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On the M-polynomial and topological descriptors of the special graph SG_n^2

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Abstract

Topological indices play a significant role in investigating and correlating the physical and chemical properties of hydrocarbon compounds. The M-polynomial has emerged as an effective mathematical tool for determining several degree-based topological descriptors associated with chemical structures. In this study, a complete graph of order 2 is employed to construct the special graph SG_n^2 through an edge-construction approach. The corresponding M-polynomial of the graph is derived and used to evaluate various degree-based topological indices, including the first Zagreb index $M_1(G)$, the second Zagreb index $M_2(G)$, and the modified Zagreb index obtained through the counting principle of 2-cycles in SG_n^2 . In addition, the symmetric sum division index $SS(G)$, the generalized Randic index $R_\alpha(G)$, and the inverse Randic index $RR_\alpha(SG_n^2)$ are computed using the obtained M-polynomial. The results demonstrate the effectiveness of the M-polynomial in determining important topological descriptors of graph-based molecular structures.

Keywords: Molecular graph, degree based topological indices, M-Polynomial, Cayley Tree, Modified Cayley Graph

Introduction

Chemical compounds can be represented effectively through graph-theoretical models, in which the structural characteristics of molecules are translated into mathematical objects. Graph theory provides a powerful framework for investigating the relationship between the structure, properties, and biological activities of chemical compounds. In chemical graph theory, atoms are represented by vertices, while chemical bonds are represented by edges. This graphical representation enables researchers to analyze molecular structures quantitatively and establish relationships between molecular descriptors and various physicochemical properties. Topological indices are numerical descriptors derived from the graph representation of a molecule. These graph invariants play an important role in studying the structural properties of chemical compounds and have found extensive applications in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR). By converting molecular structures into numerical values, topological indices provide an efficient method for predicting chemical and biological properties without performing extensive experimental investigations.

In this paper, all graphs under consideration are assumed to be simple, finite, and connected. Let $G = (V(G), E(G))$ be a graph, where $V(G)$ denotes the set of vertices and $E(G)$ denotes the set of edges. If $v \in V(G)$, then the degree of the vertex (v), denoted by $d(v)$, is defined as the number of edges incident with v .

Over the years, numerous degree-based topological indices have been developed to investigate the structural characteristics of chemical graphs. Among the most widely studied descriptors are the first Zagreb index, the second Zagreb index, the modified Zagreb index, the Randic index, and the harmonic index. These indices have been successfully applied in chemistry, pharmacology, and molecular biology to characterize chemical compounds and predict their physical, chemical, and biological properties ^[1].

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The concept of the M-polynomial was introduced by Deutsch and Klavžar in 2015 as an efficient mathematical tool for computing degree-based topological indices of chemical graphs [2]. The M-polynomial provides a unified approach for deriving several topological descriptors and has attracted considerable attention in the field of chemical graph theory. Since its introduction, many researchers have investigated its mathematical properties and demonstrated its effectiveness in evaluating various graph invariants associated with molecular structures [3, 4].

Several studies have extended the application of the M-polynomial to different classes of chemical graphs. These investigations have shown that the polynomial offers a systematic and convenient method for calculating a wide range of degree-based topological indices, thereby reducing computational complexity and providing deeper insight into the structural characteristics of chemical compounds.

In 2017, P. Gayathri and U. Priyanka determined several degree-based topological indices for the zig-zag chain of 8-cycle molecular graphs. Their study included the computation of the Randic index, geometric-arithmetic index, sum-connectivity index, harmonic index, first Zagreb index, second Zagreb index, modified second Zagreb index, inverse sum index, Albertson index, atom-bond connectivity index, symmetric division index, and augmented Zagreb index. The obtained results were expressed in terms of the parameters (a) and (n), where (a) denotes the number of hexagons and (n) represents the number of segments in the molecular graph [5].

In a graph G , M-polynomial $M(G, x, y)$, is given by

$$M(G, x, y) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(G) x^i y^j \quad (1.1)$$

where m_{ij} is total number of edges in G such that its end vertices have degree i and j , $\delta = \min\{d(u) : u \in V(G)\}$ and $\Delta = \max\{d(u) : u \in V(G)\}$. Is the minimum degree among all the vertices of graph G and is the maximum degree among all the vertices of graph G .

In this paper we have used M-polynomial to compute First Zagreb index $M_1(G)$, Second Zagreb index $M_2(G)$, the modified Zagreb index $mM_2(G)$, Randic' index $R_\alpha(G)$ and $SSD(G)$ of a special graph which are defined as follows:

$$M_1(G) = \sum_{v \in V(G)} d^2(v) \quad (1.2)$$

and

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v) \quad (1.3)$$

$$mM_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)} \quad (1.4)$$

$$R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha \quad (1.5)$$

The inverse Randic index $RR_\alpha(G)$, Symmetric sum division index $SSD(G)$ is studied in [3] and defined as follows:

$$RR_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d(u)d(v))^\alpha} \quad (1.6)$$

$$SSD(G) = \sum_{uv \in E(G)} \frac{(d^2(u)d^2(v))}{(d(u)d(v))} \quad (1.7)$$

The topological indices can be derived from M-polynomial, which are given in the preceding table:

Table 1: Relationship between topological indices and M-polynomial

Topological index	Derivation from $M(G, x, y)$
$M_1(G)$	$[(D_x + D_y)M(G, x, y)]_{x=y=1}$
$M_2(G)$	$[(D_x D_y)M(G, x, y)]_{x=y=1}$
$mM_1(G)$	$[(S_x S_y)M(G, x, y)]_{x=y=1}$
$R_\alpha(G)$	$[(D_x^\alpha D_y^\alpha)M(G, x, y)]_{x=y=1}$
$RR_\alpha(G)$	$[(S_x^\alpha S_y^\alpha)M(G, x, y)]_{x=y=1}$
$SSD(G)$	$[(S_x D_y + S_y D_x)M(G, x, y)]_{x=y=1}$

where the operators D_x , D_y , S_x , and S_y are given by

$$D_x f(x, y) = x \frac{\partial f(x, y)}{\partial x} \quad (1.8)$$

$$D_y f(x, y) = y \frac{\partial f(x, y)}{\partial y} \quad (1.9)$$

$$S_x f(x, y) = \int_0^x \frac{f(t, y)}{t} dt \quad (1.10)$$

and

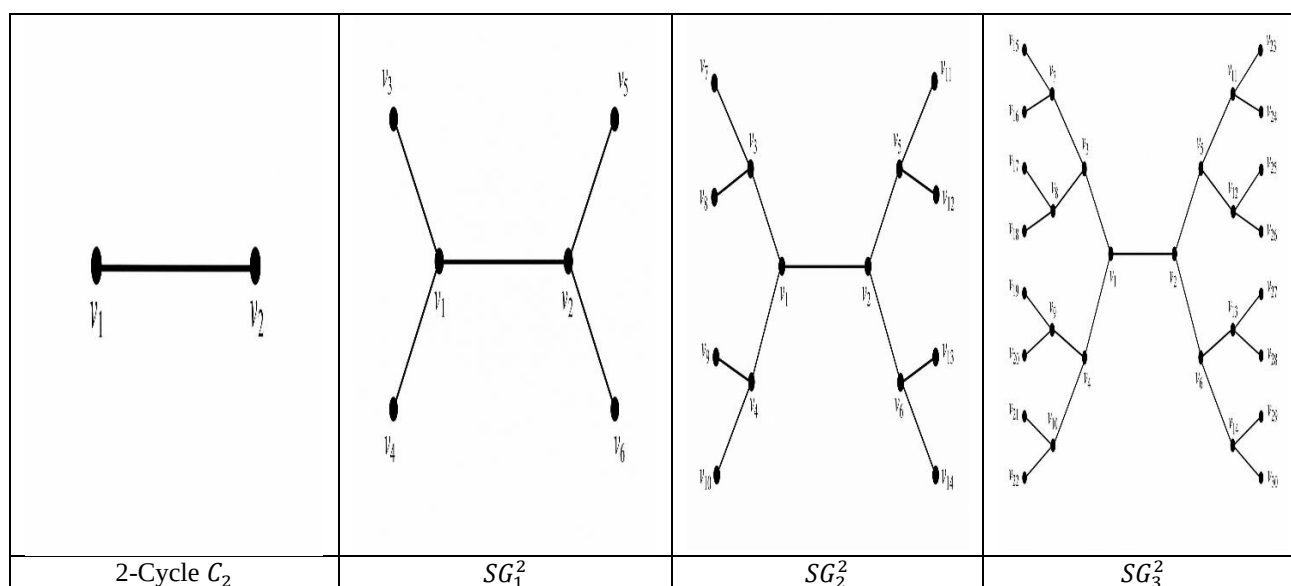
$$S_y f(x, y) = \int_0^y \frac{f(x, t)}{t} dt \quad (1.11)$$

The special graph SG_n^2 is a planar graph obtained by a recursive path-construction procedure. The construction begins with a path of order 2, which serves as the fundamental building block of the graph. New paths are successively attached to the pendent vertices of the existing graph to generate a sequence of special graphs.

In this construction, the graph SG_0^2 consists of the initial path and is referred to as the root path or level 0 of the construction. A new path is attached to each pendent vertex of SG_0^2 , producing the graph SG_1^2 . The path-construction process is then repeated by adjoining new paths to all pendent vertices created at the previous stage.

Similarly, the same procedure is applied to SG_1^2 to obtain SG_2^2 . At each successive stage, all newly created vertices are joined to form a path on the outer face of the graph, resulting in the next member of the sequence. Repeating this process n times generates the family of special graphs SG_n^2 .

Thus, SG_n^2 is constructed recursively by attaching new paths to the pendent vertices at every level. If the initial path is considered to be at level 0, then the graph obtained after the first iteration corresponds to level 1, the graph obtained after the second iteration corresponds to level 2, and so on. Consequently, after adding new edges or paths to the vertices of the preceding level, a sequence of special graphs SG_n^2 is obtained.



The recursive nature of this construction makes SG_n^2 suitable for studying graph invariants and deriving degree-based topological indices through the M-polynomial approach.

2. Results on Topological Indices of the Special Graph SG_n^2

2.1 Proposition: - Let SG_n^2 be the special graph then $|V(SG_n^2)| = 2 \cdot (2^{n+1} - 1)$ and $|E(SG_n^2)| = 2^{n+2} - 3$

Proof: - To enumerate the number of vertices we develop a counting method. We observe that 2^{n+1} levels in graph SG_n^2 and every n^{th} level has exactly n vertices.

The total number of vertices on n^{th} level $= 2 + 2^2 + 2^3 + \dots + 2^{n+1} = 2 \cdot [1 + 2 + 2^2 + \dots + 2^n]$

By geometric progression,

$$= \frac{2 \cdot [1 \cdot (2^{n+1} - 1)]}{2 - 1}$$

$$= 2 \cdot (2^{n+1} - 1)$$

So,

$$|V(SG_n^2)| = 2 \cdot (2^{n+1} - 1)$$

Also, to enumerate the number of edges we develop approach considering edges at every level and the edges between two preceding levels.

We observe that $2, 2, 2, 2^2, 2, 2^3, \dots, 2^n$ edges added at $0, 1, 2, 3, \dots, n$ levels. And $4, 8, 16, \dots, 2^n$ edges between first level and second level, second level and third level, and third level and fourth level and so on. up to n^{th} level and $(n+1)^{th}$ level respectively. So, $|E(SG_n^2)| =$ addition of on and between two consecutive levels

$$|E(SG_n^2)| = 2^{n+2} - 3$$

Next, we define the value of incidence $m_{(i,j)}$ in the graph G as total number of edges in edge set E with end vertex having degree- i and degree- j .

2.2 Lemma: - Let SG_n^2 be the special graph then the values of incidence of special graph are $m_{(1,3)} = 2^{n+1}$ where, $n \geq 1$

And $m_{(3,3)} = 2^{n+1} - 3$ where, $n \geq 1$

Proof: - From the graph we observe that at the level 1 and level 2 there are 4 edges such that their end vertices have degree-1 and degree-3.

Also, between the level n and level $n+1$ there are 2^{n+1} edges such that end vertices have degree-1 and degree-3.

$$\therefore m_{(1,3)} = 2^{n+1} \text{ where, } n \geq 1$$

Next, we count the number of edges having value of incidence $m_{(3,3)}$ at level $n+1$ there are $2^{n+1} - 3$ edges such that end vertices have degree-3 and degree-3.

$$\therefore m_{(3,3)} = 2^{n+1} - 3 \text{ where, } n \geq 1$$

2.3 Proposition: - Let SG_n^2 be the special graph then the M-polynomial of SG_n^2 is $M(SG_n^2, x, y) = 2^{n+1}xy^3 + (2^{n+1} - 3)x^3y^3$

Proof: - Employing definition of M-polynomial of SG_n^2 graph we get,

$$M(SG_n^2, x, y) = \sum_{0 \leq i \leq j \leq 4} m_{(i,j)}(SG_n^2) x^i y^j$$

$$M(SG_n^2, x, y) = m_{(1,3)}xy^3 + m_{(3,3)}x^3y^3$$

$$M(SG_n^2, x, y) = 2^{n+1}xy^3 + (2^{n+1} - 3)x^3y^3$$

Now for convenience, we denote the M-polynomial of SG_n^2 by $f(x, y)$ i.e., $f(x, y) = 2^{n+1}xy^3 + (2^{n+1} - 3)x^3y^3$

Next, we compute the operator needed for the estimation of the Next, we compute the operator needed for estimation of DBTI's

$$D_x f(x, y) = x \frac{\partial f(x, y)}{\partial x}$$

$$D_x f(x, y) = x[2^{n+1}y^3 + 3.(2^{n+1} - 3)x^2y^3]$$

$$D_x f(x, y) = 2^{n+1}xy^3 + 3.(2^{n+1} - 3)x^3y^3 \quad (2.3.1)$$

$$D_y f(x, y) = y \frac{\partial f(x, y)}{\partial y}$$

$$D_y f(x, y) = y[3.2^{n+1}xy^2 + 3.(2^{n+1} - 3)x^3y^2]$$

$$D_y f(x, y) = 3.2^{n+1}xy^3 + 3.(2^{n+1} - 3)x^3y^3 \quad (2.3.2)$$

$$S_x f(x, y) = \int_0^x \frac{f(t, y)}{t} dt$$

$$S_x f(x, y) = \int_0^x \frac{1}{t} [2^{n+1}ty^3 + (2^{n+1} - 3)t^3y^3] dt$$

$$S_x f(x, y) = \int_0^x [2^{n+1}y^3 + (2^{n+1} - 3)t^2y^3] dt$$

$$S_x f(x, y) = 2^{n+1}xy^3 + \frac{1}{3}(2^{n+1} - 3)x^3y^3 \quad (2.3.3)$$

$$S_y f(x, y) = \int_0^y \frac{f(t, y)}{t} dt$$

$$S_y f(x, y) = \int_0^y \frac{1}{t} [2^{n+1}xt^3 + (2^{n+1} - 3)x^3t^3] dt$$

$$S_y f(x, y) = \int_0^y [2^{n+1}xt^2 + (2^{n+1} - 3)x^3t^2] dt$$

$$S_y f(x, y) = \frac{1}{3} \cdot 2^{n+1}xy^3 + \frac{1}{3} \cdot (2^{n+1} - 3)x^3y^3 \quad (2.3.4)$$

$$Jf(x, y) = f(x, x) = 2^{n+1}x^4 + (2^{n+1} - 3)x^6 \quad (2.3.5)$$

2.4 Theorem:- Let SG_n^2 be the special graph then it's first Zagreb index of SG_n^2 is $M_1(SG_n^2) = 2^{n+3} + 6 \cdot (2^{n+1} - 3)$

The second Zagreb index of SG_n^3 is $M_2(SG_n^2) = 3 \cdot 2^{n+1} + 9 \cdot (2^{n+1} - 3)$

And the modified Zagreb index of SG_n^3 is $mM_2(SG_n^2) = 3 \cdot 2^{n-3} + \frac{3}{8}(3 \cdot 2^{n-2} - 1)$

Proof:- Initially computation of first Zagreb index of SG_n^2 involves the addition of equation (2.3.1) and equation (2.3.2) we have By adding equation (2.3.1) and equation (2.3.2) we have

$$(D_x + D_y)f(x, y) = [2^{n+1}xy^3 + 3 \cdot (2^{n+1} - 3)x^3y^3] + [3 \cdot 2^{n+1}xy^3 + 3 \cdot (2^{n+1} - 3)x^3y^3]$$

$$(D_x + D_y)f(x, y) = [2^{n+3}xy^3 + 6 \cdot (2^{n+1} - 3)x^3y^3]$$

Now,

$$M_1(SG_n^2) = [2^{n+3}xy^3 + 6 \cdot (2^{n+1} - 3)x^3y^3]_{x=y=1}$$

$$M_1(SG_n^2) = 2^{n+3} + 6 \cdot (2^{n+1} - 3) \quad (2.4.1)$$

We evaluate the second Zagreb index of SG_n^3

$$D_y D_x f(x, y) = D_y [2^{n+1}xy^3 + 3 \cdot (2^{n+1} - 3)x^3y^3]$$

$$D_y D_x f(x, y) = y \frac{\partial}{\partial y} [2^{n+1}xy^3 + 3 \cdot (2^{n+1} - 3)x^3y^3]$$

$$D_y D_x f(x, y) = y [3 \cdot 2^{n+1}xy^2 + 9 \cdot (2^{n+1} - 3)x^3y^2]$$

$$D_y D_x f(x, y) = [3 \cdot 2^{n+1}xy^3 + 9 \cdot (2^{n+1} - 3)x^3y^3]$$

$$M_2(SG_n^2) = [3 \cdot 2^{n+1}xy^3 + 9 \cdot (2^{n+1} - 3)x^3y^3]_{x=y=1}$$

$$M_2(SG_n^2) = 3 \cdot 2^{n+1} + 9 \cdot (2^{n+1} - 3) \quad (2.4.2)$$

The modified Zagreb index is,

$$S_x S_y f(x, y) = \int_0^x \frac{1}{t} \left[\frac{1}{3} \cdot 2^{n+1}ty^3 + \frac{1}{3} \cdot (2^{n+1} - 3)t^3y^3 \right] dt$$

$$S_x S_y f(x, y) = \int_0^x \left[\frac{1}{3} \cdot 2^{n+1}y^3 + \frac{1}{3} \cdot (2^{n+1} - 3)t^2y^3 \right] dt$$

$$S_x S_y f(x, y) = \frac{1}{3} \cdot 2^{n+1}xy^3 + \frac{1}{9} \cdot (2^{n+1} - 3)x^3y^3$$

$$mM_2(SG_n^2) = \left[\frac{1}{3} \cdot 2^{n+1}xy^3 + \frac{1}{9} \cdot (2^{n+1} - 3)x^3y^3 \right]_{x=y=1}$$

$$mM_2(SG_n^2) = \frac{1}{3} \cdot 2^{n+1} + \frac{1}{9} \cdot (2^{n+1} - 3) \quad (2.4.3)$$

2.5 Theorem: - Let SG_n^2 be the special graph then the generalized Randic index of SG_n^2 is $R_\alpha(SG_n^2) = 3^\alpha \cdot 2^{n+1} + 3^{2\alpha} \cdot (2^{n+1} - 3)$

And Inverse Randic index of SG_n^2 is $RR_\alpha(SG_n^2) = \frac{1}{3^\alpha} \cdot 2^{n+1} + \frac{1}{3^{2\alpha}} \cdot (2^{n+1} - 3)$

Proof: - We first compute the Randic index of SG_n^2

$$D_y f(x, y) = 3 \cdot 2^{n+1}xy^3 + 3 \cdot (2^{n+1} - 3)x^3y^3$$

$$D_y^\alpha f(x, y) = 3^\alpha \cdot 2^{n+1}xy^3 + 3^\alpha \cdot (2^{n+1} - 3)x^3y^3$$

$$D_x D_y^\alpha f(x, y) = x \frac{\partial}{\partial x} [3^\alpha \cdot 2^{n+1}xy^3 + 3^\alpha \cdot (2^{n+1} - 3)x^3y^3]$$

$$D_x D_y^\alpha f(x, y) = x [3^\alpha \cdot 2^{n+1}y^3 + 3 \cdot 3^\alpha \cdot (2^{n+1} - 3)x^2y^3]$$

$$D_x D_y^\alpha f(x, y) = 3^\alpha \cdot 2^{n+1}xy^3 + 3 \cdot 3^\alpha \cdot (2^{n+1} - 3)x^3y^3$$

$$D_x^\alpha D_y^\alpha f(x, y) = 1^\alpha \cdot 3^\alpha \cdot 2^{n+1}xy^3 + 3^\alpha \cdot 3^\alpha \cdot (2^{n+1} - 3)x^3y^3$$

$$D_x^\alpha D_y^\alpha f(x, y) = 3^\alpha \cdot 2^{n+1}xy^3 + 3^{2\alpha} \cdot (2^{n+1} - 3)x^3y^3$$

Thus,

$$R_\alpha(SG_n^2) = [3^\alpha \cdot 2^{n+1}xy^3 + 3^{2\alpha} \cdot (2^{n+1} - 3)x^3y^3]_{x=y=1}$$

$$R_\alpha(SG_n^2) = 3^\alpha \cdot 2^{n+1} + 3^{2\alpha} \cdot (2^{n+1} - 3) \quad (2.5.1)$$

Next we compute Inverse Randic index of special graph SG_n^3

$$S_y f(x, y) = \frac{1}{3} \cdot 2^{n+1}xy^3 + \frac{1}{3} \cdot (2^{n+1} - 3)x^3y^3$$

$$S_y^\alpha f(x, y) = \frac{1}{3^\alpha} \cdot 2^{n+1}xy^3 + \frac{1}{3^\alpha} \cdot (2^{n+1} - 3)x^3y^3$$

$$S_x S_y^\alpha f(x, y) = \int_0^x \frac{1}{t} \left[\frac{1}{3^\alpha} \cdot 2^{n+1}ty^3 + \frac{1}{3^\alpha} \cdot (2^{n+1} - 3)t^3y^3 \right] dt$$

$$S_x S_y^\alpha f(x, y) = \int_0^x \left[\frac{1}{3^\alpha} \cdot 2^{n+1}y^3 + \frac{1}{3^\alpha} \cdot (2^{n+1} - 3)t^2y^3 \right] dt$$

$$S_x S_y^\alpha f(x, y) = \frac{1}{3^\alpha} \cdot 2^{n+1}xy^3 + \frac{1}{3} \cdot \frac{1}{3^\alpha} \cdot (2^{n+1} - 3)x^3y^3$$

$$S_x^\alpha S_y^\alpha f(x, y) = \frac{1}{3^\alpha} \cdot 2^{n+1}xy^3 + \frac{1}{3^\alpha} \cdot \frac{1}{3^\alpha} \cdot (2^{n+1} - 3)x^3y^3$$

$$RR_\alpha(SG_n^2) = \left[\frac{1}{3^\alpha} \cdot 2^{n+1}xy^3 + \frac{1}{3^{2\alpha}} \cdot (2^{n+1} - 3)x^3y^3 \right]_{x=y=1}$$

$$RR_\alpha(SG_n^2) = \frac{1}{3^\alpha} \cdot 2^{n+1} + \frac{1}{3^{2\alpha}} \cdot (2^{n+1} - 3) \quad (2.5.2)$$

2.6 Theorem: - Let SG_n^2 be the special graph then the Harmonic index of SG_n^2 is

$$H(SG_n^2) = 2^{n-1} + \frac{1}{6} \cdot (2^{n+1} - 3)$$

And the inverse sum of index is

$$I(SG_n^2) = 3 \cdot 2^{n-1} + \frac{3}{2} \cdot (2^{n+1} - 3)$$

Proof: - We first compute the Harmonic index of SG_n^2

$$Jf(x, y) = 2^{n+1}x^4 + (2^{n+1} - 3)x^6$$

$$S_x Jf(x, y) = \int_0^x \frac{1}{t} [2^{n+1}t^4 + (2^{n+1} - 3)t^6] dt$$

$$S_x Jf(x, y) = \int_0^x [2^{n+1}t^3 + (2^{n+1} - 3)t^5] dt$$

$$S_x Jf(x, y) = 2^{n-1}x^4 + \frac{1}{6} \cdot (2^{n+1} - 3)x^6$$

$$H(SG_n^2) = \left[2^{n-1}x^4 + \frac{1}{6} \cdot (2^{n+1} - 3)x^6 \right]_{x=1}$$

$$H(SG_n^2) = 2^{n-1} + \frac{1}{6} \cdot (2^{n+1} - 3) \quad (2.6.1)$$

Next, the inverse sum index is determined by considering

$$D_x f(x, y) = 2^{n+1}xy^3 + 3 \cdot (2^{n+1} - 3)x^3y^3$$

$$D_y D_x f(x, y) = y \frac{\partial}{\partial y} [2^{n+1}xy^3 + 3 \cdot (2^{n+1} - 3)x^3y^3]$$

$$D_y D_x f(x, y) = y[3 \cdot 2^{n+1}xy^2 + 9 \cdot (2^{n+1} - 3)x^3y^2]$$

$$D_y D_x f(x, y) = 3 \cdot 2^{n+1}xy^3 + 9 \cdot (2^{n+1} - 3)x^3y^3$$

$$J D_y D_x f(x, y) = 3 \cdot 2^{n+1}x^4 + 9 \cdot (2^{n+1} - 3)x^6$$

$$S_x J D_y D_x f(x, y) = \int_0^x \frac{1}{t} [3 \cdot 2^{n+1}t^4 + 9 \cdot (2^{n+1} - 3)t^6] dt$$

$$S_x J D_y D_x f(x, y) = \int_0^x [3 \cdot 2^{n+1}t^3 + 9 \cdot (2^{n+1} - 3)t^5] dt$$

$$S_x J D_y D_x f(x, y) = \frac{3}{4} \cdot 2^{n+1}x^4 + \frac{3}{2} \cdot (2^{n+1} - 3)x^6$$

Now,

$$I(SG_n^2) = \left[\frac{3}{4} \cdot 2^{n+1}x^4 + \frac{3}{2} \cdot (2^{n+1} - 3)x^6 \right]_{x=1}$$

$$I(SG_n^2) = 3 \cdot 2^{n-1} + \frac{3}{2} \cdot (2^{n+1} - 3) \quad (2.6.2)$$

2.7 Theorem: - For the special graph SG_n^2 symmetric sum division index of SG_n^2 is

$$SSD(SG_n^2) = 3 \cdot 2^n + 3 \cdot 2^{n-1} + 3 \cdot 2^{n+1} + 12 \cdot (3 \cdot 2^{n-2} - 1)$$

Proof: - In order to compute the symmetric sum division index of SG_n^2 we first consider,

$$D_x f(x, y) = 2^{n+1}xy^3 + 3 \cdot (2^{n+1} - 3)x^3y^3$$

$$S_y D_x f(x, y) = \int_0^y \frac{1}{t} [2^{n+1}xt^3 + 3 \cdot (2^{n+1} - 3)x^3t^3] dt$$

$$S_y D_x f(x, y) = \int_0^y [2^{n+1} x t^2 + 3 \cdot (2^{n+1} - 3) x^3 t^2] dt$$

$$S_y D_x f(x, y) = \frac{1}{3} \cdot 2^{n+1} x y^3 + (2^{n+1} - 3) x^3 y^3$$

Now,

$$D_y f(x, y) = 3 \cdot 2^{n+1} x y^3 + 3 \cdot (2^{n+1} - 3) x^3 y^3$$

$$S_x D_y f(x, y) = \int_0^x \frac{1}{t} [3 \cdot 2^{n+1} t y^3 + 3 \cdot (2^{n+1} - 3) t^3 y^3] dt$$

$$S_x D_y f(x, y) = \int_0^x [3 \cdot 2^{n+1} y^3 + 3 \cdot (2^{n+1} - 3) t^2 y^3] dt$$

$$S_x D_y f(x, y) = 3 \cdot 2^{n+1} x y^3 + (2^{n+1} - 3) x^3 y^3$$

From the definition of symmetric sum division index we have,

$$SSD(SG_n^2) = \left[(S_y D_x f(x, y) + S_x D_y f(x, y)) M(G, x, y) \right]_{x=y=1}$$

$$SSD(SG_n^2) = \left[\frac{1}{3} \cdot 2^{n+1} x y^3 + (2^{n+1} - 3) x^3 y^3 + 3 \cdot 2^{n+1} x y^3 + (2^{n+1} - 3) x^3 y^3 \right]_{x=y=1}$$

$$SSD(SG_n^2) = \frac{5}{3} \cdot 2^{n+2} + 2^{n+2} - 6$$

$$SSD(SG_n^2) = \frac{8}{3} \cdot 2^{n+2} - 6 \quad (2.7.1)$$

3. Conclusion

Although explicit formulas provide a direct approach for evaluating topological indices, the present study employs an alternative method based on the M-polynomial to derive various degree-based topological indices of the special graph SG_n^2 . The M-polynomial offers a unified and systematic framework for computing these graph invariants and simplifies the evaluation of several important molecular descriptors. The path-construction procedure adopted in this work leads to the generation of a new family of special graphs. This construction can be extended further by repeatedly adjoining new paths to the pendent vertices and forming successive levels of the graph. Consequently, the proposed approach provides opportunities for future investigations involving different path-construction techniques and the development of other classes of recursively defined special graphs. The methodology presented in this paper can also be applied to determine additional topological indices and to explore their potential applications in chemical graph theory and related areas of mathematical chemistry.

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