MJFAS
Malaysian Journal of Fundamental and Applied Sciences

Movahedi *et al.* | Malaysian Journal of Fundamental and Applied Sciences, Vol. 20 (2024) 588-596

RESEARCH ARTICLE

Computing the Hosoya Index of Some Nanostar Dendrimers

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Abstract Dendrimers are highly branched macromolecules built up from a monomer, with new branches added in steps until a tree structure is created. The various biological characteristics of dendrimers are a good choice in chemistry, biology, the medical field, and nano-science. A topological index is a type of molecular descriptor that is calculated based on the molecular graph of a chemical structure. The Hosoya index is a well-known topological index that is used to predict some of their physico-chemical properties from the structure of molecules. The Hosoya index of a graph is defined as the total number of its independent edge sets. In this paper, we study the Hosoya index of some families of nanostar dendrimers. We obtain the formulas of the Hosoya index for two infinite classes of dendrimers, namely, nanostar dendrimer $NS_1[n]$ and tetrathiafulvalene dendrimer. We use the Mathematica program to evaluate the results and accuracy of calculations. Our results can be used in analyzing the molecular topology of these families of nanostar dendrimers.

Keywords: Topological index, Hosoya index, Dendrimers, Mathematical Chemistry.

Introduction

Mathematical chemistry is an interdisciplinary field in which molecular phenomena are modeled and studied by mathematics. One of the branches of mathematical chemistry in which the molecular structure is modeled by a simple graph known as a molecular graph where vertices correspond to atoms and the edge to the chemical bound (between the atoms) is chemical graph theory [5].

In mathematical chemistry, topological indices are defined as a vital tool for analyzing the physical properties of chemical compounds. These descriptors determine the relationship between the topology of a molecular structure and the physico-chemical properties used in the Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships [2, 4].

Haruo Hosoya first introduced the Hosoya index and showed that certain chemical and physical properties of saturated hydrocarbons are correlated with this index [6]. Some studies related to the chemical concepts of the Hosoya index can be found in [9, 10, 15].

The Hosoya index is studied in certain structures of molecular graphs involving pentagonal and hexagonal cycles. Liu *et al*. [10] characterized the tricyclic graphs with the largest Hosoya index and with the smallest Merrifield–Simmons index. In [15] the extremal unique unicyclic graph that has the maximal Hosoya index and the second maximal Hosoya index is characterized. Movahedi *et al*. [12] obtained the exact relations of the Hosoya index on some classes of cycle-related graphs namely, chain triangular cactus, Dutch windmill graph, and Barbell graph. In [13], the Hosoya polynomial for three classes of nanostar dendrimers, namely, PETIM dendrimer, POPAM dendrimer, and Nanostar dendrimer $D_3[n]$ are obtained.

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Received: 21 Nov. 2023
Accepted: 4 Feb. 2024

In chemical graph theory, chemical structures are modeled by a molecular graph to analyze underlying theoretical properties. The molecular graph of a chemical structure is a simple graph (G) where the vertices represent the atoms and the edges represent the chemical bonds between the atoms.

Let $G = (V, E)$ be a simple connected graph of order $|V| = n$ and size $|E| = m$. Two edges of G are said to be independent if they don't have a common vertex in G. A k-matching of G is a set of k mutually independent edges and the number of k-matching in G is denoted by $m(G, k)$. Let $m(G, 0) = 1$ for any graph G. Then, $Z(G)$ is defined as follows:

$$Z(G) = \sum_{k=0}^{\left\lfloor \frac{n}{2} \right\rfloor} m(G, k).$$

For graph G, the neighborhood of a vertex $u \in V$ is defined as $N_G(u) = \{ v \in V \mid uv \in E \}$. The number of edges incident to u in G is denoted by $deg_G(u)$. Two graphs G_1 and G_2 containing the same number of vertices connected in the same way are said to be isomorphic and denoted as $G_1 \simeq G_2$ [5].

Dendrimers are macromolecules with highly branched monodisperse and have complex chemical and interesting structures with a precisely tailored architecture. Applications of dendrimers are unlimited in chemistry, biology, nano-science, targeted drug delivery, and suitable subjects for interdisciplinary research. Some topological indices of these macromolecules are studied in [3, 14,16].

In this paper, we investigate the Hosoya index for two infinite classes of dendrimers nanostar dendrimer $NS_1[n]$ and tetrathiafulvalene dendrimer. The results can be used in analysing the molecular topology of these families of nanostar dendrimers.

Methodology and Main Results

In this section, we obtain the main results for computing the Hosoya index of four infinite classes of dendrimers. First, we give some lemmas that will be used in the proof of our results.

Lemma 1 [5] Let $G = (V, E)$ be a graph.

i) If $uv \in E(G)$, then $Z(G) = Z(G - uv) + Z(G - \{u, v\})$.

ii) If $v \in V(G)$, then $Z(G) = Z(G - v) + \sum_{u \in N_G(v)} Z(G - \{u, v\})$.

iii) If $G_1, G_2, \ldots, G_t$ are all components of G, then $Z(G) = \prod_{i=1}^{t} Z(G_i)$.

Lemma 2 [5] Let P_n and S_n be the path and star graph of order n, respectively. Then, for any positive integer n,

i) $Z(P_n) = F_{n+1}$,

ii) $Z(S_n) = n$,

where F_n is the n-th Fibonacci number, defined by $F_0 = 0$, $F_1 = 1$ and $F_{n+1} = F_n + F_{n-1}$.

First, we consider another type of PAMAM dendrimers, denoted by $NS_1[n]$, where $n \geq 0$ is the steps of growth (see Figure 1). This graph has $2^{n+5} - 28$ vertices and $2^{n+5} - 29$ edges [1]. In the following, we compute the Hosoya index of $NS_1[n]$ for $n \geq 0$. In doing so, we use graphs G'_n and G''_n which are shown in Figure 2.

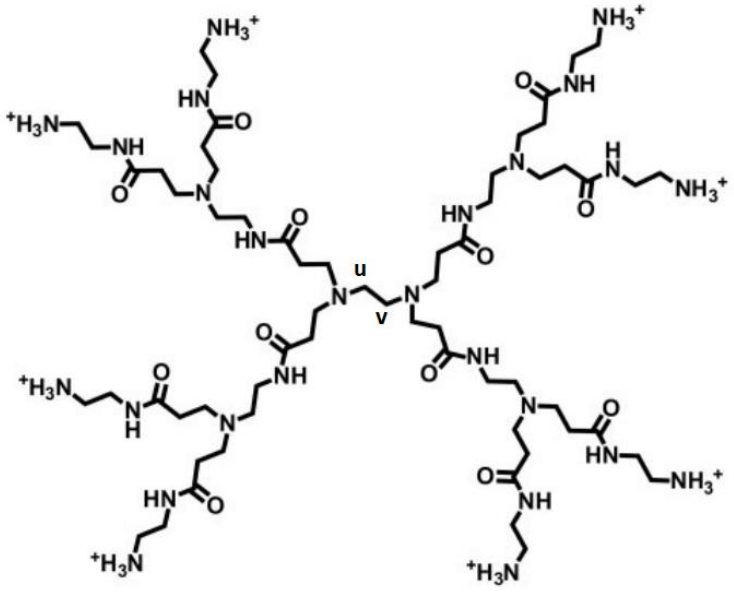


Figure 1. $NS_1[n]$ nanostar dendrimer

Theorem 1. The Hosoya index of $NS_1[n]$ for $n \geq 0$ is given by

$$Z(NS_1[n]) = Z(G_n')^2 + Z(G_n'')^2,$$

where graphs G_n' and G_n'' are shown in Figure 2 and for $n \geq 1$,

$$Z(G_n') = 456Z(G_{n-1}')^2 + 530Z(G_{n-1}')Z(G_{n-1}'') + 154Z(G_{n-1}'')^2,$$
$$Z(G_n'') = 312Z(G_{n-1}')^2 + 362Z(G_{n-1}')Z(G_{n-1}'') + 105Z(G_{n-1}'')^2,$$

with the initial conditions $Z(G_0') = 2$ and $Z(G_0'') = 1$.

Proof. By Lemma 1 and deleting the edge uv (see Figure 1), we get

$$\begin{aligned} Z(NS_1[n]) &= Z(NS_1[n] - uv) + Z(NS_1[n] - \{u, v\}) \\ &= Z(G_n')^2 + Z(G_n'')^2, \end{aligned}$$

where graphs G_n' and G_n'' are shown in Figure 2.

We apply the reduction process to G_n' and G_n'', $n \geq 1$ and delete the edges of these graphs such that the formulas are obtained in terms G_{n-1}' and G_{n-1}''. Therefore, for $n \geq 1$

$$\begin{aligned} Z(G_n') = &\Big(2(Z(P_5) + Z(P_2)^2)^2 + 2\big(Z(P_4) + Z(P_2)\big)\big(Z(P_5) + Z(P_2)^2\big)\Big) Z(G_{n-1}')^2 \\ &+2\left(2\left(Z(P_5) + Z(P_2)^2\right)\left(Z(P_4) + Z(P_2)\right)\right. \\ &\left.+\left(Z(P_4) + Z(P_2)\right)^2 + Z(S_4)(Z(P_5) + Z(P_2)^2)\right) Z(G_{n-1}')Z(G_{n-1}'') \\ &+\Big(2\left(Z(P_4) + Z(P_2)\right)^2 + 2\,Z(S_4)\left(Z(P_4) + Z(P_2)\right)\Big) Z(G_{n-1}'')^2, \end{aligned}$$

Then, by substituting for $Z(P_n)$ and $Z(S_n)$ using Lemma 2 the result follows.

Similarly, for graph G_n'',

$$\begin{aligned} Z(G_n'') = &\Big((Z(P_5) + Z(P_2)^2)^2 + 2\big(Z(P_4) + Z(P_2)\big)\big(Z(P_5) + Z(P_2)\big)\Big) Z(G_{n-1}')^2 \\ &+2\big(2\left(Z(P_5) + Z(P_2)^2\right)\left(Z(P_4) + Z(P_2)\right) \\ &\left.+\left(Z(P_4) + Z(P_2)\right)^2 + Z(S_4)(Z(P_5) + Z(P_2)^2)\right) Z(G_{n-1}')Z(G_{n-1}'') \\ &+\Big(\left(Z(P_4) + Z(P_2)\right)^2 + 2Z(S_4)\big(Z(P_4) + Z(P_2)\big)\Big) Z(G_{n-1}'')^2, \end{aligned}$$

Then, the result follows using Lemma 2.

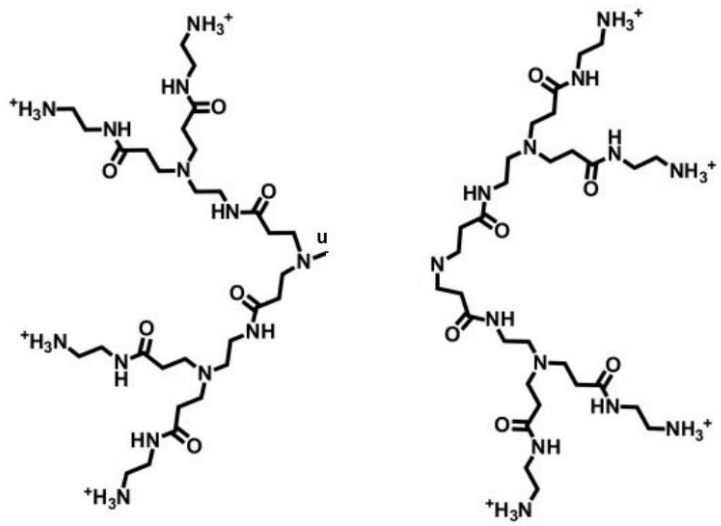
For the case $n = 0$, it is easy to see that $NS_1[0] \simeq P_1$ (see Figure 1). Therefore,

$$Z(G_0') = Z(P_2) = 2,$$

and

$$Z(G_0'') = Z(K_1) = 1.$$

This follows our result.



G'_n G''_n

Figure 2. The graphs G'_n and G''_n in Theorem 1

Finally, we shall compute the Hosoya index of another family of nanostar dendrimers as tetrathiafulvalene dendrimer of generation G_n with n growth stages, denoted by $TD_2[n]$ for $n \geq 0$. The number of vertices of $TD_2[n]$ is $31 \times 2^{n+2} - 74$ [11] as shown in Figure 3.

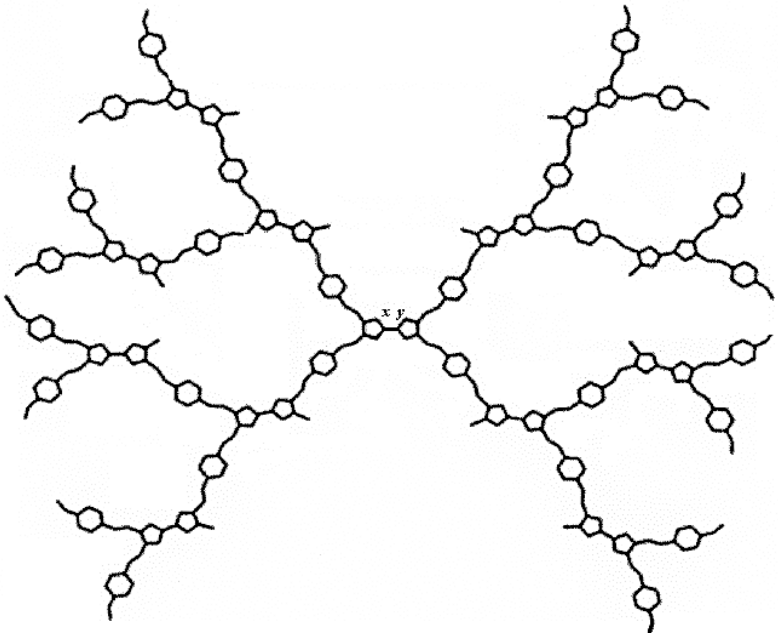


Figure 3. Tetrathiafulvalene dendrimer with 2-growth stages, $TD_2[2]$

In order to prove Theorem 2, we use two graphs G'_n and G''_n as shown in Figure 4. The number of vertices of G'_n and G''_n are $31 \times 2^{n+1} - 37$ and $31 \times 2^{n+1} - 38$, respectively. We also need in the process of proving to compute the Hosoya index of some of the certain graphs given in Figure 5 and Figure 6. Tables 1 and 2 show the Hosoya index of these graphs in Figures 5 and 6, respectively.

For computing the Hosoya index of graphs in Figure 6, we repeat Lemma 1 until the remaining graph contains components in the form of graphs in Figure 5. For example, we compute $Z(t'')$.
By starting from removing edge xy and repeating Lemma 1, we have

$$\begin{aligned} Z(t'') = &\left[(Z(P_3)^2+1)\big(Z(P_2)Z(2)+Z(5)\big)+\big(Z(P_4)+Z(P_2)\big)\big(Z(4)+Z(6)\big)\right] \\ &\times\left(\left[(Z(P_3)^2+1)\big(Z(P_2)Z(2)+Z(5)\big)+\big(Z(P_4)+Z(P_2)\big)\big(Z(4)+Z(6)\big)\right]\right. \\ &+2\left[\big(Z(P_2)+Z(P_4)\big)\big(Z(2)+Z(5)\big)+Z(P_3)\big(Z(4)+Z(6)\big)\right]\Big) \\ &+Z(P_2)\left[(Z(P_3)^2+1)Z(2)+\big(Z(P_4)+Z(P_2)\big)Z(4)\right], \end{aligned}$$

By Table 1, we have $Z(t'') = 8597596$.

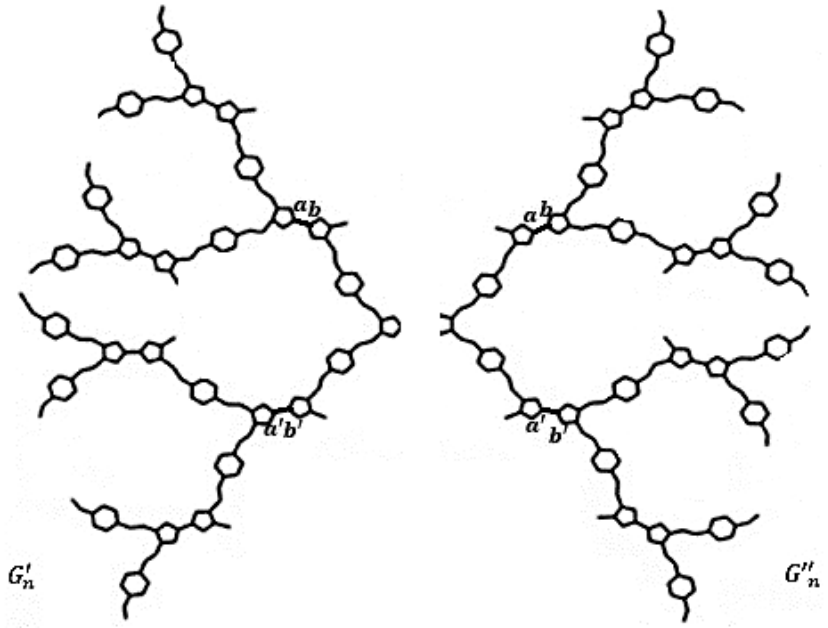


Figure 4. The graphs G'_n and G''_n in Theorem 2

Theorem 2. The Hosoya index of $TD_2[n]$ for $n \geq 0$ is obtained by the following formula,

$$Z(TD_2[n]) = Z(G'_n)^2 + Z(G''_n)^2,$$

where for $n \geq 1$,

$$\begin{aligned} Z(G'_n) &= \alpha' Z(G'_{n-1})^2 + 2\beta' Z(G'_{n-1})Z(G''_{n-1}) + \gamma' Z(G''_{n-1})^2, \\ Z(G''_n) &= \alpha'' Z(G'_{n-1})^2 + 2\beta'' Z(G'_{n-1})Z(G''_{n-1}) + \gamma'' Z(G''_{n-1})^2, \end{aligned}$$

such that $\alpha' = 84303360$, $\beta' = 28831616$, $\gamma' = 8597596$, $\alpha'' = 36774400$, $\beta'' = 14140512$, $\gamma'' = 5521204$ with the initial conditions $Z(G'_0) = 198048$ and $Z(G''_0) = 90064$.
First, we prove the following two lemmas.

Lemma 3. For $n \geq 1$,

$$Z(G'_n) = \alpha' Z(G'_{n-1})^2 + 2\beta' Z(G'_{n-1})Z(G''_{n-1}) + \gamma' Z(G''_{n-1})^2,$$

where $\alpha' = 84303360$, $\beta' = 28831616$ and $\gamma' = 8597596$.

Proof.

According to Figure 4 and Lemma 1(i) and (iii), we have

$$\begin{aligned} Z(G'_n) &= Z(G'_n - ab) + Z(G'_n - a - b) \\ &= Z(G'_{n-1})Z(H_n) + Z(G''_{n-1})Z(F_n) \end{aligned}$$

such that H_n is the graph constructed by deleting edge ab from G'_n and F_n is the graph obtained by removing the vertices a and b from G'_n.

For computing $Z(H_n)$ and $Z(F_n)$, we use Lemma 1(i) and (iii) and consider the edge $a'b'$ such that the remaining graphs be in Figure 6. Therefore, using Table 1

$$Z(H_n) = Z(t)Z(G'_{n-1}) + Z(t')Z(G''_{n-1})$$
$$= 84303360Z(G'_{n-1}) + 28831616Z(G''_{n-1}).$$

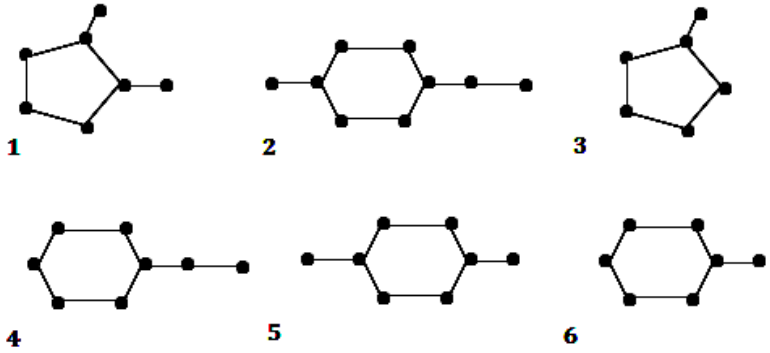


Figure 5. Some certain graphs in Theorem 5

In a similar way, for the graph F_n,

$$Z(F_n) = Z(t')Z(G'_{n-1}) + Z(t'')Z(G''_{n-1})$$
$$= 28831616Z(G'_{n-1}) + 8597596(G''_{n-1}).$$

So, by putting $\alpha' = 84303360$, $\beta' = 28831616$ and $\gamma' = 8597596$ the result completes.

■

Lemma 4. For $n \geq 1$,

$$Z(G''_n) = \alpha''Z(G'_{n-1})^2 + 2\beta''Z(G'_{n-1})Z(G''_{n-1}) + \gamma''Z(G''_{n-1})^2,$$

where $\alpha'' = 36774400$, $\beta'' = 14140512$ and $\gamma'' = 5521204$.

Proof.

According to Figure 5 and similar to the proof of Lemma 3 we have,

$$Z(G''_n) = Z(G'_{n-1})Z(H'_n) + Z(G''_{n-1})Z(F'_n)$$

where H'_n and F'_n are obtained by deleting edge ab and vertices $\{a, b\}$ in the graph G''_n, respectively.

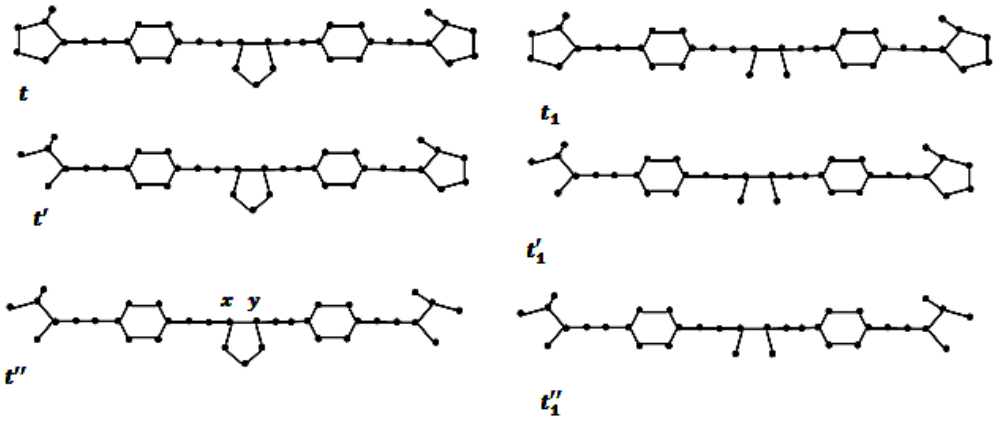


Figure 6. Some certain graphs in Lemmas 7 and 8

By Lemma 1 and by considering the edge $a'b'$ such that the remaining graphs are in Figure 6, we can compute

$$Z(H'_n) = Z(t_1)Z(G'_{n-1}) + Z(t'_1)Z(G''_{n-1})$$
$$= 36774400\, Z(G'_{n-1}) + 14140512\, Z(G''_{n-1}),$$

and

$$Z(F_n') = Z(t_1')Z(G_{n-1}') + Z(t_1'')Z(G_{n-1}'')$$
$$= 14140512Z(G_{n-1}') + 5521204Z(G_{n-1}'').$$

By Table 2, and by putting $\alpha'' = 36774400$, $\beta'' = 14140512$ and $\gamma'' = 5521204$, the proof completes.

Table 1. The Hosoya index of graphs in Figure 5

Numbers of Graphs	Hosoya index
1	24
2	64
3	16
4	44
5	38
6	26

Proof of Theorem 2. Let G_n be the graph of tetrathiafulvalene dendrimer $TD_2[n]$. Using Lemma 1 and considering edge xy in Figure 3, we have

$$Z(G_n) = Z(G_n - xy) + Z(G_n - \{x, y\})$$
$$= Z(G_n')^2 + Z(G_n'')^2,$$

where G_n' and G_n'' are shown in Figure 4. Using Lemmas 3 and 4, the formulas of the theorem hold. Thus, it is sufficient to obtain the initial conditions.

It is clear that we have $G_0' \simeq K_1''$ and $G_0'' \simeq K_2''$ (see Figure 7). For $n = 0$,

$$Z(G_0') = \big(Z(2)Z(P_3) + Z(4)Z(P_2)\big) \times \Big(\big(Z(2)Z(P_3) + Z(4)Z(P_2)\big)$$
$$+2\big(Z(2)Z(P_2) + Z(4)\big)\Big) + \big(Z(2) + Z(4)\big)^2 Z(P_6) = 198048,$$

and,

$$\big(Z(2)Z(P_3) + Z(4)Z(P_2)\big)^2 + \big(Z(2) + Z(4)\big)^2 = 90064.$$

This completes the proof. ∎

Table 2. The Hosoya index of graphs in Figure 6

Numbers of Graphs	Hosoya index
t	84303360
t'	28831616
t''	8597596
t_1	36774400
t_1'	14140512
t_1''	5521204

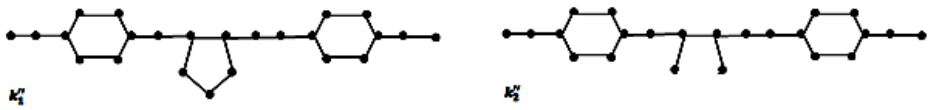


Figure 7. The graphs K_1'' and K_2'' in Theorem 2.

Numerical Results and Analysis

In the field of QSAR and QSPR studies, physico-chemical properties of the chemical compounds and their topological indices are used to predict the bioactivity of different chemical compounds. The Hosoya index is a molecular structure descriptor that is related to their physicochemical properties and is applied in the theory of conjugated π-electron systems.

Dendrimers are macromolecules with repeated growth and activation stages. Dendrimers have large and complex chemical structures and are one of the major available nanoscale building blocks. These structures are nearly perfect mono-disperse macromolecules with a regular and highly branched three-dimensional architecture.

Table 3. Numerical results related to the Hosoya index of the molecular graphs nanostar dendrimer $NS_1[n]$ and tetrathiafulvalene dendrimer

n (stages)	$Z(NS_1[n])$	$Z(TD_2[n])$
1	$1.3543 \times 1o^7$	$2.3177 \times 1o^{37}$
2	$9.9071 \times 1o^{19}$	$5.5576 \times 1o^{90}$

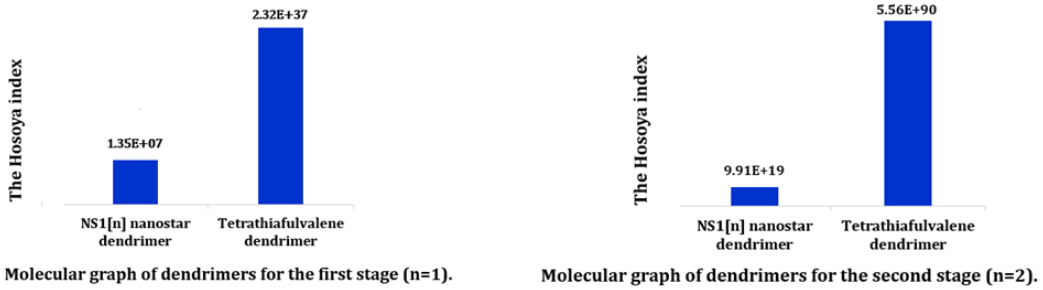


Figure 8. Comparison of the Hosoya index of the molecular graphs PAMAM, PETAA, nanostar dendrimer $NS_1[n]$ and tetrathiafulvalene dendrimer for $n = 1, 2$

In this study, we investigated the molecular structures of two infinite classes of dendrimers, namely, nanostar dendrimer $NS_1[n]$, and tetrathiafulvalene dendrimer. We obtained the formulas of the Hosoya index for these molecular structures. The numerical results of the Hosoya index of the molecular structure of studied dendrimers are shown in Table 3.

The graphical comparison of the results obtained from the Hosoya index is shown in Figure 8. It can be observed from Figure 8 and Table 3 that the value of the Hosoya index of the molecular graph $Z(TD_2[n])$ of tetrathiafulvalene dendrimer is more than others in the first and second stages ($n = 1, 2$).
Since the molecular topology structure of tetrathiafulvalene dendrimer has a more complex structure than the other studied structures, and based on Table 3 and Figure 8, it can be concluded that the Hosoya index for this structure is more than other structure at every stage.

Conclusion

The QSAR and QSPR models use parameters describing the molecular structure to give the relationship between the descriptors and biological activities. The topological index is a numerical characterization of a chemical graph that is useful in QSPR models for modeling some physico-chemical properties such as boiling point, stability, and strain energy of chemical compounds.

The Hosoya index is one of the important topological indices that is of great interest and has applications in molecular chemistry, such as boiling point, entropy, or heat of vaporization.

In this paper, the molecular structures for two infinite dendrimers, nanostar dendrimer $NS_1[n]$ and tetrathiafulvalene dendrimer based on the graph theory modeling and the edge-partition method. We

obtained the formula of the Hosoya index for the molecular graphs of these dendrimer structures. According to the numerical results, the value of the Hosoya index of the molecular graph $Z(TD_2[n])$ of tetrathiafulvalene dendrimer is more than others.

The results of this study can help to predict some physico-chemical properties, especially boiling points, entropy, or heat of vaporization of the molecular structure of the finite dendrimers.

Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

Acknowledgement

The authors would like to thank the referee for suggestions and comments which improved the paper.

References

[1] N. E. Arif, R. Hasni, A. Kalaf. (2013). Chromatic polynomial of POPAM and siloxane dendrimers. *J. Comput. Theor. Nanosci., 10*, 285-287.
[2] S. C. Basak, K. Balasubramanian, B. D. Gute, D. Mills, A. Gorczynska, S. Roszak. (2003). Prediction of cellular toxicity of halocarbons from computed chemodescriptors: A hierarchical QSAR approach. *J. Chem. Inf. Comput. Sci.*, *43*(4), 1103-1109.
[3] A. Bharali, A. Pegu, J. Buragohain and B. Deka. (2021). Generalized ISI index of certain families of nanostar dendrimers. *J. Interdiscip. Math., 24*(7), 2021-2034.
[4] J. Devillers, A. T. Balaban. (1999). *Topological indices and related descriptors in QSAR and QSPR.* Gordon and Breach, Amsterdam.
[5] I. Gutman and O. E. Polansky. (1986). *Mathematical concepts in organic chemistry.* Springer, Berlin.
[6] H. Hosoya. (1971). Topological index, a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. *Bull. Chem. Soc. Jpn., 44*, 2332-2339.
[7] H. Hosoya. (2002). The topological index Z before and after 1971. *Internet Electron. J. Mol. Des., 1*, 428-442.
[8] H. Hosoya. (2007). Important mathematical structures of the topological index Z for tree graphs. *J. Chem. Inf. Model., 47*, 744-75.
[9] H. Hosoya. (2007). Mathematical meaning and importance of the topological index Z. *Croat. Chem. Acta., 80*, 239-249.
[10] Y. Liu, W. Zhuang and Z. Liang. (2015). Largest Hosoya index and smallest Merrifield-Simmons index in tricyclic graphs. *MATCH Commun. Math. Comput. Chem., 73*, 195-224.
[11] M. Mirzagar. (2009). PI Szeged and edge Szeged polynomial of a dendrimers. *MATCH Commun. Math. Comput. Chem., 23*, 363-370.
[12] F. Movahedi, M. H. Akhbari and H. Kamarulhaili. (2021). On the Hosoya index of some families of graph. *Math. Interdisc. Res., 6*, 225-234.
[13] F. Movahedi. (2021). Matching polynomials for some Nanostar Dendrimers. *Asian-European Journal of Mathematics*, *14*(10), 2150188.
[14] F. Movahedi. (2021). Matching polynomials for some nanostar dendrimers. *Asian-Eur. J. Math., 14*(10), 2150188.
[15] J. Ou. (2009). On extremal unicyclic molecular graphs with maximal Hosoya index. *Discrete Appl. Math., 157*(2), 391-397.
[16] A. Sattar, M. Javaid and E. Bonyah. (2022). Computing connection-based topological indices of Dendrimers, *J. Chem.,* 7204641.