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SOME NEW RESULTS ON THE NULLITY OF MOLECULAR GRAPHS

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ABSTRACT. The nullity of a graph is defined as the multiplicity of eigenvalue zero of graph *G* is named the nullity of *G* denoted by $\eta(G)$. In this paper we investigate some properties of the nullity of some classes of graphs and then we compute the nullity of some infinite families of dendrimers**.**

Key Words: *characteristic polynomial, nullity, dendrimers.*

INTRODUCTION

Let $G = (V, E)$ be a graph and *e* be an arbitrary edge. Then $G\backslash e$ means a subgraph of *G* obtained by removing the edge *e* from *G*. On the other hand, the subgraph $G\backslash\{v_1,..., v_k\}$ is a graph obtained by removing the vertices $v_1,..., v_k$ from *G* and all edges incident to any of them. The line graph of *G*, denoted by $L(G)$, is the graph whose vertex set is $E(G)$ and two vertices of $L(G)$ are adjacent if the corresponding edges in *G* are incident.

The adjacency matrix $A(G)$ of graph *G* with vertex set $V(G)= \{v_1, v_2,..., v_n\}$ is a square $n \times n$ symmetric matrix $[a_{ij}]$, such that $a_{ij}= 1$ if v_i and v_j are adjacent and 0, otherwise. The characteristic polynomial $\Phi_G(\lambda)$ of *G* is defined as

$$\Phi_G(\lambda) = \det(A(G) - \lambda I) .$$

Hence, the eigenvalues of graph *G* are the roots of $\Phi_G(\lambda)$ and form the spectrum of *G*. The nullity of graph *G* is the number of zero eigenvalues in its spectrum denoted by $\eta(G)$. Suppose $r(A(G))$ be the rank of $A(G)$; it is well – known fact that $\eta(G) = n - r(A(G))$.

A null graph is a graph in which all the vertices are isolated. It is clear that $\eta(G) = n$ if and only if *G* is a null graph, see [1].

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The problem of characterizing all the graphs with zero nullity was first considered by Collatz and Sinogowitz [2]. This question is of great interest in chemistry because, if a conjugated hydrocarbon molecule is chemically stable, then its Hückel graph has zero nullity, see [3]. Computing the nullity of a graph is also an interesting problem in mathematics, since it is related to the rank of the adjacency matrix. There are many results on the nullity of trees, unicyclic graphs and bicyclic graphs, see [4-8]. Let G be a graph with edge set $E(G)$. For instance, Gutman and Sciriha [9] proved that for any tree T, $\eta(L(T)) = 0$ or 1. Some results on the nullity of line graphs can be found in [10-16].

PRELIMINARIES

We first introduce some concepts and notations of signed graphs. Recall that a set M of edges of G is a matching if every vertex of G is incident with at most one edge in M; it is a perfect matching if every vertex of G is incident with exactly one edge in M. Maximum matching is a matching with the maximum possible number of edges. The size of a maximum matching of G, *is* the maximum number of independent edges of G denoted by $\mu = \mu(G)$.

Proposition 1[1]. Let $G = G_1 \cup G_2 \cup ... \cup G_t$ where G_1, G_2, …, G_t are connected components of G. Then

$$\eta(G) = \sum_{i=1}^{t} \eta(G_i) .$$

Proposition 2[17]. Let G be a simple graph on n vertices and K_p be a subgraph of G, where $2 \le p \le n$. Then $\eta(G) \le n-p$.

Theorem 1[18]. If a bipartite graph G with $n \ge 1$ vertices does not contain any cycle of length 4s, (s = 1,2,…), then $\eta(G) = n - 2\mu(G)$.

Corollary 1 [19]. If the bipartite graph G contains a pendent vertex, and if the induced subgraph H of G is obtained by deleting this vertex together with the vertex adjacent to it, then $\eta(G) = \eta(H)$.

Corollary 2. Let G_1 and G_2 be bipartite graphs. If $\eta(G_1) = 0$ and if the graph G is obtained by joining an arbitrary vertex of G_1 by an edge to an arbitrary vertex of G_2, then $\eta(G) = \eta(G_2)$.

Theorem 2[20].

(i) A path with four vertices of degree 2 in a bipartite graph G can be replaced by an edge without changing the value of $\eta(G)$.

(ii) Two vertices and the four edges of a cycle of length 4, that lie in a bipartite graph G, can be removed without changing the value of $\eta(G)$.

Example 1. Consider graph G_r, with r hexagons depicted in Figure 1(a). By using Corollary 1, it is easy to see that $\eta(G_r) = \eta(G_{r-1})$ $(r = 1, 2, ...)$. By induction on r it is clear that $\eta(G_r) = 0$. Now consider graph H_r (Figure 1(*b*)). This graph has a pendent vertex, thus according to Corollary 2, $\eta(H_r) = \eta(T_{r-1})$. By using Corollary 2, one can see that $\eta(T_{r-1}) = \eta(H_{r-1})$. By continuing this method we see that $\eta(H_r) = \eta(H_1)$. H_1, has a pendent vertex joined to a hexagon. Corollary 2 implies that $\eta(H_1) = \eta(P_5)$ and by using Lemma 2.1, we have $\eta(H_r) = \eta(P_5) = 1$.

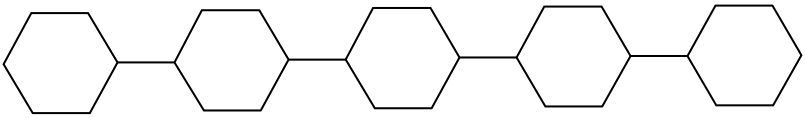


Figure 1 (*a*). Graph G_r.

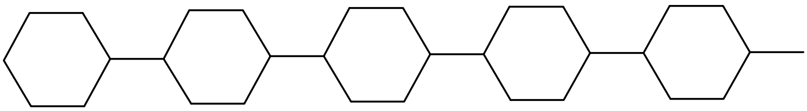


Figure 1(*b*). Graph H_r.

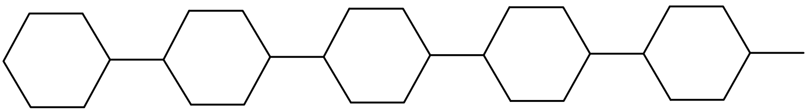


Figure 1(*c*). Graph $T_{r\text{-}1}$.

Here, by using Theorem 1, we compute the nullity of triangular benzenoid graph $G[n]$, depicted in Figure 2. By using Figure 3, one can deduce that the maximum matching can be computed as follows:

First we color the boundary edges, being exactly $3 \times n$ edges. The number of colored vertical edges in the k-th row is $k - 1$. Hence, the number of colored vertical edges is $1 + 2 + \ldots + n - 2 = (n - 1)(n - 2)/2$. By summation of these values one can see that the number of colored edges are $3n + (n - 1)(n - 2)/2 = (n^2 + 3n + 2)/2$ which is equal to the size of maximum matching. This graph has $n^2 + 4n + 1$ vertex, $3(n^2 + 3n)/2$ edges and by using Theorem 1, $\eta(G[n]) = n^2 + 4n + 1 - (n^2 + 3n + 2) = n - 1$, thus we proved the following Theorem.

Theorem 3. $\eta(G[n]) = n-1$.

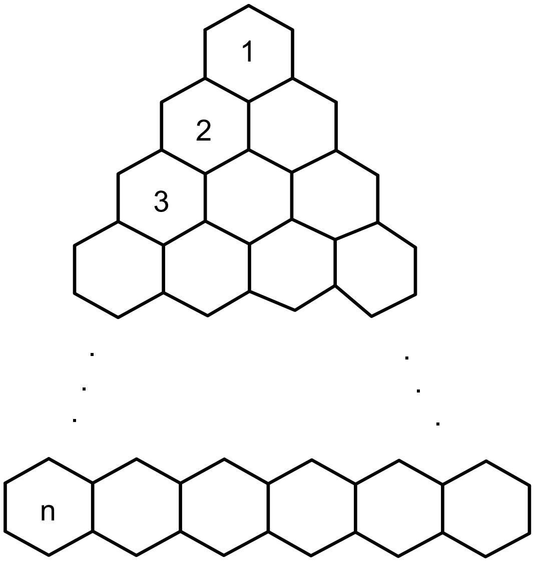


Figure 2. Graph of triangular benzenoid $G[n]$.

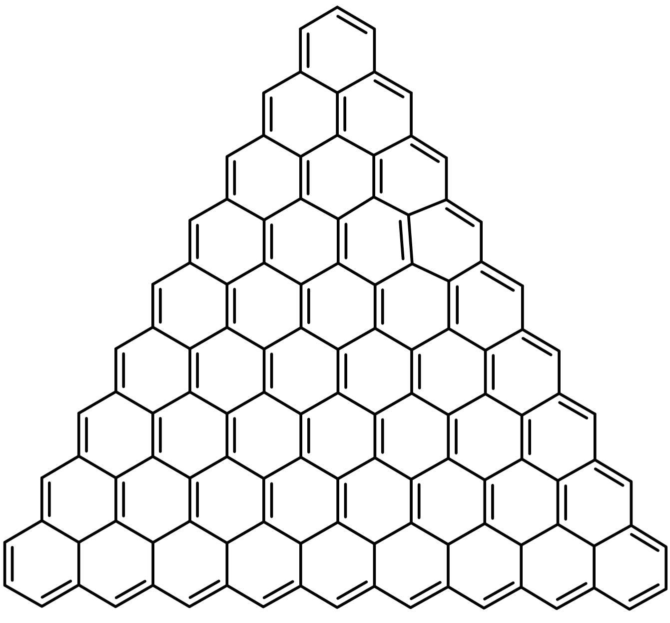


Figure 3. Graph of triangular benzenoid $G[n]$.

MAIN RESULTS

In this section, we study some theoretical properties of nullity of graphs. We recall that a clique of a simple graph G is a subset S of $V(G)$ such that $G[S]$ is complete. A clique S is maximum if G has no clique S' with $|S'| \geq |S|$.The number of vertices in a maximum clique of G is called the clique number of G and is denoted by $\omega(G)$.

The k-coloring of a graph is an assignment of k colors to the vertices of the graph so that adjacent vertices have different colors. A chromatic number is the minimum required number of colors for the vertices of a given graph denoted by $\chi(G)$.

An independent vertex set of graph G is a set of vertices such that any two vertices are not adjacent. Thus, the independence number of G is the maximum of the cardinalities of all vertex independent sets denoted by $\alpha(G)$. Here, we compute some bounds for nullity with respect to the above definitions.

Lemma 1 [21]. We have

$$\omega(G) \geq 2\chi(G) + \alpha(G) - n - 1.$$

Theorem 3. Let K_p be a induced subgraph of G, then

$$\eta(G) \leq 2n - 2\chi(G) - \alpha(G) + 1.$$

Proof. Since K_p is an induced subgraph of G, rank(G) ≥ p and thus $\eta(G) \leq n - \omega(G)$. By using Lemma 1, the proof is completed.

It is easy to see that the edge set $E(G)$ of G can be partitioned into disjoint independent sets. Let $E(G) = \bigcup_{i=1}^{s} E_i$ be a partition of disjoint elements of $E(G)$, where r_i is the number of parts of size $e_i = |E_i|$, i = 1, 2, …, s. Then we have the following result.

Lemma 2. Let G be a bipartite graph with $n \geq 1$ vertices and m edges without any cycle of length $4s$(s= 1, 2,...), then

$$n - 2\frac{m - (s-1)r_1 e_1}{r_s} \leq \eta(G) \leq n - 2\frac{m + (s-1)r_1}{r_s + (s-1)r}.$$

Proof. Since e_s is the size of maximum matching of G, $e_s = \mu(G)$ and then

$$\begin{aligned} m = \left|E(G)\right| &= r_1 e_1 + r_2 e_2 + \ldots + r_s \mu(G) \\ &\leq r_s \mu(G) + \sum_{i=1}^{s-1} r_i(\mu(G) - 1) \leq r_s \mu(G) + (\mu(G) - 1)(s-1)r_1. \end{aligned}$$

This implies that

$$\mu(G) \geq \frac{m + (s-1)r_1}{r_s + (s-1)r}.$$

For computing the lower bound it follows that:

$$m = \sum_{i=1}^{s} r_i e_i \geq (s-1) r_1 e_1 + r_s \mu(G)$$

Hence,

$$\mu(G) \leq \frac{m-(s-1)r_1 e_1}{r_s}$$

and the proof is completed.

Recall that a vertex in graph G is well-connected if it is adjacent with other vertices of G.

Lemma 3. Let v be a well – connected vertex so that $G - \{v\}$ is a connected regular graph on n vertices. Then

$$\eta(G) = \eta(G - \{v\}).$$

Proof. It is easy to see that $G = G - \{v\} + K_1$. Since $G - \{v\}$ is regular, by [22, Theorem 2.8], $rank(G) = rank(G - \{v\}) + rank(K_1)$.

This implies that

$$\eta(G) = n + 1 - rank(G) = n + 1 - [rank(G - \{v\}) + 1] = \eta(G - \{v\}).$$

Corollary 3. If G satisfies the conditions of Lemma 3, then

$$\eta(\bar{G}) = 1 + \eta(G - \{v\}).$$

Theorem 4. Let G be a connected graph and w be a vertex of G in which $N(w) = N(u) \cup N(v)$ and $N(u) \cap N(v) = \phi$ for some vertices u and v. Then

$$\eta(G) = \eta(G - \{w\}).$$

Proof. Let G satisfies the above conditions and A be adjacency matrix of G. Clearly, the sum of u-th and v-th rows equals the w-th row of A and this completes the proof.

Corollary 4. Let G be connected graph and w be a vertex of G in which $N(w) = \bigcup_{i=1}^{n} N(u_i)$ so that $N(u_i) \cap N(u_j) = \phi$ ($1 \leq i, j \leq n$). Then

$$\eta(G) = \eta(G - \{w\}).$$

Let now G and H be two connected graphs, $u \in V(G)$ and $v \in V(H)$, respectively. By connecting the vertices u and v, we obtain a bridge graph denoted by $GuvH$.

Theorem 5. We have

$$\eta(GuvH) = \min\{\eta(G), \eta(G-u)\} + \min\{\eta(H), \eta(H-v)\}.$$

Proof. It is easy to see that the characteristic polynomial of G can be written as follows:

$$\phi_G(x) = x^{\eta(G)} f(x),$$

where $f(x)$ is a polynomial of rank(G). It follows that

$$\phi(H,x) = x^{\eta(H)} g(x),\ \phi(G-u,x) = x^{\eta(G-u)} h(x) \text{ and } \phi(H-v,x) = x^{\eta(H-v)} k(x)$$

for some polynomials $g(x)$, $h(x)$ and $k(x)$, respectively. On the other hand, by [23] we have

$$\phi_{GuvH}(x) = \phi_G(x)\phi_H(x) - \phi_{G-u}(x)\phi_{H-v}(x).$$

This leads us to conclude that

$$\phi_{GuvH}(x) = x^{\eta(G)+\eta(H)} f_1(x) + x^{\eta(G-u)+\eta(H-v)} f_2(x)$$

for some polynomials $f_1(x)$ and $f_2(x)$ and this completes the proof.

Corollary 5. In Theorem 5, suppose u and v be cut vertices, G_1, G_2, …, G_k and H_1, H_2, …, H_k be respectively the components of G-u and H-v in which

$$\eta(G_1) = \eta(G_1 + u) + 1 \text{and } \eta(H_2) = \eta(H_2 + v) + 1.$$

Then

$$\eta(GuvH) = \eta(G) + \eta(H).$$

Let $G\square H$ be a graph obtained by coinciding vertex u of G by vertex v of H. Then we have:

Corollary 6. We have

$$\eta(G\square H) = \eta(G) + \eta(H) + 1.$$

Proof. By [22, Theorem 2.2.4], it is easy to see that:

$$\phi(G\square H, x) = \phi(G, x)\phi(H - v, x) + \phi(G - u, x)\phi(H, x) - x\phi(G - u, x)\phi(H - v, x)$$

$$= x^{\eta(G)+\eta(H-v)} p_1(x) + x^{\eta(G-u)+\eta(H)} p_2(x)$$

$$- x^{\eta(G-u)+\eta(H-v)+1} p_3(x)$$

where, $p_1(x)$, $p_2(x)$ and $p_3(x)$ are some polynomials. Clearly we have

$$\eta(G\square H) = \min\{\eta(G) + \eta(H - v), \eta(G - u) + \eta(H), \eta(G - u) + \eta(H - v) + 1\}$$

$$= \min\{\eta(G) + \eta(H) + 1, \eta(G) + \eta(H) + 3\}$$

$$= \eta(G) + \eta(H) + 1.$$

NULITY OF DENDRIMERS

Consider the graph C depicted in Figure 4. By using Corollary 1, $\eta(C) = \eta(C_1)$ and by Corollary 2, $\eta(C_1) = \eta(C_2)$. By continuing this method one can see that $\eta(C) = \eta(C_5) = 1$ and we can deduce the following theorem.

Theorem 6 [24]. Consider dendrimer graph $S[n]$ depicted in Figure 5. Then,

$$\eta(S[n]) = 1.$$

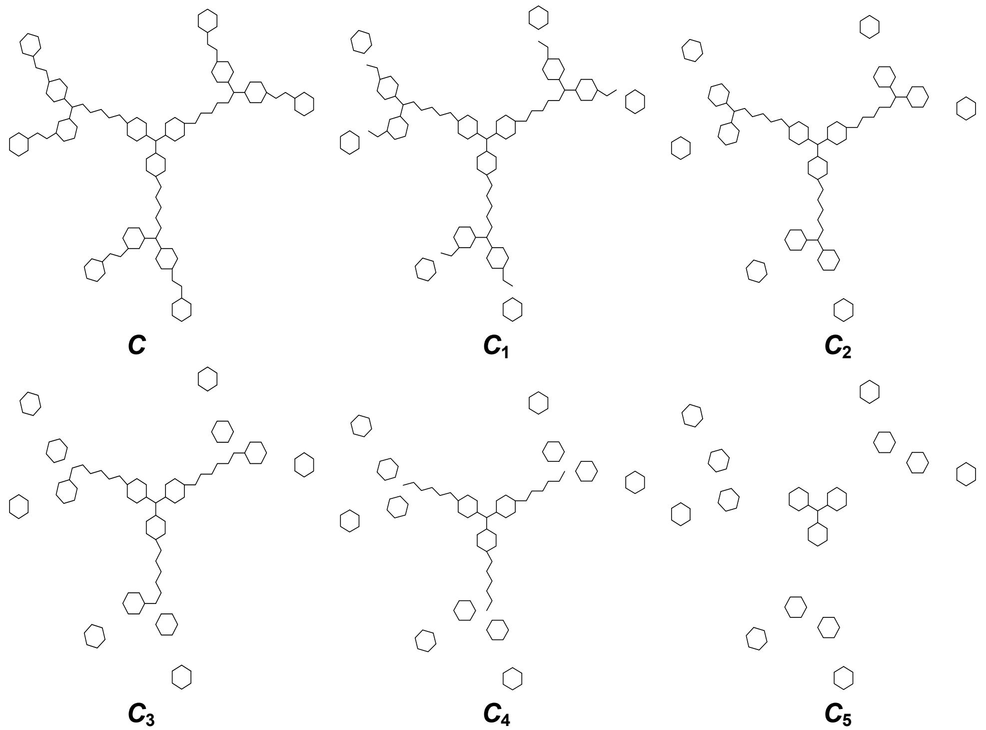


Figure 4. Computing the nullity of dendrimer *C* for n = 3.

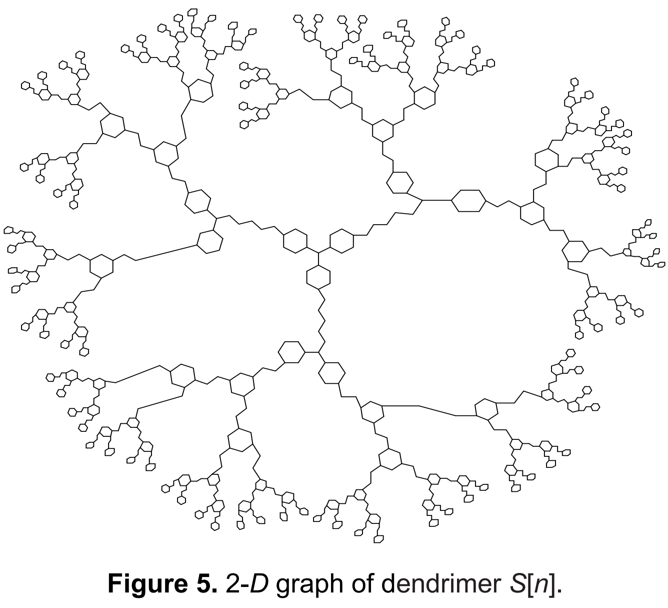


Figure 5. 2-*D* graph of dendrimer $S[n]$.

Theorem 7 [24]. Consider the nanostar dendrimer $D[n]$ in Figure 6, where n = 1, 2, … . Then

$$\eta(D[n]) = 2^{n-1}.$$

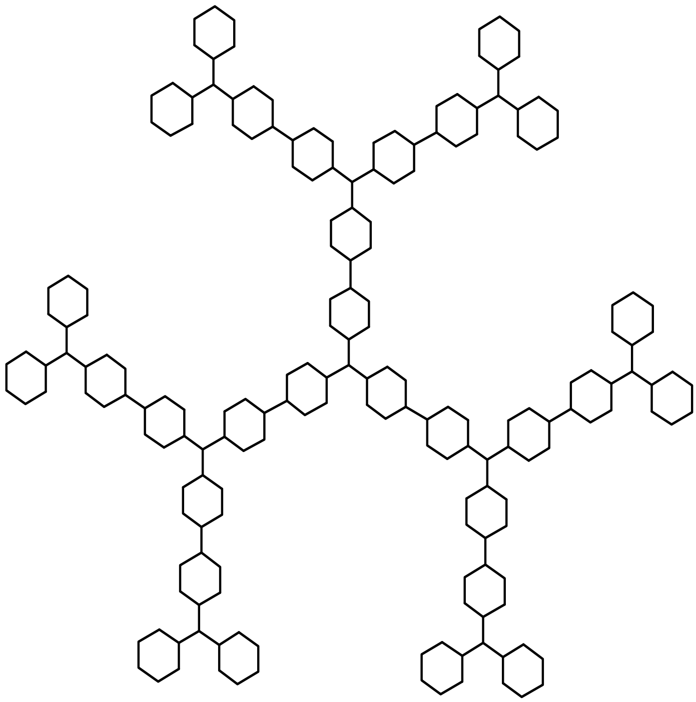
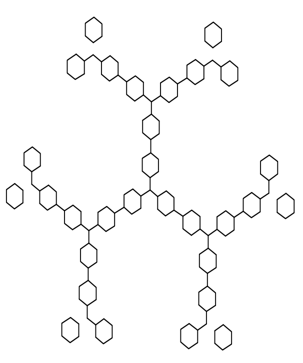
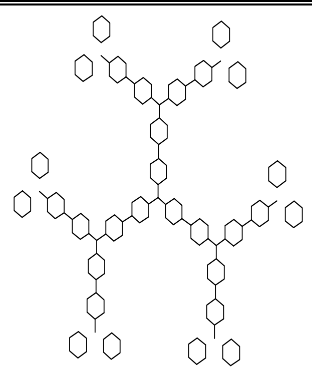
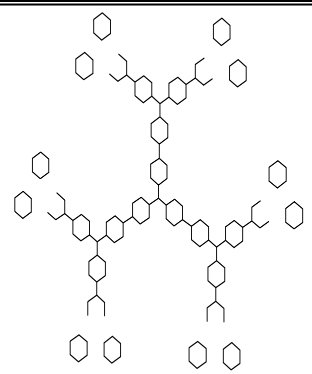


Figure 6. D graph of $D[n]$, for n = 3.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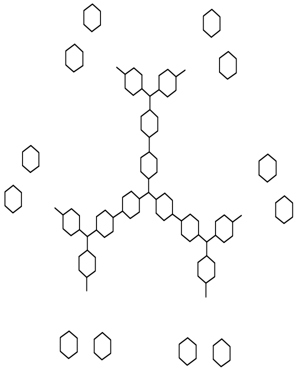	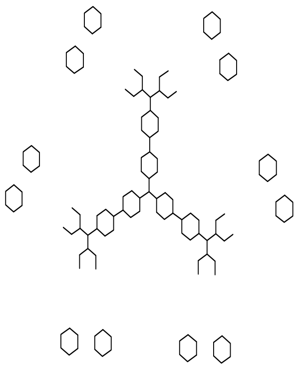	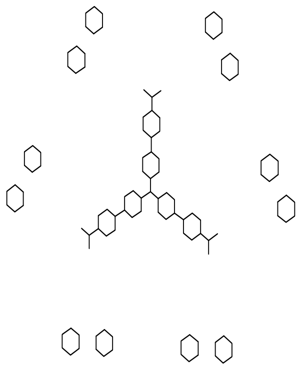
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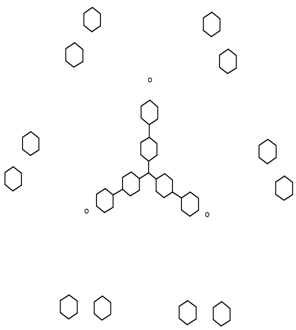	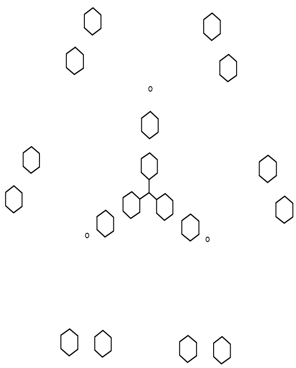	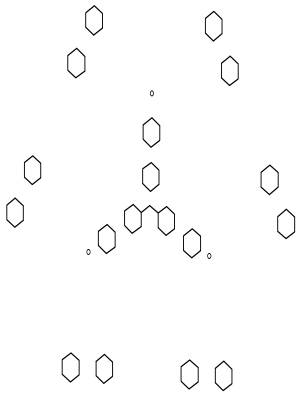
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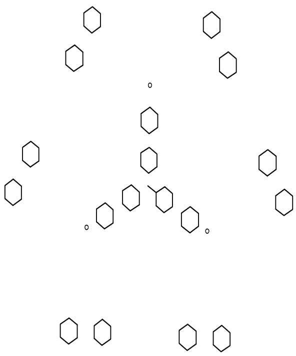	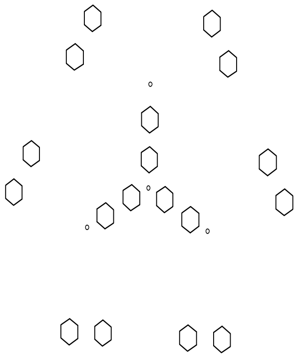	
D_9	D_{10}	

Figure 7. Computing the nullity of $D[n]$, for $n = 3$.

Here, we determine the nullity of dendrimer *T*[*n*], depicted in Figure 8. First, suppose that *n* is even. It should be noted that the number of vertices of *T* [*n*] is 2^{n+1}-1. The number of edges of a maximum matching is

$$\mu(T[n]) = 2 + 2^3 + \ldots + 2^{n-1} = (2^{n+1} - 2)/3.$$

Hence, according to Theorem 1, we have

$$\eta(T[n]) = |V(T[n])| - 2\mu(T[n]) = 2^{n+1} - 1 - 2.\frac{2^{n+1}-2}{3} = \frac{2^{n+1}+1}{3}.$$

Now suppose n is odd. Similar to the last discussion the matching number is $\mu(T[n]) = (2^{n+1} - 1)/3$ and hence

$$\eta(T[n]) = 2^{n+1} - 1 - 2.\frac{2^{n+1}-1}{3} = \frac{2^{n+1}-4}{3}.$$

Thus, we proved the following theorem.

Theorem 8. Consider the dendrimer *T*[*n*], depicted in Figure 8. Then

$$\eta(T[n]) = \begin{cases} \frac{2^{n+1}+1}{3} & 2 \mid n \\ \frac{2^{n+1}-4}{3} & 2 \nmid n \end{cases}.$$

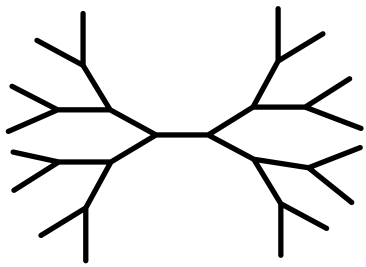

Figure8. 2-*D* graph of dendrimer *T*[*n*] for *n* = 3.

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