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A NOTE ON NULLITY OF GRAPHS

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ABSTRACT. The nullity of a graph is defined as the multiplicity of the eigenvalue zero in the spectrum of the adjacency matrix of the graph. In this paper we investigate the nullity of some classes of graphs.

Keywords*: Graph, Adjacency matrix, Nullity, Dendrimer.*

INTRODUCTION

Chemical graph theory is an important tool for studying molecular structures [1-3]. This theory had an important effect on the development of chemical sciences. All graphs considered in this paper are simple and connected. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. Let $G = (V, E)$ be a graph and $e \in E(G)$. Then the subgraph symbolized $G\backslash e$ is the subgraph of G obtained by removing the edge e from G. Denoted by $G \setminus \{v_1, \ldots, v_k\}$ it means a graph obtained by removing the vertices $v_1, \ldots, v_k$ from G and all edges incident to any of them.

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

$$\Phi(G,x) = \det(A(G) - xI).$$

The roots of the characteristic polynomial are the eigenvalues of the graph G and form the spectrum of this graph. The number of zero eigenvalues in the spectrum of the graph G is called its nullity and is denoted by $\eta(G)$. Denote by $r(A(G))$ the rank of $A(G)$. The nullity is calculated by formula: $\eta(G) = n - r(A(G))$, where n is the number of vertices in G.

For instance, the adjacency matrix of a path on two vertices is

$$A(P_2) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

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So, the characteristic polynomial of a path on two vertices is $\Phi(P_2,\lambda)=\lambda^2-1$ and the eigenvalues of P_2 are ± 1. On the other hand the rank $A(P_2)$ is 2. This implies the nullity of P_2 is zero.

For the second example consider the complete graph K_3. The adjacency matrix of K_3 is

$$A(K_3)=\begin{pmatrix}0 & 1 & 1\\ 1 & 0 & 1\\ 1 & 1 & 0\end{pmatrix}.$$

Hence, $\Phi(K_3,\lambda)=\lambda^3-3\lambda-2=(\lambda-2)(\lambda+1)^2$ and then -1, -1, 2 are its eigenvalues. This matrix is of rank 3 and so, $\eta(K_3)=0$.

The goal of this paper is computing the nullity of some dendrimer infinite classes of graphs. Throughout this paper all notations are standard and mainly taken from standard book of graph theory such as [4, 5]. We also refer the readers to consult papers [6, 7].

RESULTS AND DISCUSSION

The aim of this section is the computing of nullity of some bipartite graphs. For some graphs the spectrum is known and thereby their nullity $\eta(G)$. At first we enounce the following fundamental Lemma, useful to compute the nullity of graphs:

Lemma 1 [7 - 9]. (i) Let G be a graph on n vertices. Then $\eta(G) = n$, if and only if G is a graph without edges (a non-connected graph).

(ii) Let K_n, P_n and C_n, denote a complete graph, a path and a cycle on n vertices, respectively. Then

$$\eta(K_n)=\begin{cases}1 & n=1\\ 0 & n>1\end{cases},\quad \eta(P_n)=\begin{cases}0 & 2\mid n\\ 1 & 2\nmid n\end{cases} \text{ and } \eta(C_n)=\begin{cases}2 & n\equiv 0 (\text{mod } 4)\\ 0 & otherwise\end{cases}.$$

(ii) Let H be an induced subgraph of G. Then $r(H) \le r(G)$.

(iv) Let $G=G_1\cup G_2\cup\cdots\cup G_r$, where G_1, G_2, …, G_r are connected components of G. Then, $r(G)=\sum_{i=1}^{r} r(G_i)$, *i.e.*, $\eta(G)=\sum_{i=1}^{r}\eta(G_i)$.

(v) 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 $\eta(G)=\eta(G_2)$.

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

Now we are ready to compute the nullity of an infinite family of dendrimers graph. To do this, consider the following examples.

Example 2. Consider the graph *A* depicted in Figure 1. By using Lemma 1(v), $\eta(A)=\eta(A_1)$ and by Lemma 1(vi) $\eta(A_1)=\eta(A_2)$. Hence, $\eta(A)=0+0+0=0$.

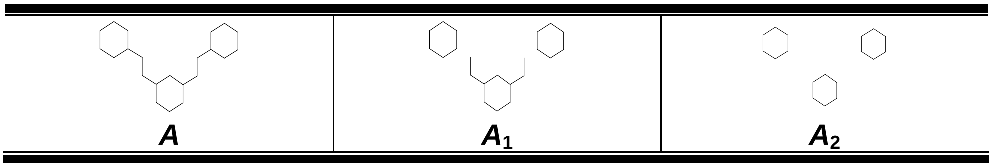


Figure 1. 2 *D* graph of *A*.

Example 3. Consider the graph *B* depicted in Figure 2. By using Lemma 1(v), $\eta(B)=\eta(B_1)$ and by Lemma 1(vi) $\eta(B_1)=\eta(B_2)$. Thus, according to Example 2, $\eta(B)=0$.

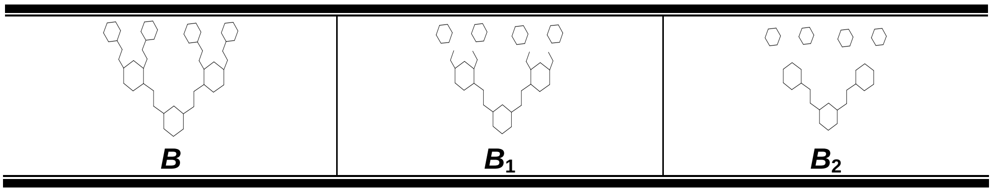


Figure 2. Computing the nullity of *B*.

Example 4. Consider the graph *C* depicted in Figure 3. By using Lemma 1(v), $\eta(C)=\eta(C_1)$ and by Lemma 1(vi) $\eta(C_1)=\eta(C_2)$. By continuing this method one can see that $\eta(C)=\eta(C_5)=1$.

By using the above method we can prove the following Theorem:

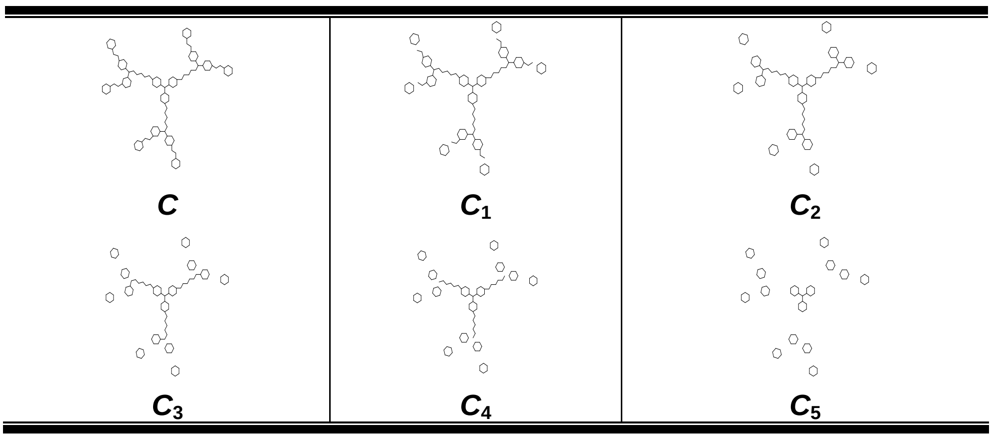


Figure 3. Computing the nullity of *C*.

Theorem 5. Consider the dendrimer graph *S*[*n*] depicted in Figure 4. Then, $\eta(S[n]) = 1$.

Proof. By using Examples 2 and 3 one can see that $\eta(S[n]) = \eta(C_5)$. According to Example 4, this value is 1 and the proof is completed.

Now, we compute the nullity of the nanostar dendrimer graph *D*[*n*] depicted in Figure 5. If *n* = 1 it is easy to see that $\eta(D[1]) = 1$. For *n* = 2, $\eta(D[2]) = 2$. In generally we have the following Theorem:

Theorem 6. Consider nanostar dendrimer *D*[*n*], then

$$\eta(D[n]) = \begin{cases} 1 & n = 1 \\ 2 & n = 2 \\ 2^{n-1} & n \neq 1, 2 \end{cases}.$$

Proof. For the cases *n* = 1, 2 the proof is clear. Suppose *n* ≥ 3, by using Lemma 1(v), one can see that $\eta(D[n]) = \eta(D) = \eta(D_1)$. On the other hand, by Lemma 1(vi), one can deduce that $\eta(D_1) = \eta(D_2) = ... = \eta(D_{10})$. In overall, the nullity of this dendrimer is related to the number of branches of *D*[*n*] and so, the proof is completed.

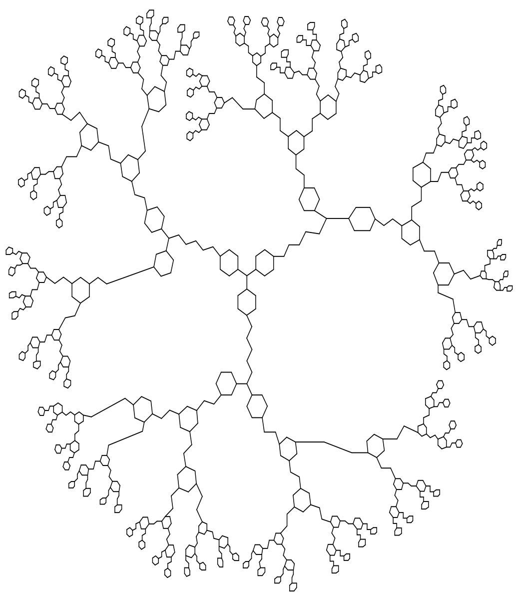


Figure 4. 2 *D* graph of *S*[*n*].

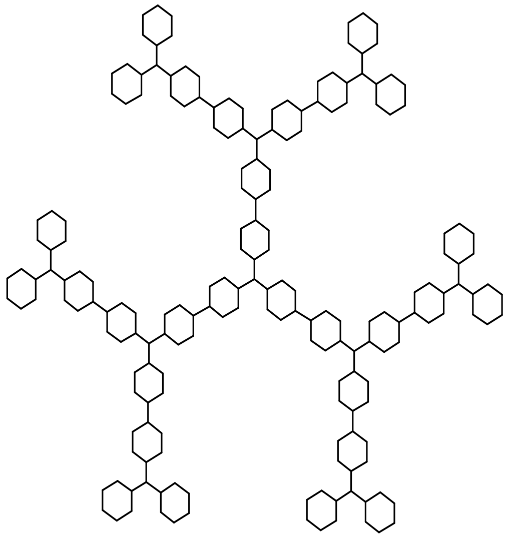
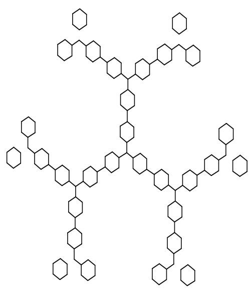
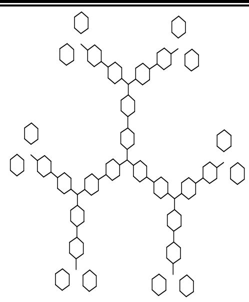
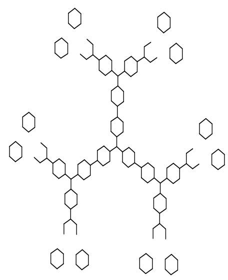


Figure 5. 2 *D* graph of *D*[*n*], for *n* = 3.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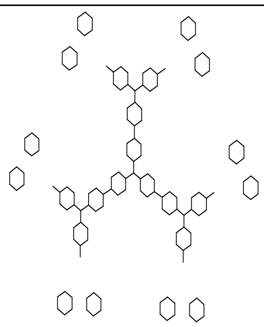
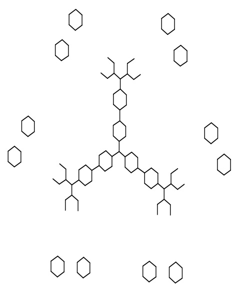
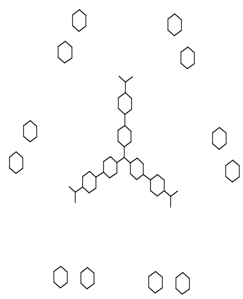
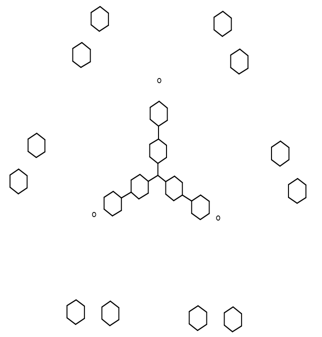
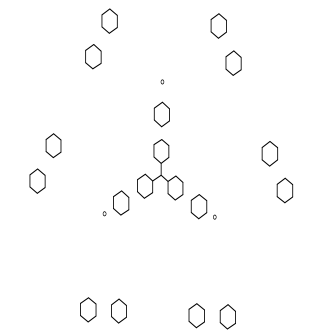
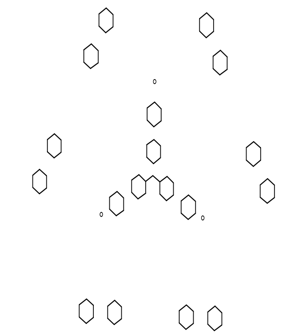
		
D_3	D_4	D_5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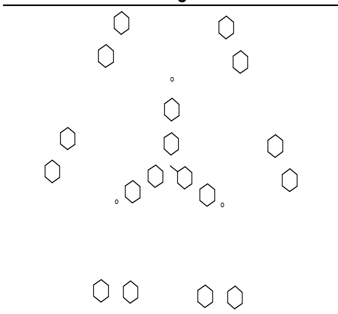	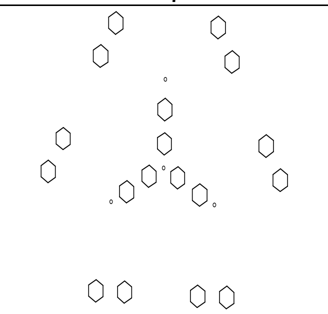	
D_9	D_{10}	

Figure 6. Computing nullity of *D*[*n*], for *n* = 3.

A hypercube (Figure 7) define as follows:

The vertex set of the hypercube H_n consist of all *n*-tuples $b_1b_2\ldots b_n$ with $b_i \in \{0,1\}$. Two vertices are adjacent if the corresponding tuples differ in precisely one place. Clearly the hypercube H_n is isomorphic to $K_2 \times \cdots \times K_2$.

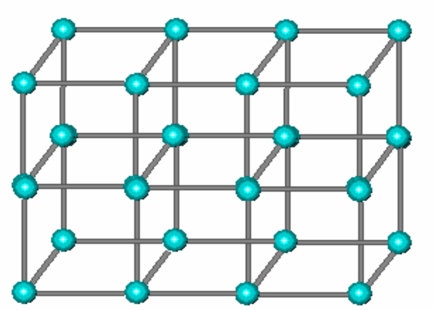

Figure 7. 3-D Graph of a Hypercube.

Theorem 7 [1]. Suppose G and H be two graph with eigenvalues λ_i $(1 \le i \le n)$ and μ_j $(1 \le j \le m)$. Then the eigenvalues of Cartesian product $G \times H$ are $\lambda_i + \mu_j$.

As a corollary of Theorem 7, we compute the nullity of the hyper cube H_n. It is well – known fact the spectrum of K_n is as follows:

$$Spec(K_n) = \begin{pmatrix} -1 & n-1 \\ n-1 & 1 \end{pmatrix}.$$

So, the eigenvalues of K_2 are ± 1 with multiplicity 1. According to Theorem 7,

$$Spec(K_2 \times K_2) = \begin{pmatrix} -2 & 0 & 2 \\ 1 & 2 & 1 \end{pmatrix}.$$

By continuing this method, one can see that the spectrum of $K_2 \times \cdots \times K_2$ is:

$$Spec(K_2 \times \cdots \times K_2) = \begin{cases} \begin{pmatrix} -n & \cdots & -2 & 0 & 2 & \cdots & n \\ 1 & \cdots & \binom{n}{(n-2)/2} & \binom{n}{n/2} & \binom{n}{(n+2)/2} & \cdots & 1 \end{pmatrix} & 2 \mid n \\ \\ \begin{pmatrix} -n & 2-n & \cdots & -1 & 1 & \cdots & n-2 & n \\ 1 & \binom{n}{1} & \cdots & \binom{n}{(n-2)/2} & \binom{n}{n/2} & \cdots & \binom{n}{n-1} & 1 \end{pmatrix} & 2 \nmid n \end{cases}.$$

This implies the nullity of K_n is as follows:

$$\eta(K_n) = \begin{cases} \binom{n}{n/2} & 2 \mid n \\ \\ 0 & 2 \nmid n \end{cases}.$$

Example 8. Consider the raph G_r, with r hexagons, depicted in Figure 8(a). By using Lemma 1(v) it is easy to see that $\eta(G_r) = \eta(G_{r-1})$ $(r = 1, 2, \ldots)$. By induction on r it is clear that $\eta(G_r) = 0$. Now consider graph H_r (Figure 8(b)). Since this graph has a pendent vertex, so by Lemma 1(vi), $\eta(H_r) = \eta(T_{r-1})$. Again we use Lemma 1(vi) and then we have $\eta(T_{r-1}) = \eta(H_{r-1})$. By continuing this method we see that $\eta(H_r) = \eta(H_1)$. H_1, has a pendent vertex joined to a hexagon. Lemma 1(vi) implies that $\eta(H_1) = \eta(P_5)$. By Lemma 1(ii) it results that $\eta(H_r) = \eta(P_5) = 1$.

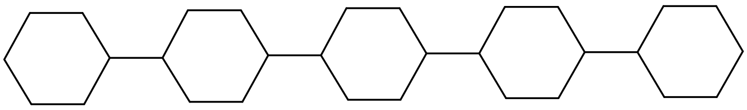

Figure 8 (*a*). Graph G_r.

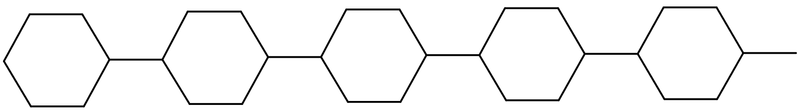

Figure 8(*b*). Graph H_r.

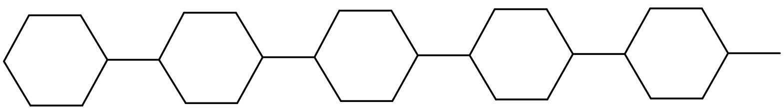

Figure 8(*c*). Graph T_{r-1}.

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* and is denoted by $m = m(G)$.

Theorem 9 [2]. If a bipartite graph *G* with $n \geq 1$ vertices does not contain any cycle of length $4s$ ($s = 1, 2, \ldots$), then $\eta(G) = n - 2m$, where *m* is the size of its maximum matching.

In this section, by using Theorem 9, we compute the nullity of triangular benzenoid graph $G[n]$, depicted in Figure 9. The maximum matching of $G[n]$ is depicted in Figure 10. In other words, to obtain the maximum matching at first we color the boundary edges, they are 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 is $3n + (n - 1)(n - 2)/2 = (n^2 + 3n + 2)/2$ which is equal to the size of maximum matching. This graph has $n^2 + 4n + 1$ vertices, $3(n^2 + 3n)/2$ edges and, by using Theorem 9, $\eta(G[n]) = n^2 + 4n + 1 - (n^2 + 3n + 2) = n - 1$, thus we proved the following Theorem:

Theorem 10. $\eta(G[n]) = n - 1$.

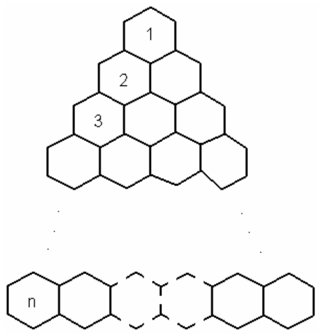

Figure 9. Graph of triangular benzenoid *G*[n].

There is an interesting result, provided by Theorem 10: the nullity of triangular benzenoid structures is very close to n, which is the value for a non-connected molecular graph. If so, this means a molecule showing such a graph cannot exist (as a bounded collection of atoms). A similar conclusion, even differently argued, was emitted by Clar [14] (see also ref. [15]).

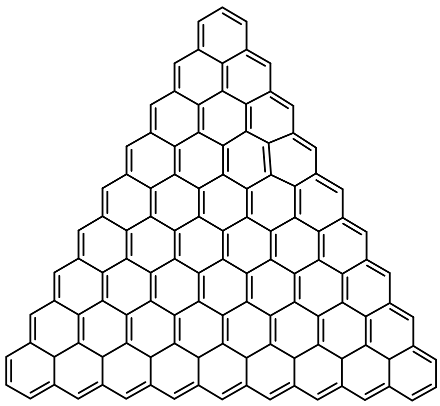

Figure 10. Graph of triangular benzenoid *G*[n].

CONCLUSION

Chemical graph theory is an important tool for studying molecular structures. This theory had an important effect on the development of the chemical sciences. In this paper we computed the nullity of some chemical graphs. This number, related to the spectral graph theory, can be informative in some extreme cases, when (quasi) non-bounded molecular graphs are predicted.

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