Hindawi
Journal of Mathematics
Volume 2024, Article ID 9941949, 12 pages
https://doi.org/10.1155/2024/9941949

Research Article

Computation of Wiener and Wiener Polarity Indices of a Class of Nanostar Dendrimer Using Vertex Weighted Graphs

Syed Ahtsham Ul Haq Bokhary,[1] **Pakeeza Bashir**,[1] **Allah Nawaz**,[1] **Shreefa O. Hilali**,[2] **Mohammed Alhagyan**,[3] **Ameni Gargouri**,[3] **and Mohammed M. A. Almazah**[4]

[1]*Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University, Multan, Pakistan*
[2]*Department of Mathematics, College of Sciences and Arts (Majardah), King Khalid University, Magardah 61937, Saudi Arabia*
[3]*Mathematics Department, College of Humanities and Science, Prince Sattam Bin Abdulaziz University, Al-Kharj, Saudi Arabia*
[4]*Department of Mathematics, College of Sciences and Arts (Muhyil), King Khalid University, Muhayil 61421, Saudi Arabia*

Correspondence should be addressed to Syed Ahtsham Ul Haq Bokhary; sihtsham@gmail.com

Received 13 August 2023; Revised 25 November 2023; Accepted 15 December 2023; Published 2 January 2024

Academic Editor: Ram Jiwari

Nanostar dendrimers are tree-like nanostructures with a well-defined, symmetrical architecture. They are built in a step-by-step, controlled synthesis process, with each layer or generation building on the previous one. Dendrimers are made up of a central core, a series of repeating units or branches, and a surface group shell. A weighted graph is a type of graph in which vertices or edges are assigned weights that represent cost, distance, and a variety of other relative measuring units. The weighted graphs have many applications and properties in a mathematical context. The topological indices are numerical values that represent the symmetry of a molecular structure. They have rich applications in theoretical chemistry. Various topological indices can be used to investigate a wide range of properties of chemical compounds with a molecular structure. They are very important in mathematical chemistry, especially in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies. In this paper, we examine the topological properties of the molecular graphs of nanostar dendrimers. For this purpose, the topological indices, namely, the Wiener index and the Wiener polarity index are computed for a class of nanostar dendrimers.

1. Introduction and Preliminary Results

1.1. Dendrimers. Dendrimers [1, 2] are hyperbranched macromolecules that carry branches from generation to generation with a central part. Dendrimers were first proposed in the late 1970s by German chemist Fritz Vögtle, who proposed highly branched macromolecules with well-defined structures. Vögtle envisioned these synthetic molecules as mimics of natural polymers such as proteins and DNA, with controlled architectures and precise properties. In the early 1980s, American chemist Donald A. Tomalia made significant contributions to the development of dendrimers. Tomalia created the first class of dendrimers, known as polyamidoamine (PAMAM) dendrimers, which is made of repetitively branched subunits of amide and amine functionality on his own. He used a divergent growth method in which he repeatedly reacted on a core molecule with a monomer, resulting in branching and the formation of a well-defined three-dimensional structure.

Dendrimers are iteratively synthesised polymers with unique properties such as polyvalency, electrostatic interaction, self-assembly, monodispersity, stability, and unimolecular micelles that make them an excellent drug delivery carrier. Dendrimer plays an important role in the biomedical field [3] and in gene delivery systems [4].

These nanostar dendrimers were created by fusing two different types of nanoparticles: gold nanostars and dendrimers. The high surface area and unique optical properties of gold nanostars make them ideal for sensing and imaging applications. Dendrimers were chosen because of their ability to transport multiple drug molecules while also targeting specific cells or tissues in the body. To make the nanostar dendrimers, the researchers first synthesised gold nanostars using a seed-mediated growth method. They then functionalized the surface of the gold nanostars with a dendritic molecule called polyamidoamine (PAMAM) dendrimers, which has a large number of functional groups on its surface that can be used to attach drug molecules. The resulting nanostar dendrimers had a core-shell structure, with the gold nanostars forming the core and the dendrimers forming the shell. The researchers demonstrated that these hybrid nanoparticles were effective at delivering drug molecules to cancer cells in vitro and that they could also be used for imaging applications. Dendrimers have received a lot of attention in scientific research and various applications.

1.2. Topological Indices. In cheminformatics, topological indices are mathematical descriptors that are used to measure and characterise molecular structure properties. These indices provide the molecular structure with a numerical depiction by encapsulating details regarding the connectivity and configuration of atoms inside a molecule. Topological indices concentrate on characteristics that are independent of particular spatial arrangements because the name "topological" refers to the study of properties that remain unchanged under continuous deformations. The topological indices are numerical values that represent the symmetry of a molecular structure. In this context, atom distribution and spatial arrangement inside a molecule are referred to as symmetry. It involves the recurrence of motifs or patterns. Because it affects several characteristics, including stability and reactivity, symmetry is a crucial component of molecular structure. They have rich applications in theoretical chemistry. Numerous characteristics of chemical compounds having a molecular structure can be examined using various kinds of topological indices. They play a very crucial role in mathematical chemistry, particularly in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship- (QSPR-) related studies. Many of these topological indices were introduced by researchers in Mathematical Chemistry, on the basis of molecular structure modelling involving graph structures. They sum up some molecular properties in a single numeric value. Topological indices have been used extensively in recent years to study the properties of dendrimers [5–9].

1.3. Wiener and Wiener Polarity Index. According to [2], the Wiener index was the first and is still the most studied topological index. It was chemistry's first application of a molecular topological index. It is demonstrated that the Wiener index number and the boiling points of alkane molecules are closely connected. Later work on quantitative structure-activity relationships revealed correlations between the critical point's parameters [10], the density, surface tension, and viscosity of its liquid phase [11], and the molecule's van der Waals surface area [5].

The Wiener index, indicated mathematically by the symbol $W(G)$, is the sum of all distances between each graph vertex.

Later on, Wiener introduced another descriptor known as the Wiener polarity index that is known to be related to the cluster coefficient of networks. The Wiener polarity index is denoted by $W_p(G)$ and is defined as the number of unordered pairs of vertices that are at distance 3 in G. In organic compounds, say paraffin, the Wiener polarity index is the number of pairs of carbon atoms which are separated by three carbon-carbon bonds. Based on the Wiener index and the Wiener polarity index, the formula

$$t_B = xW(G) + yW_p(G) + z \tag{1}$$

was used to calculate the boiling points t_B of the paraffins, where x, y, and z are constants for a given isomeric group. By using the Wiener polarity index, Lukovits and Linert demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons in [9]. Hosoya in [11] found a physical-chemical interpretation of $W_p(G)$. Actually, the Wiener polarity index of many kinds of graphs is studied, such as trees [12], unicyclic and bicyclic graphs [13], hexagonal systems, fullerenes, and polyphenylene chains [6], and lattice networks [14].

1.4. Weighted Graph. The idea of assigning weights to edges and vertices in graphs began to emerge in the early 20[th] century. Researchers recognized the need to represent relationships with different strengths or costs in various applications. Dénes Ko n̈ ig, a Hungarian mathematician, made significant contributions to the study of weighted graphs. In his book "*Theory of Graphs and Its Applications*" published in 1936, Ko n̈ ig discussed concepts such as minimum spanning trees and network flows, which involved the use of weights on edges and vertices.

A weighted graph $(G; w)$ is a graph $G = (V(G); E(G))$ together with the weight function $w: V(G) \longrightarrow \mathbb{R}^+$. The Wiener index $W(G; w)$ of the weighted graph $(G; w)$ was introduced in [15] as follows:

$$W(G) = \sum_{p,q\in V(G)} w(p)w(q)d(p,q). \tag{2}$$

For a graph G, the Djokovic–Winkler's relation on $E(G)$ Θ [16] is defined as follows:

If $d(\alpha,\beta) + d(\gamma,\sigma) \neq d(\alpha,\sigma) + d(\beta,\gamma)$, then $e = \alpha\gamma \in E(G)$ is Θ related with $f = \beta\sigma \in E(G)$. Relation Θ is reflexive and symmetric; its transitive closure Θ^* is an equivalence relation. The partition of $E(G)$ induced by Θ^* will be called the Θ^*-partition. Assume that $\mathscr{F} = \{F_i: i \in [n]\}$ denote the Θ^*-partitions of $E(G)$.

A partition $\mathscr{E} = \{E_1, \ldots, E_n\}$ of $E(G)$ is coarser than $\mathscr{F}$ if each set E_i is the union of one or more Θ^*-classes of G [16].

Theorem 1 (see [16]). *Let G be a connected weighted graph and $\mathscr{E} = \{E_1, \ldots, E_n\}$ be partition of $E(G)$ coarser than $\mathscr{F}$. Then,*

$$W(G) = \sum_{i=1}^{n} W\left(\frac{G}{E_i, w_i}\right), \tag{3}$$

where w_i: V $(G/E_i \longrightarrow \mathbb{R}^+$ is defined by $w_i(x) = \sum_{x\in C} w(x)$ for all connected components C of G/E_i.

The technique to construct the quotient graph G/E_i is to first remove all the edges of E_i from G and then shrink the vertices in each component of $G - E_i$ to one point, where vertex strength is the number of vertices in that component and edge strength is the number of edges in that component. Thus, the number of vertices in G/E_i is the number of components of $G - E_i$ and if there exists an edge between the vertices of two components in G, then an edge is formed in G/E_i. In this way, the quotient graph for each partition can be formed.

The following result gives the Wiener index of the graph composed of two subgraphs such that both the subgraphs have one vertex common.

Theorem 2 (see [17]). *Let $\mathscr{H} = \mathscr{H}_1.\mathscr{H}_2$ be a graph composed by $\mathscr{H}_1$ and $\mathscr{H}_2$ graphs such that $V(\mathscr{H}_1.\mathscr{H}_2) = V(\mathscr{H}_1) \cup V(\mathscr{H}_2)$ and $V(\mathscr{H}_1) \cap V(\mathscr{H}_2) = \{s\}$, where s is a cut vertex in $\mathscr{H}$. Let $|V(\mathscr{H}_1| = t_1$ and $|V(\mathscr{H}_2| = t_2$. If $x \in V(\mathscr{H}_1)$ and $z \in V(\mathscr{H}_2)$, then $d(x,z) = d(x,s) + d(s,z)$. And*

$$\begin{aligned} w(\mathscr{H}) = w(\mathscr{H}_1) + w(\mathscr{H}_2) + (t_1 - 1)w(s, \mathscr{H}_2) \\ + (t_2 - 1)w(s, \mathscr{H}_1). \end{aligned} \tag{4}$$

There are many types of nanostar dendrimers. Dendrimers have received a lot of attention in scientific research and various applications. Dendrimers are regarded as one of the most important, commercially available building blocks in nanotechnology. Dendrimers are used to make nanotubes, nanolatex, chemical sensors, micro- and macrocapsules, coloured glass, modified electrodes, and photon funnels, which are used to make artificial antennas. Because of its widespread application in a variety of fields, researchers have focused their efforts on determining the underlying topology of nanostar dendrimers. The F-index of nanostar dendrimers has been calculated by De and Nayeem [18]. In terms of Zagreb indices, Siddiqui et al. [19] investigated the topological properties of some nanostar dendrimers. Bokhary and Tabassum studied different graph invariants to explore different topological properties of dendrimers like the energy of some tree dendrimers [20], domination and power domination of certain dendrimers [21]. The readers are directed to [7, 9, 15, 20–26] for additional discussion in this field. The purpose of this report is to calculate the distance-based topological indices for a class of nanostar dendrimers. The first type of nanostar dendrimer that we study in this work was introduced by Dorosti et al. [25]. In this paper, they computed the Cluj index for two types of dendrimer nanostructures by analyzing the constitutive substructures of these dendrimers. In this paper, we extend this study by computing the Wiener and Wiener polarity indices of the first type of dendrimer mentioned in [25].

2. Main Results

2.1. Construction of the First Type of Nanostar Dendrimer. The stages of the first type of nanostar dendrimers can be made by connecting the multiple hexagons. There are n stages of nanostar dendrimer. In the first stage, there are seven connected hexagons which are attached with the nucleus of hexagon. The nucleus of hexagon is made up of five connected hexagons. Thus, at the first stage, there are a total of twelve hexagons. The number of vertices at stage one are $20 + 42 = 62$ and number of edges are $24 + 42 + 7 = 75$.

In the second stage of nanostar dendrimers, eight more hexagons are attached to the first stage. Thus, at the second stage, there are total twenty hexagons. The number of vertices at stage two are $20 + 42 + 48 = 62 + 48 = 110$ and the number of edges are $24 + 42 + 7 + 48 + 8 = 75 + 56 = 129$.

The first and second growing stages are different. But, from the third stage and onward, 2^i hexagons are attached to the previous stage. Let I_n be the graph of nanostar dendrimer after n stages. Thus, for $3 \le j \le n$, I_j is obtained from I_{j-1} by adding 2^j hexagons to I_{j-1}. It is easy to see that, for $n \ge 3$, the order and size of the graph I_n are $62^{n+1} + 62$ and $7.2^{n+1} - 73$, respectively. The graph of nanostar dendrimer of dimension 4 is shown in Figure 1.

2.2. Computation of Wiener Index of I_n Using Vertex Weighted Graph. Let H_n be graph having $n + 1$ stages; in the first stage, H_1 has one hexagon that is attached to an isolated vertex; after that, H_i is obtained from H_{i-1} by adding 2^{i-1} hexagons, for $2 \le i \le n + 1$. For $n \ge 1$, the order and size of the graph H_n are $62^{n+1} - 5$ and $7.2^{n+1} - 7$, respectively.

It is easy to see that, the graph H_n for $n \ge 1$ has $42^{n+1} - 4$ Θ^*-classes, which can be obtained by applying the Djoković–Winkler relation. The Θ^*-classes for the graph H_n are shown in Figure 2. Let $\{E_1, \ldots, E_n\}$ be the sets coarser than the Θ^*-classes in H_n. With the help of these sets, the quotient graphs H_n/E_i, for $1 \le i \le n + 1$, are computed. The quotient graphs H_n/E_1 and H_n/E_i are shown in Figures 3 and 4, respectively.

In the next theorem, the Wiener index of the graph H_n is computed.

Theorem 3. *Let n be the positive integer, then*

$$W(H_n) = \left(432.n - 792 + \frac{360}{2^n}\right)4^n + (252.n + 444)2^n + 30. \tag{5}$$

Proof. Let $\{E_1, \ldots, E_{n+1}\}$ be the partition of $E(H_n)$ coarser than $\mathscr{F}$. Then, from Theorem 1,

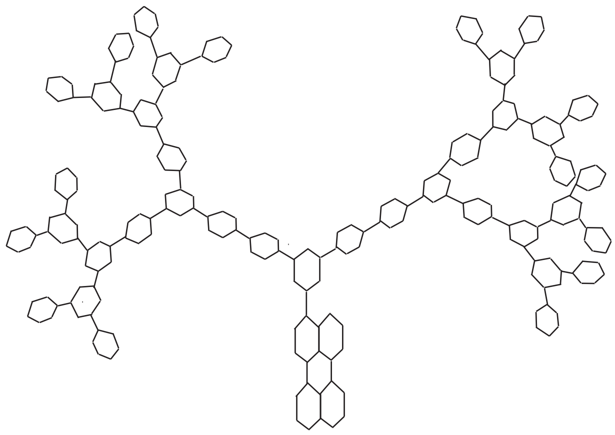

FIGURE 1: First type of nanostar dendrimers growing up to four stages.

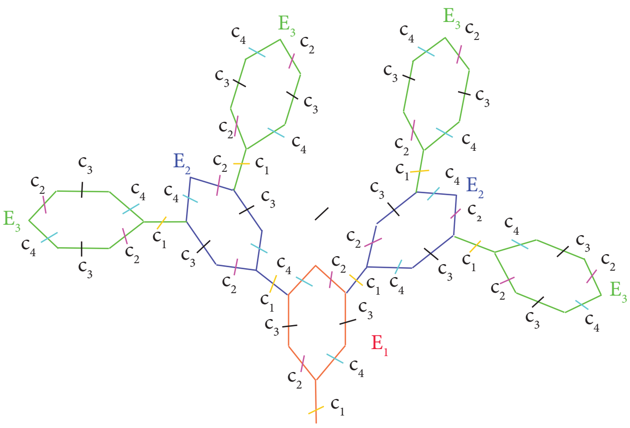

FIGURE 2: Θ^*-classes of H_2.

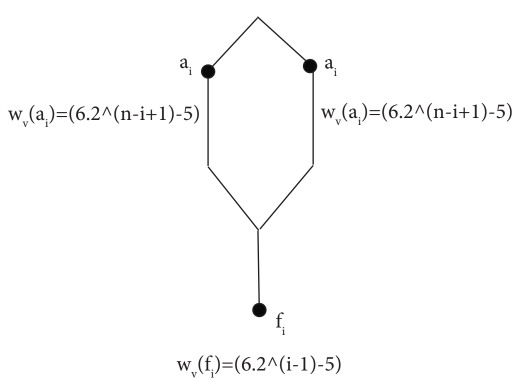

FIGURE 3: E_1 and H_n/E_1.

$$W(H_n) = \sum_{i=1}^{n+1} W\left(\frac{H_n}{E_i, w_i}\right), \tag{6}$$

where w_i: $V(H_n/E_i) \longrightarrow \mathbb{R}^+$ is defined by $w_i(x) = \sum_{x\in C} w(x)$ for all connected components C of H_n/E_i. This implies that, the weights of vertices a_1 and f_1 are $62^n - 5$ and 1, respectively, and are computed by using the quotient graph

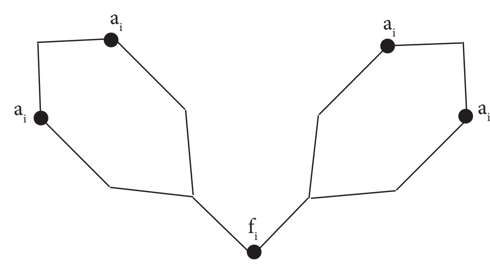

FIGURE 4: E_2 and H_n/E_2.

H_n/E_1. For $2 \le i \le n+1$, $w(a_i)$ and $w(f_i)$ in quotient graph H_n/E_i are $(6.2^{n-i+1} - 5)$ and $(6.2^{i-1} - 5)$, respectively.

Now, by using equation (2), we have

$$\begin{aligned} W\left(\frac{H_n}{E_1}\right) &= 2w(a_1)^2 + 14w(a_1) \\ &\quad + 6w(f_1)w(a_1) + 9w(f_1) + 11 \\ &= 2.(6.2^n - 5)^2 + 20(6.2^n - 5) + 20) \\ &= 2.\left(36.2^{2n} + 25 - 60.2^n\right) + 120.2^n - 80 \\ &= 72.4^n - 120.2^n + 120.2^n + 50 - 80. \end{aligned} \tag{7}$$

Thus,

$$W\left(\frac{H_n}{E_1}\right) = 72.4^n - 30. \tag{8}$$

For $2 \le i \le n+1$ and using equation (2) and Theorem 1, we have $(H_n/E_i) = 2.7w(a_i).2^{i-1} + 2.w(a_i)^2.2^{i-1} + 4.6w(a_i)^2 \binom{2^{i-1}}{2} + 3w(a_i)w(f_i).2.2^{i-1} + 9w(f_i).2^{i-1} + 11.2^{i-1} + w(a_i).\ 4.21 \binom{2^{i-1}}{2} + (13+17+17+25)\binom{2^{i-1}}{2}$.

$$
\begin{aligned}
&= 14.w(a_i) + 2^i (w(a_i)^2 + \frac{24}{2} (w(a_i)^2\left(2^{2i-2} - 2^{i-1}\right) + \frac{84}{2} (w(a_i)\left(2^{2i-2} - 2^{i-1}\right) + \left(\frac{72}{2}\left(2^{2i-2} - 2^{i-1}\right)\right.\\
&= 7.2^i.w(a_i) + 2^i\left(w(a_i)^2 + \left(12w(a_i)^2\right) + 42w(a_i) + 36\right)\left(2^{2i-2} - 2^{i-1}\right) + 3w(a_i)w(f))2^i + 9w(f).2^{i-1} + 11.2^{i-1}\\
&= w(a_i)^2\left(2^i + 12.2^{2i-2} - 12.2^{i-1}\right) + w(a_i)\left(7.2^i + 42.2^{2i-2} - 42.2^{i-1}\right)\\
&\quad + \left(36.2^{2i-2} - 25.2^{i-1}\right) + 3w(a_i)w(f)).2^i + +9w(f).2^{i-1} + 11.2^{i-1}\\
&= w(a_i)^2\left(2^i + 3.2^{2i} - 6.2^i\right) + w(a_i)\left(7.2^i + 21.2^{2i-1} - 21.2^i + 3w(f)2^i\right) + \left(9.2^{2i} - 25.2^{i-1}\right) + 9w(f).2^{i-1}.
\end{aligned} \tag{9}
$$

Thus, we have

$$
W\left(\frac{H_n}{E_i}\right) = w(a_i)^2\left(3.4^i - 5.2^i\right) + w(a_i)\left(-14.2^i + 21.2^{2i-1} + 3w(f)2^i\right) + 9.4^i - 25.2^{i-1} + 9w(f).2^{i-1}, \tag{10}
$$

where

$$
w(a_i) = \left(6.2^{n-i+1} - 5\right), w(a_i)^2 = 36.2^{2(n-i+1)} - 60.2^{n-i+1} + 25, w(f_i) = \left(6.2^{i-1} - 5\right). \tag{11}
$$

Replacing these values in equation (10), we obtain

$$
\begin{aligned}
W\left(\frac{H_n}{E_i}\right) &= \left(36.2^{2n-2i+2} - 60.2^{n-i+1} + 25\right)\left(3.2^{2i} - 5.2^i\right) + \left(6.2^{n-i+1} - 5\right)\left(-14.2^i + 21.2^{2i-1}\right.\\
&\quad \left. + 3.2^i.\left(6.2^{i-1} - 5\right) + 9.2^{2i} - 25.2^{i-1} + 9\left(6.2^{i-1} - 5\right).2^{i-1}\right.\\
&= 108.2^{2n+2} - 180.2^{2n-i+2} - 180.2^{n+i+1} + 300.2^{n+1} + 75.2^{2i} - 125.2^i - 84.2^{n+1}\\
&\quad + 126.2^{n+i} + 108.2^{n+i} - 90.2^{n+1} + 70.2^i - 105.2^{2i-1} - 90.2^{2i-1} + 75.2^i + 9.2^{2i}\\
&\quad - 25.2^{i-1} + 54.2^{2i-2} - 45.2^{i-1}\\
&= 432.4^n + (600 - 168 - 180)2^n - 720.2^{2n-i} + (-360 + 126 + 108)2^{n+i}\\
&\quad + 2^i(-125 + 75 + 70 - 35) + 2^{2i-1}(-105 - 90 + 27 + 18) + 75.4^i.
\end{aligned} \tag{12}
$$

An easy simplification implies

$$
W\left(\frac{H_n}{E_i}\right) = 432.4^n + 252.2^n - 720.2^{2n-i} - 126.2^{n+i} - 15.2^i. \tag{13}
$$

By taking summation on i, we obtain

$$
\sum_{i=2}^{n+1} W\left(\frac{H_n}{E_i}\right) = 432.4^n + 252n.2^n - 720.4^n \sum_{i=2}^{n+1}\left(\frac{1}{2^i}\right) - \left(126.2^n + 15\right)\sum_{i=2}^{n+1} 2^i. \tag{14}
$$

It is easy to compute that

$$\sum_{i=2}^{n+1}\frac{1}{2^i}=\frac{(1/4)\left(\left(1/2^n\right)-1\right)}{(-1/2)}=-\frac{1}{2}\left(\frac{1}{2^n}-1\right)=\frac{1}{2}-\frac{1}{2^{n+1}}$$
$$\sum_{i=2}^{n+1}2^i=4\left(2^n-1\right). \quad (15)$$

By putting these values in equation (14), we have

$$\begin{aligned}\sum_{i=2}^{n+1}W\left(\frac{H_n}{E_i}\right)&=432.n.4^n+252.n.2^n-720.4^n.\left(\frac{1}{2}-\frac{1}{2^{n+1}}\right)-\left(126.2^n+15\right)(4)\left(2^n-1\right)\\&=432.n.4^n+252.n.2^n-360.4^n+360.\frac{4^n}{2^n}-\left(126.2^n+15\right)\left(4.2^n-4\right)\\&=432.n.4^n+252.n.2^n-360.4^n+360.\frac{4^n}{2^n}-504.2^n+504.2^n-60.2^n+60.\end{aligned} \quad (16)$$

Hence,

$$\sum_{i=2}^{n+1}W\left(\frac{H_n}{E_i}\right)=4^n\left(432n-864+\frac{360}{2^n}\right)+(252.n+444)2^n+60. \quad (17)$$

By adding equations (8) and (17) and using Theorem 1, we obtain

$$\begin{aligned}W\left(H_n\right)&=W\left(\frac{H_n}{E_1}\right)+\sum_{i=2}^{n+1}W\left(\frac{H_n}{E_i}\right)\\&=72.4^n-30+4^n\left(432n-864+\frac{360}{2^n}\right)+(252.n+444)2^n+60.\end{aligned} \quad (18)$$

This implies that

$$W\left(H_n\right)=30+\left(432.n-792+\frac{360}{2^n}\right).4^n+(252.n+444)2^n. \quad (19)$$

This completes the proof.

For $n\geq 1$, the graph I_{n+2} has five components. One component is $H=I_2-C_6$ and let the other components be $H_{1,n}, H_{2,n}, H_{3,n}$, and $H_{4,n}$ such that $H\cap H_{i,n}=\{s_i\}$, for $1\leq i\leq 4$. Thus, I_{n+2} is obtained by the edge disjoint copies of $H_{1,n}, H_{2,n}, H_{3,n}, H_{4,n}$ and the graph H. This implies that $I_{n+2}=H\cup H_{1,n}\cup H_{2,n}\cup H_{3,n}\cup H_{4,n}$.

The partition of the graph I_{n+2} is shown in Figure 5.

Define, $K_1=H_n\cup H$, $K_2=K_1\cup H_n$, $K_3=K_2\cup H_n$, and $K_4=K_3\cup H_n$, where $H\cap H_n=\{s_1\}$, $K_1\cap H_n=\{s_2\}$, $K_2\cap H_n=\{s_3\}$, and $K_3\cap H_n=\{s_4\}$.

It is important to note that $K_4=I_{n+2}, H_{1,n}=H_{2,n}=H_{3,n}=H_{4,n}=H_n$, and $w(s_1,H_n)=w(s_2,H_n)=w(s_3,H_n)=w(s_4,H_n)$.

Further, suppose that $|H|=n_1$, $|H_{n-2}|=n_2$, $|K_1|=n_3$, $|K_2|=n_4$, $|K_3|=n_5$, and $|K_4|=n_6$.

It is easy to compute that $n_2=12.2^n-5$ and $n_1+n_3+n_4+n_5=n_1+3n_2=86+36.2^n-18=362^n+68$.

In the following lemmas, $w(s_i,H_n)$ is computed. □

Lemma 4. *Let n be the positive integer and $1\leq j\leq 4$,*

$$w\left(s_j,H_n\right)=36n.2^n-6.2^n+21. \quad (20)$$

Proof. The construction of the graph shows that the graph has $n+1$ stages, and in each stage, there are 2^{i-1} hexagons, for $1\leq i\leq n+1$. The hexagons at each stage are connected to

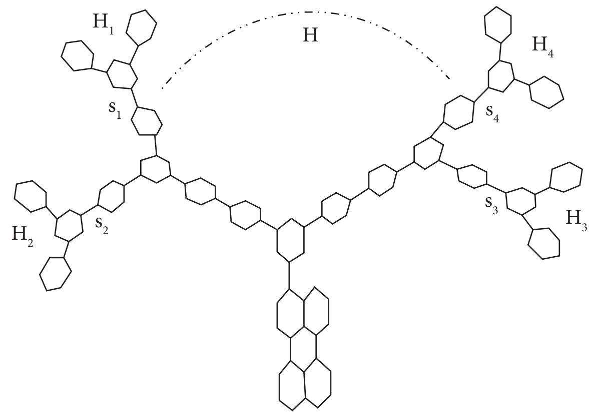

FIGURE 5: The partition of I_n into H_n and H.

two hexagons in the next stage through a vertex. Let x be a vertex connecting hexagon in $(i-1)^{\text{th}}$ stage to the hexagon at i^{th} stage. The distance of s_j to this vertex x in i^{th} stage is $3i$, where $1 \leq i \leq n+$. Further, the distance of x to the six vertices of hexagon is $1+2+2+3+3+4=15$. This implies that

$$\begin{aligned} w(s_j, H_n) &= \sum_{x \in H_n} d(x, s_i) = \sum_{i=1}^{n+1} (3(i-1)6 + 15)2^{i-1} \\ &= \sum_{i=1}^{n+1} (18i - 3)2^{i-1} = \sum_{i=1}^{n+1} 18i2^{i-1} - 3\sum_{i=1}^{n+1} 2^{i-1} \\ &= 9\sum_{i=1}^{n+1} i2^i - 3\sum_{i=1}^{n+1} 2^{i-1} \\ &= 9\left(2^{n+2}(n) + 2\right) - 3\left(2^{n+1} - 1\right) \\ &= 36n.2^n - 6.2^n + 21. \end{aligned} \tag{21}$$

□

Lemma 5. *Let n be the positive integer, then*

$$w(s_2, K_1) = 36n.2^n - 114.2^n + 1150. \tag{22}$$

Proof. Since $K_1 = H_{n-2} \cup H$, therefore, we have

$$\begin{aligned} w(s_2, K_1) &= w(s_2, H) + \sum_{i=1}^{n} d(s_1, H_{n-2}) + \sum_{i=1}^{n} d(s_2, s_1) \\ &= w(s_2, H) + w(s_1, H_{n-2}) + \sum_{i=1}^{n} d(s_1, s_2) \\ &= w(s_2, H) + w(s_1, H_{n-2}) + 10(n_2 - 1) \\ &= w(s_1, H) + W(s_1, H_{n-2}) + 10(n_2 - 1) \\ &= 1189 + 36n.2^n - 6.2^n + 21 + 10(12.2^n - 6) \\ &= 36n.2^n - 114.2^n + 1150. \end{aligned} \tag{23}$$

Hence,

$$W(s_2, K_1) = 36n.2^n - 114.2^n + 1150. \tag{24}$$

□

Lemma 6. *Let n be the positive integer, then*

$$w(s_3, K_2) = 72n.2^n + 732.2^n + 859. \tag{25}$$

Proof. Since $K_2 = H_{n-2} \cup K_1$, therefore, we have

$$\begin{aligned} w(s_3, K_2) &= \sum_{x \in K_1} d(s_3, x) + \sum_{x \in H_{n-2}} d(s_3, x) = \sum_{x \in H} d(s_3, x) + \sum_{x \in H_{1,n-1}} d(s_3, x) + \sum d(s_3, s_2) + d(s_2, x) \\ &= \sum_{x \in H} d(s_1, x) + \sum_{x \in H_{n-2}} (d(s_3, s_1) + d(s_1, x)) + \sum d(s_3, s_2) + d(s_2, x) \\ &= w(s_1, H) + 31(n_2 - 1) + w(s_1, H_{n-2}) + 31(n_2 - 1) + w(s_2, H_{n-2}) \\ &= w(s_1, H) + 62(n_2 - 1) + 2w(s_1, H_{n-2}) \\ &= 1189 + 62(12.2^n - 6) + 72n.2^n - 12.2^n + 42 \\ &= 1189 + 744.2^n - 372 + 72n.2^n - 12.2^n + 42. \end{aligned} \tag{26}$$

Hence, we have

$$w\left(s_3, K_2\right) = 72n.2^n + 732.2^n + 859, \tag{27}$$

this completes the proof. □

Lemma 6. *Let n be the positive integer, then*

$$W\left(s_4, K_3\right) = 54.n.2^n + 363.2^n + 826. \tag{28}$$

Proof. Since $K_3 = H_{n-2} \cup K_2$, therefore, we have

$$\begin{aligned} W\left(s_4, K_3\right) &= \sum_{x\in H_{3,n-2}} d\left(s_4, s_3\right) + d\left(s_3, x\right) + \sum_{x\in H} d\left(s_4, x\right) + \sum d\left(s_4, s_1\right) + d\left(s_1, x\right) + \sum d\left(s_4, s_2\right) + d\left(s_2, x\right) \\ &= 9\left(n_4 - 1\right) + w\left(s_3, H_{3,n-2}\right) + w\left(s_4, H\right) + 31\left(n_3 - 1\right) + W\left(s_2, H_{2,n-2}\right) + 31\left(n_2 - 1\right) + w\left(s_1, H\right) \\ &= 71\left(12.2^n - 6\right) + 3w\left(s_1, H_{n-2}\right) + w\left(s_1, H\right) \\ &= 852.2^n - 426 + 3.\left(36n.2^n - 6.2^n + 21\right) + 1189 \\ &= 852.2^n - 426 + 108.n.2^n - 18.2^n + 63 + 1189. \end{aligned} \tag{29}$$

Hence, we have

$$W\left(s_4, K_3\right) = 108.n.2^n + 834.2^n + 826. \tag{30}$$

This completes the proof. □

An easy computation implies that

Lemma 7. *The Wiener index of the graph H is* $W(H) = 21646$.

Now, we prove the main result of this section.

Theorem 8. *For* $n \geq 3$, $W\left(I_n\right) = 2376.n.4^n + 1116.4^n + 360.n2^n + 22872.2^n + 324.2^n\left(2^{n+1}(n-1)\right) + 2736\left(2^{n+1}(n-1)\right) + 3946$.

Proof. Since $K_1 = H \cup H_n$, $K_2 = K_1 \cup H_n$, $K_3 = K_2 \cup H_n$, and $= I_{n+2} = K_4 = K_3 \cup H_n$, therefore, by using Theorem 2, we obtain

$$\begin{aligned} W\left(K_1\right) &= W(H) + W\left(H_n\right) + \left(n_1 - 1\right)w\left(s_1, H_1\right) + \left(n_2 - 1\right)w\left(s_1, H\right), \\ W\left(K_2\right) &= W\left(H_n\right) + W\left(K_1\right) + \left(n_2 - 1\right)w\left(s_2, K_1\right) + \left(n_3 - 1\right)w\left(s_2, H_2\right), \\ W\left(K_3\right) &= W\left(H_n\right) + W\left(K_2\right) + \left(n_2 - 1\right)w\left(s_3, K_2\right) + \left(n_4 - 1\right)w\left(s_3, H_3\right), \\ W\left(K_4\right) &= W\left(H_n\right) + W\left(K_3\right) + \left(n_2 - 1\right)w\left(s_4, K_3\right) + \left(n_5 - 1\right)w\left(s_4, H_4\right). \end{aligned} \tag{31}$$

By replacing the values of $W\left(K_1\right), W\left(K_2\right)$, and $W\left(K_3\right)$ in $W\left(K_4\right)$ recursively, we obtain

$$\begin{aligned} W\left(K_4\right) &= W\left(H_n\right) + W\left(K_3\right) + \left(n_2 - 1\right)w\left(s_4, K_3\right) + \left(n_5 - 1\right)w\left(s_4, H_n\right) \\ &= W\left(H_n\right) + W\left(H_n\right) + W\left(K_2\right) + \left(n_2 - 1\right)w\left(s_3, K_2\right) + \left(n_4 - 1\right)w\left(s_3, H_n\right) + \left(n_2 - 1\right)w\left(s_4, K_3\right) + \left(n_5 - 1\right)w\left(s_4, H_n\right) \\ &= W\left(H_n\right) + W\left(H_n\right) + W\left(H_n\right) + W\left(K_1\right) + \left(n_2 - 1\right)w\left(s_2, K_1\right) \\ &\quad + \left(n_3 - 1\right)w\left(s_2, H_n\right) + \left(n_2 - 1\right)w\left(s_3, K_2\right) + \left(n_4 - 1\right)w\left(s_3, H_n\right) + \left(n_2 - 1\right)w\left(s_4, K_3\right) + \left(n_5 - 1\right)w\left(s_4, H_n\right) \\ &= W\left(H_n\right) + W\left(H_n\right) + W\left(H_n\right) + W\left(H_n\right) + W(H) + \left(n_2 - 1\right) \\ &\quad \cdot w\left(s_1, H\right) + \left(n_1 - 1\right)w\left(s_1, H_n\right) + \left(n_2 - 1\right)w\left(s_2, K_1\right) + \left(n_3 - 1\right)w\left(s_2, H_n\right) + \left(n_2 - 1\right) \\ &\quad \cdot w\left(s_3, K_2\right) + \left(n_4 - 1\right)w\left(s_3, H_n\right) + \left(n_2 - 1\right)w\left(s_4, K_3\right) + \left(n_5 - 1\right)w\left(s_4, H_n\right) \\ &= 4W\left(H_n\right) + W(H) + \left(n_2 - 1\right)\left(w\left(s_1, H\right) + w\left(s_2, K_1\right) + w\left(s_3, K_2\right) + w\left(s_4, K_3\right)\right) \\ &\quad + \left(n_5 - 1\right)w\left(s_4, H_n\right) + \left(n_4 - 1\right)w\left(s_3, H_n\right) + \left(n_3 - 1\right)w\left(s_2, H_n\right) + \left(n_1 - 1\right)w\left(s_1, H_n\right). \end{aligned} \tag{32}$$

Since $w(s_1, H_n) = w(s_2, H_n) = w(s_3, H_n) = w(s_4, H_n)$, therefore,

$$\begin{aligned} W(I_{n+2}) &= 4W(H_n) + W(H) + (n_1 + n_3 + n_4 + n_5 - 4)w(s_1, H_n) \\ &\quad + (n_2 - 1)(w(s_1, H) + w(s_2, K_1) + w(s_3, K_2) + w(s_4, K_3)). \end{aligned} \tag{33}$$

By putting values of $n_2 = 12.2^n - 5$ and $n_1 + n_3 + n_4 + n_5 = n_1 + 3n_2 = 86 + 36.2^n - 18 = 362^n + 68$ and $w(s_2, K_1)$, $w(s_3, K_2)$ and $w(s_4, K_3)$ from Lemmas 5, 6, and 7 in the above equation, we obtain

$$\begin{aligned} W(I_n) &= 4\left[\left(432.n - 792 + \frac{360}{2^n}\right)4^n + (252.n + 444)2^n + 30\right] + 21646 \\ &\quad + (36.2^n + 68 - 4)\left(9.\left(2^{n+1}(n-1) + 2\right) - 3.2^n + 3\right) + (6.2^n - 6) \\ &\quad \cdot \left(1189 + (18.n.2^n + 39.2^n + 1160) + (36.n.2^n + 330.2^n + 859) + (54.n.2^n + 363.2^n - 826)\right) \\ &= 4\left[\left(432.n - 792 + \frac{360}{2^n}\right)4^n + (252.n + 444)2^n + 30\right] + 21646 + (36.2^n + 304) \\ &\quad \cdot \left(9\left(2^{n+1}(n-1) + 2\right) - 3.2^n + 3\right) + (6.2^n - 6)(1189 + 108n.2^n + 732.2^n + 2845) \\ &= \left[\left(4.432.n.4^n - 4.4^n 792 + 4.4^n\left(\frac{360}{2^n}\right)\right) + (4.252n.2^n + 444.4.2^n + 120\right] + 21646 + (36.2^n + 304) \\ &\quad \cdot\left(9\left(2^{n+1}(n-1) + 2\right) - 3.2^n + 3\right)\big) + (6.2^n - 6)(1189 + 108n.2^n + 732.2^n + 2845) \\ &= (1728n.4^n - 3168.4^n + 1440.2^n) + 1008.n.2^n + 1776.2^n + 120 \\ &\quad + 21646 + (36.2^n + 304)\left(9\left(2^{n+1}(n-1) + 2\right) - 3.2^n + 3\right) \\ &\quad \cdot (6.2^n - 6)(1189 + 108n.2^n + 732.2^n + 2845). \\ W(I_{n=2}) &= 1728.n.4^n - 3168.4^n + 1008n.2^n + 3216.2^n + 120 + 21646 \\ &\quad + (36.2^n + 304)\left(9\left(2^{n+1}(n-1) + 2\right) - 3.2^n + 3\right) + (6.2^n - 6)(108.n.2^n + 732.2^n + 4034). \end{aligned} \tag{34}$$

Since

$$\begin{aligned} (6.2^n - 6)(108.n.2^n + 732.2^n + 4034) &= 6.2^n.108.n.2^n + 732.2^n.6.2^n + 4034.6.2^n - 6.108.n.2^n - 6.732.2^n + 6.4034 \\ &= 648.4^n.n + 4392.4^n + 24202.2^n - 648.n.2^n - 4392.2^n - 24204 \\ &= 648n.4^n + 4392.4^n - 648.n.2^n + 19812.2^n - 24204. \end{aligned} \tag{35}$$

Therefore, Wiener index of I_{n+2} reduces to $(I_{n+2}) = 1728n.4^n - 3168.4^n + 1008.n.2^n + 3216.2^n + 21766 + (36.2^n + 304)(9(2^{n+1}(n-1) + 2) - 3.2^n + 3)$ $+648.n.4^n + 4392.4^n - 648n.2^n + 19812.2^n - 24204 = 2376.n.4^n + 1224.4^n + 360.n.2^n + 23028.2^n - 24204 + 21766 + (36.2^n + 304)$ $((9(2^{n+1}(n-1) + 2) - 3.2^n + 3)$.

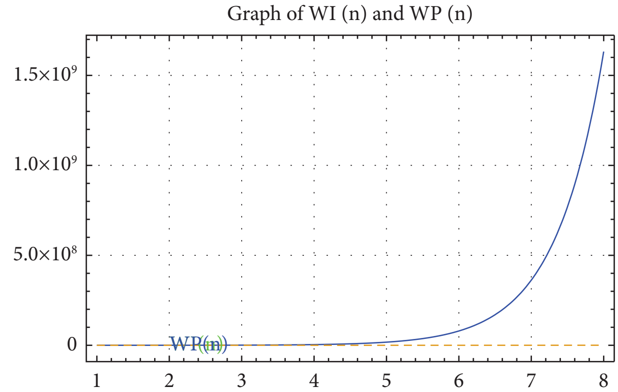

FIGURE 6: Graphical comparison of Wiener and Wiener polarity indices.

The last expression after simplification becomes

$$
\begin{aligned}
&(36.2^n + 304)\left(9\left(2^{n+1}(n-1)+2\right) - 3.2^n + 3\right)\\
&\quad = 324.2^n\left(2^{n+1}(n-1) + 2736\left(2^{n+1}(n-1) - 108.4^n - 156.2^n + 6384\,(36.2^n + 304)\left(9\left(2^{n+1}(n-1)+2\right) - 3.2^n + 3\right)\right.\right.\\
&\quad = (36.2^n + 304)\,(9\,(2n+1\,(n-1) + 9\,(2) - 3.2^n + 3) + (36.2^n + 304)\,(9\left(2^{n+1}(n-1) - 3.2^n + 21\right)\\
&\quad = 36.2^n\,(9\left(2^{n+1}\left(n-1\right) - 36.2^n.3.2^n + 36.2^n.21 + 304\left(9\left(2^{n+1}(n-1) - 304.3.2^n + 304.21\right)\right)\right.\\
&\quad = 36.2^n\left(9\left(2^{n+1}(n-1) - 108.4^n + 756.2^n\right)\right) + 2736\left(2^{n+1}(n-1) - 912.2^n + 6384\right).
\end{aligned}
\tag{36}
$$

By replacing this value, Wiener index of I_{n+2} reduces to

$$
\begin{aligned}
W\left(I_{n+2}\right) = {} & \left(2376n.4^n + 1224.4^n + 360.n.2^n + 23028.2^n - 24204\right) + 21766 + 324.2^n\left(2^{n+1}(n-1)\right)\\
& + 2736\left(2^{n+1}(n-1) - 108.4^n - 156.2^n + 6384.\right.
\end{aligned}
\tag{37}
$$

Hence, $(I_n) = 2376.n.4^n + 1116.4^n + 360.n2^n + 22872.2^n + 324.2^n\,(2^{n+1}\,(n-1)) + 2736\,(2^{n+1}\,(n-1)) + 3946.$ This completes the proof. □

2.3. Wiener Polarity Index of I_n. From the construction of the graph I_n, it is easy to see that

$$
\begin{aligned}
W_p\left(I_2\right) = {} & 2\,(2) + (2\,(2) + 4) + (3\,(2) + 3)\\
& + 2\,(3) + 2\,(3) + (3 + 2 + 1) + (3 + 2 + 1) + (2 + 1) + 3\,(13) + (18.3) + 8.2\,(2) + 8.4 = 205.
\end{aligned}
\tag{38}
$$

Theorem 9. *For $n \geq 3$,*

$$
W_p\left(I_n\right) = 3.2^{n+3} - 112. \tag{39}
$$

Proof. For $j \geq 3$, the pair of vertices at distance 3 in the hexagon is 3, and there is no vertex at distance three between two hexagons at the same stage. The pair of vertices at distance 3 between the hexagons of stages $j-1$ and j is 18, and there is no pair of vertices at distance 3 from stages $j-2$ to j. Thus,

$$
\begin{aligned}
W_p\left(I_n\right) &= W_p\left(I_2\right) + 3\left(2^3 + \cdots + 2^n\right) + 18\left(2^2 + \cdots + 2^{n-1}\right.\\
&= 205 + 3\left(2^{n+1} - 1\right) - 21 + 18\left(2^n - 1\right) - 54 = 205 + 12.2^{n+1} - 24 - 18 - 54 = 3.2^{n+3} - 112.
\end{aligned}
\tag{40}
$$

□

3. Concluding Remarks

In this article, the Wiener index and Wiener polarity index of a class of nanostar dendrimers are explored. We have computed the exact values of the Wiener index and the Wiener polarity index of the nanostar dendrimer I_n. Figure 6 shows the graphical comparison of both indices. These topological indices provide a valuable tool to measure dendrimer molecular structure, allowing for comparisons, forecasts, and comprehension of the potential effects of various structural aspects on behaviour and qualities. The solubility, stability, and reactivity of dendrimers can be shown by particular topological indices. By establishing correlations, properties dependent on the topological structure of the dendrimer can be predicted. Relationships between structure and property can be established with the help of topological indices. In future, researchers can determine which features of the dendrimer's structure have the most impact on how it behaves or performs.

Data Availability

Data from previous studies were used to support this study.

Disclosure

This work is part of the MS dissertation of one of the co-authors, Pakizah Bashir [22].

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

The authors extend their appreciation to the Deanship of Scientific Research at King Khalid University for funding this work through the Larg Groups Project under grant number RGP.2/395/44. This study was supported via funding from Prince Sattam bin Abdulaziz University project number PSAU/2023/R/1444.

References

[1] E. Abbasi, S. F. Aval, A. Akbarzadeh et al., "Dendrimers synthesis, applications, and properties," *Nanoscale Research Letters*, vol. 9, no. 1, pp. 247–310, 2014.

[2] A. A. Dobrynin, R. Entringer, and I. Gutman, "Wiener index of trees: theory and applications," *Journal of Applied Mathematics*, vol. 66, no. 3, pp. 211–249, 2001.

[3] A. Iranamanesh and N. A. Gholami, "Computing the szeged index of styrylbenzene dendrimer and triarylamine dendrimer of generation, 1-3," *Match*, vol. 62, no. 2, p. 371, 2009.

[4] F. Zeng and S. C. Zimmerman, "Dendrimers in supramolecular chemistry from molecular recognition to self-assembly," *Chemical Reviews*, vol. 97, no. 5, pp. 1681–1712, 1997.

[5] I. Gutman and T. Körtvélyesi, "Wiener indices and molecular surfaces," *Journal of Natural Research A*, vol. 50, pp. 669–671, 1995.

[6] D. A. Tomalia and J. M. J. Fréchet, "Discovery of dendrimers and dendritic polymers a brief historical perspective," *Journal of Polymer Science Part A: Polymer Chemistry*, vol. 40, no. 16, pp. 2719–2728, 2002.

[7] W. Gao, Z. Iqbal, M. Ishaq, R. Sarfraz, M. Aamir, and A. Aslam, "On eccentricity-based topological indices study of a class of porphyrin-cored dendrimers," *Biomolecules*, vol. 8, no. 3, p. 71, 2018.

[8] M. Golriz, M. R. Darafsheh, and M. H. Khalifeh, "The wiener, szeged and piindices of a phenylazomethine dendrimer," *Digest Journal of Nanomaterials and Biostructures*, vol. 6, no. 4, pp. 1545–1549, 2011.

[9] W. Hui, M. K. Siddiqui, S. Akhter, S. Hafeez, and Y. Ali, "On degree based topological aspects of some dendrimers," *Polycyclic Aromatic Compounds*, vol. 43, no. 4, pp. 3601–3612, 2022.

[10] L. I. Stiel, G. Thodos, and G. Thodos, "The normal boiling points and critical constants of saturated aliphatic hydrocarbons," *AIChE Journal*, vol. 8, no. 4, pp. 527–529, 1962.

[11] D. H. Rouvray and B. C. Crafford, "The dependence of physical-chemical properties on topological factors," *South African Journal of Science*, vol. 72, p. 47, 1976.

[12] S. Klavžar, I. Gutman, and B. Mohar, "Labeling of benzenoid systems which reflects the vertex-distance relations," *Journal of Chemical Information and Computer Sciences*, vol. 35, no. 3, pp. 590–593, 1995.

[13] H. Hosoya, "Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons," *Bulletin of the Chemical Society of Japan*, vol. 44, no. 9, pp. 2332–2339, 1971.

[14] P. S. Kowalski, A. Rudra, L. Miao, and D. G. Anderson, "Delivering the messenger: advances in technologies for therapeutic mRNA delivery," *Molecular Therapy*, vol. 27, no. 4, pp. 710–728, 2019.

[15] B. A. G. Hammer and K. Müllen, "Expanding the limits of synthetic macromolecular chemistry through polyphenylene dendrimers," *Journal of Nanoparticle Research*, vol. 20, no. 10, pp. 262–323, 2018.

[16] S. Klavžar and M. J. Nadjafi-Arani, "Wiener index in weighted graphs via unification of Θ^*-classes," *European Journal of Combinatorics*, vol. 36, pp. 71–76, 2014.

[17] S. Ashraf, M. Imran, S. A. U. H. Bokhary, and S. Akhter, "The Wiener index, degree distance index and Gutman index of composite hypergraphs and sunflower hypergraphs," *Heliyon*, vol. 8, no. 12, 2022.

[18] N. De and S. M. A. Nayeem, "Computing the F-index of nanostar dendrimers," *Pacific Science Review A: Natural Science and Engineering*, vol. 18, no. 1, pp. 14–21, 2016.

[19] M. K. Siddiqui, M. Imran, and A. Ahmad, "On Zagreb indices, Zagreb polynomials of some nanostar dendrimers," *Applied Mathematics and Computation*, vol. 280, pp. 132–139, 2016.

[20] S. A. Bokhary and H. Tabassum, "The energy of some tree dendrimers," *Journal of Applied Mathematics and Computing*, vol. 68, no. 2, pp. 1033–1045, 2022.

[21] T. Iqbal, M. Imran, and S. A. Bokhary, "Domination and power domination in certain families of nanostars dendrimers," *IEEE Access*, vol. 8, pp. 130947–130951, 2020.

[22] P. Bashir, *Distances in Nanostar Dendrimers Using Vertex Weighted Graphs, Mphill Diss*, Bahauddin Zakriya UNiversity, Multan, Pakistan, 2023.

[23] S. A. Bokhary, Adnan, M. K. Siddiqui, and M. Cancan, "On topological indices and QSPR analysis of drugs used for the treatment of breast cancer," *Polycyclic Aromatic Compounds*, vol. 42, no. 9, pp. 6233–6253, 2022.

[24] M. Adnan, S. A. Bokhary, and M. Imran, "On wiener polarity index and wiener index of certain triangular networks," *Journal of Chemistry*, vol. 2021, Article ID 2757925, 20 pages, 2021.

[25] N. Dorosti, A. Iranmanesh, and M. V. Diudea, "Computing the Cluj index of dendrimer nanostars," *Match*, vol. 62, pp. 389–395, 2009.

[26] Z. Iqbal, M. Ishaq, and M. Aamir, "On eccentricity-based topological descriptors of dendrimers," *Iranian Journal of Science and Technology Transaction A-Science*, vol. 43, no. 4, pp. 1523–1533, 2019.