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The Hosoya and Merrifield-Simmons Numbers of Water-Soluble Polyaryl Ether Dendrimer Nanostars

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ABSTRACT

A topological index of a graph G is a number $Top(G)$ which is invariant under graph isomorphism. The Hosoya index and Merrifield–Simmons index are two important topological indices applicable in nanoscience. The aim of this paper is to compute these numbers for a new class of nanostar dendrimers.

1 INTRODUCTION

Dendrimers are macromolecules comprised of a series of branches extending outward from an inner core. The word dendrimer originates from the Greek dendron, meaning “tree”. These molecules have attracted much attention because of their various electrical and optical properties. Suppose G is a simple (molecular) graph, a graph without multiple edges and loops. The set of vertices and edges of G are denoted by $V(G)$ and $E(G)$, respectively. A topological index is a numeric quantity derived from the structural graph of a molecule. The number of vertices and edges are the simplest topological indices of graphs. The concept of “topological index” was first proposed by Haro Hosoya for characterizing the topological nature of a graph.

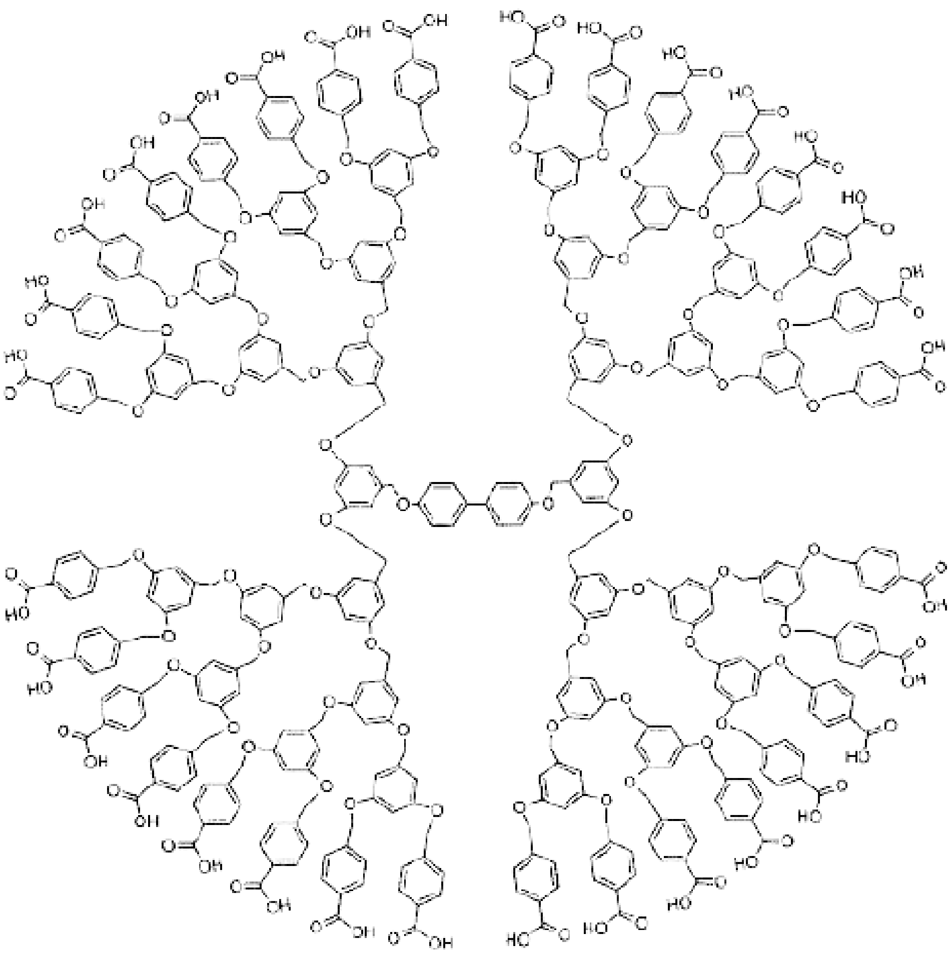
The Hosoya index of a graph G, denoted by $z(G)$, was introduced by Hosoya in 1971; it is defined as the total number of matchings (independent edge subsets), including the empty edge set, of a graph. In a series of subsequent papers, Hosoya and his coworkers showed that the “topological index” z is related with a variety of physico-chemical properties of alkanes. The molecular structure descriptor z was soon re-named into Hosoya index or Hosoya topological index, whereas the name “topological index” is nowadays used for any of the countless graph invariants that are found (or are claimed) to have some chemical applicability. Denote by $m(G,k)$, the number of ways in which k mutually independent edges can be selected in G. By definition, $m(G,0)=1$ for all graphs, and $m(G,1)$ is equal to the number of edges of G. Then

$$z = z(G) = \sum_{k\geq 0} m(G,k) .$$

From a formal point of view, the definition of the Merrifield-Simmons index is analogous to that of the Hosoya index. The Merrifield–Simmons index of a graph G, denoted by $\sigma(G)$, was introduced by Merrifield and Simmons which is defined as the total number of independent vertex sets, including the empty vertex set, of a graph. Denote by $n(G,k)$ the number of ways in which k mutually independent vertices can be selected in G. By definition, $n(G,0)=1$ for all graphs, and $n(G,1)$ is equal to the number of vertices of G. Then

$$\sigma = \sigma(G) = \sum_{k\geq 0} n(G,k) .$$

These two indices have been important topological parameters in combinatorial chemistry. A class of nanostar dendrimers is shown in Figure 1. We denote this graph by $G[n]$, which n means having of n layers.



The Molecular Graph of Dendrimer Nanostar $G[5]$.

2 LEMMAS AND RESULTS

Lemma 2.1. If $uv \epsilon E(G)$, we have $z(G) = z(G - uv) + z(G \setminus \{u, v\})$.

Proof. The proof is obvious with respect to definition.

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Definition 2.2. The disjoint union $G_1 + G_2$ of two vertex-disjoint graphs G_1 and G_2 is defined by

$V(G_1 + G_2) = V(G_1) \times V(G_2) \qquad E(G_1 + G_2) = E(G_1) \cup E(G_2)$.

Lemma 2.3. $z(G_1 + G_2) = z(G_1) \times z(G_2)$

Proof. Clearly any matching for G_1 and G_2 is a matching for $G_1 + G_2$. So the Hosoya index of disjoint union of two graphs is the sum of each Hosoya index.

■

BW. Kernighan and S. Lin. Showed that the following problem is NP-complete :

Consider a graph $G(V, E)$, where V denotes the set of vertices and E the set of edges. The standard (unweighted) version of the graph partition problem is: Given G and an integer $k > 1$, partition V into k parts (subsets) $V_1, V_2, \ldots, V_k$ such that the parts are disjoint and have equal size, and the number of edges with endpoints in different parts is minimized.

Theorem 2.5. The problem of computing the Hosoya index of $G[n]$ is NP-complete.

Proof. Any edge can be in a matching or not. By applying lemma 2.1 to edges of $G[n]$ which are between any two hexagonal shapes (see Figure 2), the problem changes to finding suitable hexagonal

graph partitions in $G[n]$. The problem is in NP since it is easy to check in polynomial time if a given set of hexagonal shapes is appropriate or not. For a number of non-appropriate hexagonal shapes, see Figure 3. To prove NP-completeness of the problem, it suffices to find a polynomial time reduction of some known NP-complete problem to this problem. Obviously by removing edges from $G[n]$, the latter problem can be reduced to this problem.
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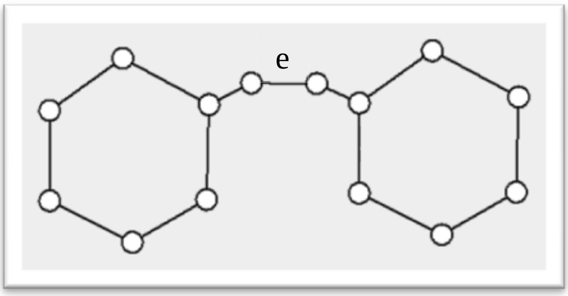

Figure 2. The position of edges between hexagons. (Except for the core of $G[n]$)

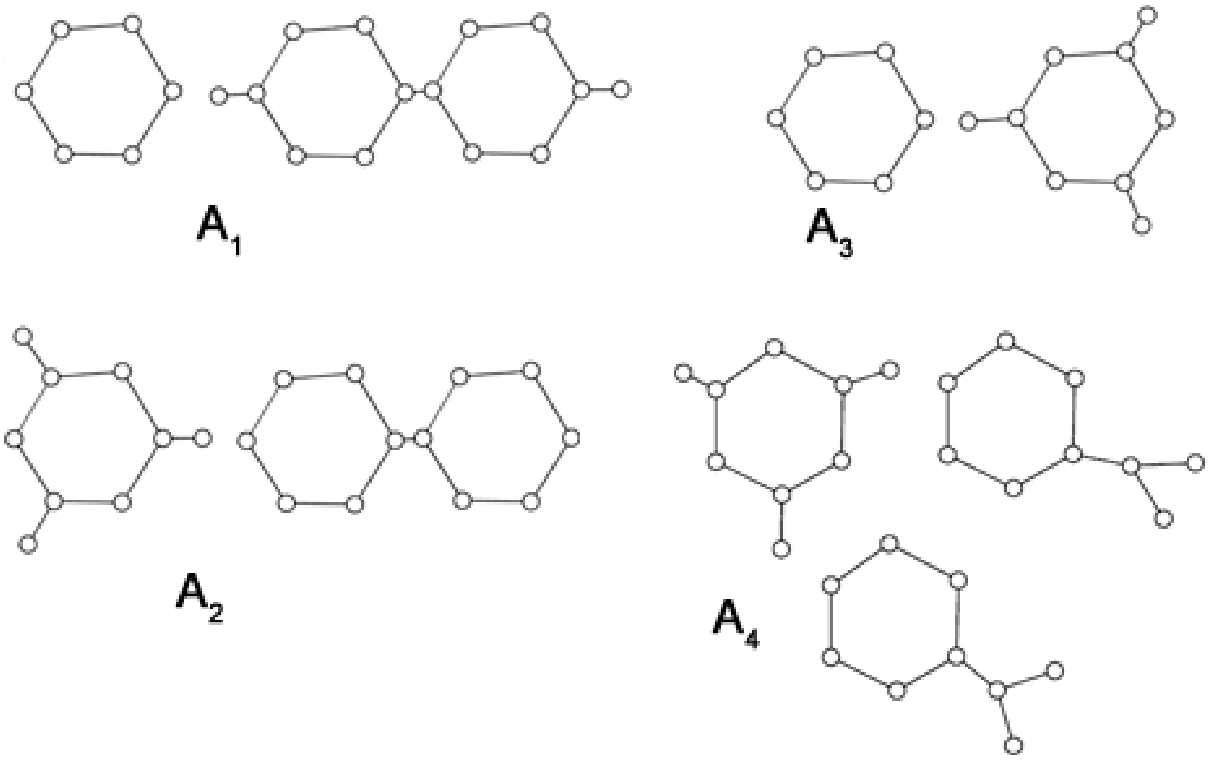

Figure 3. Non-appropriate positions.

3 A METHOD FOR SOLVING THE HOSOYA INDEX OF $G[n]$

Suppose e is the edge shown in Figure 2, and $B(G)$ is the set of all these kind of edges in $G[n]$. Every edge e can be in a matching of $G[n]$ or not. So for every $e \in B(G)$ by removing the edge e or removing incident vertices and applying lemmas 2.1 and 2.3 we have:

$$z(G[n]) = \left(z(a) + z(b) + z(c)\right) \times \left(\prod_{i=1}^{2^1+2^2+\cdots 2^n} \left(z(d) + z(e) + z(f) + z(g)\right) \right) \times \left(\prod_{i=1}^{2^{n+1}} \left(z(h) + z(i)\right)\right) - A$$

$$A = \sum_{i=1}^{t} |A_i| + \sum_{i<j} |A_i \cap A_j| + \cdots + (-1)^t |A_1 \cap A_2 \cap \ldots \cap A_t|$$

which $A_1, \ldots, A_t$ are non-appropriate positions. Some of them are shown in Figure 3. In another word, $|A_i|\ (1 \leq i \leq t)$ is the times where A_i (Figure 3) occurs by removing any edges or removing incident vertices, and $a, \ldots, i$ are positions shown in Figure 4.

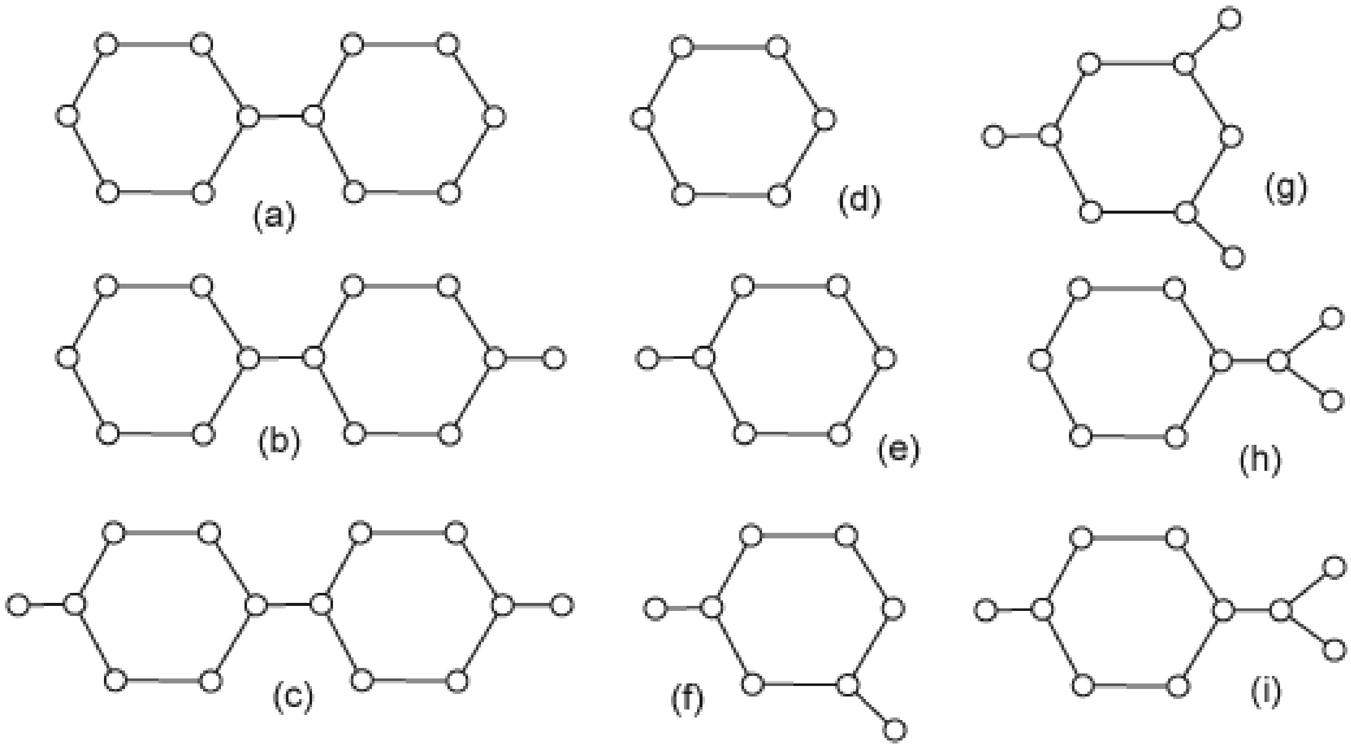

Figure 4. Different positions of hexagonal shapes.

4 LOWER BOUND

Theorem 4.1. The Hosoya index of $G[n]$ is computed as follows:

$$z(G[n]) \geq 2042 \times 133^{(2^2+2^4+\ldots+2^{n-i})} \times 32.375^{(2^1+2^3+\ldots+2^{n-j})} \times (80 \times i)^{2n}$$

where $i = 1$ and $j = 2$ if n is odd, and $i = 2$ and $j = 1$ if n is even.

Proof. Suppose $T(G[n])$ is a maximal set, consisting of the core of $G[n]$ and all hexagonal shapes that are independent from it. In another word, suppose all hexagonals as vertices (except for the core) and then $T(G[n])$ be all vertices (and incident edges) that are independent from the core. (Figure 5) Then for any $e \in B(G)$, remove the edge e or the incident vertices. It is easy to see that any $t \in T(G[n])$, can be in one of the forms of Figure 4, but others depends on hexagonal shapes that are around them. So for others, we apply the probability of occurrence.

Thus for $G[n]$, if n is odd, we have:

$$z(G[n]) \geq (z(a)+z(b)+z(c)) \times \left(\prod_{i=1}^{2^2+2^4+\dots+2^{n-1}} (z(d)+z(e)+z(f)+z(g)) \right.$$
$$\times \left(\prod_{i=1}^{2^1+2^3+\dots+2^{n-2}} \left(\frac{1}{8}z(d)+\frac{3}{8}z(e)+\frac{3}{8}z(f)+\frac{1}{8}z(g) \right) \right) \times \left(\prod_{i=1}^{2^n} \left(\frac{1}{2}z(h)+\frac{1}{2}z(i) \right) \right)$$

and if n is even, we have:

$$z(G[n]) \geq (z(a)+z(b)+z(c)) \times \left(\prod_{i=1}^{2^2+2^4+\dots+2^{n-2}} (z(d)+z(e)+z(f)+z(g)) \right.$$
$$\times \left(\prod_{i=1}^{2^1+2^3+\dots+2^{n-1}} \left(\frac{1}{8}z(d)+\frac{3}{8}z(e)+\frac{3}{8}z(f)+\frac{1}{8}z(g) \right) \right) \times \left(\prod_{i=1}^{2^n} (z(h)+z(i)) \right)$$

By enumeration of the Hosoya index of variables, we have:
$z(a) = 462, z(b) = 654, z(c) = 926, z(d) = 18, z(e) = 26, z(f) = 37, z(g) = 52, z(h) = 66, z(i) = 94$

.

So if n is odd, we have:

$$z(G[n]) \geq 2042 \times 133^{(2^2+2^4+\dots+2^{n-1})} \times 32.375^{(2^1+2^3+\dots+2^{n-2})} \times 80^{2n}$$

and if n is even, we have:

$$z(G[n]) \geq 2042 \times 133^{(2^2+2^4+\dots+2^{n-2})} \times 32.375^{(2^1+2^3+\dots+2^{n-1})} \times 160^{2n}$$

■

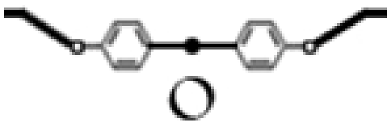

Figure 5. The core of $G[n]$.

5 MERRIFIELD-SIMMONS INDEX

Lemma 5.1. If $\epsilon V(G)$, we have $\sigma(G) = \sigma(G \setminus v) + \sigma(G \setminus N[v])$, where $N[v]$ denotes the closed neighborhood of a vertex v (v together with all its neighbors).

Proof. The proof is obvious due to the fact that any vertex either can be in an independent set or not.

■

Lemma 5.2. $\sigma(G_1 + G_2) = \sigma(G_1) \times \sigma(G_2)$.

Proof. The proof is obvious with respect to lemma 2.3.

■

Just like Hosoya index, any vertex can be in an independent set or not and computing the Merrifield-Simmons index of $G[n]$ is also NP-complete.

Theorem 5.3. The Merrifield-Simmons index of $G[n]$ is computed as follows:

$$\sigma(G[n]) \geq 1692 \times 180^{(2^2+2^4+\dots+2^{n-i})} \times 29.25^{(2^1+2^3+\dots+2^{n-j})} \times (73 \times i)^{2n}$$

where $i = 1$ and $j = 2$ if n is odd, and $i = 2$ and $j = 1$ if n is even.

Proof. Suppose $v \epsilon V(G)$ be a vertex like one of the black vertices shown in Figure 6. By applying the previous lemmas for this kind of vertices, if n is odd, we have:

$$\sigma(G[n]) \geq (\sigma(a)+\sigma(b)+\sigma(c)) \times (\prod_{i=1}^{2^2+2^4+\ldots+2^{n-1}} (\sigma(\mathrm{d})+\sigma(\mathrm{e})+\sigma(\mathrm{f})+\sigma(\mathrm{j})+\sigma(\mathrm{k})+\sigma(\mathrm{P}_4)))$$

$$\times \left(\prod_{i=1}^{2^1+2^3+\ldots+2^{n-2}} \left(\frac{1}{8}\sigma(\mathrm{d})+\frac{2}{8}\sigma(\mathrm{e})+\frac{1}{8}\sigma(\mathrm{f})+\frac{1}{8}\sigma(\mathrm{j})+\frac{2}{8}\sigma(\mathrm{k})+\frac{1}{8}\sigma(\mathrm{P}_4)\right)\right)$$

$$\times (\prod_{i=1}^{2^n} \left(\frac{1}{2}\sigma(\mathrm{h})+\frac{1}{2}\sigma(\mathrm{l})\right))$$

and if n is even, we have:

$$\sigma(G[n]) \geq (\sigma(a)+\sigma(b)+\sigma(c)) \times (\prod_{i=1}^{2^2+2^4+\ldots+2^{n-2}} (\sigma(\mathrm{d})+\sigma(\mathrm{e})+\sigma(\mathrm{f})+\sigma(\mathrm{j})+\sigma(\mathrm{k})+\sigma(\mathrm{P}_4)))$$

$$\times \left(\prod_{i=1}^{2^1+2^3+\ldots+2^{n-1}} \left(\frac{1}{8}\sigma(\mathrm{d})+\frac{2}{8}\sigma(\mathrm{e})+\frac{1}{8}\sigma(\mathrm{f})+\frac{1}{8}\sigma(\mathrm{j})+\frac{2}{8}\sigma(\mathrm{k})+\frac{1}{8}\sigma(\mathrm{P}_4)\right)\right)$$

$$\times (\prod_{i=1}^{2^n} (\sigma(\mathrm{h})+\sigma(\mathrm{l})))$$

On the other hand, we have:
$\sigma(a) = 299, \sigma(b) = 513, \sigma(c) = 880, \sigma(d) = 18, \sigma(e) = 31, \sigma(f) = 54, \sigma(j) = 41,$
$\sigma(k) = 23, \sigma(P4) = 13, \sigma(h) = 85, \sigma(l) = 61$
Thus if n is odd, we have:
$\sigma(\mathrm{G}[\mathrm{n}]) \geq 1692 \times 180^{(2^2+2^4+\ldots+2^{n-1})} \times 29.25^{(2^1+2^3+\ldots+2^{n-2})} \times 73^{2n}$
and if n is even, we have:
$\sigma(\mathrm{G}[\mathrm{n}]) \geq 1692 \times 180^{(2^2+2^4+\ldots+2^{n-2})} \times 29.25^{(2^1+2^3+\ldots+2^{n-1})} \times 146^{2n}$
which j, k and l are shown in Figure 7 and the rest are shown in Figure 4. Note that P_4 is a path graph with 4 edges.

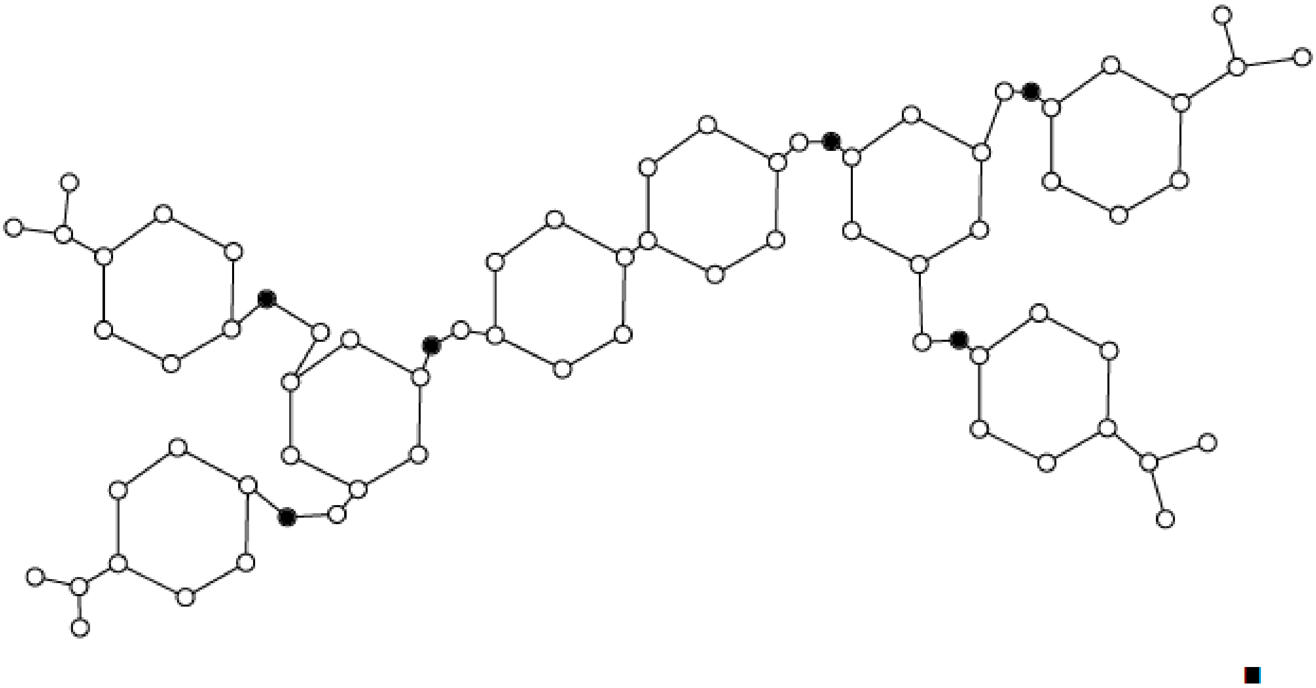

Figure 6. Different positions of vertex v.

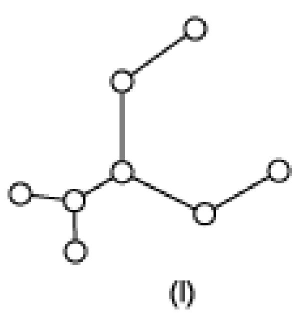

Figure 7. Different positions of hexagonal shapes.

6 CONCLUSION

By the above method, we achieved a formula that approximately computes the Hosoya and Merrifield-Simmons indices of a class of Dendrimer Nanostars. And as mentioned earlier, the Hosoya and Merrifield-Simmons indices explain a variety of physic-chemical properties of molecules.

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