Computation of Zagreb Indices on k-Gamma Graph

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Abstract-In this paper, we newly define Gamma Graph (Γ), k-Gamma Graph (Γ_k) for every $k \geq 2$ and junction vertex by using elementary graph operation. Another important graph called Swastika Graph (SW) is also defined. Additionally we shall give generalization result for n-Swastika (SW_n) for any $n \geq 1$. We shall derive Line Graph for k-Gamma Graph (Γ_k) and n-Swastika Graph(SW_n). Then we shall calculate some of topological indices namely Third Zagreb Index, First and Second Multiple Zagreb index, First and Second Zagreb polynomials for k-Gamma(Γ_k), k-Gamma Line Graph(Γ_k) where $k \geq 2$, n-Swastika Graph (SW_n) and n-Swastika Line Graph $L(SW_n)$ for any $n \geq 1$.

Index Terms-k-Gamma Graph($\boldsymbol{\Gamma_k}$), Swastika Graph($\boldsymbol{SW_n}$), Junction Vertex, Zagreb Indices.

1. INTRODUCTION

In Chemical Graph Theory, molecular graphs represent the molecular structure of a certain chemical compound and it is associated with different properties which are found in molecular graph connectivity with the corresponding chemical compounds.

A graph recognizes the easiest way of approach to understand its excellence, by means of numeric constant. Topological descriptors are based on the graph impression of the molecule and can also encode chemical information concerning atom type and bond multiplicity. The molecular descriptors is the final result of logic and the mathematical procedure which convert the chemical information fixed with in a symbolic representation of molecule in to a useful number.

The molecular structure of a drug can be considered as graph by suppressing the hydrogen atoms. The topological index of molecular graph is helpful to find properties of the drug. The drugs can be classified by using its properties. Some of the methods used for classification are Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Property Relation (QSPR) and Fuzzy Lattice Neural Networks (FLNN) etc., Thus, the topological indices are very essential tool in the field of Nanotechnology, Drug Discovery, Computer Networks, Designing Tool, Information Technology etc.,

The current researches about topological descriptors are used to qualify different chemical properties of drugs. Since, topological indices on special kinds of various graphs have been found previously which is based on the degrees of vertex and edge respectively. In this paper, we motivated to investigate a new set of graphs such as k-Gamma Graph, k-Gamma Line

Graph, Swastika Graph, n-Swastika Graph, n-Swastika Line Graph. It brings our curiosity to find some chemically interesting graphs.

2. PRELIMINARY RESULTS

Some of the well-known topological indices are defined for the simple graph G.

Definition 2.1. The Third Zagreb index [3] of a graph G, denoted by $M_3(G)$, is defined as

$$M_3(G) = \sum_{uv \in E(G)} |d(u) - d(v)| \qquad (1)$$

Definition 2.2. The First Multiple Zagreb index [5] of a graph G, denoted by $PM_1(G)$, is defined as

$$PM_1(G) = \prod_{uv \in E(G)} [d(u) + d(v)] \qquad (2)$$

Definition 2.3. The Second Multiple Zagreb index [5] of a graph G, denoted by $PM_2(G)$, is defined as

$$PM_2(G) = \prod_{uv \in E(G)} d(u)d(v) \qquad (3)$$

Definition 2.4. The First Zagreb Polynomial index [6] of a graph G, denoted by $M_1(G, x)$, is defined as

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

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Definition 2.5. The Second Zagreb Polynomial index [6] of a graph G, denoted by $M_2(G,x)$, is defined as

$$M_2(G,x) = \sum_{uv \in E(G)} x^{d(u)d(v)} \qquad (5)$$

where $d(u)$ and $d(v)$ represent the degrees of vertices of u and v in the graph G respectively.

Definition 2.6. The Line Graph [1,4,7] of a graph G is the graph $L(G)$ with the edges G as its vertices, and where two edges of G are adjacent in $L(G)$ if and if they are incident in G.

Definition 2.7. An Edge Contraction [9] is an operation which removes an edge from a graph while simultaneously merging the two vertices that it is previously joined.

The above definitions are the basic definitions which are useful in subsequent sections. The computation of topological indices of various graph families may be referred in [1, 4, 6 and 8].

3. SOME ZABREB INDICES ON k-GAMMA GRAPH AND ITS LINE GRAPH

In this section, we shall used to calculate the some of the topological indices which are defined earlier for our newly defined k- Gamma Graph and its Line Graph.

Definition 3.1. An undirected graph having three vertices and its two adjacent edges, in which edges are perpendicular is called Gamma Graph. It is denoted by Γ.
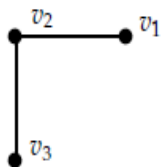
Fig. 3.1. Gamma Graph

From the above Fig.3.1. we have, v_1 = starting vertex, v_2 = incident vertex, v_3 = end vertex. Then v_1 and v_3 are pendant vertices and deg $v_2 = 2$.

Example 3.1. The Bent molecule like Silicon-di-Oxide (SiO_2) is a Gamma Graph. It helps to find the antibacterial activity.

Definition 3.2. If k- number of Gamma Graphs shares a common vertex (starting vertex), then the graph is said to be k- Gamma Graph and is denoted by Γ_k, where $k \geq 2$.

Definition 3.3. The common vertex in k- Gamma Graph is called Junction vertex. The angles between any two adjacent Gamma Graphs are equal. If θ is the angle between any two adjacency Gamma Graphs then $\theta = \frac{360}{k}$, where $k \geq 2$. The vertex set and edge set of k-Gamma Graph Γ_k is given by $|V| = 2k + 1$ and $|E| = 2k$.

Theorem 3.1. *Let Γ_k be the k- Gamma Graph, where $k \geq 2$. Then its topological indices are given by*
(1) $M_3(\Gamma_k) = 2E_2(L(\Gamma_k))$
(2) $PM_1(\Gamma_k) = 3^k(2 + k)^k$
(3) $M_2(\Gamma_k) = E(\Gamma_k)^{E(\Gamma_k)}$
(4) $M_1(\Gamma_k, x) = kx^2(x + x^k)$
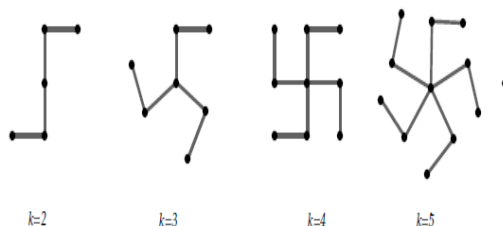(5) $M_2(\Gamma_k, x) = k(x^2 + x^{2k})$

Proof.

Fig 3.2. k- Gamma Graph (Γ_k)

Consider the k-Gamma Graph(Γ_k), for all $k \geq 2$. From the Fig. 3.2., the number of vertices and edges of Γ_k is given by $2k + 1$ and $2k$ respectively. Then the vertex set can be divided into k vertices of degree one, k vertices of degree two, and one vertex of degree k. The edge set $E(\Gamma_k)$ can be divided into two edge partitions based on the degrees of its end vertices. The first partition of edges $E_1(\Gamma_k)$ contains k edges uv, where $d_{\Gamma_k}(u) = 1, d_{\Gamma_k}(v) = 2$ and the second partition of edges $E_2(\Gamma_k)$ contains k edges uv, where $d_{\Gamma_k}(u) = 2, d_{\Gamma_k}(v) = k$. Here $d_{\Gamma_k}(u)$ and $d_{\Gamma_k}(v)$ are denoted as the degrees of its end vertices respectively. Then, we shall obtain our required results for the graph (Γ_k) as follows,
(1) The Third Zagreb index

$$M_3(\Gamma_k) = \sum_{uv \in E(\Gamma_k)} |d(u) - d(v)|$$
$$= k(k - 1)$$
$$= 2E_2(L(\Gamma_k))$$

(2) The First Multiple Zagreb index

$$PM_1(\Gamma_k) = \prod_{uv \in E(\Gamma_k)} [d(u) + d(v)]$$
$$= 3^k(2 + k)^k$$

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(3) The Second Multiple Zagreb index
$$PM_2(\Gamma_k) = \prod_{uv \in E(\Gamma_k)} d(u)d(v)$$
$$= (2)^k (2k)^k$$
$$= (2k)^{2k}$$
$$= E(\Gamma_k)^{E(\Gamma_k)}$$

(4) The First Zagreb Polynomial index
$$M_1(\Gamma_k, x) = \sum_{uv \in E(\Gamma_k)} x^{[d(u)+d(v)]}$$
$$= kx^2(x + x^k)$$

(5) The Second Zagreb Polynomial index
$$M_1(\Gamma_k, x) = \sum_{uv \in E(\Gamma_k)} x^{d(u)d(v)}$$
$$= k(x^2 + x^{2k})$$

Hence (1) – (5) holds. This completes the proof.

Theorem 3.2. *Let (Γ_k) be the Line Graph of k-Gamma Graph, where $k \geq 2$. Then its topological indices are given by*
(1) $M_3 L(\Gamma_k) = 2E_2(L(\Gamma_k))$
(2) $PM_1 L(\Gamma_k) = (1 + k)^k (2k)^{\frac{k^2-k}{2}}$
(3) $PM_2 L(\Gamma_k) = K^{E(L(\Gamma_k))}$
(4) $M_1 L(\Gamma_k, x) = E_1(L(\Gamma_k))x^{(1+k)} + E_2(L(\Gamma_k))x^{2k}$
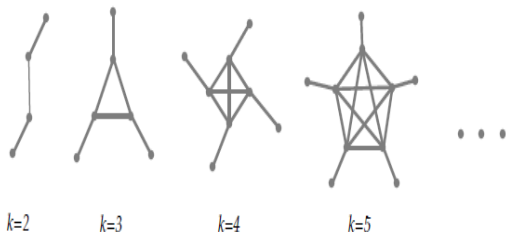(5) $M_2 L(\Gamma_k, x) = E_1(L(\Gamma_k))x^k + E_2(L(\Gamma_k))x^{k^2}$
Proof.

Fig. 3.3. Line Graph of k- Gamma Graph $L(\Gamma_k)$

Consider the Line graph of k- Gamma Graph $L(\Gamma_k)$, for any $k \geq 2$. From the Fig. 3.3., the number of vertices and edges of $L(\Gamma_k)$ is given by $2k$ vertices and $\frac{k^2+k}{2}$ edges. Then the vertex set can be divided into k vertices of degree one and k vertices of degree k. Then, the edge set $E(L(\Gamma_k))$ can be divided into two edge partitions based on the degrees of its end vertices. The first partition of edges $E_1(L(\Gamma_k))$ contains k edges uv, where $d_{L(\Gamma_k)}(u) = 1$, $d_{L(\Gamma_k)}(v) = k$. and the second partition of edges $E_2(L(\Gamma_k))$ contains $\frac{k^2-k}{2}$ edges uv, where $d_{L(\Gamma_k)}(u) = k$, $d_{L(\Gamma_k)}(v) = k$ Here $d_{L(\Gamma_k)}(u)$ and $d_{L(\Gamma_k)}(v)$ are denoted as the degrees of its end vertices respectively. Now, we shall obtain our required results for the graph $L(\Gamma_k)$ as follows,
(1) The Third Zagreb index

$$M_3(L(\Gamma_k)) = \sum_{uv \in E(L(\Gamma_k))} |d(u) - d(v)|$$
$$= k|k - 1| + \frac{k^2 - k}{2}|k - k|$$
$$= k(k - 1)$$
$$= 2E_2(L(\Gamma_k))$$

(2) The First Multiple Zagreb index
$$PM_1(L(\Gamma_k)) = \prod_{uv \in E(L(\Gamma_k))} [d(u) + d(v)]$$
$$= (1 + k)^k (2k)^{\frac{k^2-k}{2}}$$

(3) The Second Multiple Zagreb index
$$PM_2(L(\Gamma_k)) = \prod_{uv \in E(L(\Gamma_k))} d(u)d(v)$$
$$= k^{\frac{k^2+k}{2}}$$
$$= k^{E(L(\Gamma_k))}$$

(4) The First Zagreb Polynomial index
$$M_1(L(\Gamma_k)) = \sum_{uv \in E(L(\Gamma_k))} x^{[d(u)+d(v)]}$$
$$= kx^{1+k} + \frac{k^2 - k}{2}x^{2k}$$
$$= E_1(L(\Gamma_k))x^{(1+k)} + E_2(L(\Gamma_k))x^{2k}$$

(5) The Second Zagreb Polynomial index
$$M_2(L(\Gamma_k)) = \sum_{uv \in E(L(\Gamma_k))} x^{d(u)d(v)}$$
$$= kx^k + \frac{k^2 - k}{2}x^{k^2}$$
$$= E_1(L(\Gamma_k))x^k + E_2(L(\Gamma_k))x^{k^2}$$

Hence (1)-(5) holds. This completes the proof.

4. SOME ZAGREB INDICES ON SWASTIKA GRAPH AND ITS LINE GRAPH

In this section, we can calculate some of the topological indices which are defined earlier for our newly defined n- Swastika Graph (SW_n) and its Line Graph.

Definition 4.1. The four number of Gamma Graphs are joined exactly at their common vertex (starting vertex) is said to be Tetra Gamma Graph or Swastika Graph (Γ_4). The degree of Central or Junction vertex Swastika Graph ($SW(G)$) is four.

Definition 4.2. The n- number of Swastika Graph are combined by the Edge Contraction principle [9] at the pendant vertex of each Swastika Graph. The graph

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obtained is called n- Swastika Graph (SW_n) for $n \geq 1$. It contains $(7n + 2)$ vertices and $(7n + 1)$ edges.

Theorem 4.1. *Let (SW_n) be the n- Swastika Graph, where $n \geq 1$. Then its topological indices are given by*
(1) $M_3(SW_n) = 2(5n + 1)$
(2) $PM_1(SW_n) = 3^{2V(L(SW_n))}2^{2(V((SW_n))-2)}$
(3) $PM_2(SW_n) = 2^{16n}$
(4) $M_1(SW_n, x) = x^3\left[2n\left(2x^3 + \frac{x}{2} + 1\right) + (2 - x)\right]$
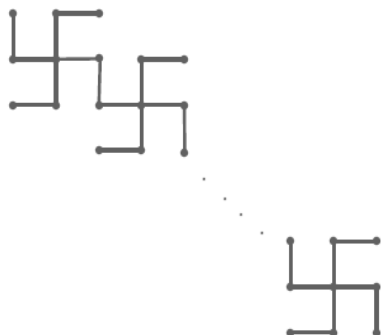(5) $M_2(SW_n, x) = x^2[n(2 + x^2 + 4x^6) + (2 - x^2)]$

Proof.

Fig.4.1. n- Swastika Graph (SW_n)

Consider the Swastika Graph SW_n, where $n \geq 1$. From the Fig.4.1, we have $(7n + 2)$ vertices and $(7n + 1)$ edges respectively. Then the vertex set, we can see that there are three vertex partitions such as, $(2n + 1)$ vertices of degree one, n vertices of degree four and 4n vertices of degree two. The edge set $E(SW_n)$ can be divided into three edge partitions based on the degrees of its end vertices. The first partition of edges $E_1(SW_n)$ contains $(2n + 2)$ edges uv, where $d_{SW_n}(u) = 1$, $d_{SW_n}(v) = 2$. The second partition of edges $E_2(SW_n)$ contains $(n - 1)$ edges uv, where $d_{SW_n}(u) = 2$, $d_{SW_n}(v) = 2$ and the third partition of edges $E_3(SW_n)$ contains $4n$ edges uv, where $d_{SW_n}(u) = 2$, $d_{SW_n}(v) = 4$. Here $d_{SW_n}(u)$ and $d_{SW_n}(v)$ are denoted as the degrees of the end vertices respectively.

Then we shall obtain our required results for the graph SW_n as follows,
(1) The Third Zagreb index
$$M_3(SW_n) = \sum_{uv \in E(SW_n)} |d(u) - d(v)|$$
$$= 2(5n + 1)$$
(2) The First Multiple Zagreb index
$$PM_1(SW_n) = \prod_{uv \in E(SW_n)} [d(u) + d(v)]$$
$$= 3^{(2n+2)}4^{(n-1)}6^{4n}$$

$$= 3^{2(3n+1)}2^{2(3n-1)}$$
$$= 3^{2V(L(SW_n))}2^{2(V((SW_n))-2)}$$
(3) The Second Multiple Zagreb index
$$PM_2(SW_n) = \prod_{uv \in E(SW_n)} d(u)d(v)$$
$$= 2^{(2n+2)}4^{(n-1)}8^{4n}$$
$$= 2^{16n}$$
(4) The First Zagreb Polynomial index
$$M_1(SW_n, x) = \sum_{uv \in E(SW_n)} x^{[d(u)+d(v)]}$$
$$= 2(n + 1)x^3 + (n - 1)x^4 + 4nx^6$$
$$= x^3\left[2n\left(2x^3 + \frac{x}{2} + 1\right) + (2 - x)\right]$$
(5) The Second Zagreb Polynomial index
$$M_2(SW_n, x) = \sum_{uv \in E(SW_n)} x^{d(u)d(v)}$$
$$= 2(n + 1)x^2 + (n - 1)x^4 + 4nx^8$$
$$= x^2[n(2 + x^2 + 4x^6) + (2 - x^2)]$$

Hence (1)-(5) holds. This completes the proof.

Theorem 4.1. *Let (SW_n) be the Line Graph of n-Swastika Graph for every integer n. Then its topological indices are given by*
(1) $M_3(L(SW_n)) = 12n$
(2) $PM_1(L(SW_n)) = 5^{4n}8^{6n}$
(3) $PM_2(L(SW_n)) = 2^{32n}$
(4) $M_1(L(SW_n, x)) = 2nx^5(3x^3 + 2)$
(5) $M_2(L(SW_n, x)) = 2nx^4(3x^{12} + 2)$
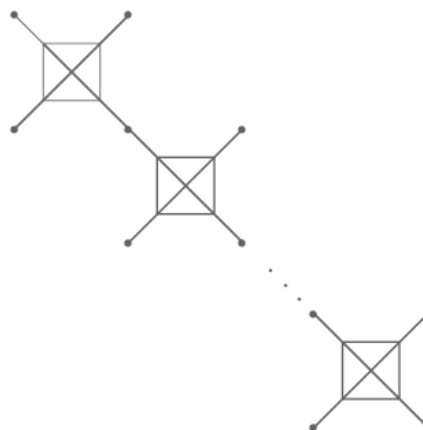
Proof.

Fig 4.2. Line Graph of n- Swastika Graph $L(SW_n)$

Consider the Line graph of Swastika Graph $L(SW_n)$, for all positive integers $n \geq 1$. From the Fig. 4.2., we get $(7n + 1)$ vertices and $(10n)$ edges. From the above Fig 4.2., the vertex set can be partitioned into $(3n + 1)$ vertices of degree one and $4n$ vertices of degree four. Then, the edge set $E(L(SW_n))$ can be divided into two edge partitions based on the degrees of its end vertices. The first edge partition

$E_1(L(SW_n))$ contains $4n$ edges uv, where $d_{L(SW_n)}(u) = 1$, $d_{L(SW_n)}(v) = 4$ and the second edge partition of edges $E_2(L(SW_n))$ contains $6n$ edges uv, where $d_{L(SW_n)}(u) = 4$, $d_{L(SW_n)}(v) = 4$. Here $d_{L(SW_n)}(u)$ and $d_{L(SW_n)}(v)$ are denoted as the degrees of the end vertices respectively. Next, we shall obtain our required results for the graph $L(SW_n)$ as follows,

(1) The Third Zagreb index
$$M_3(L(SW_n)) = \sum_{uv \in E(L(SW_n))} |d(u) - d(v)|$$
$$= 12n$$

(2) The First Multiple Zagreb index
$$PM_1(L(SW_n)) = \prod_{uv \in E(L(SW_n))} [d(u) + d(v)]$$
$$= 5^{4n} 8^{6n}$$

(3) The Second Multiple Zagreb index
$$PM_2(L(SW_n)) = \prod_{uv \in E(L(SW_n))} d(u)d(v)$$
$$= (4)^{4n}(16)^{6n}$$
$$= 2^{32n}$$

(4) The First Zagreb Polynomial index
$$M_1(L(SW_n, x)) = \sum_{uv \in E(L(SW_n))} x^{[d(u)+d(v)]}$$
$$= 4nx^5 + 6nx^8$$
$$= 2nx^5(3x^3 + 2)$$

(5) The Second Zagreb Polynomial index
$$M_2(L(SW_n, x)) = \sum_{uv \in E(L(SW_n))} x^{d(u)d(v)}$$
$$= 4nx^4 + 6nx^{16}$$
$$= 2nx^4(3x^{12} + 2)$$

Hence (1)-(5) holds. This completes the proof.

Remark 4.1. For any k- Gamma Graph, the degree of the vertex is always less than or equal to k i.e. $d(u) \le k$.

5. CONCLUSION

In this paper, we calculated some of the Zagreb types of topological indices for our newly defined k- Gamma Graph (Γ_k), k- Gamma Line Graph $L(\Gamma_k)$, n- Swastika Graph (SW_n) and n- Swastika Line Graph $L(SW_n)$. The properties of certain newly defined molecular graphs will be helpful for further studies in drug discovery system.

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