Linear Algebra and its Applications 436 (2012) 4241–4250

Contents lists available at SciVerse ScienceDirect

Linear Algebra and its Applications

journal homepage: www.elsevier.com/locate/laa

A characterization of graphs with rank 5

Gerard J. Chang[a,b,c,1], Liang-Hao Huang[d,2], Hong-Gwa Yeh[d,*,3]

[a] Department of Mathematics, National Taiwan University, Taipei 10617, Taiwan
[b] Institute for Mathematical Sciences, National Taiwan University, Taipei 10617, Taiwan
[c] National Center for Theoretical Sciences, Taipei Office, Taiwan
[d] Department of Mathematics, National Central University, Jhongli City, Taoyuan 32001, Taiwan

ARTICLE INFO

Article history:
Received 16 March 2011
Accepted 17 January 2012
Available online 21 February 2012

Submitted by R.A. Brualdi

AMS classification:
05C50
15A18
05C75
05C76

Keywords:
Nullity
Rank
Adjacency matrix
Graph
Spectrum

ABSTRACT

The rank of a graph G is defined to be the rank of its adjacency matrix. In this paper, we consider the following problem: what is the structure of a connected graph G with rank 5? or equivalently, what is the structure of a connected n-vertex graph G whose adjacency matrix has nullity $n-5$? In this paper, we completely characterize connected graphs G whose adjacency matrix has rank 5.

1. Introduction

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Throughout this paper, we only consider finite graphs with no loops or multiple edges, and use the notation and terminology of [4], unless otherwise stated. The *adjacency matrix* $A(G)$ of G having vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ is the

* Corresponding author.
E-mail addresses: gjchang@math.ntu.edu.tw (G.J. Chang), r90221003@gmail.com (L.-H. Huang), hgyeh@math.ncu.edu.tw (H.-G. Yeh).
1 Partially supported by National Science Council under Grant NSC98-2115-M-002-013-MY3.
2 Partially supported by National Science Council under Grant NSC99-2811-M-008-059.
3 Partially supported by National Science Council under Grant NSC97-2628-M-008-018-MY3.

http://dx.doi.org/10.1016/j.laa.2012.01.021

$n \times n$ symmetric matrix $[a_{ij}]$ such that $a_{ij} = 1$ if v_i is adjacent to v_j, and $a_{ij} = 0$ otherwise. The *nullity* of G, denoted by $\eta(G)$, is the multiplicity of the eigenvalue zero in the spectrum of $A(G)$. The *rank* of G, written as $r(G)$, is the number of nonzero eigenvalues in the spectrum of $A(G)$. Clearly, $r(G) + \eta(G) = |V(G)|$. A graph G is said to have nullity t (resp. rank k) if $\eta(G) = t$ (resp. $r(G) = k$). The *n-path* is the graph P_n with $V(P_n) = \{v_1, v_2, \ldots, v_n\}$ and $E(P_n) = \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n\}$. The *n-cycle* is the graph C_n with $V(C_n) = \{v_1, v_2, \ldots, v_n\}$ and $E(C_n) = \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n, v_nv_1\}$. The *complete graph* on n vertices has n vertices and $n(n-1)/2$ edges, and is denoted by K_n.

Chemistry deals with molecules and atoms. A typical atom consists of a small nucleus and a large electron cloud. As presented in most textbooks of quantum mechanics [1,2], if one wants to get an accurate determination of the structure and properties of molecules, correlations between the motions of the many electrons of the system must be included. At this point, Newton's classical mechanics no longer hold. That is, we enter the field of quantum mechanics. In quantum mechanics, all the dynamical information about a system (e.g. atom or molecule) are expressed in terms of a wavefunction by solving the Schrödinger equation. The wavefunctions for molecules are called *molecular orbitals*. However, even now, the Schrödinger equation is solvable only for systems containing one electron only; for all other systems, we use different techniques to approximate the wavefunction.

In 1931, Hückel [19] introduced a semiempirical method for approximating molecular orbitals for conjugated molecules like benzene. Essentially, Hückel theory requires the determination of eigenvectors and eigenvalues of the molecular graph. In chemistry, a conjugated hydrocarbon can be represented by its molecular graph G, where the vertices of G represent the carbon atoms, and the edges of G represent the carbon–carbon bonds of the conjugated hydrocarbon. In Hückel theory, the eigenvectors of the adjacency matrix $A(G)$ are identical to the Hückel molecular orbitals, and the eigenvalues of $A(G)$ are the energies corresponding to the Hückel molecular orbitals. The number of nonbonding molecular orbitals (NBMOs) is identical with the multiplicity of the eigenvalue zero in the spectrum of $A(G)$. It turns out that Hückel theory is essentially the same thing as graph spectral theory for planar connected graphs with maximum degree 3 (see p. 89 of [31]). If $\eta(G) > 0$, then the molecule corresponding to G have NBMOs in the Hückel spectrum, and such molecule should have open-shell ground states and be very reactive. This implies molecular instability. In this paper we aim to find a connection between the graph structure of G and the number $\eta(G)$ or, equivalently, $r(G)$.

If $\eta(G) > 0$ (resp. $\eta(G) = 0$), then G is said to be *singular* (resp. *nonsingular*). In 1957, Collatz and Sinogowitz [10] posed the problem of characterizing all singular graphs. The problem is very hard; only some particular results are known [5,6,12,13,16,17,23,25,26,28,29,32,33]. Motivated by the problem of determining the structural features that force a graph G to be singular, many papers investigated the influence of $\eta(G)$ (or, equivalently, $r(G)$) on the structure of the graph G and vice versa (see [3,5,7,17,18,20,24] for examples).

For a connected graph G on n vertices, it was shown in [27] (see also [8,18]) that $r(G) = 2$ if and only if G is isomorphic to a complete bipartite graph $K_{a,b}$, where $a + b = n$, $a, b > 0$. In the same paper it was also shown that $r(G) = 3$ if and only if G is isomorphic to a complete tripartite graph $K_{a,b,c}$, where $a + b + c = n$, $a, b, c > 0$.

After [27] many authors [14,16,18,21,30] were interested in the following question: what is the structure of a graph G with rank $r(G) = 4$? This question had not been fully answered in [14,16,18, 21,30]. In a very recent paper of ours [7], we completely resolve this question. A full characterization of connected graphs G whose adjacency matrix has rank 4 was provided in [7]. This result was also independently proved by Cheng and Liu [9].

In order to state the result proved in [7], we need to define a graph operation called multiplication of vertices (see p. 53 of [15]). Given a graph G with $V(G) = \{v_1, v_2, \ldots, v_n\}$. A subset $I \subseteq V(G)$ is called an *independent set* of G if there are no edges between any two vertices in I. Let $\mathbf{m} = (m_1, m_2, \ldots, m_n)$ be a vector of positive integers. Denote by $G \circ \mathbf{m}$ the graph obtained from G by replacing each vertex v_i of G with an independent set of m_i vertices $v_i^1, v_i^2, \ldots, v_i^{m_i}$ and joining v_i^s with v_j^t if and only if v_i and v_j are adjacent in G. We say that $\{v_i^1, v_i^2, \ldots, v_i^{m_i}\}$ is the vertices of $G \circ \mathbf{m}$ corresponding to v_i. The resulting graph $G \circ \mathbf{m}$ is said to be obtained from G by *multiplication of vertices*. Let $\mathcal{M}(G_1, G_2, \ldots, G_k)$ be the collection of all graphs H which can be constructed from one of the graphs in $\{G_1, G_2, \ldots, G_k\}$

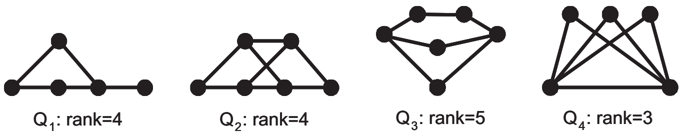

Fig. 1. The graphs Q_1, Q_2, Q_3, Q_4 and their ranks.

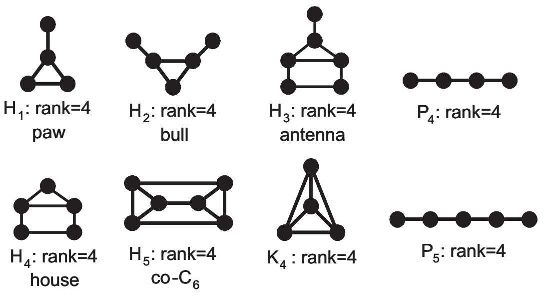

Fig. 2. The graphs $H_1, H_2, H_3, H_4, H_5, K_4, P_4, P_5$ and their ranks.

by multiplication of vertices. As examples, in Fig. 1, it can be seen that $\{Q_1, Q_2\} \subseteq \mathcal{M}(P_4), Q_3 \in \mathcal{M}(C_5)$ and $Q_4 \in \mathcal{M}(K_3)$. Now we are in a position to state the main result in [7].

Theorem 1 [7]. *Let G be a connected graph. Then $r(G) = 4$ if and only if $G \in \mathcal{M}(H_1, H_2, H_3, H_4, H_5, K_4, P_4, P_5)$, where the graphs $H_1, H_2, H_3, H_4, H_5, K_4, P_4, P_5$ are depicted in Fig. 2.*

With the notation and terminology introduced above we can restate the characterization of graphs G having $r(G) = 2$ or $r(G) = 3$ as follows:

Theorem 2 [8,18,27]. *Let G be a connected graph. Then*

(a) $r(G) = 2$ *if and only if* $G \in \mathcal{M}(K_2)$, *and*
(b) $r(G) = 3$ *if and only if* $G \in \mathcal{M}(K_3)$.

The presentations of Theorems 1 and 2 lead to a certain natural question:

Question. Given a connected graph G, is there a family of graphs $\{G_i\}_{i=1}^t$ such that $r(G) = 5$ if and only if $G \in \mathcal{M}(G_1, G_2, \ldots, G_t)$.

A complete answer to this question will give a full characterization of graphs having rank 5. In the literature, only a few partial results on the problem of characterizing graphs having rank 5 were known: A characterization of connected graph G having pendant vertices with rank $r(G) = 5$ was shown in [21,22]; in [16], Guo et al. characterized unicyclic graphs G with $r(G) = 5$ (see also [21]). A characterization of bicyclic graphs and of tricyclic graphs G for which $r(G) = 5$ was given in [21].

In Theorem 3, whose proof appears in Section 2, we answer the above question in the affirmative. All of the previous results in [16,21,22] about graphs G having $r(G) = 5$ are immediate corollaries of Theorem 3.

Theorem 3. *Let G be a connected graph. Then $r(G) = 5$ if and only if $G \in \mathcal{M}(G_1, G_2, \ldots, G_{24})$, where the graphs $G_1, G_2, \ldots, G_{24}$ are depicted in Fig. 3.*

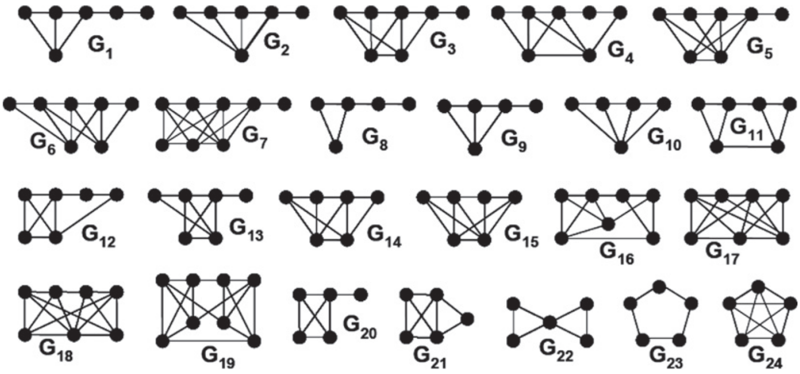

Fig. 3. $r(G_i) = 5$ for $i = 1, 2, \ldots, 24$.

2. The proof of Theorem 3

In this section we shall prove Lemmas 6–9, which imply our main result, Theorem 3, immediately. The following notation and definitions are needed in the proofs of the lemmas in this section. For a vertex x in G, the set of all vertices in G that are adjacent to x is denoted by $N_G(x)$. An edge $\{u, v\}$ between vertices u and v of G is also denoted by uv. The *distance* between u and v, denoted by $d_G(u, v)$, is the smallest length of a u, v-path in graph G. The distance between a vertex u and a subgraph H of G, denoted by $d_G(u, H)$, is defined to be the value $\min\{d_G(u, v) : v \in V(H)\}$. Given a subset $S \subseteq V(G)$. The *subgraph of G induced by S*, written as $G[S]$, is defined to be the graph with vertex set S and edge set $\{xy \in E(G) : x \in S \text{ and } y \in S\}$. For $v \in V(G) \setminus S$, we write $v \sim S$ to mean that $N_G(v) \cap S \neq \emptyset$, and write $v \nsim S$ to mean that $N_G(v) \cap S = \emptyset$. We also write $v \lhd S$ to mean $N_G(v) \supseteq S$, and write $v \ntriangleleft S$ to mean $v \sim S$ and $N_G(v) \not\supseteq S$. If $S = \{u_1, u_2, \ldots, u_t\}$, for brevity, we denote by $G[u_1, u_2, \ldots, u_t]$ the graph $G[S]$. For a subgraph H of G, let $G \setminus H$ denote the subgraph of G which is induced by the vertices of G not in H. Lemma 4 and Proposition 5 are implicitly used throughout the proofs of the results in this section. The proof of Proposition 5 is straightforward and so is omitted.

Lemma 4 [10]**.** *Suppose that G has a vertex x of degree 1. If graph H is obtained from G by deleting x together with the vertex adjacent to x, then $r(G) = r(H) + 2$.*

Proposition 5. *For graphs G and H, if $H \in \mathcal{M}(G)$, then $r(H) = r(G)$.*

Lemma 6. *Let G be a connected graph which has an induced subgraph isomorphic to C_5. Then $r(G) = 5$ if and only if $G \in \mathcal{M}(C_5)$.*

Proof. The sufficient part of this lemma is clear since $r(C_5) = 5$. To prove the necessary part we assume that $r(G) = 5$. Let H be the largest possible induced subgraph of G which can be obtained from C_5 by multiplication of vertices. Suppose that $E(C_5) = \{v_0v_1, v_1v_2, v_2v_3, v_3v_4, v_4v_0\}$. Let $V_i = \{v_i^1, v_i^2, \ldots, v_i^{m_i}\}$ be the vertices of H corresponding to v_i $(0 \leqslant i \leqslant 4)$. To prove $G = H$, assume that $V(G \setminus H) \neq \emptyset$. Since G is connected, there is a vertex $v \in V(G \setminus H)$ such that $d_G(v, H) = 1$. Let $J = \{i \in [0, 4] : v \sim V_i\}$. We now consider the cardinality of J. If $|J| = 1$ or $|J| \geqslant 3$, then it is easy to see that G contains an induced subgraph isomorphic to one of the graphs F_1, F_4, F_5, F_6, and F_7 (see Fig. 4), but this is a contradiction since all graphs F_i in Fig. 4 have $r(F_i) \geqslant 6$. It remains to consider the case that $|J| = 2$. In this case, if $v \sim V_i$ and $v \sim V_{i+1}$ for some i (subscripts are read modulo 5), then F_2 is an induced subgraph of G, a contradiction; if $v \sim V_i$ and $v \sim V_{i+2}$ for some i (subscripts are read modulo 5), then, by the choice of H, it must be $v \ntriangleleft V_i$ or $v \ntriangleleft V_{i+2}$, it follows that F_3 is an induced subgraph of G, a contradiction. This completes the proof of Lemma 6. $\square$

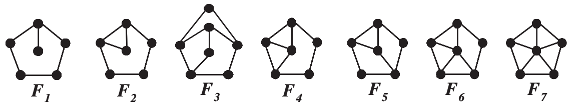

Fig. 4. $r(F_i) \geqslant 6$ for $i = 1, 2, \ldots, 7$.

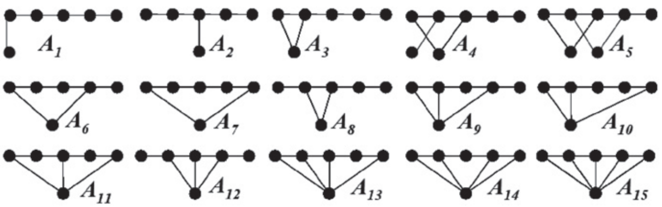

Fig. 5. $r(A_i) \geqslant 6$ for $i = 1, 2, \ldots, 15$.

Lemma 7. *Let G be a connected graph which has an induced subgraph isomorphic to P_5. Then $r(G) = 5$ if and only if $G \in \mathcal{M}(G_1, G_2, \ldots, G_7)$, where the graphs $G_1, G_2, \ldots, G_7$ are depicted in Fig. 3.*

Proof. The sufficient part of this lemma is clear. To prove the necessary part we assume that $r(G) = 5$. Let H be the largest induced subgraph of G which can be obtained from P_5 by multiplication of vertices, where $E(P_5) = \{v_1v_2, v_2v_3, v_3v_4, v_4v_5\}$. Let V_i be the vertices of H corresponding to v_i $(1 \leqslant i \leqslant 5)$. We claim that $d_G(v, H) \leqslant 1$ for all vertices $v \in V(G)$. If not, there would exist an edge $xy \in E(G \setminus H)$ such that $d_G(x, H) = d_G(y, H) + 1 = 2$. It can be seen that the subgraph of G induced by $V(H) \cup \{x, y\}$ has rank 6, a contradiction.

Next, for a vertex $v \in V(G \setminus H)$, denote by N_v the set $\{i \in [1, 5] : v \sim V_i\}$. For $J \subseteq \{1, 2, 3, 4, 5\}$, let $S_J = \{v \in V(G \setminus H) : N_v = J\}$. First, we claim that $S_{\{i\}} = \emptyset$ for $1 \leqslant i \leqslant 5$. If not the case, then by the choice of H it can be seen that G contains an induced subgraph isomorphic to one of the graphs A_1, A_2, and A_4 in Fig. 5, which contradicts to $r(G) = 5$. Second, we claim that $S_J = \emptyset$ when $|J| = 2$. If not, then by the choice of H it can be seen that G contains an induced subgraph isomorphic to one of the graphs $A_3, A_4, \ldots, A_8$ in Fig. 5, which contradicts to $r(G) = 5$. Furthermore, we claim that $S_J = \emptyset$ when $|J| = 3$ and $J \notin \{\{1, 2, 3\}, \{1, 3, 4\}, \{2, 3, 5\}, \{3, 4, 5\}\}$. If not, then we see that G contains an induced subgraph isomorphic to one of the graphs $A_9, A_{10}, A_{11}, A_{12}$ in Fig. 5, which contradicts to $r(G) = 5$. We also claim that $S_J = \emptyset$ when $|J| = 4$ and $J \notin \{\{1, 2, 3, 4\}, \{2, 3, 4, 5\}\}$. If it is not the case, then we see that G contains an induced subgraph isomorphic to one of the graphs A_{13}, A_{14} in Fig. 5, which contradicts to $r(G) = 5$. Finally, it is clear that $S_{\{1,2,3,4,5\}} = \emptyset$, since otherwise the graph A_{15} of Fig. 5 would be an induced subgraph of G, a contradiction to $r(G) = 5$.

From what we have shown above, we know that $V(G \setminus H) \subseteq \bigcup_{J \in \mathcal{I}} S_J$, where $\mathcal{I} = \{\{1, 2, 3\}, \{3, 4, 5\}, \{1, 3, 4\}, \{2, 3, 5\}, \{1, 2, 3, 4\}, \{2, 3, 4, 5\}\}$, and hence graph G is completely determined by the knowledge of S_J $(J \in \mathcal{I})$. To characterize the graph G we make the following claims (whose proofs will be given later):

Claim 1. *(a) If $x \in S_{\{1,2,3\}}$, then $N_G(x) \supseteq V_1 \cup V_2 \cup V_3$. (b) If $x \in S_{\{1,3,4\}}$, then $N_G(x) \supseteq V_1 \cup V_3 \cup V_4$. (c) If $x \in S_{\{1,2,3,4\}}$, then $N_G(x) \supseteq V_1 \cup V_2 \cup V_3 \cup V_4$.*

Claim 2. *(a) If $S_{\{1,2,3\}} \neq \emptyset$, then $S_{\{3,4,5\}} = S_{\{2,3,4,5\}} = \emptyset$. (b) If $S_{\{1,3,4\}} \neq \emptyset$, then $S_{\{2,3,5\}} = S_{\{2,3,4,5\}} = \emptyset$.*

Claim 3. *$S_{\{1,2,3\}}, S_{\{1,3,4\}}$ and $S_{\{1,2,3,4\}}$ are independent sets in G.*

Claim 4. *Suppose that $u \in S_{\{1,2,3\}}$ and $v \in S_{\{1,2,3,4\}}$. (a) We have $uv \notin E(G)$. (b) If $x \in S_{\{1,3,4\}}$, then $\{ux, vx\} \subseteq E(G)$. If $z \in S_{\{2,3,5\}}$, then $uz \in E(G)$. (c) If $y \in S_{\{2,3,4,5\}}$, then $vy \notin E(G)$.*

Proof of Claim 1. (a) Assume, to the contrary, that $N_G(x) \not\supseteq V_1 \cup V_2 \cup V_3$. It can be seen that G contains an induced subgraph isomorphic to one of the graphs B_5, B_6, B_7 depicted in Fig. 6, a contradiction to $r(G) = 5$. (b) Assume, to the contrary, that $N_G(x) \not\supseteq V_1 \cup V_3 \cup V_4$. It follows that G contains an induced subgraph isomorphic to one of the graphs B_{18}, B_{19}, B_{20} depicted in Fig. 6, a contradiction. (c) Assume,

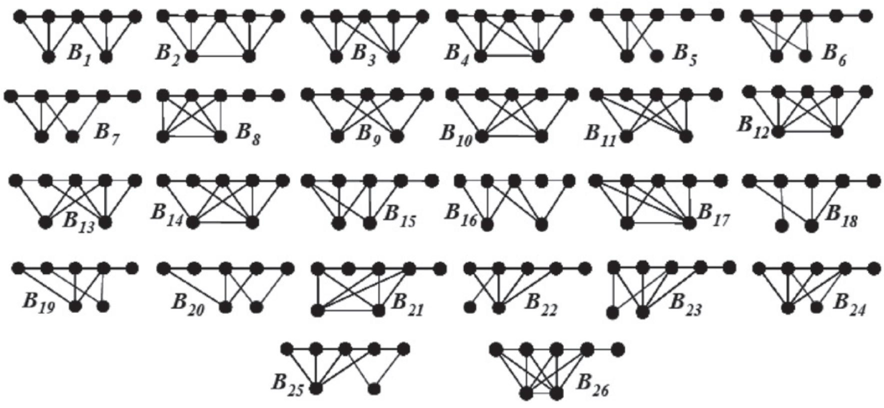

Fig. 6. $r(B_i) \geqslant 6$ for $i = 1, 2, \ldots, 26$.

to the contrary, that $N_G(x) \not\supseteq V_1 \cup V_2 \cup V_3 \cup V_4$. It can be seen that G contains an induced subgraph isomorphic to one of the graphs $B_{22}, B_{23}, B_{24}, B_{25}$ shown in Fig. 6, a contradiction to $r(G) = 5$. □

Note that Claim 1 will be implicitly used in the proofs of Claims 2–4.

Proof of Claim 2. (a) Suppose that $S_{\{1,2,3\}} \neq \emptyset$. Assume that one of the sets $S_{\{3,4,5\}}$ and $S_{\{2,3,4,5\}}$ is non-empty. It can be seen that G contains an induced subgraph isomorphic to one of the graphs B_1, B_2, B_3, B_4 shown in Fig. 6, which contradicts to $r(G) = 5$. (b) Suppose that $S_{\{1,3,4\}} \neq \emptyset$. Assume that one of the sets $S_{\{2,3,5\}}$ and $S_{\{2,3,4,5\}}$ is non-empty. It follows that G contains an induced subgraph isomorphic to one of the graphs $B_9, B_{10}, B_{13}, B_{14}$ in Fig. 6, a contradiction. □

Proof of Claim 3. Assume, to the contrary, that $S_{\{1,2,3\}}, S_{\{1,3,4\}}$ and $S_{\{1,2,3,4\}}$ are not independent sets of G. If there are two vertices x, y in $S_{\{1,2,3\}}$ such that x is adjacent to y, then B_8 shown in Fig. 6 is an induced subgraph of G, a contradiction. If there are two vertices x, y in $S_{\{1,3,4\}}$ such that x is adjacent to y, then B_{21} shown in Fig. 6 is an induced subgraph of G, a contradiction. If there are two vertices x, y in $S_{\{1,2,3,4\}}$ such that x is adjacent to y, then B_{26} shown in Fig. 6 is an induced subgraph of G, a contradiction. □

Proof of Claim 4. (a) Assume, to the contrary, that $uv \in E(G)$. It follows that B_{17} (see Fig. 6) is an induced subgraph of G, a contradiction. (b) Assume, to the contrary, that $\{ux, uz, vx\} \not\subseteq E(G)$. It can be seen that G contains an induced subgraph isomorphic to one of the graphs B_{11}, B_{15}, B_{16} shown in Fig. 6, a contradiction. (c) Assume, to the contrary, that $vy \in E(G)$. It can be seen that B_{12} of Fig. 6 is an induced subgraph of G, a contradiction. □

Since H can be obtained from P_5 by multiplication of vertices, due to symmetry, the following result is equivalent to Claim 2.

Claim 2′. *(a) If $S_{\{3,4,5\}} \neq \emptyset$, then $S_{\{1,2,3\}} = S_{\{1,2,3,4\}} = \emptyset$. (b) If $S_{\{2,3,5\}} \neq \emptyset$, then $S_{\{1,3,4\}}$ $S_{\{1,2,3,4\}} = \emptyset$.*

Now, by Claims 1,2,2′,3,4 and by symmetry of the graph H, we see that G is isomorphic to one of the graphs H, $G[V(H) \cup S_{\{1,2,3\}}]$, $G[V(H) \cup S_{\{1,3,4\}}]$, $G[V(H) \cup S_{\{1,2,3,4\}}]$, $G[V(H) \cup S_{\{1,2,3\}} \cup S_{\{1,3,4\}}]$, $G[V(H) \cup S_{\{1,2,3\}} \cup S_{\{2,3,5\}}]$, $G[V(H) \cup S_{\{1,2,3\}} \cup S_{\{1,2,3,4\}}]$, $G[V(H) \cup S_{\{1,3,4\}} \cup S_{\{1,2,3,4\}}]$, $G[V(H) \cup S_{\{1,2,3,4\}} \cup S_{\{2,3,4,5\}}]$, $G[V(H) \cup S_{\{1,2,3\}} \cup S_{\{1,3,4\}} \cup S_{\{1,2,3,4\}}]$. Note that $G[V(H) \cup S_{\{1,2,3\}} \cup S_{\{1,3,4\}}]$ is isomorphic to $G[V(H) \cup S_{\{1,2,3\}} \cup S_{\{1,2,3,4\}}]$. Since $r(H) = r(G[V(H) \cup S_{\{1,3,4\}}]) = 4$ and $r(G) = 5$, it follows that $G \in \mathcal{M}(G_1, G_2, \ldots, G_7)$. This completes the proof of the lemma. □

Lemma 8. *Let G be a connected graph which contains no induced C_5 or P_5 and contains an induced P_4. Then $r(G) = 5$ if and only if $G \in \mathcal{M}(G_8, G_9, \ldots, G_{19})$, where $G_8, G_9, \ldots, G_{19}$ are depicted in Fig. 3.*

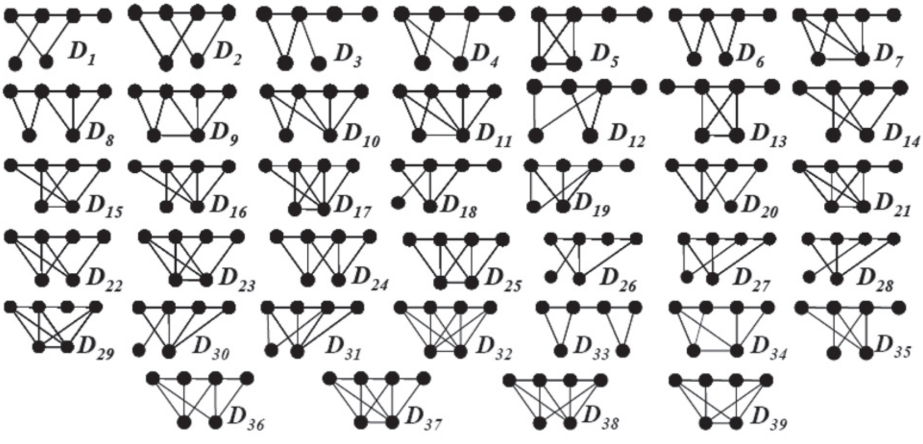

Fig. 7. $r(D_i) \geqslant 6$ for $i = 1, 2, \ldots, 39$.

Proof. The sufficient part of this lemma is clear. To prove the necessary part, given a connected graph G which contains no induced C_5 or P_5, we assume that $r(G) = 5$. Let H be the largest induced subgraph of G which can be obtained from P_4 by multiplication of vertices, where $E(P_4) = \{v_1v_2, v_2v_3, v_3v_4\}$. Let V_i be the vertices of H corresponding to v_i ($1 \leqslant i \leqslant 4$). We claim that $d_G(v, H) \leqslant 1$ for all vertices $v \in V(G)$. If not, there would exist an edge $xy \in E(G \setminus H)$ such that $d_G(x, H) = d_G(y, H) + 1 = 2$. It can be seen that $G[V(H) \cup \{x, y\}]$ has rank 6, a contradiction to $r(G) = 5$.

For a vertex $v \in V(G \setminus H)$, denote by N_v the set $\{i \in [1, 4] : v \sim V_i\}$. For $J \subseteq \{1, 2, 3, 4\}$, let $S_J = \{v \in V(G \setminus H) : N_v = J\}$. With this notation, we claim that $S_{\{1\}} = S_{\{4\}} = \emptyset$, since G contains no induced P_5. Next, we claim that $S_{\{2\}} = S_{\{3\}} = \emptyset$. If not the case, say $v \in S_{\{2\}}$, then by the choice of H it can be seen that $v \not\lhd V_2$, and hence G contains an induced subgraph D_1 shown in Fig. 7, a contradiction to $r(G) = 5$. Since G contains no induced C_5, it follows that $S_{\{1,4\}} = \emptyset$. Furthermore, we claim that $S_{\{1,3\}} = S_{\{2,4\}} = \emptyset$. If not, say $v \in S_{\{1,3\}}$, then by the choice of H we see that either $v \not\lhd V_1$ or $v \not\lhd V_3$. It follows that G contains an induced subgraph isomorphic to one of the graphs D_1, D_2 depicted in Fig. 7, a contradiction.

From what we have proved so far, we know that $V(G \setminus H) \subseteq \bigcup_{J \in \mathcal{I}} S_J$, where $\mathcal{I} = \{\{1, 2\}, \{3, 4\}, \{2, 3\}, \{1, 2, 3\}, \{2, 3, 4\}, \{1, 2, 4\}, \{1, 3, 4\}, \{1, 2, 3, 4\}\}$, and hence graph G is completely determined by the knowledge of S_J ($J \in \mathcal{I}$). To characterize the graph G we make the following claims:

Claim 1. *(a) If $x \in S_{\{1,2\}}$, then $N_G(x) \supseteq V_1 \cup V_2$. (b) If $x \in S_{\{2,3\}}$, then $N_G(x) \supseteq V_2 \cup V_3$. (c) If $x \in S_{\{1,2,3\}}$, then $N_G(x) \supseteq V_1 \cup V_2 \cup V_3$. (d) If $x \in S_{\{1,2,4\}}$, then $N_G(x) \supseteq V_1 \cup V_2 \cup V_4$. (e) If $x \in S_{\{1,2,3,4\}}$, then $N_G(x) \supseteq V_1 \cup V_2 \cup V_3 \cup V_4$.*

Claim 2. *S_J is an independent set in G for any $J \subseteq \{1, 2, 3, 4\}$.*

Claim 3. *(a) If $S_{\{1,2\}} \neq \emptyset$, then $S_{\{2,3\}} = S_{\{1,2,3\}} = S_{\{2,3,4\}} = S_{\{1,2,3,4\}} = \emptyset$. (b) If $S_{\{2,3\}} \neq \emptyset$, then $S_{\{1,2,4\}} = S_{\{1,3,4\}} = S_{\{1,2,3,4\}} = \emptyset$. (c) If $S_{\{1,2,3\}} \neq \emptyset$, then $S_{\{1,2,4\}} = S_{\{2,3,4\}} = \emptyset$.*

Claim 4. *(a) If $u \in S_{\{1,2\}}$ and $x \in S_{\{3,4\}} \cup S_{\{1,2,4\}}$, then $ux \in E(G)$. If $u \in S_{\{1,2\}}$ and $x' \in S_{\{1,3,4\}}$, then $ux' \notin E(G)$. (b) If $u \in S_{\{2,3\}}$ and $x \in S_{\{1,2,3\}} \cup S_{\{2,3,4\}}$, then $ux \in E(G)$. (c) If $u \in S_{\{1,2,3\}}$ and $x \in S_{\{1,3,4\}}$, then $ux \in E(G)$. If $u \in S_{\{1,2,3\}}$ and $x' \in S_{\{1,2,3,4\}}$, then $ux' \notin E(G)$. (d) If $u \in S_{\{1,2,4\}}$ and $x \in S_{\{1,2,3,4\}}$, then $ux \in E(G)$. If $u \in S_{\{1,2,4\}}$ and $x' \in S_{\{1,3,4\}}$, then $ux' \notin E(G)$.*

Proof of Claim 1. (a) Assume, to the contrary, that $N_G(x) \not\supseteq V_1 \cup V_2$. It follows that G contains an induced subgraph isomorphic to D_3 or D_4 (see Fig. 7), a contradiction to $r(G) = 5$. (b) Assume, to the contrary, that $N_G(x) \not\supseteq V_2 \cup V_3$. It follows that D_{12} of Fig. 7 is an induced subgraph of G, a contradiction. (c) Assume, to the contrary, that $N_G(x) \not\supseteq V_1 \cup V_2 \cup V_3$. It follows that G contains an induced subgraph isomorphic to one of the graphs D_{18}, D_{19}, D_{20} depicted in Fig. 7, a contradiction. (d) Assume, to the contrary, that $N_G(x) \not\supseteq V_1 \cup V_2 \cup V_4$. It follows that G contains an induced subgraph isomorphic to one of the graphs D_{26}, D_{27}, D_{28} depicted in Fig. 7. That is a contradiction. (e) Assume, to the contrary, that

$N_G(x) \not\supseteq V_1 \cup V_2 \cup V_3 \cup V_4$. It can be seen that either D_{30} or D_{31} (see Fig. 7) is an induced subgraph of G, a contradiction to $r(G) = 5$. □

Proof of Claim 2. Since H can be obtained from P_4 by multiplication of vertices, from what we have already proved and by the symmetry of H, it suffices to consider the sets S_J, where $J \in \{\{1, 2\}, \{2, 3\}, \{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 3, 4\}\}$. To show this, let us assume to the contrary that $x, y \in S_J$ and $xy \in E(G)$. It can be seen that G contains an induced subgraph isomorphic to one of the graphs $D_5, D_{13}, D_{21}, D_{29}, D_{32}$ shown in Fig. 7, a contradiction to $r(G) = 5$. □

Proof of Claim 3. (a) Suppose that $S_{\{1,2\}} \neq \emptyset$. Assume, to the contrary, that one of the sets $S_{\{2,3\}}, S_{\{1,2,3\}}, S_{\{2,3,4\}}, S_{\{1,2,3,4\}}$ is non-empty. It can be seen that G contains an induced subgraph isomorphic to P_5 or to one of the graphs $D_6, D_7, \ldots, D_{11}$ shown in Fig. 7, which is a contradiction to the fact that G contains no induced P_5 and $r(G) = 5$. (b) Suppose that $S_{\{2,3\}} \neq \emptyset$. Assume, to the contrary, that one of the sets $S_{\{1,2,4\}}, S_{\{1,3,4\}}, S_{\{1,2,3,4\}}$ is non-empty. It follows that one of the graphs $D_{14}, D_{15}, D_{16}, D_{17}$ depicted in Fig. 7 is an induced subgraph of G, a contradiction. (c) Suppose that $S_{\{1,2,3\}} \neq \emptyset$. Assume, to the contrary, that either $S_{\{1,2,4\}}$ or $S_{\{2,3,4\}}$ is non-empty. It follows that G contains an induced subgraph isomorphic to one of the graphs $D_{22}, D_{23}, D_{24}, D_{25}$ depicted in Fig. 7, a contradiction to $r(G) = 5$. □

Proof of Claim 4. To prove this claim we assume, to the contrary, that either $ux \notin E(G)$ or $ux' \in E(G)$. (a) In the case of $ux \notin E(G)$ and $x \in S_{\{3,4\}}$, we see that D_{33} depicted in Fig. 7 is an induced subgraph of G. In the case of $ux \notin E(G)$ and $x \in S_{\{1,2,4\}}$, we see that P_5 is an induced subgraph of $G[V(H) \cup \{u, x\}]$. In the case of $ux' \in E(G)$ and $x' \in S_{\{1,3,4\}}$, we see that D_{34} depicted in Fig. 7 is an induced subgraph of G. In any case, we obtain a contradiction to the fact that G contains no induced P_5 and $r(G) = 5$. (b) By hypothesis, we see that D_{35} is an induced subgraph of G. That is a contradiction to $r(G) = 5$. (c) By hypothesis, we see that either D_{36} or D_{37} is an induced subgraph of G. This is a contradiction. (d) By hypothesis, we see that either D_{38} or D_{39} (see Fig. 7) is an induced subgraph of G, a contradiction arises. □

Since H can be obtain from P_4 by multiplication of vertices, by Claims 1–4 together with symmetry of the graph H , we see that G is isomorphic to one of the graphs H, $G[V(H) \cup S_{\{1,2\}}]$, $G[V(H) \cup S_{\{2,3\}}]$, $G[V(H) \cup S_{\{1,2,3\}}]$, $G[V(H) \cup S_{\{1,2,4\}}]$, $G[V(H) \cup S_{\{1,2,3,4\}}]$, $G[V(H) \cup S_{\{1,2\}} \cup S_{\{3,4\}}]$, $G[V(H) \cup S_{\{1,2\}} \cup S_{\{1,2,4\}}]$, $G[V(H) \cup S_{\{1,2\}} \cup S_{\{1,3,4\}}]$, $G[V(H) \cup S_{\{2,3\}} \cup S_{\{1,2,3\}}]$, $G[V(H) \cup S_{\{2,3\}} \cup S_{\{2,3,4\}}]$, $G[V(H) \cup S_{\{1,2,3\}} \cup S_{\{1,3,4\}}]$, $G[V(H) \cup S_{\{1,2,3\}} \cup S_{\{1,2,3,4\}}]$, $G[V(H) \cup S_{\{1,2,4\}} \cup S_{\{1,3,4\}}]$, $G[V(H) \cup S_{\{1,2,4\}} \cup S_{\{1,2,3,4\}}]$, $G[H \cup S_{\{1,2\}} \cup S_{\{3,4\}} \cup S_{\{1,2,4\}}]$, $G[H \cup S_{\{1,2\}} \cup S_{\{1,2,4\}} \cup S_{\{1,3,4\}}]$, $G[H \cup S_{\{1,2,3\}} \cup S_{\{1,3,4\}} \cup S_{\{1,2,3,4\}}]$, $G[H \cup S_{\{1,2,4\}} \cup S_{\{1,3,4\}} \cup S_{\{1,2,3,4\}}]$, $G[H \cup S_{\{1,2\}} \cup S_{\{3,4\}} \cup S_{\{1,2,4\}} \cup S_{\{1,3,4\}}]$.

Since $r(H) = r(G[V(H) \cup S_{\{2,3\}}]) = r(G[V(H) \cup S_{\{1,2,4\}}]) = r(G[V(H) \cup S_{\{1,2,4\}} \cup S_{\{1,3,4\}}]) = 4$, $G[V(H) \cup S_{\{1,2\}} \cup S_{\{1,3,4\}}] \cong G_{11}$, $G[V(H) \cup S_{\{1,2,3\}} \cup S_{\{1,2,3,4\}}] \cong G_{14}$, and $G[V(H) \cup S_{\{1,2\}} \cup S_{\{1,2,4\}} \cup S_{\{1,3,4\}}] \cong G_{16}$, by what we have proved so far, it can be seen directly that $G \in \mathcal{M}(G_8, G_9, \ldots, G_{19})$. □

Lemma 9. *Let G be a connected graph which contains no induced P_4. Then $r(G) = 5$ if and only if $G \in \mathcal{M}(G_{20}, G_{21}, G_{22}, G_{24})$, where $G_{20}, G_{21}, G_{22}, G_{24}$ are depicted in Fig. 3.*

Proof. The sufficient part of this lemma is clear. To prove the necessary part we assume that $r(G) = 5$. Let t be the maximum size of a complete subgraph in G. It is clear that $t \leqslant 5$, since $r(K_6) = 6 > r(G)$. Let H be the largest induced subgraph of G which can be obtained from K_t by multiplication of vertices, where $V(K_t) = \{v_1, v_2, \ldots, v_t\}$. Let V_i be the vertices of H corresponding to v_i $(1 \leqslant i \leqslant t)$. For a vertex $v \in V(G \setminus H)$, denote by N_v the set $\{i \in [1, t] : v \sim V_i\}$. For $J \subseteq \{1, 2, \ldots, t\}$, let $S_J = \{v \in V(G \setminus H) : N_v = J\}$. Now let us observe that the following property holds for every vertex $v \in V(G \setminus H)$.

Property $\mathcal{P}$**.** If $v \sim V_i$ and $v \nsim V_j$ for some $1 \leqslant i, j \leqslant t$, then $v \lhd V_i$.

To prove Property $\mathcal{P}$, assume that $\{x, y\} \subseteq V_i$ such that $vx \in E(G)$ and $vy \notin E(G)$. For any $z \in V_j$, it can be seen that $G[v, x, z, y]$ is an induced P_4 in G, a contradiction. We remark that, in the sequel, Property $\mathcal{P}$ will be used without explicit reference to it.

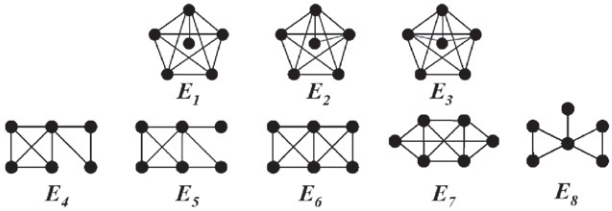

Fig. 8. $r(E_i) \geqslant 6$ for any $i = 1, 2 \ldots, 8$.

When $t = 5$, we claim that $G \cong H$. If this is not the case, then there is a vertex $v \in V(G \setminus H)$ such that $d_G(v, H) = 1$. By the choice of H, we see that $v \notin S_J$ when $|J| = 4$. It follows that G contains an induced subgraph isomorphic to one of the graphs E_1, E_2, E_3 shown in Fig. 8. That is a contradiction to $r(G) = 5$. Therefore, $G \in \mathcal{M}(G_{24})$ provided that $t = 5$.

Now the remaining proof of Lemma 9 is divided into two parts according to the value of t.

Part I. Suppose that $t = 4$. First note that $d_G(v, H) \leqslant 1$ for any $v \in V(G)$. If this is not the case, there would exist an edge $xy \in E(G \setminus H)$ such that $d_G(x, H) = d_G(y, H) + 1 = 2$. It can be seen that $G[V(H) \cup \{x, y\}]$ has rank 6, a contradiction to $r(G) = 5$. Next, by the choice of H and $t = 4$, we see that $S_{\{1,2,3\}} = S_{\{1,2,4\}} = S_{\{1,3,4\}} = S_{\{2,3,4\}} = S_{\{1,2,3,4\}} = \emptyset$.

Claim 1. *(a) If $S_{\{1\}} \neq \emptyset$, then $S_J = \emptyset$, where $|J| \leqslant 2$ and $J \neq \{1\}$. (b) If $S_{\{1,2\}} \neq \emptyset$, then $S_{\{3,4\}} = S_{\{2,3\}} = \emptyset$.*

Proof of Claim 1. (a) When $x \in S_{\{1\}}$ and $y \in S_{\{2\}} \cup S_{\{2,3\}}$, we see that either $G[\{x\} \cup V_1 \cup V_2 \cup \{y\}]$ or $G[\{y, x\} \cup V_1 \cup V_4]$ contains an induced P_4, that is a contradiction. When $x \in S_{\{1\}}$ and $y \in S_{\{1,2\}}$, we see that if $xy \in E(G)$, then $G[\{x, y\} \cup V_2 \cup V_3]$ contains an induced P_4, a contradiction; if $xy \notin E(G)$, then E_5 (see Fig. 8) is an induced subgraph of G, a contradiction again. This completes the proof. (b) When $x \in S_{\{1,2\}}$ and $y \in S_{\{3,4\}}$, we see that if $xy \notin E(G)$ then $G[\{x\} \cup V_2 \cup V_3 \cup \{y\}]$ contains an induced P_4, a contradiction; if $xy \in E(G)$, then E_7 (see Fig. 8) is an induced subgraph of G, a contradiction again. When $x \in S_{\{1,2\}}$ and $y \in S_{\{2,3\}}$, we see that if $xy \in E(G)$, then $G[\{x, y\} \cup V_3 \cup V_4]$ contains an induced P_4, a contradiction; if $xy \notin E(G)$, then $G[\{x\} \cup V_1 \cup V_3 \cup \{y\}]$ contains an induced P_4, a contradiction again. $\square$

Claim 2. *$S_{\{1\}}$ and $S_{\{1,2\}}$ are independent sets in G.*

Proof of Claim 2. Suppose that $xy \in E(G)$. If $x, y \in S_{\{1\}}$, then E_4 shown in Fig. 8 is an induced subgraph of G, a contradiction to $r(G) = 5$. If $x, y \in S_{\{1,2\}}$, then E_6 depicted in Fig. 8 is an induced subgraph of G, a contradiction. This completes the proof of this claim. $\square$

Now, by Claim 1, Claim 2 and symmetry of the graph H, we see that G is isomorphic to one the graphs H, $G[V(H) \cup S_{\{1\}}]$ and $G[V(H) \cup S_{\{1,2\}}]$. Since $r(H) = 4$, it must be $G \in \mathcal{M}(G_{20}, G_{21})$. This completes the proof of Part I of the lemma.

Part II. Suppose that $t = 3$. Since G contains no induced P_4, it follows that $d_G(v, H) \leqslant 1$ for any $v \in V(G)$. Note that $S_{\{1,2,3\}} = \emptyset$, since $t = 3$.

Claim. *(a) $S_{\{1,2\}} = S_{\{1,3\}} = S_{\{2,3\}} = \emptyset$. (b) If $S_{\{1\}} \neq \emptyset$, then $S_{\{2\}} = \emptyset$.*

Proof of the Claim. (a) Assume, to the contrary, that $x \in S_{\{1,2\}}$. Recall that if $v \sim V_i$ and $v \nsim V_j$ for some $1 \leqslant i, j \leqslant 3$, then $v \lhd V_i$. Therefore $G[V(H) \cup \{x\}]$ can be obtained from K_3 by multiplication of vertices, a contradiction to the choice of H. (b) If $x \in S_{\{1\}}$ and $y \in S_{\{2\}}$, then either $G[\{x\} \cup V_1 \cup V_2 \cup \{y\}]$ or $G[\{x, y\} \cup V_2 \cup V_3]$ contains an induced P_4, a contradiction. $\square$

Note that G is not isomorphic to H, since $r(H) = 3$ and $r(G) = 5$. The above claim shows that $V(G)$ is equal to $V(H) \cup S_{\{i\}}$ for some $i \in \{1, 2, 3\}$. Without loss of generality, say $V(G) = V(H) \cup S_{\{1\}}$. Clearly $S_{\{1\}}$ is not an independent set of G, since $r(G) = 5$. Let xy be an edge in the subgraph of G induced by $S_{\{1\}}$. We claim that if $z \in S_{\{1\}} \setminus \{x, y\}$, then z is adjacent to exactly one vertex in $\{x, y\}$. Indeed, if $\{zx, zy\} \subseteq E(G)$, then K_4 is a subgraph of G, a contradiction to $t = 3$; if $\{zx, zy\} \cap E(G) = \emptyset$, then E_8 shown in Fig. 8 is an induced subgraph of G, a contradiction to $r(G) = 5$. Denote by S_x the set $\{v \in S_{\{1\}} \setminus \{x, y\} : vx \in E(G)\}$, and denote by S_y the set $\{v \in S_{\{1\}} \setminus \{x, y\} : vy \in E(G)\}$. Note that S_x (and hence S_y) is an independent set of G, since $t = 3$. For $u \in S_x$ and $v \in S_y$, we claim that u is adjacent to v. If this is not the case, then $G[u, x, y, v]$ is an induced P_4, a contradiction. From what we have proved so far, we see that $G[S_x \cup S_y]$ is a complete bipartite graph. Now we can conclude that $G \in \mathcal{M}(G_{22})$. This completes the proof of Part II of the lemma. □

Acknowledgements

The authors thank the anonymous referee for very careful reading and for constructive comments which help to improve the presentation of the paper.

References

[1] P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, Oxford University Press, 2005.
[2] P.W. Atkins, J. de Paula, Physical Chemistry, eighth ed., Oxford University Press, 2006.
[3] F. Ashraf, H. Bamdad, A note on graphs with zero nullity, MATCH 60 (2008) 15–19.
[4] J.A. Bondy, U.S.R. Murty, Graph theory, in: Graduate Texts in Mathematics, vol. 244, Springer-Verlag, New York, 2008.
[5] B. Borovićanin, I. Gutman, Nullity of graphs, in: D. Cvetković, I. Gutman (Eds.), Applications of Graph Spectra, Math. Inst., Belgrade, 2009, pp. 107–122.
[6] M. Brown, J.W. Kennedy, B. Servatius, Graph singularity, Graph Theory Notes N. Y. 25 (1993) 23–32.
[7] Gerard J. Chang, L.H. Huang, H.G. Yeh, A characterization of graphs with rank 4, Linear Algebra Appl. 434 (2011) 1793–1798.
[8] B. Cheng, B. Liu, On the nullity of graphs, Electron. J. Linear Algebra 16 (2007) 60–67.
[9] B. Cheng, B. Liu, On the nullity of tricyclic graphs, Linear Algebra Appl. 434 (2011) 1799–1810.
[10] L. Collatz, U. Sinogowitz, Spektren endlicher Grafen, Abh. Math. Sem. Univ. Hamburg 21 (1957) 63–77.
[11] D. Cvetković, I. Gutman, N. Trinajstić, Graphical studies on the relations between the structure and reactivity of conjugated system: the role of non-bonding molecular orbitals, J. Mol. Struct. 28 (1975) 289–303.
[12] D. Cvetković, M. Doob, H. Sachs, Spectra of Graphs – Theory and Application, Academic Press, New York, 1980.
[13] S. Fiorini, I. Gutman, I. Sciriha, Trees with maximum nullity, Linear Algebra Appl. 397 (2005) 245–251.
[14] Y.-Z. Fan, K.-S. Qian, On the nullity of bipartite graphs, Linear Algebra Appl. 430 (2009) 2943–2949.
[15] M.C. Golumbic, Algorithmic Graph Theory and Perfect Graphs, second ed., Elsevier, 2004.
[16] J.-M. Guo, W. Yan, Y.-N. Yeh, On the nullity and the matching number of unicyclic graphs, Linear Algebra Appl. 431 (2009) 1293–1301.
[17] I. Gutman, I. Sciriha, On the nullity of line graphs of trees, Discrete Math. 232 (2001) 35–45.
[18] S. Hu, X. Tan, Bolian Liu, On the nullity of bicyclic graphs, Linear Algebra Appl. 429 (2008) 1387–1391.
[19] E. Hückel, Grundzüge der Theorie ungesäutigter und aromatischer Verbindungen, Verlag Chemie, Berlin, 1940.
[20] W. Li, A. Chang, On the trees with maximum nullity, MATCH 56 (2006) 501–508.
[21] S. Li, On the nullity of graphs with pendent vertices, Linear Algebra Appl. 429 (2008) 1619–1628.
[22] B. Liu, Y. Huang, S. Chen, On the characterization of graphs with pendent vertices and given nullity, Electron. J. Linear Algebra 18 (2009) 719–734.
[23] M. Nath, B.K. Sarma, On the null-spaces of acyclic and unicyclic singular graphs, Linear Algebra Appl. 427 (2007) 42–54.
[24] G.R. Omidi, On the nullity of bipartite graphs, Graphs Combin. 25 (2009) 111–114.
[25] I. Sciriha, On the construction of graphs of nullity one, Discrete Math. 181 (1998) 193–211.
[26] I. Sciriha, On singular line graphs of trees, Congr. Numer. 135 (1998) 73–91.
[27] I. Sciriha, On the rank of graphs, in: Y. Alavi, D.R. Lick, A. Schwenk (Eds.), Combinatorics, Graph Theory, and Algorithms, vol. II, New Issue Press, Western Michigan University, Kalamazoo, Michigan, 1999, pp. 769–778.
[28] I. Sciriha, A characterization of singular graphs, Electron. J. Linear Algebra 16 (2007) 451–462.
[29] I. Sciriha, P.W. Fowler, On nut and core singular fullerenes, Discrete Math. 308 (2008) 267–276.
[30] X. Tang, B. Liu, On the nullity of unicyclic graphs, Linear Algebra Appl. 408 (2005) 212–220.
[31] N. Trinaistic, Chemical Graph Theory, second ed., CRC Press, 1992.
[32] R. Wilson, Singular graphs, in: V.R. Kulli (Ed.), Recent Studies in Graph Theory, Vishwa Int. Publications, Gulbarga, 1989, pp. 228–236.
[33] Y.N. Yeh, I. Gutman, C.M. Fu, Graph transformations which preserve the multiplicity of an eigenvalue, Discrete Appl. Math. 67 (1996) 221–228.