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A Note on the Nullity of Unicyclic Graphs

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Abstract The number of zero eigenvalues in the spectrum of the graph G is called its nullity and is denoted by $\eta(G)$. In this paper, we determine the all extremal unicyclic graphs achieving the fifth upper bound $n-6$ and the sixth upperbound $n-7$.

Keywords eigenvalues; nullity; unicyclic graphs.

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1. Introduction

Let $G=(V,E)$ be a simple undirected graph, having vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$. The adjacency matrix $A(G)$ of a graph G 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 eigenvalues $\lambda_1,\lambda_2,\ldots,\lambda_n$ of $A(G)$ are said to be the eigenvalues of the graph G, and to form the spectrum of this graph, denoted by $\mathrm{Spec}(G)$. The number of zero eigenvalues in the spectrum of the graph G is called its nullity and is denoted by $\eta(G)$.

For any $v\in V$, denote by $N(v)$ the neighborhood of v. The disjoint union of two graph G_1 and G_2 is denoted by $G_1\cup G_2$. As usual, the star, cycle and the complete graph of order n are denoted by S_n, C_n, and K_n, respectively. An isolated vertex is sometimes denoted by K_1. We shall use $K_{s,t}$ and $K_{r,s,t}$ to denote the complete bipartite and the complete tripartite graph, respectively.

A connected simple graph with n vertices is said to be acyclic if it has $n-1$ edges, unicyclic if it has n edges. Denote by $\mathscr{T}_n$, $\mathscr{U}_n$ the set of all n-vertex trees and unicyclic graphs, respectively. Let $\mathscr{G}_n$ be the set of all n-vertex graphs. A subset N of $\{0,1,2,\ldots,n\}$ is said to be the nullity set $\mathscr{G}_n$ of provided that for any $k\in N$, there exists at least one graph $G\in\mathscr{G}_n$ such that $\eta(G)=k$.

Collatz and Sinogowitz [3] first posed the problem of characterizing all graphs which satisfy $\eta(G)>0$. This question is of great interest in chemistry, because, as has been shown in [11], for a bipartite graph G (corresponding to an alternated hydrocorbon), if $\eta(G)>0$, the molecule is unstable. In addition, the nullity of a graph is related to the singularity of $A(G)$. However, the problem has not yet been solved completely. Some results on trees and bipartite graphs

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are known [2, 9, 10]. Some nullity results on acyclic, unicyclic, bicyclic and tricyclic graphs are known [1, 2, 6–10, 12].

Cheng and Liu [2] characterized the extremal graphs attaining the upper bound $n-2$ and the second upper bound $n-3$. Li [8] characterized the extremal graphs with pendent vertices achieving the third upper bound $n-4$ and the forth upper bound $n-5$.

In this paper, as the continuance of them, we determine the all extremal unicyclic graphs achieving the fifth upper bound $n-6$ and the sixth upper bound $n-7$.

In Section 2, we list some known results needed in this paper. In Section 3, we improve Li's Theorems. In Section 4, we characterize the extremal unicyclic graphs achieving the fifth upper bound $n-6$ and the sixth upper bound $n-7$.

2. Some Lemmas

In this section, we will present some lemmas which are required in the proof of the main results.

Lemma 1 ([4]) *Let v be a pendent vertex of a graph G and u be its neighbor. Then $\eta(G) = \eta(G - \{u, v\})$, where $G - \{u, v\}$ is the induced subgraph of G obtains by deleting u and v.*

Lemma 2 ([7]) *Let $G = G_1 \cup G_2 \cup \cdots \cup G_t$, then*

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

where $G_1, G_2, \ldots, G_t$ is connected components of G.

Lemma 3 ([7]) *Let G be a graph on n vertices. Then $\eta(G) = n$ iff G is a null graph.*

Lemma 4 ([12]) *If $n \equiv 0 \pmod 4$, then $\eta(C_n) = 2$; otherwise, $\eta(C_n) = 0$.*

Lemma 5 ([12]) *The nullity set of $\mathscr{U}_n$ $(n \geq 5)$ is $\{0, 1, \ldots, n-4\}$.*

Note that if $U \in \mathscr{U}_n$ and $|V(U)| = 3$, then $U = C_3$. If $U \in \mathscr{U}_n$ and $|V(U)| = 4$, then $U = C_4$ or $U = C'$, where C' is obtained by appending a cycle C_3 to a vertex of a path P_2.

Lemma 6 ([5]) *Let $T \in \mathscr{T}_n$, then $\eta(T) \leq n-2$, the equality holds iff $T \cong S_n$.*

Lemma 7 ([8]) *Let $T \in \mathscr{T}_n$, then $\eta(T) = n-4$, iff $T \cong T_1^*$ or $T \cong T_2^*$, where T_1^* and T_2^* are shown in Figure 1.*

Figure 1 $\eta(T) = n-4$

Lemma 8 ([8]) *The nullity set of $\mathscr{T}_n$ is $\{0, 2, 4, \ldots, n-4, n-2\}$ if n is even, otherwise is*

$\{1, 3, 5, \ldots, n-4, n-2\}$.

Lemma 9 ([12]) *Let $U \in \mathscr{U}_n$ $(n \geq 5)$. Then $\eta(U) = n-4$ iff $U \cong U_1^*$ or $U \cong U_2^*$ or $U \cong U_3^*$, where U_1^*, U_2^* and U_3^* are depicted in Figure 2.*

Lemma 10 ([8]) *Let $U \in \mathscr{U}_n$ $(n \geq 5)$. Then $\eta(U) = n-5$ iff $U \cong U_4^*$, where U_4^* are depicted in Figure 2.*

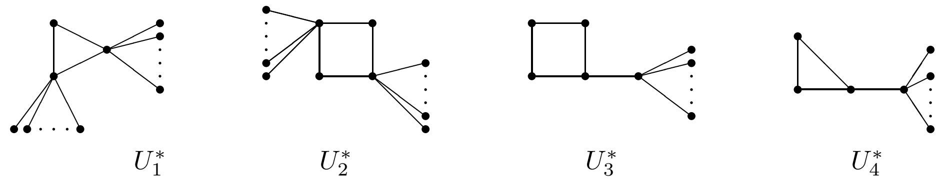

Figure 2 $\eta(U) = n-4$ and $\eta(U) = n-5$

3. Improved results for Li's Theorems

Let G_2^* be an n-vertex graph obtained from a complete bipartite graph $K_{r,s}$ and a star $K_{1,t}$ by identifying a vertex of $K_{r,s}$ with the center of $K_{1,t}$, where $r, s, t \geq 1$ and $r+s+t = n$. Let $K_{1,l,m}$ be a complete tripartite graph with the maximal degree vertex v, where l, $m > 0$. Then let G_1 be an n-vertex graph created from $K_{1,l,m}$ and a star $K_{1,p}$ by identifying the vertex v with the center of $K_{1,p}$, where $l, m, p \geq 1$ and $l+m+p+1 = n$. G_1 and G_2^* are depicted in Figure 3.

Let G_4^* be an n-vertex graph obtained from a complete tripartite graph $K_{r,s,t}$ and a star $K_{1,q}$ by identifying a vertex of $K_{r,s,t}$ with the center of $K_{1,q}$, where $r, s, t, q > 0$ and $r+s+t+q = n$. Let $K_{1,l,m,p}$ be a tetrapartite graph with the maximal degree vertex v, where $l, m, p > 0$. Then let G_3 be an n-vertex graph created from $K_{1,l,m,p}$ and a star $K_{1,d}$ by identifying the vertex v and the center of $K_{1,d}$, where $l, m, p, d > 0$ and $l+m+p+d+1 = n$. G_3 and G_4^* are depicted in Figure 3.

Li [8] obtains Theorem A and Theorem B, they are described in the following:

Theorem A ([8]) *Let G be a connected n-vertex graph with pendent vertices. Then $\eta(G) = n-4$ iff $G \cong G_1^*$ or $G \cong G_2^*$, where G_1^* is a connected spanning subgraph of G_1 (see Figure 3) and contains $K_{l,m}$ as its subgraph, G_2^* is depicted in Figure 3.*

Theorem B ([8]) *Let G be a connected n-vertex graph with pendent vertices and G has no isolated vertex, Then $\eta(G) = n-5$ iff $G \cong G_3^*$ or $G \cong G_4^*$, where is G_3^* is a connected spanning subgraph of G_3 (see Figure 3) and contains $K_{l,m,p}$ as its subgraph, G_3^* is depicted in Figure 3.*

However, they can be briefly described Theorem A' and Theorem B' in the following. Because if the maximal degree vertex v is not adjacent to the second partita vertices in G_1 (see Figure 3), then we can obtain G_2^*, where G_2^* is a connected spanning subgraph of G_1 (see Figure 3) and contains $K_{l,m}$ as its subgraph. So is Theorem B.

Theorem A′ *Let G be a connected n-vertex graph with pendent vertices. Then $\eta(G) = n-4$*

iff $G \cong G_1^*$, *where* G_1^* *is a connected spanning subgraph of* G_1 *(see Figure 3) and contains* $K_{l,m}$ *as its subgraph.*

Theorem B′ *Let* G *be a connected* n*-vertex graph with pendent vertices and* G *has no isolated vertex. Then* $\eta(G) = n - 5$ *iff* $G \cong G_3^*$, *where* G_3^* *is a connected spanning subgraph of* G_3 *(see Figure 3) and contains as* $K_{l,m,p}$ *its subgraph.*

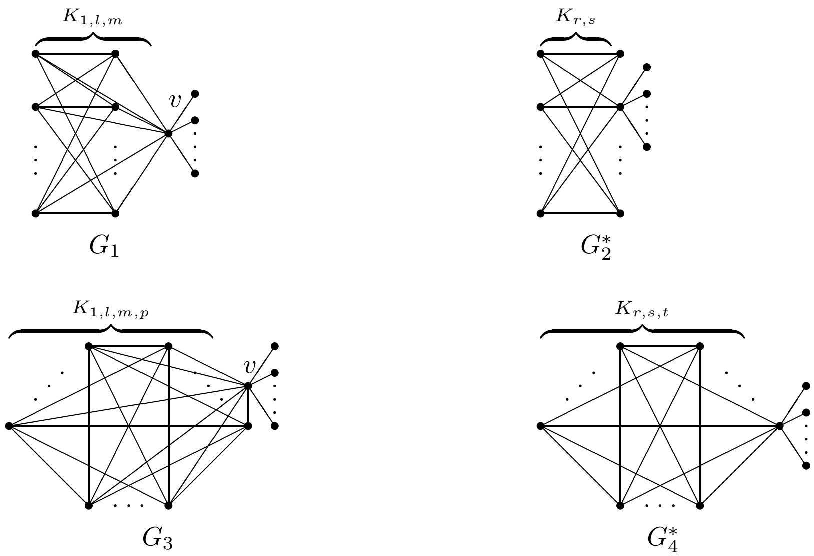

Figure 3 $\eta(G) = n - 4$ and $\eta(G) = n - 5$

Meanwhile, Li [8] thinks that he obtains U_3' and $T_{G_{11}}$ where U_3' (see Figure 4) is a extremal unicyclic graph with $\eta(U_3') = n - 4$ and $T_{G_{11}}$ (see Figure 4) is a extremal tricyclic graph with $\eta(T_{G_{11}}) = n - 5$. Actually, he makes a mistake. We can directly calculate by Lemmas 1, 2, and 3 that $\eta(U_3') = n - 6$, $\eta(U_3'') = n - 4$ and $\eta(T_{G_{11}}') = n - 5$. However, $T_{G_{11}}$ is a bicyclic graph. Thus, U_3' and $T_{G_{11}}$ should be replaced by U_3'' and $T_{G_{11}}'$, respectively.

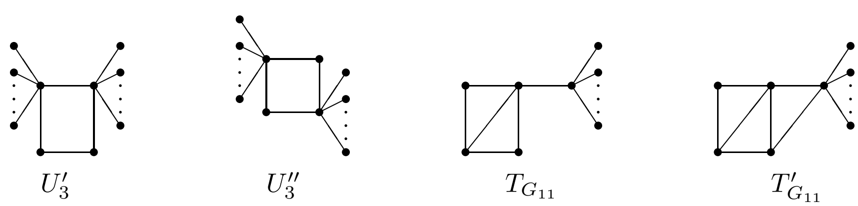

Figure 4 Two graphs should be replaced

4. Main results

Theorem 1 *Let* $U \in \mathscr{U}_n$ $(n \geq 6)$ *be a unicyclic graph. Then* $\eta(U) = n - 6$ *iff* $U \cong C_6$, $U \cong C_8$ *or* $U \cong U_i$ $(i = 1, 2, \ldots, 15)$, *where* U_i *are shown in Figure 5.*

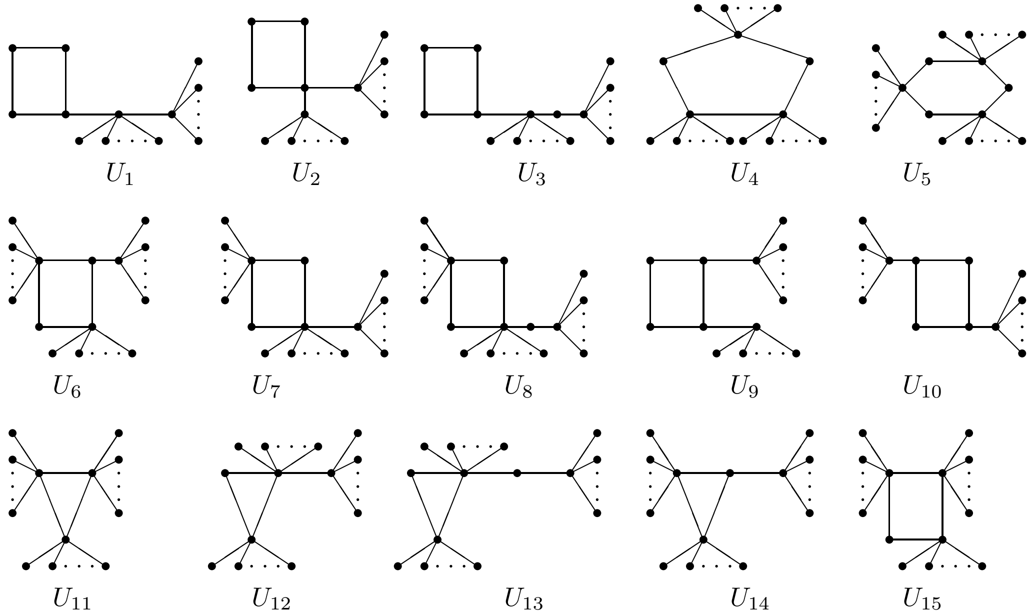

Figure 5 $\eta(U) = n - 6$

Proof "$\Longleftarrow$". If $U \cong C_6$, $U \cong C_8$ and $U \cong U_i^*$ $(i = 1, 2, \ldots, 15)$, it is easy to check directly by Lemmas 1-4 that $\eta(U) = n - 6$.

"$\Longrightarrow$". Assume that $\eta(U) = n - 6$. If there is no pendent vertex in U, by Lemma 4, then $U \cong C_6$ or $U \cong C_8$. Otherwise, we can find a pendent vertex, say x, in U. Let $N(x) = y$. Delete x, y from U, let the resultant graph be $G_1 = U - \{x, y\} = G_{11} \cup G_{12} \cup \cdots \cup G_{1p}$, where $G_{11}, G_{12}, \ldots, G_{1p}$ are connected components of G_1. Some of these components may be trivial, that is, K_1. But not all components are trivial, otherwise, adding x, y to G_1 gives a star, a contradiction to Lemma 6.

Obviously, there is at most a connected unicyclic component of G_1. Meanwhile, other connected components are trees except for trivial component in G_1. Actually, there is a unique nontrivial connected unicyclic component or two nontrivial tree components except for trivial component in G_1. Thus, $G_1 = U_0 \cup T_1 \cup T_2 \cup \cdots \cup T_{p_1} \cup sK_1$ or $G_1 = T_1 \cup T_2 \cup \cdots \cup T_{q_1} \cup s'K_1$. We consider the following cases:

Case 1 $G_1 = U_0 \cup T_1 \cup T_2 \cup \cdots \cup T_{p_1} \cup sK_1$.

Subcase 1.1 If $|V(U_0)| \geq 5$, then by Lemmas 1–5,

$$\begin{aligned}\eta(U) &= \eta(U_0) + \sum_{i=1}^{p_1} \eta(T_i) + s\eta(K_1) \leq (|V(U_0)| - 4) + (\sum_{i=1}^{p_1} |V(T_i)| - 2p_1) + s \\ &= (|V(U_0)| + \sum_{i=1}^{p_1} |V(T_i)| + s) - 4 - 2p_1 = n - 6 - 2p_1\end{aligned}$$

where s is the number of isolated vertices in G_1 and the above equality holds iff U_0 is unicyclic graph and all of $T_1, T_2, \ldots, T_{p_1}$ are stars. If $p_1 \geq 1$, then $\eta(U) \leq n - 6 - 2p_1 \leq n - 8$, a contradiction. So $G_1 = U_0 \cup sK_1$ ($|V(U_0)| \geq 5$).

Subcase 1.2 If $|V(U_0)| = 4$, then $U_0 = C_4$ or $U_0 = C'$.

(a) $U_0 = C'$. That is to say, $G_1 = C' \cup T_1 \cup T_2 \cup \cdots \cup T_{p_1} \cup tK_1$. Then

$$\begin{aligned}\eta(U) &= \eta(C') + \sum_{i=1}^{p_1} \eta(T_i) + t\eta(K_1) \leq (|V(C')| - 4) + (\sum_{i=1}^{p_1} |V(T_i)| - 2p_1) + t \\ &= (|V(C')| + \sum_{i=1}^{p_1} |V(T_i)| + t) - 4 - 2p_1 = n - 6 - 2p_1\end{aligned}$$

where t is the number of isolated vertices in G_1, and the above equality holds iff all of $T_1, T_2, \ldots, T_{p_1}$ are stars. If $p_1 \geq 1$, then $\eta(U) \leq n - 6 - 2p_1 \leq n - 8$, a contradiction. So $G_1 = C' \cup tK_1$.

(b) $U_0 = C_4$. That is to say, $G_1 = C_4 \cup T_1 \cup T_2 \cup \cdots \cup T_{p_1} \cup rK_1$. Then

$$\begin{aligned}\eta(U) &= \eta(C_4) + \sum_{i=1}^{p_1} \eta(T_i) + r\eta(K_1) \leq (|V(C_4)| - 2) + (\sum_{i=1}^{p_1} |V(T_i)| - 2p_1) + r \\ &= (|V(C_4)| + \sum_{i=1}^{p_1} |V(T_i)| + r) - 2 - 2p_1 = n - 4 - 2p_1,\end{aligned}$$

where r is the number of isolated vertices in G_1, and the above equality holds iff all of $T_1, T_2, \ldots, T_{p_1}$ are stars. If $p_1 \geq 2$, then $\eta(U) \leq n - 6 - 2p_1 \leq n - 8$, a contradiction. So $p_1 = 0$ or $p_1 = 1$, that is to say, $G_1 = C_4 \cup rK_1$ or $G_1 = C_4 \cup T_1 \cup r'K_1$.

Subcase 1.3 If $|V(U_1)| = 3$, then $U = C_3$. That is to say, $G_1 = C_3 \cup T_1 \cup T_2 \cup \cdots \cup T_{p_1} \cup uK_1$. Then

$$\begin{aligned}\eta(U) &= \eta(C_3) + \sum_{i=1}^{p_1} \eta(T_i) + u\eta(K_1) \leq (|V(C_3)| - 3) + (\sum_{i=1}^{p_1} |V(T_i)| - 2p_1) + u \\ &= (|V(C_4)| + \sum_{i=1}^{p_1} |V(T_i)| + u) - 3 - 2p_1 = n - 5 - 2p_1\end{aligned}$$

where u is the number of isolated vertices in G_1, and the above equality holds iff all of $T_1, T_2, \ldots, T_{p_1}$ are stars. If $p_1 \geq 1$, then $\eta(U) \leq n - 5 - 2p_1 \leq n - 7$, a contradiction. So $G_1 = C_3 \cup uK_1$.

Case 2 $G_1 = T_1 \cup T_2 \cup \cdots \cup T_{q_1} \cup s'K_1$. Then by Lemmas 1–3, 5 and 6,

$$\eta(U) = \sum_{i=1}^{q_1} \eta(T_i) + s'\eta(K_1) \leq (\sum_{i=1}^{q_1} |V(T_i)| - 2q_1) + s' = n - 2 - 2q_1,$$

where s' is the number of isolated vertices in G_1 and the above equality holds iff all of $T_1, T_2, \ldots, T_{q_1}$ are stars. If $q_1 \geq 3$, then $\eta(U) \leq n - 6 - 2p_1 \leq n - 8$, a contradiction. So $q_1 = 1$ or $q_2 = 2$, that is to say, $G_1 = T_1 \cup s'K_1$ or $G_1 = T_1 \cup T_2 \cup s''K_1$.

Combining above discussion, we obtain $G_1 = U_0 \cup sK_1$ ($|V(U_0)| \geq 5$) or $G_1 = T_1 \cup s'K_1$ or $G_1 = T_1 \cup T_2 \cup s''K_1$ or $G_1 = C' \cup tK_1$ or $G_1 = C_4 \cup rK_1$ or $G_1 = C_4 \cup T_1 \cup r'K_1$ or $G = C_3 \cup uK_1$. Now, we consider the following cases for G_1:

Case i If $G_1 = U_0 \cup sK_1$ ($|V(U_0)| \geq 5$), then

$$\eta(U) = \eta(U_0) + s\eta(K_1) \leq (|V(U_0)| - 4) + s = n - 6$$

the above equality holds iff U_0 is unicyclic graph and $\eta(U_0) = n_1 - 4$, where U_0 has n_1 vertices, by Lemma 9, that is, $U_0 \cong U_1^*$ or $U_0 \cong U_2^*$ or $U_0 \cong U_3^*$.

Case ii If $G_1 = T_1 \cup s'K_1$, then

$$\eta(U) = \eta(T_1) + s'\eta(K_1) \leq (|V(T_1)| - 4) + s' = n - 6$$

the above equality holds iff T_1 is tree and $\eta(T_1) = n_1 - 4$, where T_1 has n_1 vertices, by Lemma 7, that is, $T_1 \cong T_1^*$ or $T_1 \cong T_2^*$.

Case iii If $G_1 = T_1 \cup T_2 \cup s''K_1$, then

$$\eta(U) = \eta(T_1) + \eta(T_2) + s''\eta(K_1) \leq (|V(T_1)| - 2) + (|V(T_2)| - 2) + s'' = n - 6$$

the above equality holds iff both T_1 and T_2 are stars, by Lemma 6, that is, $T_1 \cong S_{n_1}$ or $T_1 \cong S_{n_2}$.

Case iv If $G_1 = C' \cup tK_1$, then

$$\eta(U) = \eta(C') + t\eta(K_1) = (|V(T_1)| - 4) + t = n - 6.$$

Case v If $G_1 = C_4 \cup rK_1$, then

$$\eta(U) = \eta(C_4) + r\eta(K_1) = (|V(C_4)| - 2) + r = n - 4$$

this is a contradiction to $\eta(U) = n - 6$.

Case vi If $G_1 = C_4 \cup T_1 \cup r'K_1$, then

$$\eta(U) = \eta(C_4) + T_1 + r'\eta(K_1) \leq (|V(C_4)| - 2) + (|V(T_1)| - 2) + r' = n - 6$$

the above equality holds iff T_1 is star, by Lemma 6, that is, $T_1 \cong S_{n_1}$.

Case vii If $G_1 = C_3 \cup uK_1$, then

$$\eta(U) = \eta(C_3) + u\eta(K_1) \leq (|V(C_3)| - 3) + u = n - 5$$

this is a contradiction to $\eta(U) = n - 6$.

In order to recover U, to add x, y to G_1, we need to insert edges from y to each of $n - n_1 - 2$ isolated vertices of G_1 and the vertex x, where $n_1 = s$ or $n_1 = s'$ or $n_1 = s''$. This gives a star S_{n_2}, where $n_2 = n - n_1$. If $G_1 = U_1^* \cup n_1K_1$ or $G_1 = U_2^* \cup n_1K_1$ or $G_1 = U_3^* \cup n_1K_1$, where U_1^*, U_2^* and U_3^* are depicted in Figure 2, then the resultant graphs are isomorphic to U_1-U_3, U_6-U_{10}, U_{12}-U_{14}, where U_i (i = 1-3, 6-10, 12-14) are depicted in Figure 5. If $T_1 \cong T_1^*$ or $T_1 \cong T_2^*$, where T_1^* and T_2^* are depicted in Figure 1, then the resultant graphs are isomorphic to U_4-U_8, U_{11}-U_{15}, where U_i (i = 4-8, 11-15) are depicted in Figure 5. If $T_1 \cong S_{n_1'}$ or $T_1 \cong S_{n_2'}$, where both $S_{n_1'}$ and $S_{n_2'}$ are the stars with order n_1' and n_2', respectively, then the resultant graphs are isomorphic to U_7, U_8, U_{12}, U_{13}, where U_i ($i = 7, 8, 12, 13$) are depicted in Figure 5. If $G_1 = C' \cup tK_1$, then the resultant graphs are isomorphic to U_{11}' or U_{12}', where U_{11}' and U_{12}' are subgraph of U_{11} and U_{12}, respectively. If $G_1 = C_4 \cup S_{n_1''} \cup r'K_1$, where $S_{n_1''}$ is the star with order n_1'', then the resultant graphs are isomorphic to U_1 or U_3, where both U_1 and U_3 are depicted in Figure 5.

This completes the proof of Theorem 1. □

Theorem 2 *Let $U \in \mathscr{U}_n$ $(n \geq 7)$ be a unicyclic graph. Then $\eta(U) = n - 7$ iff $U \cong C_7$ or $U \cong U_i$ $(i = 16, 17, 18, 19, 20)$, where U_i are shown in Figure 6.*

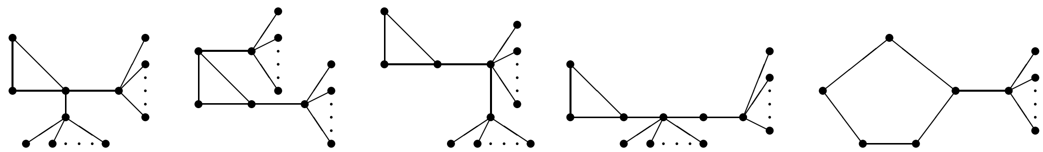

Figure 6 $\eta(U) = n - 7$

Proof This Theorem is similar to the pervious Theorem by Lemmas 1–5, 8 and 10. Thus, the resultant graphs are isomorphic to C_7 or U_{16}-U_{20}, where U_i $(i =$ 16-20$)$ are depicted in Figure 6. □

References

[1] ASHRAF F, BAMDAD H. *A note on graphs with zero nullity* [J]. MATCH Commun. Math. Comput. Chem., 2008, **60**(1): 15–19.
[2] CHENG Bo, LIU Bolian. *On the nullity of graphs* [J]. Electron. J. Linear Algebra, 2007, **16**: 60–67.
[3] COLLATZ L, SINGOWITZ U. *Spektren endlicher Grafen* [J]. Abh. Math. Sem. Univ. Hamburg, 1957, **21**: 63–77. (in German)
[4] CVETKOVIĆ D M, DOOB M, SACHS H. *Spectra of Graphs-Theory and Application* [M]. Academic Press, New York, 1980.
[5] ELLINGHAM M N. *Basic subgraphs and graph spectra* [J]. Australas. J. Combin., 1993, **8**: 247–265.
[6] FIORINI S, GUTMAN I, SCIRIHA I. *Trees with maximum nullity* [J]. Linear Algebra Appl., 2005, **397**: 245–251.
[7] HU Shengbiao, TAN Xuezhong, LIU Bolian. *On the nullity of bicyclic graphs* [J]. Linear Algebra Appl., 2008, **429**(7): 1387–1391.
[8] LI Shuchao. *On the nullity of graphs with pendent vertices* [J]. Linear Algebra Appl., 2008, **429**(7): 1619–1628.
[9] LI Wei, CHANG An. *On the trees with maximum nullity* [J]. MATCH Commun. Math. Comput. Chem., 2006, **56**(3): 501–508.
[10] LI Shuchao, LI Xuechao, ZHU Zhongxun. *On tricyclic graphs with minimal energy* [J]. MATCH Commun. Math. Comput. Chem., 2008, **59**(2): 397–419.
[11] LONGUET-HIGGINS H C. *Resonance structures and MO in unsaturated hydrocarbons* [J]. J. Chem. Phys., 1950, **18**: 265–273.
[12] TAN Xuezhong, LIU Bolian. *On the nullity of unicyclic graphs* [J]. Linear Algebra Appl., 2005, **408**: 212–220.