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Neighbour degree connectivity indices of graphs and its applications to the octane isomers

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Abstract

The sum of neighbour degrees $\delta_G(u)$ of a vertex u is defined as the sum of the degrees of all neighbour vertices of u of a graph G. In this paper, we obtained neighouhourhood version of Zagreb indices of line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$ and graphene sheet.

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1 Introduction

Let G be a simple, undirected, connected graph of order n and size m. Let $V(G)$ be the vertex set and $E(G)$ be the edge set of G. The edge joining the vertices u and v is denoted by uv. The *degree* of a vertex u is the number of edges incident to it and is denoted by $d_G(u)$. The *nighbour* of a vertex $u \in V(G)$ is defined as the number of adjacent vertices of vertex u of graph G. The sum of neighbour degrees $\delta_G(u)$ of a vertex u is defined as the sum of the degrees of all neighbour vertices of u of a graph G, that is

$$\delta_G(u) = \sum_{u \in N_G(u)} d_G(u)$$

For a graph theoretic terminology, we refer the books [1, 6].

The first and second *Zagreb indices* of a graph G are defined as [5]

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)] \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v).$$

The Zagreb indices were used in the structure property model. Recent results on the Zagreb indices can be found in [2, 3, 4, 7, 10, 11, 12]. Sourav Monadl et. al, introduced neighbourhood versions of some topological indices, among those the first and second neighbourhood Zagreb indices defined as follows [8],

$$M_1^*(G) = \sum_{uv \in E(G)} [\delta(u) + \delta(v) = 2M_2(G)] \tag{1}$$

and

$$M_2^*(G) = \sum_{uv \in E(G)} \delta(u)\delta(v). \tag{2}$$

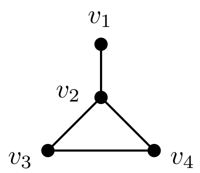

Figure 1

For a graph given in Fig. 1, $\delta(v_1) = 3$, $\delta(v_2) = 5$, $\delta(v_3) = 5$, $\delta(v_4) = 5$. Therefore $M_1^*(G) = 38$ and $M_2^*(G) = 90$.

2 Computation of First and second neighbourhood version of Zagreb indices of some class of graphs

Lemma 2.1. *Let G be r-regular graph. Then*

$$M_1^*(G) = 2mr^2$$
$$M_2^*(G) = mr^4$$

Lemma 2.2. *For $n > 4$, let P_n be a path with n-vertices. Then*

$$M_1^*(G) = 8(n-2)$$
$$M_2^*(G) = 16n - 44$$

Lemma 2.3. *Let S_n be a star with n-vertices. Then*

$$M_1^*(G) = 2(n-1)^2$$
$$M_2^*(G) = (n-1)^3$$

3 First and second neighbourhood version of Zagreb indices of line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p, q]$

Nadeem et al.,computed genralized Randic, general Zagreb and sum connevtivity indices, atom-bond connectivity index $ABC(G)$ with $ABC_4(G)$ and geometric arithmatic index $GA(G)$ with $GA_5(G)$ indices of the line graphs of subdivision graph of $2D-$lattice, nanotube and nanotorus $TUC_4C_8[p, q]$. Here number of sqares in row denoted by p, number of rows of squares by q in $2D$-lattice and nanotube. For structure and more information one can refer [9]

Theorem 3.1. *Let G be the line graph of the subdivision graph of 2D-lattice of TUC4C8[p, q]. Then*

$$M_1^*(G) = \begin{cases} 324pq - 134p - 134q + 8 & \text{if } p > 1, \; q > 1 \\ 190p - 126 & \text{if } p > 1, \; q = 1. \end{cases}$$
$$M_2^*(G) = \begin{cases} 145pq - 753p - 753q + 172 & \text{if } p > 1, \; q > 1 \\ 707p - 581 & \text{if } p > 1, \; q = 1. \end{cases}$$

Proof. $|V(G)| = 2[6pq - p - q]$ and $|E(G)| = 18pq - 5p - 5q$. Partition the edge set of G is given in the Table 1 and Table 2:

Table 1: Edge partition of line graph of the subdivision graph of 2D-lattice of TUC4C8[p, q] when $p > 1$ and $q > 1$

$(\delta(u), \delta(v))uv \in E(G)$	(4, 4)	(4 ,5)	(5, 5)	(5, 8)	(8, 9)	(9, 9)
Number edges	4	8	2(p+q-4)	4(p+q-2)	8(p+q-2)	2(9pq+10)-19(p+q))

Table 2: Edge partition of line graph of the subdivision graph of 2D-lattice of TUC4C8[p, q] when $p > 1$ and $q = 1$

$(\delta(u), \delta(v))uv \in E(G)$	(4, 4)	(4 ,5)	(5, 5)	(5, 8)	(8, 8)	(8, 9)	(9, 9)
Number edges	6	4	2(p-2)	4(p-1)	2(p-1)	4(p-1)	p-1

Case 1: when $p > 1$ and $q > 1$,

$$\begin{aligned} M_1^*(G) &= \sum_{uv \in E(G)} [\delta(u) + \delta(v)] \\ &= 4(4+4) + 8(4+5) + 2(p+q-4)(5+5) + 4(p+q-2)(5+8) \\ &\quad +8(p+q-2)(8+9) + (2(9pq+10) - 19(p+q))(9+9) \\ &= 324pq - 134p - 134q + 8. \end{aligned}$$

$$\begin{aligned} M_2^*(G) &= \sum_{uv \in E(G)} \delta(u)\delta(v) \\ &= 4(4 \times 4) + 8(4 \times 5) + 2(p+q-4)(5 \times 5) + 4(p+q-2)(5 \times 8) \\ &\quad +8(p+q-2)(8 \times 9) + (2(9pq+10) - 19(p+q))(9 \times 9) \\ &= 145pq - 753p - 753q + 172. \end{aligned}$$

Case 2: when $p > 1$ and $q = 1$,

$$\begin{aligned} M_1^*(G) &= \sum_{uv \in E(G)} [\delta(u) + \delta(v)] \\ &= 6(4+4) + 4(4+5) + 2(p-2)(5+5) + 4(p-1)(5+8) + 2(p-1)(8+8) \\ &\quad +4(p-1)(8+9) + (p-1)(9+9) \\ &= 190p - 126. \end{aligned}$$

$$\begin{aligned} M_2^*(G) &= \sum_{uv \in E(G)} \delta(u)\delta(v) \\ &= 6(4 \times 4) + 4(4 \times 5) + 2(p-2)(5 \times 5) + 4(p-1)(5 \times 8) + 2(p-1)(8 \times 8) \\ &\quad +4(p-1)(8 \times 9) + (p-1)(9 \times 9) \\ &= 707p - 581. \end{aligned}$$

□

4 First and second neighbourhood version of Zagreb indices of line graph of the subdivision graph of $TUC_4C_8[p, q]$ nanotube

Theorem 4.1. *Let H be the line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$ nanotube. Then*

$$M_1^*(H) = \begin{cases} 324pq - 134p & \text{if } \ p > 1, \ q > 1 \\ 190p & \text{if } \ p > 1, \ q = 1. \end{cases}$$

$$M_2^*(H) = \begin{cases} 1458pq - 753p & \text{if } \ p > 1, \ q > 1 \\ 707p & \text{if } \ p > 1, \ q = 1. \end{cases}$$

Proof. $|V(H)| = 12pq - 2p$ and $|E(G)| = 18pq - 5p$. Partition the edge set of G is given in the Table 3 and Table 4:

Case 1: when $p > 1$ and $q > 1$,

$$\begin{aligned} M_1^*(H) &= \sum_{uv \in E(G)} [\delta(u) + \delta(v)] \\ &= 2p(5+5) + 4p(5+8) + 8p(8+9) + (18pq - 19p)(9+9) \\ &= 324pq - 134p. \end{aligned}$$

Table 3: Edge partition of line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p, q]$ nanotube when $p > 1$ and $q > 1$

$(\delta(u), \delta(v))uv \in E(H)$	(5, 5)	(5 , 8)	(8, 9)	(9, 9)
Number edges	$2p$	$4p$	$8p$	$18pq - 19p$

Table 4: Edge partition of line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p, q]$ nanotube when $p > 1$ and $q = 1$

$(\delta(u), \delta(v))uv \in E(H)$	(5, 5)	(5 , 8)	(8, 8)	(8, 9)	(9, 9)
Number edges	$2p$	$4p$	$2p$	$4p$	p

$$\begin{aligned} M_2^*(H) &= \sum_{uv \in E(G)} \delta(u)\delta(v) \\ &= 2p(5 \times 5) + 4p(5 \times 8) + 8p(8 \times 9) + (18pq - 19p)(9 \times 9) \\ &= 1458pq - 753p. \end{aligned}$$

Case 2: when $p > 1$ and $q = 1$,

$$\begin{aligned} M_1^*(H) &= \sum_{uv \in E(G)} [\delta(u) + \delta(v)] \\ &= 2p(5 + 5) + 4p(5 + 8) + 2p(8 + 8) + 4p(8 + 9) + p(9 + 9) \\ &= 190p. \end{aligned}$$

$$\begin{aligned} M_2^*(H) &= \sum_{uv \in E(G)} \delta(u)\delta(v) \\ &= 2p(5 \times 5) + 4p(5 \times 8) + 2p(8 \times 8) + 4p(8 \times 9) + p(9 \times 9) \\ &= 707p. \end{aligned}$$

□

5 First and second neighbourhood version of Zagreb indices of graphene sheet

Graphene is a planar sheet of carbon atoms that is densely placed in a honeycomb crystal lattice. It is the main element of certain carbon allotropes. The structure of graphene $G(p, q)$ with p rows and q columns. It has pq hexogons.

Theorem 5.1. *Let $G(m, n)$ be graphene sheet, with $p, q > 1$, then*

$$\begin{aligned} M_1^*(G(p, q)) &= 14p + 12q + 54pq - 34. \\ M_2^*(G(p, q)) &= -11p - 30q + 243pq - 147. \end{aligned}$$

$$\begin{aligned} M_1^*(G(p, q)) &= \sum_{uv \in E(G)} [\delta(u) + \delta(v)] \\ &= 4(4 + 5) + p(5 + 5) + 8(5 + 7) + (2p - 4)(5 + 8) + (4q - 8)(6 + 7) + 2q(7 + 9) + (p - 2)(8 + 8) \\ &\quad + (2p - 4)(8 + 9) + (3pq - 4q - 4p + 5)(9 + 9) \\ &= 14n + 12m + 54mn - 34 \end{aligned}$$

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Table 5: Edge partition of graphene sheet $G(p,q)$ and $p,q>1$

$(\delta(u),\delta(v))uv \in G(p,q)$	(4, 5)	(5 , 5)	(5, 7)	(5, 8)	(6, 7)	(7, 9)	(8, 8)	(8, 9)	(9, 9)
Number edges	4	p	8	$2p-4$	$4q-8$	$2q$	$p-2$	$2p-4$	$3pq-4p-4q+5$

$$\begin{aligned} M_2(G(p,q)) &= \sum_{uv\in E(G)} \delta(u)\delta(v) \\ &= 4(4\times 5)+p(5\times 5)+8(5\times 7)+(2p-4)(5\times 8)+(4q-8)(6\times 7)+2q(7\times 9)+(p-2)(8\times 8) \\ &\quad +(2p-4)(8\times 9)+(3pq-4q-4p+5)(9\times 9) \\ &= -11p-30q+243pq-147 \end{aligned}$$

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