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Computational Study of Sombor Index on Generalized Abid–Waheed Graphs for Polymer Modeling

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Abstract

This study investigates the topological properties of generalized Abid Waheed graphs. Development of theoretical models in chemistry, reducing computational complexity while analysing large molecules or networks Abid Waheed graphs play a significant role. Motivated by these findings, the research was extended to encompass generalized Abid Waheed graphs, characterized by r cycles of order s. A notable similarity between Abid Waheed graphs and Jahangir graphs was observed. The potential applications of these findings in network topology and optimization are explored, leveraging the degree-based indices on Abid Waheed graphs as a model for networking systems. In this study, we further examined the topological characteristics of nano star dendrimers through the framework of chemical graph theory by employing Abid Waheed graph models. Nano star dendrimers, a class of star-shaped polymers, possess highly branched and symmetrical structures, making them particularly well-suited for mathematical representation via recursive and hierarchical graphs. Abid Waheed graphs, recognized for effectively capturing the complexity of molecular architectures, were adapted to model various generations of such dendritic polymers. Our analysis focused on two significant graph-theoretic descriptors: the Sombor index, introduced by Gutman et al. in 2021, and the M-polynomial. The Sombor index, defined as: $SO(G) = \sum_{e=xy \in E(G)} \sqrt{d_x^2 + d_y^2}$ *Our findings reveal that both the Sombor index and the M-polynomial are responsive to structural variations in dendrimer generations, displaying consistent and interpretable growth patterns as the dendritic network expands. This work establishes a novel and meaningful connection between topological indices and polymer nanostructures, contributing to the development of computational tools for predicting physicochemical properties and supporting applications in nanomaterial design, drug delivery, and materials science. Furthermore, the Sombor index, through the encoding of degree-based structural properties, is a sensitive indicator of molecular complexity and branching that are directly linked to the physicochemical behaviour of dendritic polymers including nano star dendrimers.*

Keywords: Topological index, degree, polymer abid waheed graph, jahangir graph, network topology, sustainable networking

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INTRODUCTION

Graph theory plays a crucial role in modeling and analyzing various real-world systems, including networks, chemical compounds, and social structures. Topological indices, which are numerical graph invariants, provide valuable insights into the structural properties of these systems. Among these indices, the Sombor index has gained recent attention due to its efficacy in predicting various physicochemical properties of molecules [1]. This research focuses on applying the Sombor index to analyze Abid Waheed graphs, a family of graphs with unique structural characteristics. Abid Waheed graphs, denoted as AW (r, s), consist of *r* cycles of order *s* that share a common vertex. These graphs exhibit interesting topological properties and bear resemblance to Jahangir graphs [2] [3]. The provided text focuses on the application of topological indices, particularly the Sombor index, in predicting physicochemical properties of chemical compounds and exploring their potential in drug discovery, specifically for antituberculosis drugs. It mentions [4], which discusses degree-based topological indices and QSPR analysis of antituberculosis drugs. The initial phase of this study involved analyzing the Sombor index for standard Abid Waheed graphs.

Building upon these results, the research was extended to generalized Abid Waheed graphs, where the number of cycles and their order can vary. The primary objective of this paper is to explore the potential applications of the Sombor index on Abid Waheed graphs in the context of network topology and optimization [5]. By modeling networking systems using Abid Waheed graphs, we aim to investigate how the Sombor index can be utilized to analyze and optimize network performance. This research contributes to the growing body of knowledge on topological indices and their applications in diverse fields.

The subsequent sections will detail the methods employed, present the results obtained, discuss their implications, and highlight potential applications in network analysis. The Sombor index, proposed by Ivan Gutman, is a recently introduced degree-based topological index that has gained significant attention in the field of chemical graph theory. This index has been shown to have strong predictive capabilities for various physicochemical properties of molecules. The Sombor index captures the structural information of a graph by considering the degree of each vertex and its neighboring vertices [6]. Gutman's work on the Sombor index has laid the foundation for understanding its mathematical properties and exploring its applications. The average Sombor index has been recognized as a measure of graph irregularity, providing insights into the structural diversity of networks.

Abid Waheed graphs are a family of graphs characterized by their unique structure, comprising r cycles of order s that share a common vertex. Previous studies have investigated the topological properties of Abid Waheed graphs, including the computation of the Hosaya polynomial and Wiener index [7]. These studies have demonstrated the potential of Abid Waheed graphs in modeling and analyzing various systems, particularly in the field of computer networking. The present study aims to bridge the gap between the Sombor index and Abid Waheed graphs, exploring the generalization of Abid Waheed graphs and their applications in network topology and optimization. The study is divided into two main phases: analysis of the Sombor index for standard Abid Waheed graphs, and extension to generalized Abid Waheed graphs. The initial phase involved computing the Sombor index for standard Abid Waheed graphs, denoted as AW (r, s), where s represents the order of the cycles and r represents the number of cycles. The Sombor index of these graphs was calculated using the formula provided by Gutman [8].

In the second phase, the research was extended to generalized Abid Waheed graphs, where the order of the cycles (s) and the number of cycles (r) were allowed to vary. This generalization was motivated by the observed similarities between Abid Waheed graphs and Jahangir graphs. The Sombor index of these generalized Abid Waheed graphs was computed and analyzed, revealing interesting patterns and insights. [9] explores the Atom-Bond Connectivity Index (ABC4) and the Geometric Arithmetic Index (GA5) for specific *nano star dendrimers*. Although both deal with topological indices and complex graph structures, they analyze different indices and graph families. The potential applications of the Sombor index on Abid Waheed graphs were explored in the context of network topology and optimization. Specifically, the Sombor index was investigated as a measure of network irregularity and its potential to model and analyze sustainable networking strategies. This study employed a combination of theoretical and computational approaches to analyze the Sombor index of Abid Waheed graphs. generalized Abid Waheed graphs using the Sombor index. [10] discusses efficiency in network topologies for data centers, focusing on arithmetic studies of various designs. For example, one could explore whether the Sombor index correlates with the efficiency coefficient (η) mentioned in [10]. The study presents the computation of the Hosaya polynomial and Wiener index for Abid Waheed graphs

$(AW)_p^6$, where $p \geq 1$. This work establishes the mathematical foundations for understanding the topological properties of these graphs. The generalization of Abid Waheed graphs explored in this study expands the potential applications of these structures in modelling and analyzing complex networks.

The analysis of the Sombor index for these generalized graphs provides insights into the structural characteristics and irregularity of the networks they represent. [11] focuses on computing multiplicative degree-based topological indices of the Jahangir graph. While Jahangir graphs and Abid Waheed graphs share similarities, the study in [7], which provides insights into the Wiener and Hyper-Wiener indices of Abid Waheed graphs. These indices are closely related to the Sombor index, and understanding their properties could inform the analysis and interpretation of the Sombor index results. [12] advocates for using graph theory to model and analyze environmental sustainability in supply chains, offering a unique perspective on optimizing complex networks for ecological impact. This complements your application of graph theory to network topology analysis. [13] demonstrates a practical application of graph theory in urban planning by analyzing green space connectivity.

This supports the broader applicability of graph-based methods for network optimization in diverse fields, aligning with your exploration of the Sombor index for similar purposes. It also applies graph theory to analyze urban green space connectivity in Bhopal, India. It uses various indices like Intra Connectivity, Betweenness Centrality, and Integral Index Connectivity to assess and improve green space network functionality. This aligns well with work on the Sombor index, as both explore graph-based approaches to understanding network structure and optimization, albeit with different indices and application contexts.

POLYMERS IN NANO STAR DENDRIMER

A polymer is a material either natural or synthetic whose molecules consist of many repeating small chemical units called monomers, connected in a consistent arrangement. Polymers are generally semi-crystalline, possessing both crystalline and amorphous regions within their structure. The degree of polymerization refers to the average number of monomer units (mers) in a polymer molecule. Depending on how these monomers combine, polymer molecules can form three-dimensional networks, two-dimensional planar structures, or one-dimensional linear chains. Organic polymers are typically one-dimensional in structure. In addition to carbon and hydrogen, polymer molecules may also contain atoms such as oxygen, nitrogen, chlorine, fluorine, silicon, phosphorus, and sulphur. These atoms are bonded together through covalent bonds. In some cases, adjacent polymer chains are linked by secondary interactions, known as cross-links, which are weaker than covalent bonds. These cross-links provide flexibility to the polymer by preventing the sliding of adjacent chains when the material is stretched. A branched polymer consists of molecules that have side chains (branches) attached to the main chain. A copolymer, on the other hand, is composed of two or more different types of monomer units. In such dendritic structures Parameters such as the level of branching, local connectivity and edge distribution have been found to have a substantial influence on the polymer compactness, surface reactivity and encapsulation efficiency. Since the Sombor index is sensitive to local changes in degree, it is a useful quantitative descriptor correlated with such molecular-level behaviours and thus it shows potential as a QSPR analysis in polymer chemistry.

METHODOLOGY

Figure1 $\mathcal{D}_n$ – Nano star Dendrimer which resembles Abid Waheed graph $(AW)_3^6$, [9] Nano star Dendrimer $\mathcal{D}_n$ for n = 1 whose vertices are 15 in number and categorized based on their degree association as 15 vertices of degree 2 and 4 vertices of degree 3. Also, the edges are 21 in number which are again categorized degree relationship with end vertices as: 12 edges of degree (2,2), 6 edges of degree (2,3) and 3 edges of degree (3,3). The calculated Sombor index and M-polynomial are not mere mathematical descriptors, but they are also used as polymer structure indicators. In particular, the degree formulation of the Sombor index mirrors branching complexity of dendritic polymers, where a higher-degree vertex represents a central or branch point. In the same manner, edge partitions are connectivity patterns, which provide information on the way monomer units are connected.

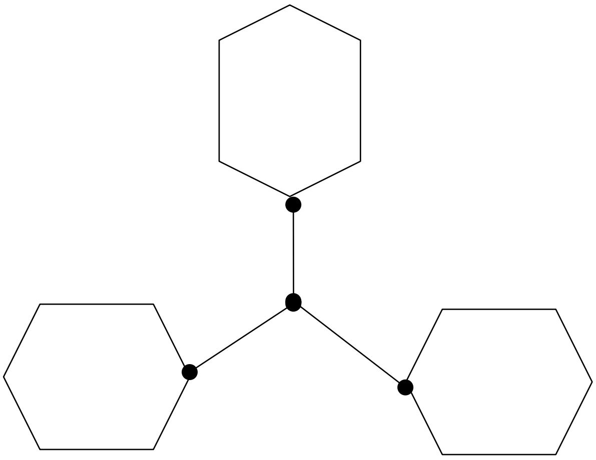

Figure 1. Nano star dendrimer $\mathcal{D}_n$ for n = 1 and Abid Waheed graph: $(AW)_3^6$

These correlations are used to give a theoretical justification to interpret molecular compactness and network topology of real nano star dendrimers.

FIGURES AND TABLES

Definition of $\mathcal{M}$ POLYNOMIAL:

Let G = (V, E) be a simple, undirected graph, where V(G) is the set of vertices and E(G) is the set of edges. For each edge $e = xy \in E(G)$, let d_x and d_y be the degrees of vertices u and v, respectively. Let $m_{i,j}$ denote the number of edges $uv \in E(G)$ such that $\{d_x, d_y\} = \{i, j\}$, where $i \leq j$. Then the

$\mathcal{M}$ polynomial of the graph G is defined as: $\mathcal{M}(G; x, y) = \sum_{i \leq j} m_{i,j} x^i y^j$. This is a bivariate polynomial that encodes the distribution of edge degrees in the graph.

$\mathcal{M}$ polynomial of $\mathcal{D}_n$ @ n = 1 is $\mathcal{M}\ (\mathcal{D}_1\colon x, y) = 12x^2y^2 + 6x^2y^3 + 3x^3y^3$
$D_x = 24xy^2 + 12xy^3 + 9x^2y^3$
$x\,D_x = 24x^2y^2 + 12x^2y^3 + 9x^3y^3$
$D_x^2 = 48xy^2 + 24xy^3 + 27x^2y^3$
$x\,D_x^2 = 48x^2y^2 + 24x^2y^3 + 27x^3y^3$
$D_y = 24x^2y + 18x^2y^2 + 9x^3y^2$
$y\,D_y = 24x^2y^2 + 18x^2y^3 + 9x^3y^3$
$D_y^2 = 48x^2y + 54x^2y^2 + 27x^3y^2$
$y\,D_y^2 = 48x^2y^2 + 54x^2y^3 + 27x^3y^3$
$SO(\mathcal{D}_1) = \sqrt{D_x^2 + D_y^2} = 96x^2y^2 + 78x^2y^3 + 54x^3y^3$

$SO(\mathcal{D}_1)$ @ $x = y = 1$ is $12\sqrt{8} + 6\sqrt{13} + 3\sqrt{18}$
$SO(AW)_3^6 = 12\sqrt{8} + 6\sqrt{13} + 3\sqrt{18}$
$SO(\mathcal{D}_n) = SO(AW)_3^6$, @ $x = y = 1$. ■

Theorem 1: Let $\mathcal{D}_n$ be the Nano star dendrimer then whose M-polynomial is

$$\mathcal{M}(\mathcal{D}_n\ ; x, y) = 12(2 * 2^{n-1} - 1)x^2y^2 + 6(5 * 2^{n-1} - 4)x^2y^3 + (12 * 2^{n-1} - 9)x^3y^3.$$

Proof: The generalization of Abid Waheed graph for 'r' cycles of order 's' where $r \geq 1$ and $s \geq 3$.

So, the procedure started with 'r' cycles of order 4 as we already discussed it for order 3. ■'r' cycles each of order 4:

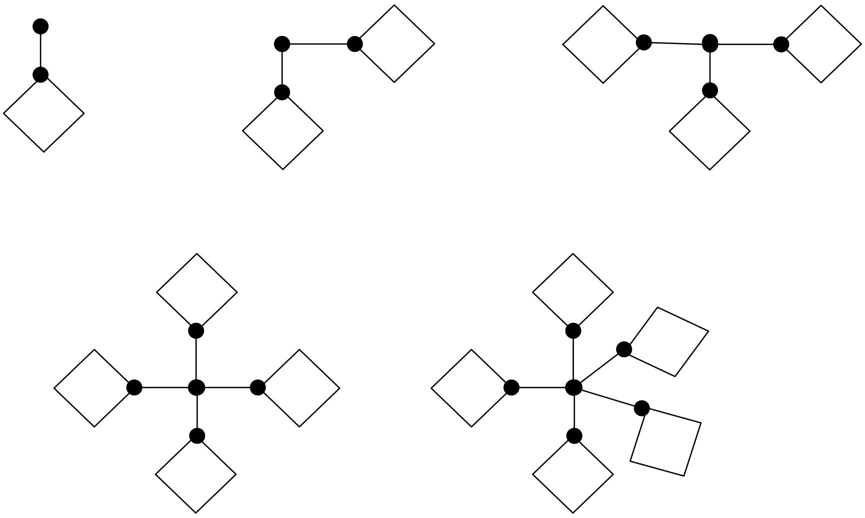

Figure 2. 1,2,3,4 and 5 cycle/s of order 4 respectively.

Case 1: r =1, s=4 as in Figure 2
Here, total vertices, V = rs + 1= 5, total edges, E = r (s + 1) = 5

$$V_{\{2\}}=3, V_{\{3\}}=1, V_{\{1\}}=1. E_{2,2}=2, E_{2,3}=2, E_{1,3}=1$$

$$\mathrm{SO(AW)}_1^4 = 2\sqrt{2^2+2^2}+2\sqrt{2^2+3^2}+1\sqrt{1^2+3^2}=2\sqrt{8}+2\sqrt{13}+\sqrt{10}$$

Case 2: r =2, s=4
Here, total vertices, V = rs + 1= 9, total edges, E = r (s + 1) = 10

$$V_{\{2\}}=7, V_{\{3\}}=2\,.E_{2,2}=4, E_{2,3}=6$$

$$\mathrm{SO(AW)}_2^4 = 6\sqrt{2^2+2^2}+4\sqrt{2^2+3^2}=6\sqrt{8}+4\sqrt{13}$$

Case 3: r =3, s=4
Here, total vertices, V = rs + 1= 13, total edges, E = r (s + 1) = 15

$$V_{\{2\}}=9, V_{\{3\}}=4. E_{2,2}=6, E_{2,3}=6, E_{3,3}=3$$

$$\mathrm{SO(AW)}_3^4 = 6\sqrt{2^2+2^2}+6\sqrt{2^2+3^2}+3\sqrt{3^2+3^2}=6\sqrt{8}+6\sqrt{13}+9\sqrt{2}$$

Case 3: r =4, s=4
Here, total vertices, V = rs + 1= 17, total edges, E = r (s + 1) = 20

$$V_{\{2\}}=12, V_{\{3\}}=4, V_{\{4\}}=1\ E_{2,2}=8, E_{2,3}=8, E_{3,4}=4$$

$$\mathrm{SO(AW)}_4^4 = 8\sqrt{2^2+2^2}+8\sqrt{2^2+3^2}+4\sqrt{3^2+4^2}=8\sqrt{8}+8\sqrt{13}+4\sqrt{5}$$

Case 3: r =5, s=4
Here, total vertices, V = rs + 1= 21, total edges, E = r (s + 1) = 25

$$V_{\{2\}}=15, V_{\{3\}}=5, V_{\{5\}}=1\ E_{2,2}=10, E_{2,3}=10, E_{3,5}=5$$

$$\mathrm{SO(AW)}_4^4 = 10\sqrt{2^2+2^2}+10\sqrt{2^2+3^2}+5\sqrt{3^2+5^2}=10\sqrt{8}+10\sqrt{13}+5\sqrt{34}\ \blacksquare$$

Theorem 2: $\mathrm{(AW)}_r^s, r \geq 1, s \geq 3$, ‘r’ cycles of order ‘s’ generalization is as follows:
In general, $\mathrm{(AW)}_r^s$ graph, edge partitions are categorized as follows:
For, if r = 1; $E_{1,3}=1, E_{2,2}=s-2, E_{2,3}=2$
if r = 2; $E_{2,2}=r(s-2), E_{2,3}=3$
if r ≥ 3; $E_{2,2}=r(s-2), E_{2,3}=2r, E_{3,r}=r$

Proof: Tabulating the above information and extending it for different values of ‘r’ and s = 4 we get the following tabulation as in Table 1.

Table 1. Generalization of edge partitions for different values of ‘r’ and s = 4.

r, s	**V**	**E**	**(1, 3)**	**(2, 2)**	**(2, 3)**	**(3, 3)**	**(3, 4)**	**(3, 5)**	**(3, 6)**	**(3, 7)**
1, 4	5	5	1	2	2					
2, 4	9	10		4	6					
3, 4	13	15		6	6	3				
4, 4	17	20		8	8		4			
5, 4	21	25		10	10			5		
6, 4	25	30		12	12				6	
7, 4	29	35		14	14					7

Table 2. Generalization of edge partitions for different values of ‘r’ and s = 3.

r, s	**V**	**E**	**(1, 3)**	**(2, 2)**	**(2, 3)**	**(3, 3)**	**(3, 4)**	**(3, 5)**	**(3, 6)**
1, 3	4	4	1	1	2				
2, 3	7	8		2	6				
3, 3	10	12		3	6	3			
4, 3	13	16		4	8		4		
5, 3	16	20		5	10			5	
6, 3	19	24		6	12				6

Table 3. Generalization of edge partitions of Abid Waheed Graphs for different values of ‘r’ and ‘s’.

	$(\mathbf{AW})_\mathbf{r}^\mathbf{3}$	$(\mathbf{AW})_\mathbf{r}^\mathbf{4}$	$(\mathbf{AW})_\mathbf{r}^\mathbf{5}$	$(\mathbf{AW})_\mathbf{r}^\mathbf{6}$
	(1,3) (2,2) (2,3) (3,r)	(1,3) (2,2) (2,3) (3,r)	(1,3) (2,2) (2,3) (3,r)	(1,3) (2,2) (2,3) (3,r)
r = 1	r r 2r	r 2r 2r	r 3r 2r	r 4r 2r
r = 2	r 3r	2r 3r	3r 3r	4r 3r
r = 3	r 2r r	2r 2r r	3r 2r r	4r 2r r

As ‘r’ increases by 1, vertex set V increases by ‘s’ 9 (i.e by 4) and edge set E increases by ‘s’+1 (i.e by 5). In a similar fashion we try to get it for different values of ‘r’ and s = 3 we get the following tabulation as shown in Table 2.

Analyzing the above tables and validating with few results on it we obtained an observation on general results which is been done for ‘r’ cycles for s = 3, 4, 5, 6, .as listed in Table 3.

Hence our findings on general edge partitions of Abid Waheed graphs $(\mathrm{AW})_\mathrm{r}^\mathrm{s}$ is as follows if r = 1; $\mathrm{E}_{1,3} = 1, \mathrm{E}_{2,2} = \mathrm{s} - 2, \mathrm{E}_{2,3} = 2$, if r = 2; $\mathrm{E}_{2,2} = \mathrm{r}(\mathrm{s} - 2), \mathrm{E}_{2,3} = 3$ and
for r ≥ 3; $\mathrm{E}_{2,2} = \mathrm{r}(\mathrm{s} - 2),\ \mathrm{E}_{2,3} = 2\mathrm{r}, \mathrm{E}_{3,\mathrm{r}} = \mathrm{r}$. ∎

Sombor, Reduced Sombor and Average Sombor index for Abid Waheed graphs $(AW)_r^s$:

$$\mathrm{SO(G)} = \sum_{e = xy\, \in E(G)} \sqrt{d_x^2 + d_y^2}$$

1. For if r = 1; $E_{1,3} = 1, E_{2,2} = s - 2, E_{2,3} = 2$, we have,
   $SO(AW)_1^s = 1\sqrt{1^2 + 3^2} + (s-2)\sqrt{2^2 + 2^2} + 2\sqrt{2^2 + 3^2} = \sqrt{10} + (s-2)\sqrt{8} + 2\sqrt{13}$
2. When r = 2; $SO(AW)_2^s = 2(s-2)\sqrt{2^2 + 2^2} + 3\sqrt{2^2 + 3^2} = 2(s-2)\sqrt{8} + 3\sqrt{13}$
3. Similarly, when r ≥ 3,

$$SO(AW)_r^s = r(s-2)\sqrt{2^2 + 2^2} + 2r\sqrt{2^2 + 3^2} + r\sqrt{3^2 + r^2}$$
$$= r(s-2)\sqrt{8} + 2r\sqrt{13} + r\sqrt{3^2 + r^2} \blacksquare$$

$$\mathrm{RSO(G)} = \sum_{\mathrm{e=\, xy\in E(G)}} \sqrt{(d_{\mathrm{x}}-1)^2+(\mathrm{d}_y-1)^2}$$

1. For if r = 1; $E_{1,3} = 1, E_{2,2} = s-2, E_{2,3} = 2$, we have,
   $$RSO(AW)_1^s = 1\sqrt{0^2+2^2}+(s-2)\sqrt{1^2+1^2}+2\sqrt{1^2+2^2} = \sqrt{4}+(s-2)\sqrt{2}+2\sqrt{5}$$
2. If r = 2; $E_{2,2} = r(s-2), E_{2,3} = 3$ which implies the reduced sombor index
   $$RSO(AW)_2^s = r(s-2)\sqrt{1^2+1^2}+3\sqrt{1^2+2^2} = 2(s-2)\sqrt{2}+3\sqrt{5}$$
3. Similarly, when r $\geq$ 3, $SO(AW)_r^s = r(s-2)\sqrt{1^2+1^2}+2r\sqrt{1^2+2^2}+r\sqrt{2^2+(r-1)^2} = r(s-2)\sqrt{2}+2r\sqrt{5}+r\sqrt{4+(r-1)^2}$ ■

$$ASO(G) = \sum_{xy\in E(G)} \sqrt{(d_x-\tfrac{2m}{n})^2+(d_y-\tfrac{2m}{n})^2}$$

1. For if r = 1; $E_{1,3} = 1, E_{2,2} = s-2, E_{2,3} = 2$, we have,
   $$ASO(AW)_1^s = 1\sqrt{(1-\tfrac{2m}{n})^2+(3-\tfrac{2m}{n})^2}+(s-2)\sqrt{(2-\tfrac{2m}{n})^2+(2-\tfrac{2m}{n})^2}+ 2\sqrt{(2-\tfrac{2m}{n})^2+(3-\tfrac{2m}{n})^2}$$
2. When r = 2;
   $$ASO(AW)_2^s = 2(s-2)\sqrt{(2-\tfrac{2m}{n})^2+(2-\tfrac{2m}{n})^2}+3\sqrt{(2-\tfrac{2m}{n})^2+(3-\tfrac{2m}{n})^2}$$
3. Similarly, when r ≥ 3,
   $$SO(AW)_r^s = r(s-2)\sqrt{(2-\frac{2m}{n})^2+(2-\frac{2m}{n})^2}+2r\sqrt{(2-\frac{2m}{n})^2+(3-\frac{2m}{n})^2} + r\sqrt{(3-\frac{2m}{n})^2+(r-\frac{2m}{n})^2} \blacksquare$$

CONCLUSIONS

In this study, we have presented a generalization of the Abid Waheed graph and investigated its properties using the Sombor topological index. Specifically, we developed an edge partitioning scheme to systematically analyze the Sombor index of Abid Waheed graphs. Derived closed-form expressions for the Sombor index of the generalized Abid Waheed graphs, capturing the contributions of different edge classes. Explored the potential applications of the Sombor index in network topology analysis and optimization, highlighting its utility in modeling sustainable networking strategies. The results obtained in this study provide a deeper understanding of the structural properties of Abid Waheed graphs and their generalized counterparts. Furthermore, the Sombor index has shown promise as a tool for characterizing the efficiency and robustness of network topologies, which could have important implications for the design and management of communication networks. In addition to theoretical analysis, we extended the applicability of the generalized Abid Waheed graph model to represent polymers in nano star dendrimers. Due to their hierarchical, highly branched architecture, nano star dendrimers can be effectively modeled using recursive graph structures such as Abid Waheed graphs. The study of their Sombor index provided insight into the topological complexity, connectivity, and branching behavior of these dendritic polymer networks. This implies that the Sombor index not only encodes abstract topological data but also encodes essential chemical properties of molecular symmetry, accessibility and stability which are crucial to functional performance of nano-dendrimers in practical applications.

Future work could involve investigating the correlation between the Sombor index and other network performance metrics, as well as exploring the application of these insights to real-world network optimization problems.

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