

# Computation of M-Polynomial and Topological Indices of Some Cycle Related Graphs

S. Rajeswari and N. Parvathi\*

**Abstract**—Topological indices provide valuable insights into various physical, chemical, and biological properties of molecules. Topological indices are correlated with various physicochemical properties of molecules, including boiling point, melting point, stability, distortion, strain energy, and ultimately biological activity. QSAR models utilize statistical techniques to establish quantitative relationships between these descriptors and the observed biological activity of compounds. By analyzing a dataset of molecules with known biological activities and their corresponding topological indices, QSAR models can predict the activity of new compounds based solely on their structural features. The M-polynomial provides information about the closed form of topological indices based on the degrees of the molecular graph. In this paper, we compute the M-polynomial of some families of graphs, tadpole, helm, gear, friendship, and fan graph. Further, we compute various topological indices for the above-mentioned graph in M-polynomial.

**Index Terms**—Chemical graph theory, Topological indices, M-polynomial, Tadpole, Helm, Gear, Fan, Friendship graph.

## I. INTRODUCTION

GRAPH theory has widespread applications across various disciplines, owing to its ability to model relationships and structures such as physics, biology, operation research, optimization theory, statistical mechanics, computer science, engineering, and even chemistry. In each field, graph theory provides powerful tools for modeling, analyzing, and solving a wide range of problems, making it a versatile and indispensable area of study. One of the most important sub-fields of mathematical chemistry is chemical graph theory which originated by Ante Graovac, Milan Randić, Alexander Balaban, Haruo Hosoya, Nenad Trinajstić, and Ivan Gutman. Chemical graph theory is indeed a field within graph theory that deals specifically with the study of molecular graphs[1]. In this field, chemical structures are represented using graphs, where atoms are represented as vertices and chemical bonds as edges. By applying concepts and techniques from graph theory, researchers in chemical graph theory aim to understand various properties of molecules, such as their connectivity, symmetry, stability, and reactivity. This interdisciplinary approach is fundamental in chemistry, biochemistry, and computational chemistry for understanding molecular behavior and designing new compounds with desired properties. Molecular descriptors are fundamental

in Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) modeling. These descriptors are numerical representations of molecular properties that help establish relationships between the structure of chemical compounds and their various physical, chemical, and biological activities. The first known application to find the physical properties of a chemical structure in 1947 is often attributed to the development of computational quantum chemistry methods[2].

Molecular descriptors are quantitative representations of molecular structures that encode various physicochemical properties or structural features of molecules. These descriptors are crucial in computational chemistry, drug design, and cheminformatics. It depends on the distance between the two vertices, the eigenvalues of the graph, the vertex of the graph, etc. In their study, Gao et al. might have investigated how topological indices can be utilized to understand aspects such as the molecular size, shape, branching patterns, or other structural features of nanostar dendrimers[3]. These indices could offer valuable information for predicting various properties of nanostar dendrimers, including solubility, stability, reactivity, or biological activity. In chemical graph theory, molecules are often represented as graphs, where atoms are represented by vertices (nodes), and chemical bonds between atoms are represented by edges connecting these vertices. The topological index used for a molecular graph is indeed a numerical representation derived from mathematical and logical operations applied to the structural features of a molecule. These indices are utilized in quantitative structure-activity relationship (QSAR) studies, molecular modeling, and cheminformatics to correlate molecular structure with various properties and activities. These indices provide a quantitative representation of the molecular structure, capturing physicochemical properties that are relevant for various applications in chemistry, including drug design, material science, and environmental studies. The topological descriptors are derived from hydrogen-suppressed molecular graphs. In cheminformatics, quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) are widely used to study the relationship between the structure of chemical compounds and their biological activity or physical properties, respectively. Mathematical modeling plays a significant role in analyzing major concepts in chemistry. The general form of degree-based topological indices of a graph can vary depending on the specific index being considered. However, many degree-based topological indices can be expressed in terms of the degrees of vertices in the graph

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$$TI(\Omega) = \sum_{gh \in E(\Omega)} t(d_{\Omega}(\mu_g)d_{\Omega}(\mu_h))$$

where  $t = t(g, h)$  is a function appropriately chosen for the computation.

Mathematical chemistry has excellent tools such as polynomials, and functions that can predict the properties of chemical compounds successfully. Topological indices are widely utilized in various fields such as network theory and chemistry due to their ability to provide valuable insights into the structure and properties of complex systems. In network theory, topological indices help characterize the connectivity patterns of networks, which is crucial for understanding phenomena such as information flow, robustness, and resilience of networks. In chemistry, they provide quantitative measures of molecular topology, which are often correlated with physical and chemical properties such as boiling points, melting points, solubility, and reactivity. For example, the Hosoya polynomial, also called the Wiener polynomial, is a significant tool in chemical graph theory [4]. It calculates distance-dependent topological indices, which are numerical descriptors of molecular structure based on graph theory concepts. There are many polynomials such as the pi polynomial, Theta polynomial, PI polynomial [5], Tutte polynomial [6], matching [7], Schultz [8], Zang-Zang polynomial [9], etc. In the realm of degree-based topological indices, the M-polynomial serves a comparable function by facilitating the computation of closed expressions for numerous degree-based topological indices. Consequently, the computation of degree-based topological indices simplifies to the evaluation of a singular polynomial. Furthermore, a thorough analysis of this polynomial can provide fresh insights into understanding degree-based topological indices.[10], [11]. The theory concerning the Szeged index on polynomial chains was discussed by Gao et al. [12]. Throughout this article, we employ the concept of a molecular graph, which refers to a connected graph devoid of loops and parallel edges, where vertices and edges represent atoms and chemical bonds within the compound [13]. Shao et al. discussed hued colorings of cartesian products of cycles and paths [14]. A graph  $\Omega$  with vertex set  $V(\Omega)$  and edge set  $E(\Omega)$  is connected if there exists a connection between any pair of vertices in  $G$ . The degree of a vertex  $v \in V(\Omega)$  of a graph  $\Omega$ , denoted by  $\delta_v$  is the total number of edges incident with  $v$ .

*Definition 1.1:* [15] Let  $\Omega$  be the graph the  $M$  polynomial is represented by the following

$$M(\Omega; g, h) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(\Omega)g^i h^j$$

where  $\delta = \text{Min}(\mu_h): h \in V(\Omega)$ ,  $\Delta = \text{Max}(\mu_h): h \in V(\Omega)$

$$D_g = g \frac{\partial t(g, h)}{\partial g}$$

$$D_h = h \frac{\partial t(g, h)}{\partial h}$$

$$S_g = \int_0^g \frac{t(f, h)}{f} df$$

$$S_h = \int_0^h \frac{t(g, f)}{f} df$$

$$J(t(g, h)) = t(g, g) \cdot Q_{\alpha} t(g, h) = g^{\alpha} t(g, h); \neq 0$$

*Definition 1.2:* [16] Zagreb indices was introduced by Gutman and Trinajstić in 1998[14]

The first Zagreb index is

$$M_1(\Omega) = \sum_{gh \in E(\Omega)} (\mu_g + \mu_h)$$

*Definition 1.3:* [16] The second Zagreb index is defined as

$$M_2(\Omega) = \sum_{gh \in E(\Omega)} (\mu_g \cdot \mu_h)$$

*Definition 1.4:* [17] The second modified Zagreb index is defined as

$${}^m M_2(\Omega) = \sum_{gh \in E(\Omega)} \frac{1}{\mu_g \cdot \mu_h}$$

*Definition 1.5:* [18] The general randic index is defined as

$$R_{\alpha}(\Omega) = \sum_{gh \in E(\Omega)} (\mu_g \cdot \mu_h)^{\alpha}$$

*Definition 1.6:* [19], [20] The inverse randic index is

$$RR_{\alpha}(\Omega) = \sum_{gh \in E(\Omega)} \frac{1}{(\mu_g \cdot \mu_h)^{\alpha}}$$

*Definition 1.7:* [21] The harmonic index is defined as

$$H(\Omega) = \sum_{gh \in E(\Omega)} \frac{2}{\mu_g + \mu_h}$$

*Definition 1.8:* [22] Symmetric division deg index of a connected graph  $(\Omega)$  is defined as

$$SDD(\Omega) = \sum_{gh \in E(\Omega)} \frac{\min(\mu_g, \mu_h)}{\max(\mu_g, \mu_h)} + \frac{\max(\mu_g, \mu_h)}{\min(\mu_g, \mu_h)}$$

*Definition 1.9:* [23] The inverse sum index is

$$ISI(\Omega) = \sum_{gh \in E(\Omega)} \frac{\mu_g \cdot \mu_h}{\mu_g + \mu_h}$$

*Definition 1.10:* [24] The forgotten topological index is defined as

$$F(\Omega) = \sum_{gh \in E(\Omega)} (\mu(g)^2 + \mu(h)^2)$$

*Definition 1.11:* [25] The augmented zagreb index of  $G$  proposed by Furtula et.al is defined as

$$A(\Omega) = \sum_{gh \in E(\Omega)} \left( \frac{\mu_g \cdot \mu_h}{\mu_g + \mu_h - 2} \right)^3$$

TABLE I  
THE RELATIONSHIP BETWEEN THE M POLYNOMIAL AND TOPOLOGICAL INDICES

Molecular descriptors	Mathematical expression	Derivation from $(M(\Omega) : g, h)$
First Zagreb index	$\mu_g + \mu_h$	$(D_g + D_h) (M(\Omega) : g, h)$
Second Zagreb index	$\mu_g \cdot \mu_h$	$(D_g \cdot D_h) (M(\Omega) : g, h)$
Second Modified Zagreb index	$\frac{1}{\mu_g \cdot \mu_h}$	$(S_g \cdot S_h) (M(\Omega) : g, h)$
Harmonic index	$\frac{2}{\mu_g + \mu_h}$	$2S_g J(M(\Omega) : g, h)$
Symmetric division index	$\frac{\min(\mu_g \cdot \mu_h)}{\max(\mu_g \cdot \mu_h)} + \frac{\max(\mu_g \cdot \mu_h)}{\min(\mu_g \cdot \mu_h)}$	$(D_g S_h + S_g D_h) (M(\Omega) : g, h)$
Inverse sum index	$\frac{\mu_g \cdot \mu_h}{\mu_g + \mu_h}$	$S_g J D_g D_h (M(\Omega) : g, h)$
Forgotten topological index	$[\mu(g)^2 + \mu(h)^2]$	$(D_g^2 + D_h^2) (M(\Omega) : g, h)$
Augmented Zagreb index	$\left(\frac{\mu_g \cdot \mu_h}{\mu_g + \mu_h - 2}\right)^3$	$S_g^3 Q_{-2} J D_g^3 D_h^3 (M(\Omega) : g, h)$

II. MAIN RESULTS

To calculate degree-based topological indices for graphs such as tadpole, helm, gear, friendship, and fan graph. We first drew these graphs and then we divided the edge sets based on the degree of the end vertices and computed their cardinality. Based on this edge partition, we computed the M-polynomials of the families of graphs. Then using the table.1 we determined several topological indices. In this section, we give our main computational results and divide the section into five subsections.

Tadpole graph

Definition 2.1: A tadpole graph is denoted by  $T_{m,n}$  we mean the graph is obtained by joining a cycle  $C_m$  to a path graph  $P_n$  with a bridge [26].

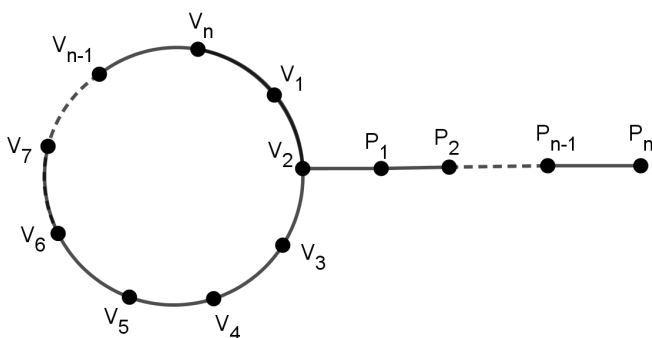


Fig. 1. Tadpole graph

Theorem 2.2: Let  $T_{m,n}$  be a tadpole of order  $m + n$  and size  $m + n$ , then

$$M(T_{m,n}; g, h) = gh^2 + (m + n - 4)g^2h^2 + 3g^2h^3$$

Proof: The tadpole has  $m + n$  vertices and  $m + n$  edges.

The edge set of  $T_{m,n}$  can be partitioned as

$$|E_{12}| = e = gh \in E(T_{m,n}); \mu_g = 1, \mu_h = 2 \Rightarrow |E_{12}| = 1$$

$$|E_{22}| = e = gh \in E(T_{m,n}); \mu_g = 2, \mu_h = 2 \Rightarrow |E_{22}| = n + m - 4$$

$$|E_{23}| = e = gh \in E(T_{m,n}); \mu_g = 1, \mu_h = 2 \Rightarrow |E_{23}| = 3$$

The following result is obtained by applying the interpretation of M-polynomial, let

$$M(\Omega; g, h) = t(g, h)$$

$$\begin{aligned} M(\Omega; g, h) &= \sum_{i \leq j} m_{ij} ((\Omega)g^i h^j) \\ &= \sum_{1 \leq 2} (m_{ij}(H_n)g^i h^j) + \sum_{2 \leq 2} (m_{ij}(H_n)g^i h^j) \\ &\quad + \sum_{2 \leq 3} (m_{ij}(H_n)g^i h^j) \\ &= |E_{1,2}|gh^2 + |E_{2,2}|g^2h^2 + |E_{2,3}|g^2h^3 \\ M(T_{m,n}; g, h) &= gh^2 + (m + n - 4)g^2h^2 + 3g^2h^3 \end{aligned}$$

Hence the proof. ■

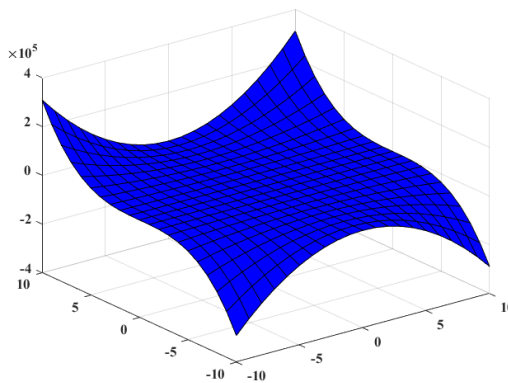


Fig. 2. 3D-Plots of M-Polynomial of Tadpole graph

Now using this M-polynomial, we compute some degree based topological index of the tadpole graph in the following

theorem using Table 1.

**Theorem 2.3:** If  $T_{m,n}$  is a tadpole, then

1.  $M_1(T_{m,n}) = 4(m+n) + 2$
2.  $M_2(T_{m,n}) = 4(m+n) + 4$
3.  ${}^m M_2(T(m,n)) = \frac{m+n}{4}$
4.  $H(T_{m,n}) = \frac{m+n}{4} - \frac{2}{15}$
5.  $SDD(T_{m,n}) = 2(m+n) + 1$
6.  $ISI(T_{m,n}) = (m+n) + \frac{4}{15}$
7.  $F(T_{m,n}) = 8m + 8n - 12$
8.  $A(T_{m,n}) = 8(m+n)$

*Proof:* Let  $t(g, h) = gh^2 + (m+n-4)g^2h^2 + 3g^2h^3$

**1. First Zagreb index**

$$t(g, h) = gh^2 + (m+n-4)g^2h^2 + 3g^2h^3$$

$$D_g t(g, h) = gh^2 + 2(m+n-4)g^2h^2 + 6g^2h^3$$

$$D_h t(g, h) = 2gh^2 + 2(m+n-4)g^2h^2 + 9g^2h^3$$

$$(D_g + D_h)t(g, h) = 3gh^2 + 4(m+n-4)g^2h^2 + 15g^2h^3$$

$$M_1[T_{m,n}] = (D_g + D_h)t(g, h)|_{g=h=1} = 4(m+n) + 2$$

**2. Second Zagreb index**

$$t(g, h) = gh^2 + (m+n-4)g^2h^2 + 3g^2h^3$$

$$D_g t(g, h) = gh^2 + 2(m+n-4)g^2h^2 + 6g^2h^3$$

$$D_h t(g, h) = 2gh^2 + 2(m+n-4)g^2h^2 + 9g^2h^3$$

$$(D_g + D_h)t(g, h) = 3gh^2 + 4(m+n-4)g^2h^2 + 15g^2h^3$$

$$M_1[T_{m,n}] = (D_g + D_h)t(g, h)|_{g=h=1} = 4(m+n) + 2$$

**3. Second Modified Zagreb index**

$$t(g, h) = gh^2 + (m+n-4)g^2h^2 + 3g^2h^3$$

$$S_h(t(g, h)) = \frac{gh^2}{2} + \frac{(m+n-4)}{2}g^2h^2 + g^2h^3$$

$$(S_g \cdot S_h)(t(g, h)) = \frac{gh^2}{2} + \frac{(m+n-4)}{4}g^2h^2 + \frac{g^2h^3}{2}$$

$${}^m M_2(G)[T_{m,n}] = (S_g \cdot S_h)t(g, h)|_{g=h=1} = \frac{m+n}{4}$$

**4. Harmonic index**

$$t(g, h) = gh^2 + (m+n-4)g^2h^2 + 3g^2h^3$$

$$Jt(g, h) = g^3 + (m+n-4)g^4 + 3g^5$$

$$S_g Jt(g, h) = \frac{g^3}{3} + \frac{(m+n-4)}{4}g^4 + \frac{3}{5}g^5$$

$$2S_g Jt(g, h) = \frac{2}{3}g^3 + \frac{(m+n-4)}{2}g^4 + \frac{6}{5}g^5$$

$$H[T_{m,n}] = 2S_g Jt(g, h)|_{g=h=1} = \frac{m+n}{4} - \frac{2}{15}$$

**5. Symmetric division index**

$$t(g, h) = gh^2 + (m+n-4)g^2h^2 + 3g^2h^3$$

$$S_h(t(g, h)) = \frac{gh^2}{2} + \frac{(m+n-4)}{2}g^2h^2 + \frac{3}{3}g^2h^3$$

$$D_g \cdot S_h(t(g, h)) = \frac{gh^2}{2} + (m+n-4)g^2h^2 + 2g^2h^3 \cdot 4$$

$$D_h(t(g, h)) = 2gh^2 + 2(m+n-4)g^2h^2 + 9g^2h^3$$

$$S_g D_h t(g, h) = 2gh^2 + (m+n-4)g^2h^2 + \frac{9}{2}g^2h^3$$

$$(D_g S_h + S_g D_h)t(g, h) = \frac{5}{2}gh^2 + 2(m+n-4)g^2h^2 + \frac{13}{2}g^2h^3$$

$$SDD[T_{m,n}] = (D_g S_h + S_g D_h)t(g, h)|_{g=h=1} = 2(m+n) + 1$$

**6. Inverse sum index**

$$t(g, h) = gh^2 + (m+n-4)g^2h^2 + 3g^2h^3$$

$$D_h t(g, h) = 2gh^2 + 2(m+n-4)g^2h^2 + 9g^2h^3$$

$$D_g D_h t(g, h) = 2gh^2 + 4(m+n-4)g^2h^2 + 18g^2h^3$$

$$J D_g D_h t(g, h) = 2g^3 + 4(m+n-4)g^4 + 18g^5$$

$$S_g J D_g D_h t(g, h) = \frac{2}{3}g^3 + (m+n-4)g^4 + \frac{18}{5}g^5$$

$$ISI[T_{m,n}] = S_g J D_g D_h t(g, h)|_{g=h=1} = (m+n) + \frac{4}{15}$$

**7. Forgotten topological index**

$$t(g, h) = gh^2 + (m+n-4)g^2h^2 + 3g^2h^3$$

$$D_g^2 t(g, h) = gh^2 + 4(m+n-4)g^2h^2 + 12g^2h^3$$

$$D_h^2 t(g, h) = 4gh^2 + 4(m+n-4)g^2h^2 + 27g^2h^3$$

$$(D_g^2 + D_h^2)t(g, h) = 5gh^2 + 8(m+n-4)g^2h^2 + 39g^2h^3$$

$$F[T_{m,n}] = (D_g^2 + D_h^2)t(g, h)|_{g=h=1} = 8m + 8n - 12$$

**8. Augmented Zagreb index**

$$t(g, h) = gh^2 + (m+n-4)g^2h^2 + 3g^2h^3$$

$$D_h^3 t(g, h) = 8gh^2 + 8(m+n-4)g^2h^2 + 81g^2h^3$$

$$D_g^3 D_h^3 t(g, h) = 8gh^2 + 64(m+n-4)g^2h^2 + 648g^2h^3$$

$$J D_g^3 D_h^3 t(g, h) = 8g^3 + 64(m+n-4)g^4 + 648g^5$$

$$Q_{-2} J D_g^3 D_h^3 t(g, h) = 8g + 64(m+n-4)g^2 + 648g^3$$

$$S_g^3 Q_{-2} D_g^3 D_h^3 t(g, h) = 8g + 8(m+n-4)g^2 + 24g^3$$

$$A[T_{m,n}] = S_g^3 Q_{-2} D_g^3 D_h^3 t(g, h)|_{g=h=1} = 8(m+n)$$

Hence the proof. ■

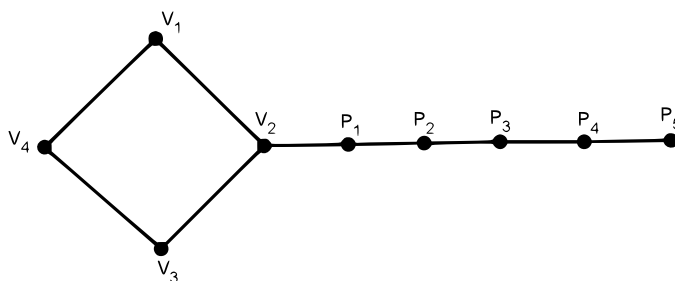


Fig. 3. Example of Tadpole graph  $T_{4,5}$

Let us examine the tadpole graph  $T_{4,5}$  as depicted in Fig.3 and we calculated the topological indices as follows.

TABLE II  
NUMERICAL VALUES OF TADPOLE GRAPH

Topological Indices	Numerical values
First zagreb index	38
Second zagreb index	40
Second modified zagreb index	2.25
Harmonic index	4.367
Symmetric division deg index	9
Inverse sum index	9.267
Forgotten topological index	84
Augmented zagreb index	37

**Helm graph**

*Definition 2.4:* The Helm graph is obtained by joining a pendant edge attached to each vertex of  $C_n$  of the wheel graph [26].

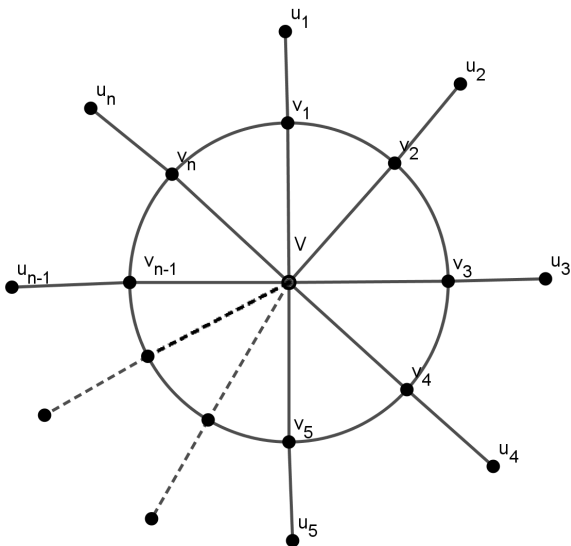


Fig. 4. Helm graph

*Theorem 2.5:* Let  $H_n$  be a Helm graph of order  $2n + 1$  and size  $3n$ , then

$$M(H_n; g, h) = ngh^4 + ng^4h^4 + ng^4h^4 + ng^4h^n$$

*Proof:* From the figure of  $H_n$ , we can say that the edge partition has divided into three partitions,

$$\begin{aligned} |E_{1,4}| &= |gh\epsilon E(H_n); \mu_g = 1, \mu_h = 4| \Rightarrow |E_{1,4}| = n \\ |E_{4,4}| &= |gh\epsilon E(H_n); \mu_g = 4, \mu_h = 4| \Rightarrow |E_{4,4}| = n \\ |E_{4,n}| &= |gh\epsilon E(H_n); \mu_g = 4, \mu_h = n| \Rightarrow |E_{4,n}| = n \end{aligned}$$

By using the definition of M-Polynomial

$$\begin{aligned} M(\Omega; g, h) &= t(g, h) \\ M(\Omega; g, h) &= \sum_{i \leq j} m_{ij} ((\Omega)g^i h^j) \\ &= \sum_{1 \leq 4} (m_{ij}(H_n)g^i h^j) + \sum_{4 \leq 4} (m_{ij}(H_n)g^i h^j) \\ &\quad + \sum_{4 \leq n} (m_{ij}(H_n)g^i h^j) \\ &= |E_{1,4}|gh^4 + |E_{4,4}|g^4h^4 + |E_{4,n}|g^4h^n \\ M(H_n; g, h) &= ngh^4 + ng^4h^4 + ng^4h^n \end{aligned}$$

Hence the proof. ■

*Theorem 2.6:* If  $H_n$  is a Helm, then

1.  $M_1(H_n) = n^2 + 17n$
2.  $M_2(H_n) = 4n(n + 5)$
3.  ${}^m M_2(H_n) = \frac{9n}{16}$
4.  $H(H_n) = \frac{13n}{20} + \frac{2n}{n+4}$
5.  $SDD(H_n) = \frac{n^2}{4} + \frac{25n}{4} + 4$
6.  $I(H_n) = \frac{14n}{5} + \frac{4n^2}{4+n}$
7.  $F(H_n) = n^3 + 65n$

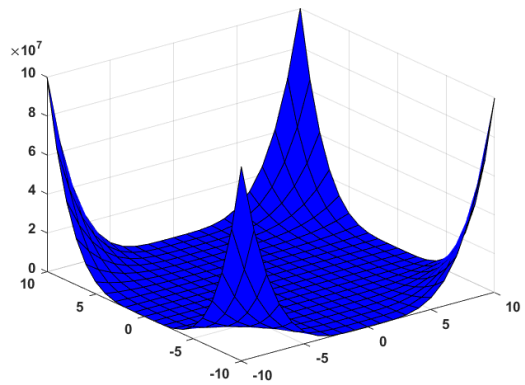


Fig. 5. 3D-Plots of M-Polynomial of Helm graph

8.  $A(H_n) = 16n^4 + 128n$

*Proof:* Let  $t(g, h) = ngh^4 + ng^4h^4 + ng^4h^n$ . Then we have

**1. First Zagreb index**

$$\begin{aligned} t(g, h) &= ngh^4 + ng^4h^4 + ng^4h^n \\ D_g t(g, h) &= ngh^4 + ng^4h^4 + ng^4h^n \\ D_h t(g, h) &= 4ngh^4 + 4ng^4h^4 + n^2g^4h^n \\ (D_g + D_h)t(g, h) &= 5ngh^4 + 8ng^4h^4 + (4n + n^2)g^4h^n \\ M_1[H_n] &= (D_g + D_h)t(g, h)|_{g=h=1} = n^2 + 17n \end{aligned}$$

**2. Second Zagreb index**

$$\begin{aligned} t(g, h) &= ngh^4 + ng^4h^4 + ng^4h^n \\ D_h t(g, h) &= 4ngh^4 + 4ng^4h^4 + n^2g^4h^n \\ D_g \cdot D_h t(g, h) &= 4ngh^4 + 16ng^4h^4 + 4n^2g^4h^n \\ M_2[H_n] &= D_g \cdot D_h t(g, h)|_{g=h=1} = 4n(n + 5) \end{aligned}$$

**3. Second Modified Zagreb index**

$$\begin{aligned} t(g, h) &= ngh^4 + ng^4h^4 + ng^4h^n \\ S_h t(g, h) &= \frac{n}{4}gh^4 + \frac{n}{4}g^4h^4 + \frac{n}{4}g^4h^n \\ (S_g \cdot S_h)t(g, h) &= \frac{n}{4}gh^4 + \frac{n}{16}g^4h^4 + \frac{n}{4}g^4h^n \\ {}^m M_2[H_n] &= (S_g \cdot S_h)t(g, h)|_{g=h=1} = \frac{9n}{16} \end{aligned}$$

**4. Harmonic index**

$$\begin{aligned} t(g, h) &= ngh^4 + ng^4h^4 + ng^4h^n \\ Jt(g, h) &= ng^5 + ng^8 + ng^{4+n} \\ S_g Jt(g, h) &= \frac{n}{5}g^5 + \frac{n}{8}g^8 + \frac{n}{4+n}g^{4+n} \\ 2S_g Jt(g, h) &= \frac{2n}{5}g^5 + \frac{n}{4}g^8 + \frac{2n}{4+n}g^{4+n} \\ H[H_n] &= 2S_g Jt(g, h)|_{g=h=1} = \frac{13n}{20} + \frac{2n}{n+4} \end{aligned}$$

**5. Symmetric division index**

$$\begin{aligned} t(g, h) &= ngh^4 + ng^4h^4 + ng^4h^n \\ S_h t(g, h) &= \frac{n}{4}gh^4 + \frac{n}{4}g^4h^4 + \frac{n}{n}g^4h^n \\ (D_g \cdot S_h)t(g, h) &= \frac{n}{4}gh^4 + \frac{4n}{4}g^4h^4 + 4g^4h^n \\ D_h t(g, h) &= 4ngh^4 + 4ng^4h^4 + n^2g^4h^3 \end{aligned}$$

$$S_g \cdot D_h t(g, h) = 4ngh^4 + ng^4h^4 + \frac{n^2}{4}g^4h^3$$

$$(D_g \cdot S_h + S_g \cdot D_h)t(g, h) = (\frac{n}{4} + 4n)gh^4 + 2ng^4h^4$$

$$+ (4 + \frac{n^2}{4})g^4h^3$$

$$SDD[H_n] = (D_g \cdot S_h + S_g \cdot D_h)t(g, h)|_{g=h=1}$$

$$SDD[H_n] = \frac{n^2 + 25n + 16}{4}$$

6. Inverse Sum index

$$t(g, h) = ngh^4 + ng^4h^4 + ng^4h^n$$

$$D_h t(g, h) = 4ngh^4 + 4ng^4h^4 + n^2g^4h^n$$

$$D_g \cdot D_h t(g, h) = 4ngh^4 + 16ng^4h^4 + 4n^2g^4h^n$$

$$JD_g \cdot D_h t(g, h) = 4ng^5 + 16ng^8 + 4n^2g^{4+n}$$

$$S_g JD_g \cdot D_h t(g, h) = \frac{4n}{5}g^5 + \frac{16n}{8}g^8$$

$$+ \frac{4n^2}{n+4}g^{4+n}$$

$$ISI[H_n] = S_g JD_g \cdot D_h t(g, h)|_{g=h=1} = \frac{14n}{5} + \frac{4n^2}{4+n}$$

7. Forgotten topological index

$$t(g, h) = ngh^4 + ng^4h^4 + ng^4h^n$$

$$D_g^2 t(g, h) = ngh^4 + 16ng^4h^4 + 16ng^4h^n$$

$$D_h^2 t(g, h) = 16ngh^4 + 16ng^4h^4 + n^3g^4h^3$$

$$(D_g^2 + D_h^2)t(g, h) = (16 + n)gh^4 + 32ng^4h^4$$

$$+ 16ng^4h^n + n^3g^4h^3$$

$$F[H_n] = (D_g^2 + D_h^2)t(g, h)|_{g=h=1} = n^3 + 65n$$

8. Augmented Zagreb index

$$t(g, h) = ngh^4 + ng^4h^4 + ng^4h^n$$

$$D_h^3 t(g, h) = 64ngh^4 + 64ng^4h^4 + n^4g^4h^n$$

$$D_g^3 \cdot D_h^3 t(g, h) = 64ngh^4 + 4096ng^4h^4 + 64n^4g^4h^n$$

$$JD_g^3 \cdot D_h^3 t(g, h) = 64ng^5 + 4096ng^8 + 64n^4g^{4+n}$$

$$Q_{-2} JD_g^3 \cdot D_h^3 t(g, h) = 64ng^2 + 4096ng^6 + 64n^4g^2$$

$$S_g^3 Q_{-2} JD_g^3 \cdot D_h^3 t(g, h) = 64ng^2 + 64ng^6 + 16n^4g^2$$

$$A[H_n] = S_g^3 Q_{-2} JD_g^3 \cdot D_h^3 t(g, h)|_{g=h=1} = 16n^4 + 128n$$

Hence the proof. ■

Let us consider the example of the helm graph  $H_5$ , as illustrated in Fig. 6

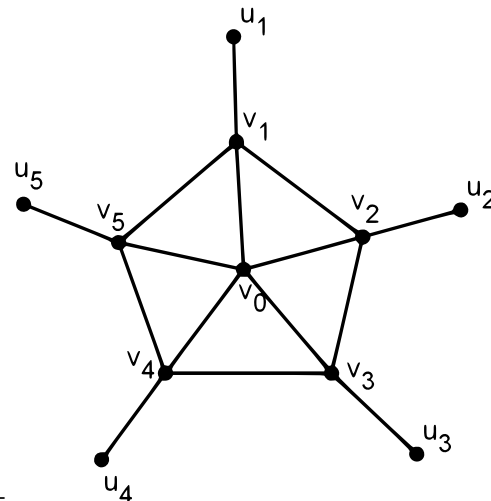


Fig. 6. Example of Helm graph  $H_5$

Gear graph

Definition 2.7: The gear graph is obtained by a vertex added between each pair of adjacent vertices of  $C_n$  of the wheel graph [27].

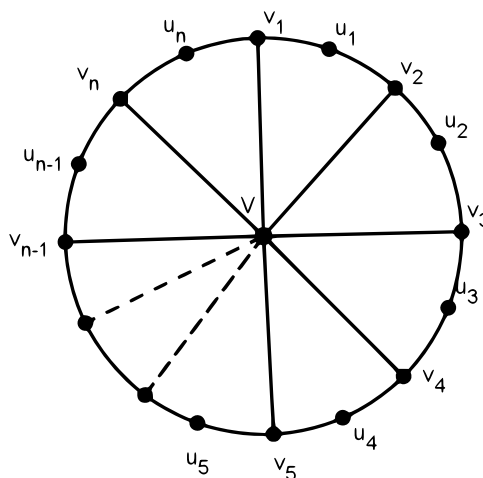


Fig. 7. Gear graph

TABLE III  
NUMERICAL VALUES OF HELM GRAPH

Topological Indices	Numerical values
First zagreb index	110
Second zagreb index	200
Second modified zagreb index	1.812
Harmonic index	4.362
Symmetric division deg index	11
Inverse sum index	25.12
Forgotten topological index	450
Augmented zagreb index	223.8

Theorem 2.8: Let  $G_n$  be a gear graph of order  $2n + 1$  and size  $3n$  edges, then  $M(G_n; g, h) = 2ng^2h^3 + ng^3h^n$

Proof: The graph  $G_n$  has  $2n + 1$  vertices and  $3n$  edges. We can divide the edge set  $G_n$  into the following three classes depending on each edge at the degree of end vertices.

$$|E_{(2,3)}| = |gh \in E(H_n); \mu_g = 2, \mu_h = 3| \Rightarrow |E_{2,3}| = 2n$$

$$|E_{(3,n)}| = |gh \in E(H_n); \mu_g = 3, \mu_h = n| \Rightarrow |E_{3,n}| = n$$

By using the definition of M-polynomial

$$\begin{aligned}
 M(\Omega; g, h) &= t(g, h) \\
 M(\Omega; g, h) &= \sum_{i \leq j} m_{ij} ((\Omega)g^i h^j) \\
 &= \sum_{2 \leq 3} (m_{ij}(H_n)g^i h^j) + \sum_{3 \leq n} (m_{ij}(H_n)g^i h^j) \\
 &= |E_{2,3}|g^2 h^3 + |E_{3,n}|g^3 h^n \\
 M(G_n; g, h) &= 2ng^2 h^3 + ng^3 h^n
 \end{aligned}$$

Hence the proof.

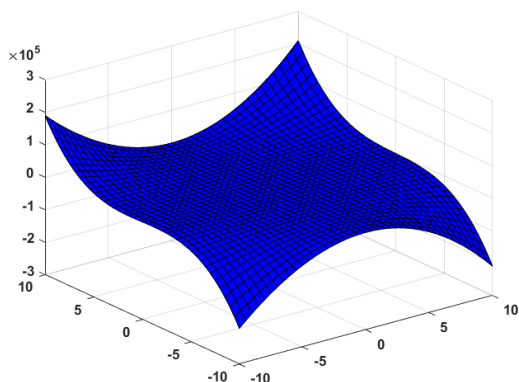


Fig. 8. 3D-plots of M-polynomial of Gear graph

**Theorem 2.9:** If  $G_n$  is a gear, then

1.  $M_1(G_n) = n^2 + 4n$
2.  $M_2(G_n) = 12n + 3n^2$
3.  ${}^m M_2(G_n) = \frac{n+1}{3}$
4.  $H(G_n) = \frac{4n}{5} + \frac{2n}{3+n}$
5.  $SDD(G_n) = \frac{6}{26n+18}$
6.  $I(G_n) = \frac{12n}{5} + \frac{3n^2}{3+n}$
7.  $F(G_n) = n^3 + 35n$
8.  $A(G_n) = n^4 + 54n$

*Proof:* Let  $t(g, h) = 2ng^2 h^3 + ng^3 h^n$

**1. First Zagreb index**

$$\begin{aligned}
 D_g t(g, h) &= 4ng^2 h^3 + 3ng^3 h^n \\
 D_h t(g, h) &= 6ng^2 h^3 + n^2 g^3 h^n \\
 (D_g + D_h)(t(g, h)) &= 10ng^2 h^3 + (3n + n^2)g^3 h^n \\
 M_1[G_n] &= (D_g + D_h)(t(g, h))|_{g=h=1} = n^2 + 13n
 \end{aligned}$$

**2. Second Zagreb index**

$$\begin{aligned}
 t(g, h) &= 2ng^2 h^3 + ng^3 h^n \\
 D_h t(g, h) &= 6ng^2 h^3 + n^2 g^3 h^n \\
 D_g \cdot D_h t(g, h) &= 12ng^2 h^3 + 3n^2 g^3 h^n \\
 M_2[G_n] &= D_g \cdot D_h t(g, h)|_{g=h=1} = 12n + 3n^2
 \end{aligned}$$

**3. Second Modified Zagreb index**

$$\begin{aligned}
 t(g, h) &= 4ng^2 h^3 + ng^3 h^n \\
 S_h t(g, h) &= \frac{2n}{3}g^2 h^3 + \frac{n}{n}g^3 h^n \\
 S_g \cdot S_h t(g, h) &= \frac{n}{3}g^2 h^3 + \frac{1}{3}g^3 h^n \\
 {}^m M_2[G_n] &= S_g \cdot S_h t(g, h)|_{g=h=1} = \frac{n}{3} + \frac{1}{3}
 \end{aligned}$$

**4. Harmonic index**

$$\begin{aligned}
 t(g, h) &= 2ng^2 h^3 + ng^3 h^n \\
 Jt(g, h) &= 2ng^5 + ng^{3+n} \\
 S_g Jt(g, h) &= \frac{2n}{5}g^5 + \frac{n}{3+n}g^{3+n} \\
 2S_g Jt(g, h) &= \frac{4n}{5}g^5 + \frac{2n}{3+n}g^{3+n} \\
 H[G_n] &= 2S_g Jt(g, h)|_{g,h=1} = \frac{4n}{5} + \frac{2n}{3+n}
 \end{aligned}$$

**5. Symmetric division index**

$$\begin{aligned}
 t(g, h) &= 2ng^2 h^3 + ng^3 h^n \\
 S_h t(g, h) &= \frac{4n}{3}g^2 h^3 + 3g^3 h^n \\
 D_g \cdot S_h t(g, h) &= 4ng^2 h^3 + 3ng^3 h^n \\
 D_h t(g, h) &= 4ng^2 h^3 + 3ng^3 h^n \\
 S_g \cdot D_h t(g, h) &= \frac{4n}{2}g^2 h^3 + \frac{3n}{3}g^3 h^n \\
 (D_g \cdot S_h + S_g \cdot D_h)(t(g, h)) &= \frac{4n}{3}g^2 h^3 \\
 &+ 3g^3 h^n + \frac{4n}{2}g^2 h^3 + ng^3 h^n \\
 SDD[G_n] &= (D_g \cdot S_h + S_g \cdot D_h)(t(g, h))|_{g,h=1} \\
 SDD[G_n] &= \frac{26n+18}{6}
 \end{aligned}$$

**6. Inverse sum index**

$$\begin{aligned}
 t(g, h) &= 2ng^2 h^3 + ng^3 h^n \\
 D_h t(g, h) &= 6ng^2 h^3 + n^2 g^3 h^n \\
 D_g \cdot D_h t(g, h) &= 12ng^2 h^3 + 3n^2 g^3 h^n \\
 JD_g \cdot D_h t(g, h) &= 12ng^5 + 3n^2 g^{3+n} \\
 S_g JD_g \cdot D_h t(g, h) &= \frac{12}{n}g^5 + \frac{3n^2}{3+n}g^{3+n} \\
 ISI[G_n] &= S_g JD_g \cdot D_h t(g, h)|_{g,h=1} = \frac{12n}{5} + \frac{3n^2}{3+n}
 \end{aligned}$$

**7. Forgotten topological index**

$$\begin{aligned}
 t(g, h) &= 2ng^2 h^3 + ng^3 h^n \\
 D_g^2 t(g, h) &= 8ng^2 h^3 + 9ng^3 h^n \\
 D_h^2 t(g, h) &= 18ng^2 h^3 + n^3 g^3 h^n \\
 (D_g^2 + D_h^2)t(g, h) &= 26ng^2 h^3 + (9n + n^2 + n^3)g^3 h^n \\
 F[G_n] &= (D_g^2 + D_h^2)t(g, h)|_{g,h=1} = n^3 + 35n
 \end{aligned}$$

8. Augmented Zagreb index

$$t(g, h) = 2ng^2h^3 + ng^3h^n$$

$$D_h^3 t(g, h) = 54ng^2h^3 + n^4g^3h^n$$

$$D_g^3 . D_h^3 t(g, h) = 432ng^2h^3 + 27n^4g^3h^n$$

$$JD_g^3 . D_h^3 t(g, h) = 432ng^5 + 27n^4g^{3+n}$$

$$Q_{-2} JD_g^3 . D_h^3 t(g, h) = 432ng^3 + 27n^4g^{n+1}$$

$$S_g^3 Q_{-2} JD_g^3 . D_h^3 t(g, h) = 54ng^3 + n^4g^{n+1}$$

$$A[G_n] = S_g^3 Q_{-2} JD_g^3 . D_h^3 t(g, h)|_{g,h=1} = n^4 + 54n$$

Hence the proof. ■

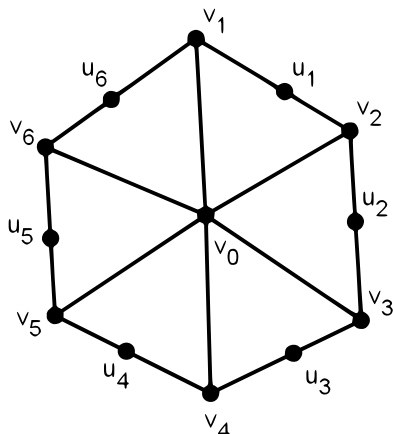


Fig. 9. Example of Gear graph  $G_6$

Consider a gear graph  $G_6$  as depicted in Fig. 9

TABLE IV  
NUMERICAL VALUES OF GEAR GRAPH

Topological Indices	Numerical values
First zagreb index	114
Second zagreb index	180
Second modified zagreb index	3.17
Harmonic index	6.14
Symmetric division deg index	13
Inverse sum index	26.4
Forgotten topological index	426
Augmented zagreb index	198.014

Friendship graph

Definition 2.10: The friendship graph is obtained by deleting the alternate edges of the cycle  $C_{2n}$  of  $W_{2n}$  [27]

Theorem 2.11: Let  $Fr_n$  is a friendship graph, then  $n \geq 3$ , M-polynomial of  $Fr_n$  is  $M(Fr_n; g, h) = ng^2h^2 + 2ng^2h^{2n}$

Proof: The friendship graph has  $2n + 1$  vertices and  $3n$  edges. From the figure of  $Fr_n$ , the edge sets divided into two partitions.

$$|E_{2,2}| = |gh \in E(G); \mu_g = 2, \mu_h = 2| \Rightarrow |E_{2,2}| = n$$

$$|E_{2,2n}| = |gh \in E(G); \mu_g = 2, \mu_h = 2n| \Rightarrow |E_{2,2n}| = 2n$$

From the definition of M-polynomial, we have

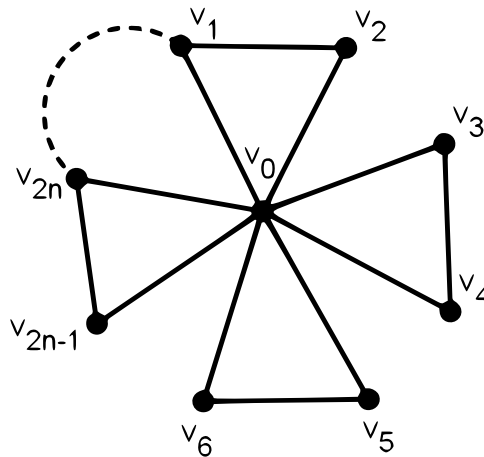


Fig. 10. Friendship graph

$$M(\Omega; g, h) = t(g, h)$$

$$M(\Omega; g, h) = \sum_{i \leq j} m_{ij} ((\Omega)g^i h^j)$$

$$= \sum_{2 \leq 2} (m_{ij}(H_n)g^i h^j) + \sum_{2 \leq 2n} (m_{ij}(H_n)g^i h^j)$$

$$= |E_{2,2}|g^2 h^2 + |E_{2,2n}|g^2 h^{2n}$$

$$M(Fr_n; g, h) = ng^2 h^2 + 2ng^2 h^{2n}$$

Hence the proof. ■

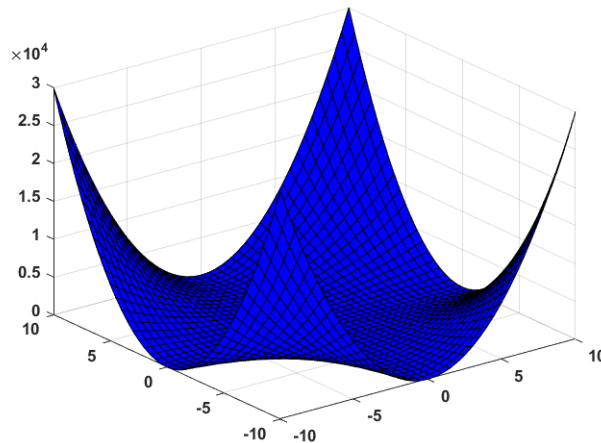


Fig. 11. 3D-Plots of M-Polynomial of Friendship graph

Theorem 2.12: If  $Fr_n$  is a friendship, then

- $M_1(Fr_n) = 4n^2 + 18n$
- $M_2(Fr_n) = 6n(2n + 1)$
- ${}^m M_2(Fr_n) = \frac{n}{4} + \frac{1}{2}$
- $H(Fr_n) = \frac{n}{2} + \frac{2n}{n+1}$
- $SDD(Fr_n) = 9n$
- $I(Fr_n) = \frac{10n^2 + 2n}{2n + 2}$
- $F(Fr_n) = 8n^3 + 16n$
- $A(fr_n) = 16n^4 + 8n$



**Proof: 1. First Zagreb index**

$$\begin{aligned}
 t(g, h) &= ng^2h^2 + 2ng^2h^{2n} \\
 D_g t(g, h) &= 2ng^2h^2 + 4ng^2h^{2n} \\
 D_h t(g, h) &= 2ng^2h^2 + 4n^2g^2h^{2n} \\
 (D_g + D_g)(t(g, h)) &= 4ng^2h^2 + (4n^2 + 4n)g^2h^{2n} \\
 M_1[Fr_n] &= (D_g + D_g)(t(g, h))|_{g=h=1} = 4n^2 + 8n
 \end{aligned}$$

**2. Second Zagreb index**

$$\begin{aligned}
 t(g, h) &= ng^2h^2 + 2ng^2h^{2n} \\
 D_h t(g, h) &= 2ng^2h^2 + 4n^2g^2h^{2n} \\
 D_g \cdot D_h t(g, h) &= 4ng^2h^2 + 8n^2g^2h^{2n} \\
 M_2[Fr_n] &= D_g \cdot D_h t(g, h) = 6ng^2h^2 + 12n^2g^2h^{2n}
 \end{aligned}$$

**3. Second Modified Zagreb index**

$$\begin{aligned}
 t(g, h) &= ng^2h^2 + 2ng^2h^{2n} \\
 S_h t(g, h) &= \frac{n}{2} \frac{2n}{2n} g^2h^{2n} \\
 S_g \cdot S_h t(g, h) &= \frac{n}{4} g^2h^2 + \frac{1}{2} g^2h^{2n} \\
 {}^m M_2[Fr_n] &= S_g \cdot S_h t(g, h)|_{g=h=1} = \frac{n}{4} + \frac{1}{2}
 \end{aligned}$$

**4. Harmonic index**

$$\begin{aligned}
 t(g, h) &= ng^2h^2 + 2ng^2h^{2n} \\
 Jt(g, h) &= ng^4 + 2ng^{2+2n} \\
 S_g Jt(g, h) &= \frac{n}{4} g^4 + \frac{2n}{2+2n} g^{2+2n} \\
 2S_g Jt(g, h) &= \frac{n}{2} g^4 + \frac{2n}{n+1} g^{2+2n} \\
 H[Fr_n] &= 2S_g Jt(g, h)|_{g,h=1} = \frac{n}{2} + \frac{2n}{n+1}
 \end{aligned}$$

**5. Symmetric division index**

$$\begin{aligned}
 t(g, h) &= ng^2h^2 + 2ng^2h^{2n} \\
 S_h t(g, h) &= \frac{n}{2} g^2h^2 + \frac{2n}{2n} g^2h^{2n} \\
 D_g \cdot S_h t(g, h) &= \frac{2n}{2} g^2h^2 + 2g^2h^{2n} \\
 D_h t(g, h) &= 2ng^2h^2 + 4ng^2h^{2n} \\
 S_g \cdot D_h t(g, h) &= ng^2h^2 + 2ng^2h^{2n} \\
 (D_g \cdot S_h + S_g \cdot D_h)(t(g, h)) &= 3ng^2h^2 + 6ng^2h^{2n} \\
 SDD[Fr_n] &= (D_g \cdot S_h + S_g \cdot D_h)(t(g, h))|_{g,h=1} = 9n
 \end{aligned}$$

**6. Inverse sum index**

$$\begin{aligned}
 t(g, h) &= ng^2h^2 + 2ng^2h^{2n} \\
 D_h t(g, h) &= 2ng^2h^2 + 4n^2g^2h^{2n} \\
 D_g \cdot D_h t(g, h) &= 4ng^2h^2 + 8n^2g^2h^{2n} \\
 JD_g \cdot D_h t(g, h) &= 4ng^4 + 8n^2g^2g^{2n} \\
 S_g JD_g \cdot D_h t(g, h) &= ng^4 + \frac{8n^2}{2n+2} g^{2n+2} \\
 ISI[Fr_n] &= S_g JD_g \cdot D_h t(g, h)|_{g,h=1} = n + \frac{8n^2}{2n+2}
 \end{aligned}$$

**7. Forgotten topological index**

$$\begin{aligned}
 t(g, h) &= ng^2h^2 + 2ng^2h^{2n} \\
 D_g^2 t(g, h) &= 4ng^2h^2 + 8ng^2h^{2n} \\
 D_h^2 t(g, h) &= 4ng^2h^2 + 8n^3g^2h^{2n} \\
 (D_g^2 + D_h^2)(t(g, h)) &= 8ng^2h^2 + (8n^3 + 8n)g^2h^{2n} \\
 F[Fr_n] &= (D_g^2 + D_h^2)(t(g, h))|_{g=h=1} = 8n^3 + 16n
 \end{aligned}$$

**8. Augmented Zagreb index**

$$\begin{aligned}
 t(g, h) &= ng^2h^2 + 2ng^2h^{2n} \\
 D_h^3 t(g, h) &= 8ng^2h^2 + 16ng^2h^{2n} \\
 D_g^3 \cdot D_h^3 t(g, h) &= 64ng^2h^2 + 128n^4g^2h^{2n} \\
 JD_g^3 \cdot D_h^3 t(g, h) &= 64ng^4 + 128n^4g^2h^{2n} \\
 Q_{-2} JD_g^3 \cdot D_h^3 t(g, h) &= 64ng^2h^2 + 128n^4g^{2n} \\
 S_g^3 Q_{-2} JD_g^3 \cdot D_h^3 t(g, h) &= 8ng^2 + 16n^4g^{2n} \\
 A[Fr_n] &= S_g^3 Q_{-2} JD_g^3 \cdot D_h^3 t(g, h)|_{g=h=1} = 16n^4 + 8n
 \end{aligned}$$

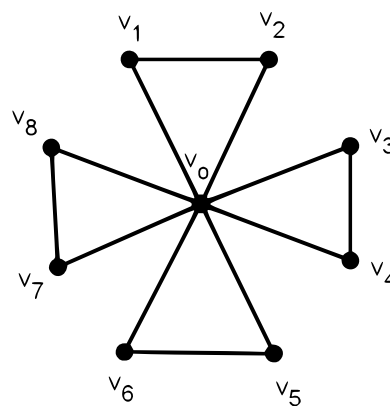


Fig. 12. Example of Friendship graph  $Fr_4$

Let us explore the friendship graph  $Fr_4$  as depicted in Fig.12

TABLE V  
NUMERICAL VALUES OF FRIENDSHIP GRAPH

Topological Indices	Numerical values
First zagreb index	64
Second zagreb index	80
Second modified zagreb index	2.334
Harmonic index	4.667
Symmetric division deg index	10
Inverse sum index	14.67
Forgotten topological index	192
Augmented zagreb index	96

**Fan graph**

The fan graph  $F_n$ , ( $n \geq 3$ ) is defined as the graph  $K_1 + P_n$ , where  $K_1$  is singleton graph and  $P_n$  is the path on  $n$  vertices [28].

*Theorem 2.13:* Let  $F_n$  be a fan graph of order  $n + 1$  and size  $2n - 1$ , then the M-polynomial of  $F_n$  is

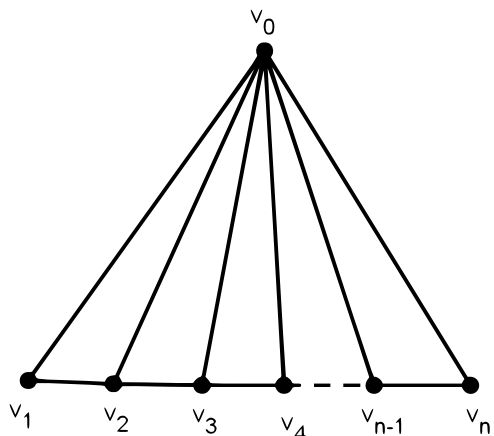


Fig. 13. Fan graph

$$M(F_n; g, h) = 2g^2h^3 + 2g^2h^n + (n - 3)g^3h^3 + (n - 2)g^3h^n$$

*Proof:* Let  $F_n$  be a fan has  $2n + 1$  vertices and  $2n - 1$  edges. The edge set has divided into four partitions as,

$$\begin{aligned} |E_{2,3}| &= |gh \in E(G); \mu_g = 2, \mu_h = 3| \Rightarrow |E_{2,3}| = 2 \\ |E_{2,n}| &= |gh \in E(G); \mu_g = 2, \mu_h = n| \Rightarrow |E_{2,n}| = 2 \\ |E_{3,3}| &= |gh \in E(G); \mu_g = 3, \mu_h = 3| \Rightarrow |E_{3,3}| = n - 3 \\ |E_{3,n}| &= |gh \in E(G); \mu_g = 3, \mu_h = n| \Rightarrow |E_{3,n}| = n - 2 \end{aligned}$$

By using the definition of M-polynomial

$$\begin{aligned} M(\Omega; g, h) &= \sum_{i \leq j} m_{ij} ((\Omega)g^i h^j) \\ &= \sum_{2 \leq 3} (m_{ij}(H_n)g^i h^j) + \sum_{2 \leq n} (m_{ij}(H_n)g^i h^j) \\ &\quad + \sum_{3 \leq 3} (m_{ij}(H_n)g^i h^j) + \sum_{3 \leq n} (m_{ij}(H_n)g^i h^j) \\ &= |E_{2,3}|g^2h^3 + |E_{2,n}|g^2h^n + |E_{3,3}|g^3h^3 \\ &\quad + |E_{3,n}|g^3h^n \end{aligned}$$

$$M(F_n; g, h) = 2g^2h^3 + 2g^2h^n + (n - 3)g^3h^3 + (n - 2)g^3h^n$$

Hence the proof. ■

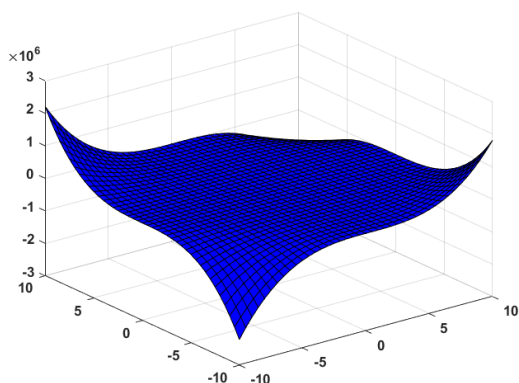


Fig. 14. 3D-Plots of M-Polynomial of Fan graph

**Theorem 2.14:** If  $F_n$  is a fan, then

1.  $M_1(F_n) = n^2 + 9n - 10$
2.  $M_2(F_n) = 3n^2 + 7n - 15$
3.  ${}^m M_2(F_n) = \frac{n^2 + 3n + 3}{9n}$

4.  $H(F_n) = \frac{4}{5} + \frac{4}{2+n} + \frac{n-3}{3} + \frac{4n-4}{3+n}$
5.  $SDD(F_n) = \frac{n^2 - 2n + 13}{n^2 - 2n + 13} + \frac{n^2 + 3n - 2}{n^2 + 3n - 2} + (2n - 6)$
6.  $ISI(F_n) = \frac{3n(n-2)}{n+3} + \frac{4n}{n+2} + \frac{15n-21}{10}$
7.  $F(F_n) = n_3 + 27n - 38$
8.  $A(F_n) = n^4 - 52n^3 + 27n - 27$

**Proof: 1. First Zagreb index**

$$\begin{aligned} t(g, h) &= 2g^2h^3 + 2g^2h^n + (n - 3)g^3h^3 + (n - 2)g^3h^n \\ D_g t(g, h) &= 4g^2h^3 + 4g^2h^n + 3(n - 3)g^3h^3 \\ &\quad + 3(n - 2)g^3h^n \end{aligned}$$

$$\begin{aligned} D_h t(g, h) &= 6g^2h^3 + 2ng^2h^n + 3(n - 3)g^3h^3 \\ &\quad + n(n - 2)g^3h^n \end{aligned}$$

$$\begin{aligned} (D_g + D_h)(t(g, h)) &= 10g^2h^3 + (2n + 4)g^2h^n \\ &\quad + 6(n - 3)g^3h^3 + (n + 3)(n - 2)g^3h^n \end{aligned}$$

$$M_1[F_n] = (D_g + D_h)(t(g, h))|_{g=h=1} = n^2 + 9n - 10$$

**2. Second Zagreb index**

$$\begin{aligned} t(g, h) &= 2g^2h^3 + 2g^2h^n + (n - 3)g^3h^3 + (n - 2)g^3h^n \\ D_h t(g, h) &= 6g^2h^3 + 2ng^2h^n + 3(n - 3)g^3h^3 \\ &\quad + n(n - 2)g^3h^n \end{aligned}$$

$$\begin{aligned} D_g \cdot D_h t(g, h) &= 12g^2h^3 + 4ng^2h^n \\ &\quad + 9(n - 3)g^3h^3 + 3n(n - 2)g^3h^n \end{aligned}$$

$$M_2[F_n] = D_g \cdot D_h t(g, h)|_{g=h=1} = 3n^2 + 7n - 15$$

**3. Second Modified Zagreb index**

$$\begin{aligned} t(g, h) &= 2g^2h^3 + 2g^2h^n + (n - 3)g^3h^3 + (n - 2)g^2h^n \\ S_h t(g, h) &= \frac{2}{3}g^2h^2 + \frac{2}{n}g^2h^n \\ &\quad + \frac{(n - 3)}{3}g^3h^3 + \frac{n - 2}{n}g^3h^3 \end{aligned}$$

$$\begin{aligned} S_g \cdot S_h t(g, h) &= \frac{1}{3}g^2h^3 + \frac{1}{n}g^2h^n \\ &\quad + \frac{n - 3}{9}g^3h^3 + \frac{n - 2}{3n}g^3h^3 \end{aligned}$$

$${}^m M_2[F_n] = S_g \cdot S_h t(g, h)|_{g=h=1} = \frac{n^2 + 3n + 3}{9n}$$

**4. Harmonic index**

$$\begin{aligned} t(g, h) &= 2g^2h^3 + 2g^2h^n + (n - 3)g^3h^3 + (n - 2)g^3h^n \\ Jt(g, h) &= 2g^5 + 2g^{2+n} + (n - 3)g^6 + (n - 2)g^{3+n} \end{aligned}$$

$$\begin{aligned} S_g Jt(g, h) &= \frac{2}{5}g^5 + \frac{2}{2+n}g^{2+n} \\ &\quad + \frac{n - 3}{6}g^6 + \frac{n - 2}{3+n}44g^{3+n} \end{aligned}$$

$$\begin{aligned} 2S_g Jt(g, h) &= \frac{4}{5}g^5 + \frac{2}{2+n}g^{2+n} \\ &\quad + \frac{n - 3}{3}g^6 + \frac{2(n - 2)}{3+n}g^{3+n} \end{aligned}$$

$$H[F_n] = 2S_g Jt(g, h)|_{g=h=1}$$

$$H[F_n] = \frac{4}{5} + \frac{4}{2+n} + \frac{n-3}{3} + \frac{4n-4}{3+n}$$

5. Symmetric division deg index

$$\begin{aligned}
 t(g, h) &= 2g^2h^3 + 2g^2h^n + (n - 3)g^3h^3 + (n - 2)g^3h^n \\
 S_{ht}(g, h) &= \frac{2}{3}g^2h^3 + \frac{2}{n}g^2h^n + \frac{n-3}{3}g^3h^3 + \frac{n-2}{n}g^3h^n \\
 D_g S_{ht}(g, h) &= \frac{4}{3}g^2h^3 + \frac{4}{n}g^2h^n + (n - 3)g^3h^3 \\
 &+ 3\left(\frac{n-2}{n}\right)g^3h^n \\
 D_{ht}(g, h) &= 6g^2h^3 + 2ng^2h^n \\
 &+ 3(n - 3)g^3h^3 + n(n - 2)g^3h^n \\
 S_g D_{ht}(g, h) &= 3g^2h^3 + ng^2h^n \\
 &+ (n - 3)g^3h^3 + \frac{n(n-2)}{3}g^3h^n \\
 SDD[F_n] &= D_g S_h + S_g D_h|_{g=h=1} \\
 SDD[F_n] &= \frac{n^2 - 2n + 13}{3} + \frac{n^2 + 3n - 2}{n} + (2n - 6)
 \end{aligned}$$

6. Inverse sum index

$$\begin{aligned}
 t(g, h) &= 2g^2h^3 + 2g^2h^n + (n - 3)g^3h^3 + (n - 2)g^3h^n \\
 D_{ht}(g, h) &= 6g^2h^3 + 2ng^2h^n \\
 &+ 3(n - 3)g^3h^3 + n(n - 2)g^3h^n \\
 D_g \cdot D_{ht}(g, h) &= 12g^2h^3 + 4ng^2h^n \\
 &+ 9(n - 3)g^3h^3 + 3n(n - 2)g^3h^n \\
 JD_g \cdot D_{ht}(g, h) &= 12g^5 + 4ng^{n+2} \\
 &+ 9(n - 3)g^6 + 3n(n - 2)g^{n+3} \\
 S_g JD_g \cdot D_{ht}(g, h) &= \frac{12}{5}g^5 + \frac{4n}{n+2}g^{n+2} + \frac{9(n-3)}{6}g^6 \\
 &+ \frac{3n(n-2)}{3+n}g^{3+n} \\
 ISI[F_n] &= S_g JD_g \cdot D_{ht}(g, h)|_{g,h=1} \\
 ISI[F_n] &= \frac{3n(n-2)}{n+3} + \frac{4n}{n+2} + \frac{15n-21}{10}
 \end{aligned}$$

7. Forgotten topological index

$$\begin{aligned}
 t(g, h) &= 2g^2h^3 + 2g^2h^n \\
 &+ (n - 3)g^3h^3 + (n - 2)g^3h^n \\
 D_g^2 t(g, h) &= 8g^2h^3 + 8g^2h^n \\
 &+ 9(n - 3)g^3h^3 + 9(n - 2)g^3h^n \\
 D_h^2 t(g, h) &= 18^2h^3 + 2n^2g^2h^n \\
 &+ 9(n - 3)g^3h^3 + n^2(n - 2)g^3h^n \\
 D_g^2 + D_h^2 t(g, h) &= 26g^2h^3 + (2n^2 + 8)g^2h^n \\
 &+ 18(n - 3)g^3h^3 + (n^2 + 9)(n - 2)g^3h^n \\
 F[F_n] &= D_g^2 + D_h^2 t(g, h)|_{g=h=1} = n^3 + 27n - 38
 \end{aligned}$$

8. Augmented Zagreb index

$$\begin{aligned}
 t(g, h) &= 2g^2h^n + 2g^2h^3 + (n - 3)g^3h^3 + (n - 2)g^3h^n \\
 D_h^3 t(g, h) &= 54g^2h^3 + 2n^3g^2h^n \\
 &+ 27(n - 3)g^3h^3 + n^3(n - 2)g^3h^n \\
 D_g \cdot D_h^3 t(g, h) &= 432g^2h^3 + 16n^3g^3h^n + 729(n - 3)g^2h^3 \\
 &+ (27n^4 - 54n^3)g^3h^n \\
 JD_g \cdot D_h^3 t(g, h) &= 432g^5 + 16n^3g^{2+n} + 729ng^5 - 2187g^5 \\
 &+ 27n^4g^{n+1} - 145n^3g^{3+n} \\
 Q_{-2} JD_g \cdot D_h^3 t(g, h) &= 432g^3 + 16n^3g^n + 729ng^3 - 2187g^3 \\
 &+ 27n^4g^{n+1} - 1458n^3g^{n+1} \\
 S_g Q_{-2} JD_g \cdot D_h^3 t(g, h) &= 54g^3 + 2n^3g^n + 27ng^3 - 81g^3 \\
 &+ n^4g^{n+1} - 54n^3g^{n+1} \\
 S_g Q_{-2} JD_g \cdot D_h^3 t(g, h)|_{g,h=1} & \\
 A[F_n] &= n^4 - 52n^3 + 27n - 27
 \end{aligned}$$

Hence the proof. ■

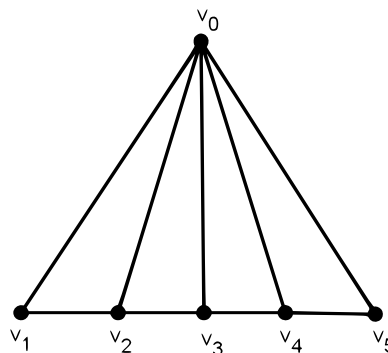


Fig. 15. Example of Fan graph  $F_5$

In Fig.15, the Fan graph  $F_5$  is depicted, with the following calculated topological indices:

TABLE VI  
NUMERICAL VALUES OF FAN GRAPH

Topological Indices	Numerical values
First zagreb index	60
Second zagreb index	95
Second modified zagreb index	0.956
Harmonic index	2.788
Symmetric division deg index	6
Inverse sum index	13.822
Forgotten topological index	222
Augmented zagreb index	159.774

III. CONCLUSION

Topological indices are numerical descriptors derived from the molecular graph of a chemical compound. These indices encode structural information about the molecule in a way that is often useful for predicting various properties or activities of the compound. They are widely used in quantitative structure-activity relationship (QSAR) studies, which aim to correlate the structure of a molecule with its biological activity, chemical reactivity, or other properties. The M-polynomial and topological indices are commonly used in

mathematical chemistry to describe the molecular structure of chemical compounds. Being able to forecast the properties of compounds can have significant implications across various industries, from pharmaceuticals to materials science and beyond. Predictive modeling in chemistry can help streamline the discovery and development process of new compounds, potentially leading to breakthroughs in areas like drug design, materials engineering, and environmental remediation. For example, the Zagreb indices are used to calculate total  $\pi$ -electronic energy, the harmonic index is used for medication configuration, the symmetric division deg index is a good predictor of the total surface area, and the augmented Zagreb index is a good predictor of the heat of information.

REFERENCES

- [1] J.A. Bondy, U.S.R Murthy, Graph Theory with applications, Macmillan Press, New York USA, 1976.
- [2] M.Naeem, M.K.Siddiqui, J.L.G. Guirao, W.Gao, "New and Modified Eccentric indices of Octagonal Grid  $O_{mn}$ ," *Applied Mathematics and Nonlinear Sciences*, vol. 3, no. 1, pp. 209-228, 2018.
- [3] W. Gao, L. Shi and M.R. Farahani, "Distance-based indices for some families of dendrimer nanostars," *IAENG International Journal of Applied Mathematics*, vol.46, no.2, pp.168-186, 2016.
- [4] I.Gutman, "Some properties of the Wiener polynomials," *Graph Theory Notes, Newyork*, vol. 44, pp. 13-18, 1993.
- [5] A.R. Ashrafi, B. Manoochehrian, and H.Yousefi-Azari, "On the PI polynomial of a graph" *Util Math.*, vol. 71, pp. 97-108, 2006.
- [6] T. Doslic, "Planar polycyclic graphs and their tutte polynomials," *J. Math. Chem.*, vol. 51, pp. 1599-1607, 2013.
- [7] E.J. Farrell, "An introduction to matching polynomials," *J. Combin. Theory Ser. B*, vol. 27, pp. 75-86, 1979.
- [8] F. Hassani, A. Iranmanesh and S. Mirzaie, "Schultz and modified Schultz polynomials of  $C_{100}$  fullerene," *MATCH Commun. Math. Comput. Chem.*, vol. 69, pp. 87-92, 2013.
- [9] H.Zhang, F.Zhang, "The clar covering polynomial of hexagonal systems I," *Discrete Appl. Math.*, vol. 69, pp. 147-167, 1996.
- [10] V. Alamian, A. Bharami, and B. Edalatzadeh, "PI polynomial of V-Phenylenic of nanotubes and nanotori," *Int. J. Mole. SCI*, vol. 9, no. 3, pp. 229-234, 2008.
- [11] A.T.Balaban, "Highly discriminating distance based numerical descriptor," *Chemical Physics Letters*, vol. 89, no. 5, pp.399-404, 1982.
- [12] W.Gao and L.Shi, "Szeged related indices of unilateral polyomino chain and unilateral hexagonal chain," *IAENG International Journal of Applied Mathematics*, vol. 45, no.2, pp. 138-150, 2015.
- [13] S.Fajtlowicz, "On Conjectures of graffitti II. Congr," *Chemical Physics Letters*, vol. 860, pp. 189-197, 1987.
- [14] R.Shao and L.Zuo, "Hued colorings of cartesian products of square of cycles with paths," *IAENG International Journal of Applied Mathematics*, vol. 48, no.3, pp.258-267, 2018.
- [15] E.Deutsch, and S.Klavzar, "M-Polynomial and degree-based topological indices," *Iran J. Math. Chem.*, vol. 6, no. 2, pp. 93-102, 2015.
- [16] I. Gutman, N.Trinajstic, "Graph Theory and molecular orbitals, total  $\pi$  electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535-538, 1972.
- [17] A. Milicevic, S. Nikolic, N.Trinajstic, "On reformulated zagreb indices," *Mol. Divers*, vol. 8, pp. 393-399, 2004.
- [18] Y.Hu, X.Li, Y.Shi, T.Xu, and I.Gutman, "On molecular graphs with smallest and greatest zeroth-order general randic index," *MATCH Commun. Math. Chem*, vol. 54, pp. 425-434, 2005.
- [19] G.Caporossi, I.Gutman, P.Hansen, and L.Pavlovic, "Graphs with maximum connectivity index," *Comput. Biol. Chem.*, vol. 27, 2003.
- [20] X.Li, I.Gutman, "Mathematical aspects of Randic-type molecular structure descriptors," *Mathematical Chemistry Monographs, No.1 Publisher, University of Kragujevac*,2006.
- [21] B.S. Shetty, V.Lokesha, P.S.Ranjini, "On the harmonic index of graph operations," *Trans. Combin*, vol. 4, pp. 5-14, 2015.
- [22] V.K.Gupta, V.Lokesha, S.B. Shwetha, and P.S.Ranjini, "On the Symmetric division deg index of graph," *Southeast Asian Bull.Math*, vol. 40, pp. 59-80, 2016.
- [23] Jelena Sedlar, Dragan Stevanovic, Alexander vasilyev, "On the inverse sum indeg index," *Discrete Applied Mathematics*, vol. 184, pp. 202-212, 2015.
- [24] B.Furtula, I.Gutman, "A forgotten topological indices," *Journal of Mathematical Chemistry*, vol. 53, no. 4, pp. 1184-1190, 2015.
- [25] B.Furtula, A. Gravoac, and D.Vukicevic, "Augmented Zagreb index," *Journal of Mathematical Chemistry*, vol. 48, pp. 370-380, 2010.
- [26] O.Ozgecolakoglu, "NM-Poynomials and Topological indices of some cycle-related graphs," *Symmetry*, vol. 14, 2022.
- [27] A.Alsini, A.Alwardi, M.R.Farahani, S.Nandappad, "On  $\psi_k$  polynomial of graph," *Eurasian Chemical Communication*, vol. 3, no. 4, pp. 219-226, 2022.
- [28] J.A.Gallian, "A dynamic survey of graph labelling," *Electron. J. Combin*, vol. 502, pp. 1-623, 2018.