S.; Jummanner, R.B. Note on forgotten topological index of chemical structure in drugs. *Appl. Math. Nonlinear Sci.* 2016, 1, 369–374. [CrossRef]
- [14] Gao, W.; Imran, M.; Siddiqui, M.K.; Naeeme, M.; Jamil, F. Molecular Description of Copper (I) Oxide and Copper (II) Oxide. *Quimica Nova* 2018, 41, 874–879. [CrossRef]
- [15] Baig, A.Q.; Imran, M.; Khalid, W.; Naeem, M. Molecular description of carbon graphite and crystal cubic carbon structures. *Can. J. Chem.* 2017, 95, 674–686. [CrossRef]
- [16] Balaban, A.T.; Quintas, L.V. The smallest graphs, trees, and 4-trees with degenerate topological index. *J. Math. Chem.* 1983, 14, 213–233.
- [17] Graovac, A.; Ghorbani, M.; Hosseinzadeh, M.A. Computing fifth geometric-arithmetic index for nanostar dendrimers. *J. Math. Nanosci.* 2011, 1, 33–42.
- [18] Gutman, I.; Polansky, O.E. *Mathematical Concepts in Organic Chemistry*; Springer: New York, NY, USA, 1986.

*Corresponding author.

E-mail address: m.v.surseshpari@ gmail.com