JOURNAL OF MECHANICS OF CONTINUA AND MATHEMATICAL SCIENCES
www.journalimcms.org

ISSN (Online) : 2454 -7190 Vol.-19, No.-4, April (2024) pp 12-28 ISSN (Print) 0973-8975

SPECIAL GRAPHS AND THEIR ZAGREB INDICES: A COMPARATIVE STUDY

A. P. Pushpalatha[1], S. Suganthi[2]

[1,2] Department of Mathematics, Velammal College of Engineering and Technology (Autonomous), Madurai, India.

Email: [1]app@vcet.ac.in, [2]skh@vcet.ac.in

Corresponding Author: **A. P. Pushpalatha**

https://doi.org/10.26782/jmcms.2024.04.00002

(Received: February 06, 2024; Revised: March 26, 2024; Accepted: April 05, 2024)

Abstract

A simple, finite and connected graph is denoted by $G = (V, E)$. The primary Zagreb index, denoted as $M_1(G)$, characterizes the graph topologically by representing a squared degree sum of their vertices. Similarly, $M_2(G)$ denotes a second Zagreb index, that offers a topological measure of summing the degree of the product for adjacent vertices of graph G, We investigate a study of this topological indices $M_1(G)$&$M_2(G)$ and got some interesting results also.

Keywords: Zagreb indices, first Zagreb index, second Zagreb index, Fan graph, Barbell graph, Thorn graph.

I. Introduction

In this paper, we derive expressions for $M_1(G)$ termed the primary Zagreb index & $M_2(G)$ a second Zagreb index about a specific graph. Our formulations are based on the number of vertices and certain positive integers denoted as a and b. Our investigation involves an exploration of the properties of these topological indices, $M_1(G)$ and $M_2(G)$, leading to the discovery of intriguing results. In this document, our focus is exclusively on simple connected graphs free of loops and several boundaries. Intended for the given graph G, the term $V(G)$ and $E(G)$ signifies all vertices set and edges correspondingly. From the context of graph G, v a vertex degree was defined as an edge count incident to v, denoted by all vertices and edges set, correspondingly. In a graph G a vertex degree v is defined as an edge count that occurred to v, signified as $deg_G(v)$.

The graphical invariant, often signified as the fixed number under the graph automorphisms, is a numerical property associated with a graph that remains unchanged despite structural variations. These numbers of invariants were termed as the topological directories alternatively in a chemical graph theory field. A Wiener index stands as a straightforward and versatile topological index, proving to be an invaluable tool for characterizing the structure and properties of molecules. Widely employed in an area of pharmacology, chemistry, and materials science. Weiner index was referred to as a total distance among each vertices pair in the corresponding graph. The $M_1(G) and\, M_2(G)$ Zagreb indices were presented in the work [I] and were developed further in work [II]. In [III, IV, V], a primary characteristic of $M_1(G) and M_2(G)$were outlined.

These two topological indices serve as indicators for the splitting degrees within the essential carbon atom of the molecule. As noted in [VIII], path and star emerges as a tree thus exhibiting smaller and larger $M_2(G)$ values, correspondingly. Thorn graph idea was introduced initially by Gutman et al. [XI] and subsequently discovered to have diverse chemical applications in [VIII, XII, XIII, XIX, XX, XXI]. The characteristics of both the first & second Zagreb indices that were among the first descriptors of a molecular structure have undergone extensive research. Many mathematicians working in chemistry have recently been interested in the concept of Zagreb coindices are established through the definitions of the first Zagreb index, signified as $M_1(G)$, & second Zagreb index signified by $M_2(G)$, which is shown below:

$$M_1(G) = \sum_{u,v\in E(G)}[deg(u) + deg(v)] \tag{1}$$

$$M_2(G) = \sum_{u,v\in E(G)}[deg(u). deg(v)] \tag{2}$$

In the work [XIV], $M_1(G)\ and\ M_2(G)$ Zagreb indices were introduced, and key properties of these indices were summarized. Subsequent research, reported in [XVI], delves into recent findings on Zagreb indices, providing references to prior mathematical investigations in this domain. In recent years, there has been an exploration of novel variants of traditional Zagreb indices including the multiplicative sum Zagreb index, multiplicative Zagreb indices,multiplicative Zagreb coindices, and Zagreb coincides [VII, VIII, XIV, XVII]. Notably, both the first and second Zagreb coindices of graph G are denoted as:

$$\overline{M_1} = \overline{M_1(G)} = \sum_{u\neq v\in E(G)}[deg(u) + deg(v)] \tag{3}$$

$$\overline{M_2} = \overline{M_2(G)} = \sum_{u\neq v\in E(G)}[deg(u)deg(v)] \tag{4}$$

We refer to Harary et al. [XXIII] for the theoretical nomenclature and notations for any graph. [VIII, IX, X, XIII], report a few recent studies regarding Zagreb indices and include references to earlier mathematical studies in this field. You may think of these indices as molecular structure descriptors because they show how much the molecular carbon-atom skeleton has branched.

For information on the historical context, computational approaches, and mathematical characteristics of Zagreb indices, we recommend that the reader study [XIIIX XIX, XX, XXI]. Numerous topological indices currently capturing attention in mathematical chemistry are formulated depending on the degree of vertex within the molecular graph.

II. Literature Survey

Kinkar Ch Das, Kexiang XU et al [XIV] developed several lower and upper bounds in the first and second Zagreb indices for the graph. The characteristics of the two Zagreb indices, which are among the first descriptors of molecular structure, have undergone extensive research. Many mathematicians working in chemistry have recently been interested in the concept of Zagreb indices.

We have uncovered compelling results concerning the Thorn graph about the number of vertices and positive integers a and b. These findings are noteworthy, even in light of the many elegant results previously achieved on this matter. The initial Zagreb index, represented as $M_1(G)$, is a graph theoretical parameter that characterizes the degree and size distribution of graph G. This index reflects the graph's complexity and can offer insights into its structural properties. The second Zagreb index, labeled $M_2(G)$, is another topological index used to analyze the chemical and physical properties of molecules in chemistry. This index can provide information about the branching and connectivity of the graph.

Numerous investigations have examined the characteristics and uses of the Zagreb indices. In [XIV], researchers investigated the relationship between these indices and various graph properties, such as stability, chromatic number, and eigenvalues. These indices can be thought of as molecular structure descriptors because they show how branching the molecular carbon atom skeleton is [XXIV]. In other works, we have applied Zagreb indices in chemical and mathematical contexts, shedding light on their significance in different domains.

Overall, the first and second Zagreb indices serve as valuable tools for graph analysis and have found applications in diverse fields due to their ability to capture key aspects of a graph's structure and behavior. Further research in this area could involve exploring their applications in different contexts and extending their utility in graph theory and related disciplines.

The complexity and topological characteristics of molecules are measured in chemistry and computer science using the topological Zagreb indices. These indices can be used to forecast physical and chemical characteristics like boiling points, toxicity, and biological activity, which can be useful in the development of new drugs and the study of new materials. Scientists can enhance their understanding of a molecule's behavior and characteristics through the utilization of Zagreb indices. These indices effectively encapsulate the distribution of atoms and bonds within a molecule. We have discovered some intriguing findings for thorn graphs about the number of points and positive integers like a and b, even though many beautiful results on this issue have already been attained.

This manuscript is structured as shown: In the section 3, the structural properties of the Thorn graph are presented and the first and second Zagreb indices of the Thorn graph $T_{a,b}(P_n)$ are computed, for any value of $a\ and\ b$. In section 4, here is the estimation of the first and second Zagreb indices of the Barbell graph $B(K_n,\ K_n)$ & a the first and second Zagreb indices of the fan graph. We present a comparative research of the Topological Zagreb indices that are produced mathematically and manually. We found that the two values were the same.

III. The Thorn graph's First & Second Zagreb Indices of Path

III.i. Definition of Thorn graph of a Path [XI, XXII]

Consider any pair of distinct positive integers, denoted as a and b where a ≠ b. Let $P_n(n\ \geq\ 3)$ represent a path on n vertices, namely $v_1, v_2, \dots, v_n$.The Thorn graph of $P_n$is symbolized as $T_{a,b}(P_n)$, achieved by appending $ad_i\ +\ b$, a pendant vertices number to each $P_n$vertex, at which deg_i denotes a vertex degree v_1, $1\ \leq\ i\ \leq\ n$.

III.ii. Illustration

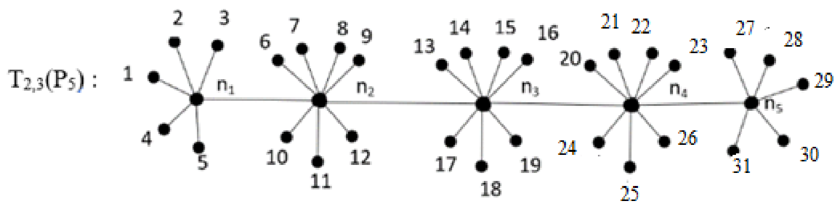

Fig.1.

III.iii. Structural Properties of Thorn graph

1. $|V\ [T_{a,b}(P_n)]| = |V\ (P_n)| + 2(a\ +\ b) + (n\ -\ 2)(2a\ +\ b)$
   $|V\ [T_{a,b}(P_n)]| = 2a(n\ -\ 1) + n(1\ +\ b)$
2. $|E[T_{a,b}(P_n)]| = |E(Pn)| + 2(a\ +\ b) +\ (n\ -\ 2) + (2a + b)$
   $|E[T_{a,b}(P_n)]| = n\ -\ 1 - 2a + n(2a + b)$
3. $\omega[T_{a,b}(P_n)] = 2$, where $\omega(G)$ is the clique number.6
4. $\chi[T_{a,b}(P_n)] = 2$, where $\chi(G)$ is the coloring number. since $[T_{a,b}(P_n)]$ is a tree.
5. $\kappa[T_{a,b}(P_n)] = 1$ where $\kappa(G)$ is vertex connectivity number.
6. $T_{a,b}(P_n)$is a [1, a + b, 2a + 2b + 2, 2a + b] - regular graph.
7. $\gamma[T_{a,b}(P_n)] = n$, at which$\gamma(G)$denotes the domination number G.

Let's compute the indices of the topology of the Thorn graph that are derived from the path.

III.vi. First Zagreb index of $T_{a,b}$ (P_n)

$$M_1\left(T_{a,b}(P_n)\right) = (4n\text{-}6)a^2 + (4n\text{-}4)ab + nb^2 + a(10n\text{-}14) + b(5n\text{-}4) + (4n - 6),$$

$n \geq 3$ (5)

Proof:

Let $n_1, n_2, \ldots, n_n$ be the vertices of P_n. Let $n_1', n_1'', \ldots, n_1^{a+b}$ are the pendant vertices attached with n_1; let $n_2', n_2'', \ldots, n_2^{2a+b}$ are the pendant vertices attached with n_2; …let $n_{n-1}', n_{n-1}'', \ldots, n_{n-1}^{2a+b}$ are the pendant vertices attached with n_{n-1}; and let $n_n', n_n'', \ldots, n_n^{a+b}$ are the pendant vertices attached with n_n respectively.

Degree of all the vertices of $T_{a,b}(P_n)$ is given by

$$\deg(v) = \begin{cases} a+b+1, if \ \ v \text{ is the terminal vertex of } P_n \\ 1, if \ \ v \text{ is the pendant vertex of } T_{a,b}(P_n) \\ 2a+b+2, if \ \ v \text{ is the internal vertex of } P_n \end{cases} \quad (6)$$

In the thorn graph $T_{a,b}$ (P_n), there are two points of degree a + b + 1. These are the two vertices that are connected to the two new vertices that are added to the path P_n to form the thorn graph. The thorn graph $T_{a,b}$ (P_n), also has 2a(n − 1) + nb, pendant vertices. These are the vertices that are connected to the 2a vertices that are added to the n − 1 edges of the path P_n to form the thorn graph. The remaining (n−2) vertices of the thorn graph are internal vertices, and they have a degree of 2a + b + 2. This is because these vertices are connected to the two new vertices that are added to the path P_n to form the thorn graph, and they are also connected to 2a of the vertices that are added to the n − 1 edges of the path P_n to form the thorn graph.

$$M_1\left(T_{a,b}(P_n)\right) = [deg(n_1) + deg(n_1')] + [deg(n_1) + deg(n_1'')] + \cdots + \left[deg(n_1) + deg\left(n_1^{(a+b)}\right)\right] + [deg(n_1) + d(n_2)] + [deg(n_2) + d(n_2')] + [deg(n_2) + deg(n_2'')] + \cdots + \left[deg(n_2) + deg(n_2)^{(2a+b)}\right] + [deg(n_2) + deg(n_3)] + \cdots + [deg(n_{n-1}) + deg(n_{n-1}')] + [deg(n_{n-1}) + deg(n_{n-1}'')] + \cdots + \left[deg(n_{n-1}) + deg\left(n_{n-1}^{(2a+b)}\right)\right] + [deg(n_{n-1}) + deg(n_n)] + [deg(n_n) + deg(n_n')] + [deg(n_n) + deg(n_n'')] + \cdots + \left[deg(n_n) + deg\left(n_n^{(a+b)}\right)\right] \quad (7)$$

$$= [(a+b)(a+b+2) + (a+b+1) + (a+b+2)] + (n-3)[(2a+b)(2a+b+3) + 2(2a+b+2)] + [(2a+b)(2a+b+3)] + (3a+2b+3)] + [(a+b+2)(a+b)] \quad (8)$$

$$M_1\left(T_{a,b}(P_n)\right) = (4n-6)a^2 + (4n-4)ab + nb^2 + a(10n-14) + b(5n-4) + (4n-6), n \geq 3 \quad (9)$$

III.v. Illustration:

Consider $T_{2,2}(P_6)$. Here $a = b = 2;\ n = 6$

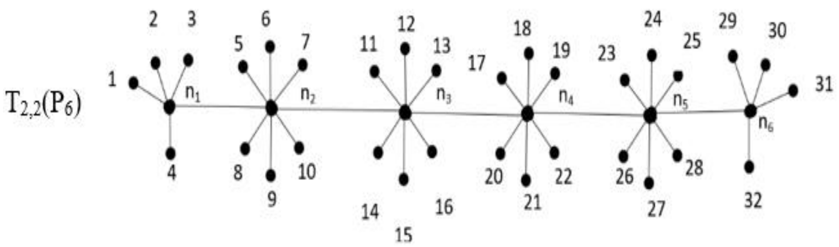

Fig. 2.

The degree of all the vertices of $T_{a,b}(P_n)$ are given below;

(i) n_1, n_6 are of degree $a + b + 1 = 5$

(ii) $(n-2)$ Points are of degree $2a + b + 2 = 8$

(iii) All the pendant points are of degree $(2a + b)n - 2a = 32$

$$M_1\left(T_{a,b}(P_n)\right) = (4n-6)a^2 + (4n-4)ab + nb^2 + a(10n-14) + b(5n-4) + (4n-6) \quad (10)$$

$$M_1\left(T_{2,2}(P_6)\right) = 338 \quad (11)$$

For $T_{2,2}(P_6)$, $M_1[T_{2,2}(P_6)]$ can be calculated manually:

Table : 1.

•	n_1	n_2	n_3	n_4	n_5	n_6	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	M(G)
n_1		13					6	6	6	6																													37
n_2			16								9	9	9	9	9	9																							70
n_3				16													9	9	9	9	9	9																	70
n_4					16																		9	9	9	9	9	9											70
n_5						13																							9	9	9	9	9	9					67
n_6																																			6	6	6	6	24
M(G)																																							338

The Topological index $M_1[T_{a,b}(P_n)]$ calculated manually and by using the formula appears to be same.

III.vi. Second Zagreb index of $T_{a,b}$(Pn)

The second Zagreb index is

$$M_2(G) = (8n-14)a^2 + (8n-10)ab + b^2(2n-1) + a(12n-22) + b(6n-8) + (4n-8),\ n \geq 3 \quad (12)$$

Proof:

Let $n_1, n_2, \ldots, n_n$ be the vertices of P_n.. Let $n_1', n_1'', \ldots, n_1^{a+b}$ are the pendant vertices attached n_1; let $n_2', n_2'', \ldots, n_2^{2a+b}$ are the pendant vertices attached with n_2; . . . let $n_{n-1}', n_{n-1}'', \ldots, n_{n-1}^{2a+b}$ are the pendant vertices attached with n_{n-1}; and let $n_n', n_n'', \ldots, n_n^{a+b}$ are the pendant vertices attached with n_n respectively. The second Zagreb index is

$$M_1(T_{a,b}(P_n)) = [deg(n_1).deg(n_1')] + [deg(n_1).deg(n_1'')] + \cdots + \left[deg(n_1).deg\left(n_1^{(a+b)}\right)\right] + [deg(n_1).deg(n_2)] + [deg(n_2).deg(n_2')] + [deg(n_2).deg(n_2'')] + \cdots + \left[deg(n_2).deg(n_2)^{(2a+b)}\right] + [deg(n_2).deg(n_3)] + \cdots + [deg(n_{n-1}).deg(n_{n-1}')] + [deg(n_{n-1}).deg(n_{n-1}'')] + \cdots + \left[deg(n_{n-1}).deg\left(n_{n-1}^{(2a+b)}\right)\right] + [deg(n_{n-1}).deg(n_n)] + [deg(n_n).deg(n_n')] + [deg(n_n).deg(n_n'')] + \cdots + \left[deg(n_n).deg\left(n_n^{(a+b)}\right)\right] \quad (13)$$

$$=[(a+b)(a+b+1) + (a+b+1)(2a+b+2)] + (n-3)[(2a+b)(2a+b+2)+(2a+b+2)^2] + [(2a+b)(2a+b+2) + (a+b+1)(2a+b+2)] + [(a+b+1)(a+b)] \quad (14)$$

$$M_2(G) = (8n-14)a^2 + (8n-10)ab+b^2(2n-1)+a(12n-22)+b(6n-8) +(4n-8),\ n \geq 3 \quad (15)$$

III.vii. Illustration

Consider $T_{2,1}(P_6)$.

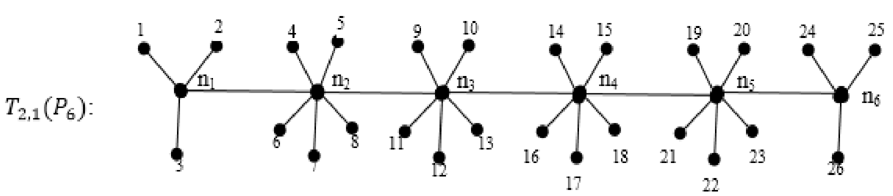

Fig. 3.

Consider $T_{2,1}(P_6)$

(i) In $T_{2,1}(P_6)$, n_1, n_6 are of degree a + b + 1 = 4

(ii) (n − 2) points are of degree 2a + b + 2 = 7

(iii) All the pendant vertices are of degree (2a + b)n − 2a = 26

Then,

M_2[Ta,b(Pn)] = (8n − 14)a 2 + (8n − 10)ab + b 2 (2n − 1) + a(12n − 22) + b(6n − 8) + (4n − 8) (16)

$M_2[T_{2,1}(P_6))] = 367$ (17)

$M_2[T_{2,1}(P_6)]$ can be calculated manually

Table : 2

*	n_1	n_2	n_3	n_4	n_5	n_6	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	$M_2(G)$
n_1	*	28					4	4	4																								40
n_2		*	49							7	7	7	7	7																			84
n_3			*	49											7	7	7	7	7														84
n_4				*	49															7	7	7	7	7									84
n_5					*	28																			7	7	7	7	7				63
n_6						*																								4	4	4	12
$M_2(G)$																																	367

The Topological index $M_2[T_{2,1}(P_6)]$ calculated manually and through the formula are the same.

IV. Barbell Graph's First and Second Zagreb

IV.i. Barbell graph definition: [XXII]

An n-Barbell graph is the straightforward graph that is formed on linking two indices of the complete graph K_n with bridge. This is signified by $B(K_n, K_n)$ where n is greater than or equal to 3.

IV.ii. The structural properties of the n-Barbell graph

1. Vertices: The n-Barbell graph has 2n vertices.

2. Edges: The n-Barbell graph has n 2 − n + 1 edges.

3. Degrees: vertices (2n − 2) were of n − 1 degree & two vertices were of n − degree

IV.iii. Illustration

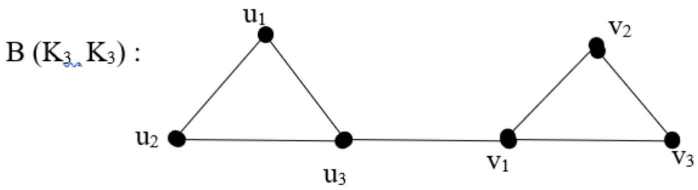

Fig. 4.

IV.iv. Result

In Barbell graph B(Kn, Kn)

(i) $M_1[B(K_{n,}K_n)]=2(n-1)[n^2-n+1], n\geq 3$ (18)

(ii) $M_2[B(K_{n,}K_n)]=(n-1)^2[n^2-n+2], n\geq 3$ (19)

Proof:

Let $B(K_{n,}K_n)$ denotes the Barbell graph having vertex sets $\{u_1,u_2,\dots u_n\}$ and assume $\{v_1,v_2,\dots v_n.\}$ will be another vertex set that has vertices disjoint complete graph $K_{n,}$.

Join $u_{i,}$ $1\leq i\leq n$ with any one of the $\{v_1,v_2,\dots v_n.\}$ vertex disjoint complete graph $K_{n,}$, say v_i , $1\leq i\leq n$.

Let u_1 [which is of degree n − 1] be the vertex which is adjacent to $u_2, u_3, \dots, u_{n-1}$ are of degree $(n-1)$ and $u_1$will be adjacent to u_n, which is of nvdegree . The index of 1st Zagreb's Barbell graph $B(K_{n,}K_n)$ can be determined by computing the contributions of the edges with regard to vertex u_1 as

$$[deg(u_1)+deg(u_2)]+[deg(u_1)+deg(u_3)]+\cdots+[deg(u_1)+deg(u_{n-1})]+[deg(u_1)+deg(u_n)]=2(n-1)(n-2)+(2n-1) \quad (20)$$

Also, vertex u_2 be the vertex which is adjacent to $u_3, u_4, \dots u_{n-1}$ with each degree n−1 respectively. The contributions of the edges Concerning vertex u_2 to the first Zagreb index of $B(K_{n,}K_n)$ can be calculated as follows:

$$[deg(u_2)+deg(u_3)]+[deg(u_2)+deg(u_4)]+\cdots+[deg(u_2)+deg(u_{n-1})]+[deg(u_2)+deg(u_n)]=2(n-1)(n-3)+(2n-1) \quad (21)$$

The impact of the edges concerning the vertex u_3 to the first Zagreb index of $B(K_{n,}K_n)$are calculated using a similar approach to vertex u_2.

$$[deg(u_3)+deg(u_4)]+[deg(u_3)+deg(u_5)]+\cdots+[deg(u_3)+deg(u_{n-1})]+[deg(u_3)+deg(u_n)]=2(n-1)(n-4)+(2n-1) \quad (22)$$

For the vertex u_{n-2}, the contributions of the edges with respect to vertex u_{n-2} to the 1stZagreb index of $B(K_{n,}K_n)$ are calculated as

$$[(n-1)+(n-1)]+[(n-1)+n] = 2(n-1)+(2n-1) \quad (23)$$

For vertex u_{n-1}, the contributions of the edges concerning vertex u_{n-1} to the 1stZagreb index of $B(K_{n,}K_n)$ are calculated as;

$$[deg(u_{n-1})+deg(u_n) = n-1+n= 2n-1 \quad (24)$$

For the vertex u_n, the contributions of the edges concerning vertex un to the first Zagreb index $B(K_{n,}K_n)$are calculated as;

$$[deg(u_n)+deg(v_1)] = n+n = 2n \quad (25)$$

For the vertex v_1, the contributions of the edges concerning vertex v_1 to the first Zagreb index of $B(K_{n,}K_n)$are calculated as;

$$[deg(v_1)+deg(v_2)]+[deg(v_1)+deg(v_3)]+\cdots+[deg(u_1)+deg(v_{n-1})]+[deg(v_1)+deg(v_n)] = 2(n-1)(n-2)+(2n-1) \quad (26)$$

For a vertex v_2 ,the contributions of the edges with respect to vertex $v_2$to the first Zagreb index of $B(K_{n,}K_n)$are calculated as;

$$[deg(v_2)+deg(v_3)]+[deg(v_2)+deg(v_4)]+\cdots+[deg(v_2)+deg(v_{n-1})]+[deg(v_2)+deg(v_n)] = 2(n-1)(n-3)+(2n-1) \quad (27)$$

For a vertex v_{n-1}, the contributions of the edges with respect to vertex v_{n-1} to the first Zagreb index of $B(K_{n,}K_n)$ are calculated as;

$$[deg(v_{n-1})+deg(v_n)]=n-1+n = 2n-1 \quad (28)$$

$$M_1[B(K_{n,}K_n)] = 2\{2(n-1)[(n-2)+(n-3)+\ldots+3+2+1]\}+2(n-1)(2n-1)+2n \quad (29)$$

$$M_2[B(K_{n,}K_n))] = 2(n-1)[n^2-n+1]+2n, n\geq 3 \quad (30)$$

IV.v. Illustration:

B (K5 , K5) :

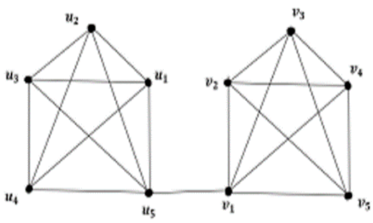

Fig. 5.

$$M_1[B(K_{n,}K_n)] = 2(n-1)[n^2 - n + 1] + 2n \quad (31)$$

$$M_1[B(K_{5,}K_5)] = 2(5-1)[5^2 - 5 + 1] + 2 * 5 = 178 \quad (32)$$

For B (K_5, K_5), $M_1[B(K_5, K_5)]$ can be calculated manually

Table : 3

	u_1	u_2	u_3	u_4	u_5	v_1	v_2	v_3	v_4	v_5	$M_1[B(K_{5,}K_5)]$
u_1	*	8	8	8	9						33
u_2			8	8	9						25
u_3				8	9						17
u_4					9						9
u_5						10					10
v_1							9	9	9	9	36
v_2								8	8	8	24
v_3									8	8	16
v_4										8	8
v_5										*	
											178

The Topological index of $M_1[B(K_5, K_5)]$ calculated both methods follow the same underlying principles and use the same formula, they should produce identical results.

IV.vi. Second Zagreb index of B(K_n, K_n)

$$M_2[B(K_n, K_n)]=2\{[(n-2)(n-1)^2 + n(n-1)] + [(n-3)(n-1)^2 + n(n-1)] + [(n-4)(n-1)^2 + n(n-1)] + \cdots + [1.(n-1)^2] + n(n-1)\} + n^2 \quad (33)$$

$$= 2(n-1)^2\{(n-2) + (n-3) + \cdots + 3 + 2 + 1\} + 2n(n-1)(n-1) + n^2 \quad (34)$$

$$= 2(n-1)^2[(n-2)(n-1)/2] + 2n(n-1)^2 + n^2 \quad (35)$$

$$M_2[B(K_n, K_n)] = (n-1)^2[n^2 - n + 2] + n^2, \; n \geq 3 \quad (36)$$

IV.vii. Illustration:

$$M_2[B(K_n, K_n)] = (n-1)^2[n^2 - n + 2] + n^2, \; n \geq 3 \quad (37)$$

Here $n = 5$, $M_2[B(K_5, K_5)] = (5-1)^2[5^2 - 5 + 2] + 5^2 = 377$ (38)

For $M_2[B(K_5, K_5)]$ can be calculated manually

Table : 4

	u_1	u_2	u_3	u4	u_5	v_1	v_2	v_3	v_4	v_5	M_2[B (K_5, K_5)]
u_1	*	16	16	16	20						68
u_2			16	16	20						52
u_3				16	20						36
u_4					20						20
u_5						25					25
v_1							20	20	20	20	80
v_2								16	16	16	48
v_3									16	16	32
v_4										16	16
v_5										*	
											377

The Topological index $M_2(\mathrm{B}(\mathrm{K}_5,\mathrm{K}_5))$calculated manually and through the formula are the same.

IV.viii. Result

For the regular graph $G(p,q)$, at which p denotes vertices number and q signifies number of edges, $first\ Zagreb\ index M_1(G)$ will be equivalent to 2qr, and the second Zagreb index is $M_2(G)$ equal to qr^2.

IV.ix. Illustration

For a Petersen graph G, p = 10, q = 15, r = 3

$$M_1(G) = \sum_{\mathbf{u,v} \in \mathbf{E}(G)} [\boldsymbol{d(u)} + \boldsymbol{d(v)}] = 2qr = 90 \quad (39)$$

$$M_2(G) = \sum_{\mathbf{u,v} \in \mathbf{E}(G)} [\boldsymbol{d(u)}.\boldsymbol{d(v)}] = qr^2 = 135 \quad (40)$$

In the Petersen graph, each vertex has a degree of 3, $M_1(G)$and $M_2(G)$ are calculated manually:

Table : 5

	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8	v_9	v_{10}	$M_1(G)$
v_1			6	6		6					18
v_2				6	6		6				18
v_3					6		6				12
v_4									6		6
v_5										6	6
v_6							6			6	12
v_7								6			6
v_8									6		6
v_9										6	6
v_{10}											
$M_1(G)$											90

$M_2(G)$ are calculated manually:

Table : 6

	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8	v_9	v_{10}	$M_2(G)$
v_1			9	9		9					27
v_2				9	9		9				27
v_3					9		9				18
v_4									9		9
v_5										9	9
v_6							9			9	18
v_7								9			9
v_8									9		9
v_9										9	9
v_{10}											
$M_2(G)$											135

The Topological indices $M_1(G)$ and $M_2(G)$, manually and through the formula, both methods should yield the same results.

IV.x. Theorem

Let G be a Fan graph, $F_{n+1}(= P_n + K_1)$, $n \geq 3$. Attach k pendant vertices with the full degree vertex u of G, The resulting graph is represented by G_1. Then

$$M_1(G_1) = k(k + 2n + 1) + n(n + 9) - 10 \qquad (41)$$

and

$$M_2(G_1) = k(k + 4n - 2) + n(3n + 7) - 15 \qquad (42)$$

Proof:

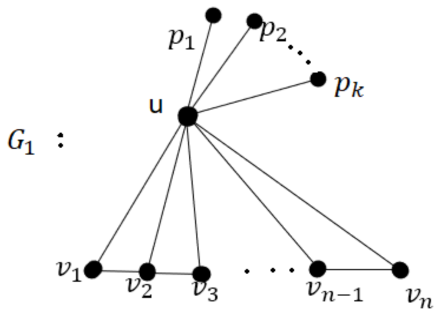

Fig. 6.

Consider G as F_{n+1} having $v_1, v_2, \ldots, v_{n-1}, v_n$ as its vertices and u be the only one full degree vertex in G. (ie) $\Delta(G) = deg_G(u) = n$.

Attach k-pendant vertices at u and those points are labeled as $p_1, p_2, \ldots, p_k$. Then the resultant graph is denoted by G_1.Then $\Delta(G_1) = \deg_{G_1}(u) = n + k$.

The 1st Zagreb index of the graph is computed as

$$M_1(G_1) = k(k + 2n + 1) + n(n + 9) - 10 \quad (43)$$

$$M_1(G_1) = k(k + 2n + 1) + n(n + 9) - 10, n \geq 3 \quad (44)$$

The second Zagreb index of graph is computed as

$$M_2(G_1) = k(k + 4n - 2) + n(3n + 7) - 15, n \geq 3 \quad (45)$$

IV.xi. Illustration

Let $G = F_5$. Attach five pendant vertices with u. The resultant graph is G_1.

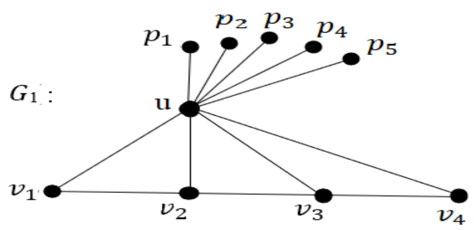

Fig. 7.

$$M_1(G_1) = k(k + 2n + 1) + n(n + 9) - 10 \quad (46)$$

Here n = 4, k = 5.

$$M_1(G_1) = 5(14) + 4(13) - 10 = 112 \quad (47)$$

$$M_2(G_1) = k(k + 4n - 2) + n(3n + 7) - 15 \quad (48)$$

Here n = 4, k = 5

$$M_2(G_1) = 5(19) + 4(19) - 15 = 156 \quad (49)$$

$M_1(G_1)$ is calculated manually:

Table : 7

	v_1	v_2	v_3	v_4	u	p_1	p_2	p_3	p_4	p5	$M_1(G1)$
v_1		5									5
v_2			6								6
v_3				5							5
v_4											
u	11	12	12	11		10	10	10	10	10	96
	Total										112

$M_2(G_1)$ is calculated manually:

Table : 8

	v_1	v_2	v_3	v_4	u	p_1	p_2	p_3	p_4	p5	$M_2(G1)$
v_1		6									6
v_2			9								9
v_3				6							6
v_4											
u	18	27	27	18		9	9	9	9	9	135
	Total										156

The Topological indices $M_1(G_1)$ and $M_2(G_1)$ calculated manually and through the formula are the same.

V. Conclusion

This article has successfully derived expressions for the first and second Zagreb indices of the Thorn graph from path Pn, and has also presented calculations for the first and second Zagreb indices of Barbell graph B (K_n, K_n) and Fan graph F_n. These findings not only contribute to our understanding of graph theory but also pave the way for further exploration across various families of graphs in different directions. The results of this research indicate numerous possibilities for extending the study to encompass additional graph families and explore diverse research trajectories. This opens up new avenues for investigation and potential applications in various branches of Engineering. Overall, the insights gained from this study have the potential to make significant contributions to the field of graph theory and its practical applications, highlighting the importance of continued research and exploration in this area.

Conflict of Interest

The author declares that there was no conflict of interest regarding this paper.

References

I. Akhtar, S., Imran, M., Gao, W. and Farahani, M. R., : 'On topological indices of honeycomb networks of graphene networks. Hacet.' *J. Math. Stat.* 2018, 47(1) 19-35. 10.15672/HJMS.2017.464

II. Balaban A. T., Motoc I., Bonchev D., Mekenyan O., : 'Topological indices for structure activity correlations.' Topics Curr Chem,1983, 114:21-55

III. Das K. C., : 'On comparing Zagreb indices of graphs.' MATCH commun math comput Chem, 2010, 63: 433-440.

IV. Das, K. C, : 'Maximizing the sum of the squares of the degrees of a graph.' Discrete Math., 285, (2004), 57–66.

V. Das, K. C., Gutman, I. and Zhou, B., : 'New upper bounds on Zagreb indices.' *J. Math. Chem.*, 46, (2009), 514–521.

VI. De, N., : 'The vertex Zagreb index of some graph operations.' Carpathian Math. Publ. 2016, 8(2), 215-223.

VII. Eliasi M, Iranmanesh A, Gutman I., : 'Multiplicative versions of first Zagreb index., MATCH Commun Math comput chem, 2012, 68:217-230.

VIII. Farahani, M. R. and Kanna, M. R. (2015), : 'Generalized Zagreb Index of V-Phenylenic Nanotubes and Nanotori.' *Journal of Chemical and Pharmaceutical Research*, 7(11), 241-245.

IX. Gutman I., : 'Multiplicative Zagreb indices of trees. Bull Soc Math Banja luka, 2011, 18:17-23.

X. Gutman I., Das K. C., : 'The first Zagreb index 30 years after.' MATCH Commun Math Comput Chem, 2004, 50: 83-92.

XI. Gutman, I., : 'Distance in thorny graph.' Publ. Inst. Math Beograd 63 (1998) 31-36.

XII. Gutman I., : 'Trinajstic, N.G.T and molecular orbitals totalπ −electron energy of alternant hydrocarbons.' chem. phys. Lett, 1972,17, 535-535.

XIII. Gupta C. K., Lokesha,v. Shwetha B. S. and Ranjini.P. S., : 'Graph operations on the symmetric division deg index of ghs.' *Palestine. J. Math*. 2017, 6(1), 280-286.

XIV. Khalifcha, M. H., : 'Yousefi-Azaria, H., Ashrafi, A. R., : 'The first and second Zagreb indices of some graph operations.' Discret. Appl. Math. 2009, 157, 804-811.

XV. Kexiang XU, : 'The Zagreb indices of graphs with a given clique number.' Applied Mathematics Letters , Volume 6, Issue 11 (2011), Pages1026-1030.

XVI. Kinkar Ch. Das, Kexiang XU, Junki Nam., : 'Zagreb indices of graphs' Frontiers of Mathematics 2015.

XVII. K. C. Das, I. Gutman and B. Horoldagva (2012). : 'Comparison between Zagreb indices and Zagreb coindices.' MATCH Commun. Math. Comput. Chem., 68, pp.189 – 198

XVIII. K. C. Das, I. Gutman and B. Zhou (2009). : 'New Upper Bounds on Zagreb Indices.' *J. Math. Chem*.,46, pp. 514 - 521.

XIX. Lokesha, V., Deepika, T., : 'Symmetric division deg index of tricyclic tetracyclic graphs.' *Int. J. Sci. Eng*. Res.2016 ,7(5), 53-55.

XX. R. Pradeep Kumar, Soner Nandappa D., M. R. Rajesh Kanna., : 'Redefined Zagreb, Randic, harmonic and GA indices of graphene.' *International Journal of Mathematical Analysis* Vol.11, (2017), no.10, 493- 502. 10.12988/ijma.2017.7454

XXI. Sridhara G., Kanna , M. R. R. and Indumathi, R. S. : 'Computation of topological indices of graphene.' *J. Nanometrial* (2015) ID 969348.

XXII. K. Thilagavathi and A. Sangeetha Devi, : 'Harmonious coloring and Proceedings of International Conference on Mathematical and Computer Science.' Department of Mathematics Loyola College Chennai. (ICMCS 2009) Page no 50-52.

XXIII. F. Harary, : 'Graph Theory.' Addision Wesley, Reading Mass (1972).

XXIV. Yan, Z., Liu, H. and Liu, H., : 'Sharp bounds for the second Zagreb index of unicyclic graphs.' *J. Math. Chem*., 42, (2007), 565–574. 10.1007/s10910-006-9132-7

XXV. Zhou, B. and Gutman, I., : 'Further properties of Zagreb indices.' MATCH Commun. Math. Comput. Chem., 4, (2005),233–239.