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Eccentricity based Topological Indices of $L(CNC_3[2])$ and $L(CNC_4[2])$ Graphs

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Abstract: ***The eccentricity of a vertex is the maximum distance from it to any other vertex, ec(u) = max{d(u, v)|∀u∈V(G)}. In this paper we compute total eccentricity index, average eccentricity index, different versions of eccentricity-based Zagreb indices($M_1^*(G), M_1^{**}(G), M_2^*(G)$), fourth GA eccentricity index, fifth ABC eccentricity index, eccentric connectivity index and eccentric connectivity polynomial of line graphs of $CNC_3[2]$ and $CNC_4[2]$ carbon nanocones.***

Keywords: Carbon nanocone, eccentricity, eccentric Zagreb index, line graph, topological index

1. Introduction

Let G be a finite, simple, connected graph with vertex set V(G) and edge set E(G). Let d_v be the degree of a vertex v in a graphG and is the number of vertices adjacent to v. The edge connecting the vertices u and v is denoted by uv. A molecular graph is are presentation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the chemical compound and edges correspond to chemical bonds [1]. The 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 [2]. Topological indices of a simple graph are numerical descriptors that are derived from graph of chemical compounds. The distance d(u, v) between two vertices u and v of a graph G is defined as the length of a shortest path connecting them [3]. For a vertex u∈V(G) its eccentricity (ec(u)) is defined as

$$ec(u) = max\{d(u, v)|\forall u \in V(G)\}. \qquad (1)$$

The first Zagreb eccentricity index is defined as the sum of the squares of the eccentricities of the vertices, and the second Zagreb eccentricity index is defined as the sum of the products of the eccentricities of pairs of adjacent vertices [4-6].

The graphical structure of $CNC_k[n]$ carbon nanocones have a cycle of k-length at its central part and n levels of hexagons positioned at the conical exterior around its part. F-indices and F-polynomials of carbon nanocones $CNC_k[n]$ were investigated in [7]. Degree based topological indices of carbon nanocones were discussed in detail by considering different carbon nanocones in [8]. Different versions of harmonic indices of certain nanotubes were studied in [9]. The line graph of G is denoted by L(G) and is obtained from G by associating a vertex with each edge of the graph and connecting two vertices with an edge if and only if the corresponding edges have a vertex in common [10]. Let G be a (p, q) graph. Then L(G) has q vertices and $\frac{1}{2}\sum_{i=1}^{p} d_G x(u_i)^2 - q$ edges [11]. The eccentric connectivity index is deeply connected to the average eccentricity, but for each vertex v, eccentric connectivity index takes one local property and one global property into account [12]. Different versions of Nirmala indices of chloroquine, hydroxychloroquine and remdesivir was investigated by V.R.Kulli [13]. Nirmala indices of carbon nanocones were discussed in [14]. In [15] the eccentric connectivity index of nanosheets and nanotube of SiO_2 were computed. Distance eccentric connectivity index of the line graph of linear chain of benzene was discussed in [16].The eccentricity based topological indices of diamond graphs was studied by M. O. Turaci [17]. Some edge degree based topological indices, since the edge degree of a graph is the vertex degree of its line graph, were computed by K. B. Sudhakara et al. for line graph of graphene [18]. The eccentric connectivity index provides good correlations with regard to both physical and biological properties [19]. A formula of third Zagreb index ($M_1^*(G)$) for an infinite family of linear polycene parallelogram of benzenoid by using cut method was obtained in [20].

The maximum and minimum degree of a vertex among vertices of G are denoted by $\Delta = \max\{d_v|v\in V(G)\}$, $\delta = \min\{d_v|v\in V(G)\}$ respectively. In [21] M. Bhanumati and E. J. Rani introduced the Harmonic eccentric index and it is defined as

$$HEI(G) = \sum_{uv\in E(G)} \frac{2}{ec(u)+ec(v)}.$$

The formulas used to study eccentricity based topological indices are taken from [22-24].

Total eccentricity index

$$\zeta(G) = \sum_{v\in V(G)} ec(v). \qquad (2)$$

Average eccentricity index

$$avec(G) = \frac{1}{n}\sum_{v\in V(G)} ec(v) \qquad (3)$$

Eccentricity versions of Zagreb indices

$$M_1^*(G) = \sum_{uv\in E(G)} [ec(u) + ec(v)] \qquad (4)$$

$$M_1^{**}(G) = \sum_{v\in V(G)} ec(v)^2 \qquad (5)$$

$$M_2^*(G) = \sum_{uv\in E(G)} [ec(u)ec(v)] \qquad (6)$$

Fourth GA eccentricity index

$$GA_4(G) = \sum_{uv\in E(G)} \frac{2\sqrt{ec(u)ec(v)}}{ec(u)+ec(v)} \quad (7)$$

Fifth ABC eccentricity index

$$ABC_5(G) = \sum_{uv\in E(G)} \sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}} \quad (8)$$

Eccentric connectivity index

$$\xi(G) = \sum_{v\in V(G)} d_v ec(v) \quad (9)$$

Eccentric connectivity polynomial [25-26]

$$ECP(G,x) = \sum_{v\in V(G)} d_v x^{ec(v)} \quad (10)$$

In this paper total eccentricity index, average eccentricity index, eccentricity versions of Zagreb indices $(M_1^*(G), M_1^{**}(G), M_2^*(G))$, fourth GA eccentricity index, fifth ABC eccentricity index, eccentric connectivity index and eccentric connectivity polynomial are studied for line graphs of CNC_3 [2] and CNC_4 [2] carbon nanocones. All the symbols and notations used in this paper are standard and taken mainly from books of graph theory [28-30].

2. Materials and Methods

A molecular graph G(V, E) is constructed by representing each atom of molecule by vertex and bonds between them by edges. Let V(G) be vertex set and E(G) be edge set. The subdivision graph S(G) is the graph obtained from G by replacing each of its edge by a path of length2, by inserting an additional vertex in to each edge of G. The line graph is denoted by L(G) whose vertices are the edges of G and connecting two vertices with an edge if and only if the corresponding edges have a vertex in common. The line graphs of carbon nanocones CNC_3 [2] and CNC_4 [2] are shown in figures 1 and 2 respectively [27].

In this paper total eccentricity index, average eccentricity index, eccentricity versions of Zagreb indices $(M_1^*(G), M_1^{**}(G), M_2^*(G))$, fourth GA eccentricity index, fifth ABC eccentricity index, eccentric connectivity index and eccentric connectivity polynomial are computed for line graphs of $CNC_3[2]$ and $CNC_4[2]$ carbon nanocones by using equations (2-10).

3. Results and Discussion

The line graphs of CNC_3 [2] and $CNC_4[2]$ carbon nanocones are shown in figures 1 and 2 respectively. The vertex degree, eccentricity of all vertices and edges of $L(CNC_3$ [2]) and $L(CNC_4[2])$ are represented in table (1-2) and are used to compute the eccentricity based topological indices. In this section we compute the eccentricity based topological indices by using equations (2-10).

3.1 Eccentricity based topological indices of $L(CNC_3[2])$

Theorem 1: Let G be the line graph of $(CNC_3[2])$ carbon nanocone, then

(i)Total eccentricity index of $L(CNC_3[2])$ is 225.
(ii)Average eccentricity index of $L(CNC_3[2])$ is 6.25.
(iii)$M_1^*(G)$of $L(CNC_3[2])$ is 774.
(iv)$M_1^{**}(G)$of $L(CNC_3[2])$ is 1425.
(v)$M_2^*(G)$of $L(CNC_3[2])$ is 2394.

Proof: By using figure 1, equations (2-6) and table 1 we can prove the theorems (i-v).

Theorem 2: Fourth GA eccentricity index of $L(CNC_3[2])$ is 63.

Proof: By using figure 1, equation (7) and table 1, we have

$$GA_4(G) = \sum_{uv\in E(G)} \frac{2\sqrt{ec(u)ec(v)}}{ec(u)+ec(v)}$$

$$=15\frac{2\sqrt{7\times7}}{7+7} + 12\frac{2\sqrt{6\times7}}{6+7} + 15\frac{2\sqrt{6\times6}}{6+6} + 3\frac{2\sqrt{5\times5}}{5+5} + 18\frac{2\sqrt{5\times6}}{5+6}$$

$= 63.$

Theorem 3: Fifth ABC eccentricity index of $L(CNC_3[2])$ is 33.

Proof: By using figure 1, equation (8) and table 1, we have

$$ABC_5(G) = \sum_{uv\in E(G)} \sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}}$$

$$=15\sqrt{\frac{7+7-2}{7\times7}} + 12\sqrt{\frac{6+7-2}{6\times7}} + 15\sqrt{\frac{6+6-2}{6\times6}} + 3\sqrt{\frac{5+5-2}{5\times5}} + 18\sqrt{\frac{5+6-2}{5\times6}}$$

$= 33.$

Theorem 4: Eccentric connectivity index of $L(CNC_3[2])$ is774.

Proof: By using figure 1, equation (9) and table 1, we have

$\xi(G) = \sum_{v\in V(G)} d_v ec(v)$
$= 3(2\times7) + 12(3\times7) + 15(4\times6) + 6(4\times5)$
$= 774.$

Theorem 5: Eccentric connectivity polynomial of $L(CNC_3[2])$ is$42x^7+60x^6+24x^5$.

Proof: By using figure 1, equation (10) and table 1, we have

$ECP(G,x) = \sum_{v\in V(G)} d_v x^{ec(v)}$
$= 3\times2x^7+12\times3x^7+15\times4x^6+6\times4x^5$
$= 42x^7+60x^6+24x^5.$

3.2 Eccentricity based topological indices of $L(CNC_4[2])$

Theorem 6. Let G be the line graph of $(CNC_4[2])$ carbon nanocone, then

(i) Total eccentricity index of $L(CNC_4[2])$ is 312.
(ii) Average eccentricity index of $L(CNC_4[2])$ is 6.5.
(ii) $M_1^*(G)$of $L(CNC_4[2])$ is 1131.
(iv) $M_1^{**}(G)$of $L(CNC_4[2])$ is 2496.
(v) $M_2^*(G)$of $L(CNC_4[2])$ is 4970.

Proof: By using figure 2, equations (2-6) and table 2 we can prove the theorems (i-v).

Theorem 7: Fourth GA eccentricity index of $L(CNC_4[2])$ is 85.

Proof: By using figure 2, equation (7) and table 2, we have

$$GA_4(G) = \sum_{uv\in E(G)} \frac{2\sqrt{ec(u)ec(v)}}{ec(u)+ec(v)}$$

$=4\frac{2\sqrt{7\times7}}{7+7}+\ 16\frac{2\sqrt{8\times9}}{8+9}+\ 20\frac{2\sqrt{8\times8}}{8+8}+\ 8\ \frac{2\sqrt{9\times10}}{9+10}+\ 16\frac{2\sqrt{7\times8}}{7+8}$
$+7\frac{2\sqrt{6\times7}}{6+7}+12\frac{2\sqrt{6\times6}}{6*6}$
$=85.$

Theorem 8: Fifth ABC eccentricity index of L(CNC_4[2]) is 40.

Proof: By using figure 1, equation (8) and table 2, we have

$$ABC_5(G)=\sum_{uv\in E(G)}\sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}}$$

$$=4\sqrt{\frac{7+7-2}{7\times7}}+\ 16\sqrt{\frac{8+9-2}{8\times9}}+\ 20\sqrt{\frac{8+8-2}{8\times8}}+$$
$$8\sqrt{\frac{9+10-2}{9\times10}}+16\sqrt{\frac{7+8-2}{7\times8}}+7\sqrt{\frac{6+7-2}{6\times7}}+12\sqrt{\frac{6+6-2}{6\times6}}$$
= 4o.

Theorem 9: Eccentric connectivity index of L(CNC_4[2]) is 1096.

Proof: By using figure 2, equation (9) and table 2, we have

$\xi(G)=\sum_{v\in V(G)} d_v ec(v)$
$= 8(4\times6)+8(4\times7)+12(4\times8)+8(3\times9)+4(2\times10)$
$= 1096.$

Theorem 10: Eccentric connectivity polynomial of L(CNC_4[2]) is
$8x^{10}+24x^9+48x^8+32x^7+32x^6$.

Proof: By using figure 2, equation (10) and table 2, we have

$ECP(G,x)=\sum_{v\in V(G)} d_v x^{ec(v)}$
$= 8\times4x^6+8\times4x^7+12\times4x^8+8\times3x^9+4\times2\ x^{10}$
$= 8x^{10}+24x^9+48x^8+32x^7+32x^6.$

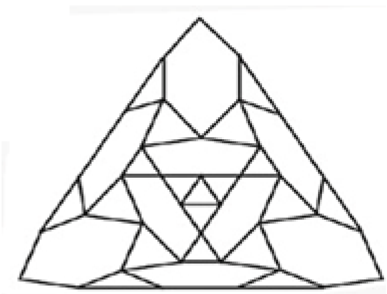

Figure 1: Graph of L(CNC_3[2])

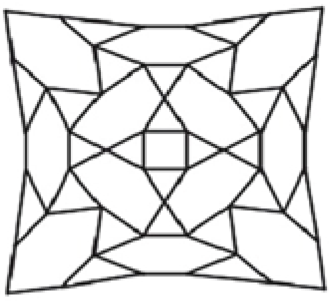

Figure 2: Graph of L(CNC_4[2])

Table 1: Vertex degree partition of line graph of CNC_3[2] carbon nanocone with eccentricity and frequency

Ec (u)	d_u	d_u	d_u
	2	3	4
7	3	12	--
6	--	--	15
5	--	--	6

(ec(u), ec(v))	(7, 7)	(6, 7)	(6, 6)	(5, 5)	(5, 6)
frequency	15	12	15	3	18

Table 2: Vertex degree partition of line graph of CNC_4[2] carbon nanocone with eccentricity and frequency

ec(u)	d_u	d_u	d_u
	2	3	4
6	--	--	8
7	--	--	8
8	--	8	12
9	--	8	--
10	4	--	--

(ec(u), ec(v))	(7, 7)	(9, 8)	(8, 8)	(9, 10)	(7, 8)	(6, 7)	(6, 6)
frequency	4	16	20	8	16	7	12

4. Conclusion

Total eccentricity index, average eccentricity index, eccentricity versions of Zagreb indices ($M_1^*(G), M_1^{**}(G), M_2^*(G)$), fourth GA eccentricity index, fifth ABC eccentricity index, eccentric connectivity index and eccentric connectivity polynomial are studied for line graphs of CNC_3[2] and CNC_4[2] carbon nanocones.

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