

GRAPHS WITH SMALL NEGATIVE INERTIA INDEX

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Abstract: For a graph G with order n , the number of positive and negative eigenvalues of G , denoted by $p(G)$ and $n(G)$, respectively, are called the positive and negative inertia indices of G . The inertia indices are closely related to the nullity of the graph, which has important applications in chemistry, and is intensively studied, especially for molecular graphs. The main objective of this paper is to determine the structure of graphs with small negative inertia index. By utilizing vertex multiplications, we obtain a characterization for graphs G with $n(G) \leq 2$, as well as for graphs G with pendent vertices and with $n(G) \leq 3$.

Keywords: positive inertia index; negative inertia index; multiplication of vertices

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1 Introduction

We consider finite simple graphs in this paper. Undefined concepts and notations will follow [1], and so we write $G = (V(G), E(G))$ to denote a simple graph with vertex set $V(G)$ and edge set $E(G)$. As in [1], for a vertex subset $U \subseteq V(G)$, $G[U]$ is the subgraph of G induced by U . For a vertex $u \in V(G)$, define $N_G(u) = \{v \in V(G) \mid v \text{ is adjacent to } u \text{ in } G\}$ to be the neighborhood of vertex u in G , and $d_G(u) = |N_G(u)|$ as the degree of u in G . For integers $n, n_1, \dots, n_t > 0$, K_n, C_n and $K_{n_1, n_2, \dots, n_t}$ denote the complete graph on n vertices, the n -cycle and the complete multipartite graph, respectively. If G and H are two vertex disjoint graphs, then $G \cup H$ denotes the disjoint union of G and H .

Throughout this paper, the vertices of a graph G are often labeled as $V(G) = \{v_1, v_2, \dots, v_n\}$, where $n = |V(G)|$. As in [1], the adjacency matrix of G is an $n \times n$ matrix $A(G) = (a_{ij})_{n \times n}$, where a_{ij} is the number of edges joining v_i and v_j in G . The eigenvalues $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n$ of $A(G)$ are said to be the eigenvalues of the graph G and to form the spectrum of this graph. The number of positive, negative and zero eigenvalues in the spectrum of G are called positive inertia index, negative inertia index and nullity of the graph G , and are denoted by $p(G)$, $n(G)$ and $\eta(G)$, respectively. Obviously $p(G) + n(G) + \eta(G) = n$. The rank of G , written as $r(G)$, is the number of nonzero eigenvalues in the spectrum of G . It follows from the definitions that $r(G) = p(G) + n(G) = n - \eta(G)$.

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In chemistry, a conjugated hydrocarbon molecule can be modeled 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 molecule. The nullity (as well as the rank) of a molecular graph G has a number of important applications in chemistry. For example, it is known [2] that $\eta(G) = 0$ is a necessary condition for the molecule represented by G to be chemically stable. More studies on nullity or rank of graphs can be found in [3–28], among others. To the best of our knowledge, very few studies on the positive and negative inertia indices of graphs were conducted. In [29], Hoffman showed that a graph has exactly one negative eigenvalue if and only if its non-isolated vertices form a complete bipartite graph. In [30], Smith showed that a graph has exactly one positive eigenvalue if and only if its non-isolated vertices form a complete multipartite graph. In [31], graph G is characterized with $p(G) \geq n - 2$, where $n = |V(G)|$. It raises the problem of characterizing graph G with small negative inertia indices.

This motivates the current research. In this paper, we present a complete characterization for graphs G with $n(G) \leq 2$, and for graphs G with both $\delta(G) = 1$ and $n(G) \leq 3$, where $\delta(G)$ is the smallest degree of G .

This paper is organized as follows: in Section 2, preliminary lemmas will be presented. A Characterization for graph G with $n(G) \leq 2$, and for graph G with pendent vertices and with $n(G) \leq 3$ are given in Sections 3 and 4. The characterization of graph G with $n(G) \leq 2$ extends the former result of Hoffman in [29].

2 Preliminaries

Lemma 2.1 Let G and H be graphs. Then

$$p(G \cup H) = p(G) + p(H); \quad n(G \cup H) = n(G) + n(H).$$

Lemma 2.2 (see [30]) A graph G has exactly one positive eigenvalue if and only if its non-isolated vertices form a complete multipartite graph.

Lemma 2.3 (see [9, 32]) (the Cauchy inequalities) Let A be Hermtian matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, B be one of its principal submatrices and B have eigenvalues $\mu_1 \geq \dots \geq \mu_m$. Then the inequalities $\lambda_{n-m+i} \leq \mu_i \leq \lambda_i (i = 1, \dots, m)$ hold.

Lemma 2.4 Let H be a vertex-induced subgraph of G . Then

(1) $r(H) \leq r(G)$, $p(H) \leq p(G)$ and $n(H) \leq n(G)$.

(2) If $r(H) = r(G)$, then $p(H) = p(G)$ and $n(H) = n(G)$.

Proof Lemma 2.4 follows from Lemma 2.3 and from the inequality $r(H) = p(H) + n(H) \leq p(G) + n(G) = r(G)$.

Lemma 2.5 (see [33]) Let G be a connected graph with rank k (≥ 2). Then there exists a vertex-induced subgraph H (of G) on k vertices such that $r(H) = k$.

As in [1], a vertex subset $I \subseteq V(G)$ of a graph G is an independent set (also referred as a stable set) of G if $G[I]$, the subgraph induced by I , is edgeless. Let $m = (m_1, m_2, \dots, m_n)$ be a vector of positive integers. Denote by $G \circ m$ the graph obtained from G by replacing

each vertex v_i of G with an independent set of m_i vertices $v_i^1, v_i^2, \dots, v_i^{m_i}$ and joining v_i^s with v_j^t if and only if v_i and v_j are adjacent in G ($1 \leq s \leq m_i, 1 \leq t \leq m_j$). The resulting graph $G \circ m$ is said to be obtained from G by multiplication of vertices.

Let Ω be the set of some graphs, we denote by $\mathcal{M}(\Omega)$ the class of all graphs that can be constructed from one of the graphs in Ω by multiplication of vertices.

Lemma 2.6 (see [5, 6]) Let G and H be graphs. If $G \in \mathcal{M}(\{H\})$, then $r(G) = r(H)$. Furthermore, in this case, we have both $p(G) = p(H)$ and $n(G) = n(H)$.

A graph is called a basic graph if it has no isolated vertex and can not be obtained from other graphs by multiplication of vertices. By definition, a graph with no isolated vertices is not a basic graph if and only if it has two vertices which have same neighborhoods. By Lemma 2.6, it suffices to study basic graphs when we investigate graph invariants such as the rank, the positive inertia index and the negative inertia index.

Lemma 2.7 (see [19]) Let G be a graph containing a pendant vertex, and let H be the induced subgraph of G obtained by deleting the pendant vertex together with the vertex adjacent to it. Then $p(G) = p(H) + 1$ and $n(G) = n(H) + 1$.

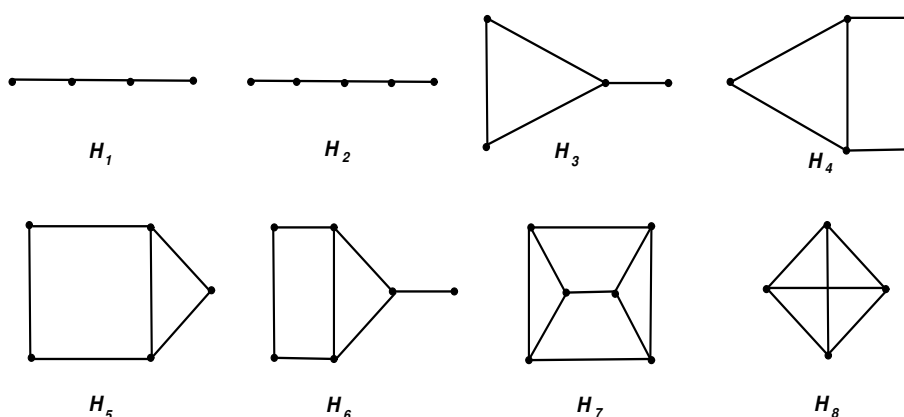


Figure 1: the connected basic graph with $r(H) = 4$

Lemma 2.8 (see [5,6,8]) Let G be a connected graph. Then

- (a) $r(G) = 2$ if and only if $G \in \mathcal{M}(\{K_2\})$,
- (b) $r(G) = 3$ if and only if $G \in \mathcal{M}(\{K_3\})$,
- (c) $r(G) = 4$ if and only if $G \in \mathcal{M}(\Omega_1)$, where $\Omega_1 = \{H_1, H_2, \dots, H_8\}$,
- (d) $r(G) = 5$ if and only if $G \in \mathcal{M}(\Omega_2)$, where $\Omega_2 = \{G_1, G_2, \dots, G_{24}\}$,

where graphs H_i ($i = 1, 2, \dots, 8$) are depicted in Figure 1 and graphs G_i ($i = 1, 2, \dots, 24$) are depicted in Figure 2.

Lemma 2.9 (see [31]) Let G be a graph of order n , then $p(G) = n - 2$ if and only if one of the following holds

- (1) $n = 2$, $G \cong 2K_1$; or
- (2) $n = 3$, $G \cong K_1 \cup K_2$, $K_{1,2}$ or K_3 ; or
- (3) $n = 4$, $G \cong F_1, F_2$ or F_3 ; or

(4) $n = 5$, $G \cong C_5$,
 where graphs $F_i (i = 1, 2, 3)$ are depicted in Figure 3.

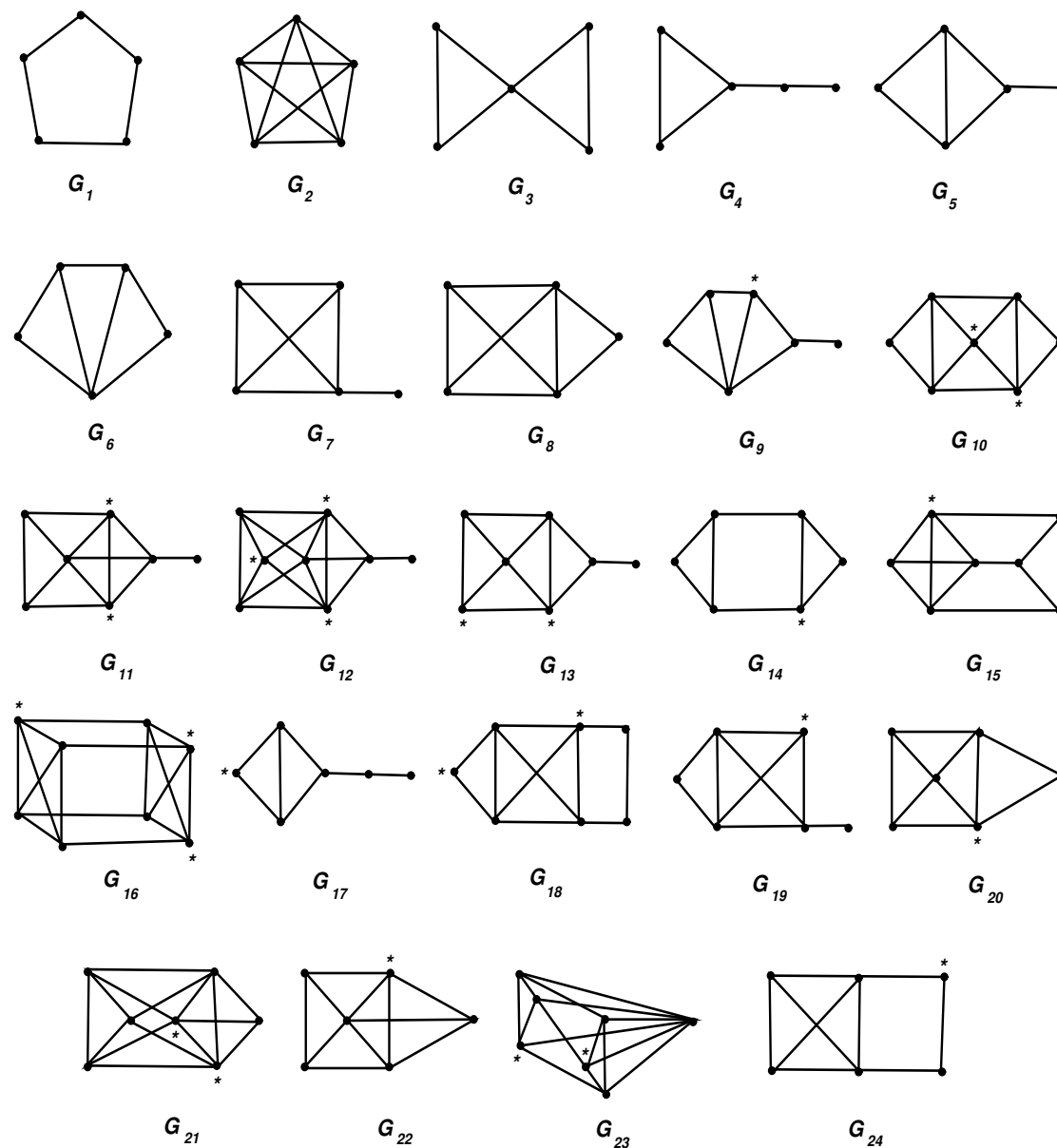
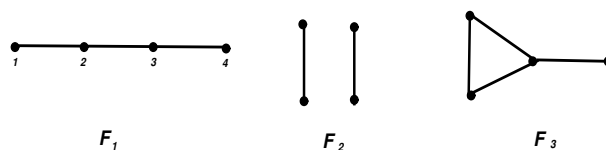


Figure 2: the connected basic graph with $r(G) = 5$

3 Characterization of Graphs G with $n(G) \leq 2$

The following lemmas will be needed in our characterization.

Lemma 3.1 (see [29]) A graph has exactly one negative eigenvalue if and only if its non-isolated vertices form a complete bipartite graph. In other words, if G is a connected

Figure 3: The graph G with four vertices and $p(G) = 2$

graph, then $n(G) = 1$ if and only if $G \in \mathcal{M}(\{K_2\})$.

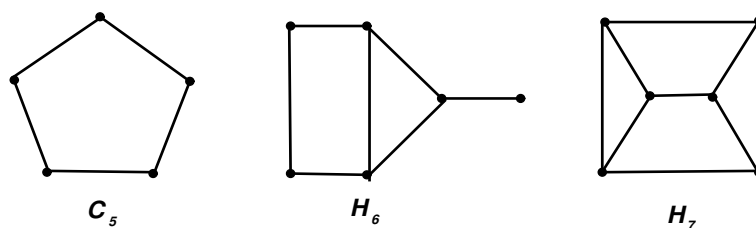
Lemma 3.2 Let G be a connected graph. Then $n(G) = 2$ if and only if $G \in \mathcal{M}(\Omega_3)$, where $\Omega_3 = \{K_3, C_5, H_1, H_2, \dots, H_7\}$, and the graphs H_i ($i = 1, 2, \dots, 7$) are defined in Figure 1.

Proof It is routine to verify that $n(G) = 2$ for $G \in \{K_3, C_5\} \cup \{H_i | 1 \leq i \leq 7\}$. Thus the sufficiency follows from Lemma 2.6.

To prove the necessity, we note that $r(G) > n(G) = 2$. If $r(G) = 3$, then by Lemma 2.8 (b), $G \in \mathcal{M}(\{K_3\})$. If $r(G) = 4$, then by Lemma 2.8 (c), $G \in \mathcal{M}(\{H_1, H_2, \dots, H_8\})$. However, as direct computation yields $n(H_8) = 3$, we must have $G \in \mathcal{M}(\{H_1, H_2, \dots, H_7\})$.

If $r(G) = 5$, then by Lemma 2.8 (d), $G \in \mathcal{M}(\{G_1, G_2, \dots, G_{24}\})$. Direct computation yields $n(G_2) = 4$. To determine the values of the other $n(G_i)$'s, we utilize Table 1 of [9] to find $n(G_i) = 3$, $3 \leq i \leq 8$. By deleting the vertices which be marked * in graphs depicted in Figure 2, we observe that each G_i , $9 \leq i \leq 18$, has a vertex-induced subgraph isomorphic to G_4 , that each of G_{19}, G_{20} and G_{21} has a vertex-induced subgraph isomorphic to G_5 , that each of G_{22} and G_{23} has a vertex-induced subgraph isomorphic to G_6 , and that G_{24} has a vertex-induced subgraph isomorphic to G_7 . It follows by Lemma 2.4 (2) that $n(G_i) = 3$, $9 \leq i \leq 24$. Hence in this case, $G \in \mathcal{M}(\{G_1\}) = \mathcal{M}(\{C_5\})$.

If $r(G) = k \geq 6$, then by Lemma 2.5, there exists a vertex-induced subgraph H (of G) on k vertices such that $r(H) = k$. Furthermore, by Lemma 2.4(2), we have $n(H) = 2$ and $p(H) = k - 2$. However, there does not exist such a graph H by Lemma 2.9. This means that there does not exist graph G with $r(G) = k \geq 6$ and $n(G) = 2$.

Figure 4: basic extremal graphs with respect to $n(G) = 2$.

A graph G is called basic extremal graph with respect to $n(G) = 2$, if G is a basic graph with $n(G) = 2$, and G is not a proper vertex-induced subgraph of any other basic graphs H with $n(H) = 2$. By definition, since K_3 is a proper vertex-induced subgraph of H_6 , hence K_3 is not a basic extremal graph with respect to $n(G) = 2$, the same graphs H_i ($i = 1, 2, 3, 4, 5$) are not basic extremal graph with respect to $n(G) = 2$. However, it is routine to verify that

the graphs G in Figure 4 are basic extremal graphs with respect to $n(G) = 2$.

Theorem 3.1 now follows from Lemma 3.1 and Lemma 3.2.

Theorem 3.1 Let G be a graph. Then $n(G) \leq 2$ if and only if $G \in \mathcal{M}(\Omega_4)$, where Ω_4 is the set of all vertex-induced subgraph of each graph in $\Theta_1 = \{C_5 \cup K_1, H_6 \cup K_1, H_7 \cup K_1\}$, and C_5, H_6, H_7 are depicted in Figure 4.

4 Characterization of Graphs G with Pendent Vertices and $n(G) \leq 3$

Let H be a graph with $V(H) = \{v_1, v_2, \dots, v_n\}$ and $m = (m_1, m_2, \dots, m_n)$ be a vector with $m_i = 1$ or 2 , ($i = 1, 2, \dots, n$). Then $V(H)$ can be divided into two sets: $V_1 = \{v_i \in V(H) \mid m_i = 1\}$ and $V_2 = \{v_i \in V(H) \mid m_i = 2\}$. Let v_i^1 and v_i^2 be the vertices in $H \circ m$ by multiplying the vertex v_i in H when $m_i = 2$. For a subset $U \subseteq V_1$, we construct a graph $(H \circ m)^U$ as follows

$$\begin{aligned} V((H \circ m)^U) &= \{x, y\} \cup V(H \circ m), \\ E((H \circ m)^U) &= \{(x, y)\} \cup \{(y, v_i^1) \mid \forall m_i = 2\} \cup \{(y, v_i) \mid v_i \in U\} \cup E(H \circ m). \end{aligned}$$

By the definition, $(H \circ m)^U$ has a pendent vertex x .

Lemma 4.1 If H is a basic graph, then $(H \circ m)^U$ is also a basic graph.

Proof For any $i, j \in \{1, 2, \dots, n\}$, if $i \neq j$, as H is a basic graph, then $N_H(v_i) \neq N_H(v_j)$. So $N_{(H \circ m)^U}(v_i^s) \neq N_{(H \circ m)^U}(v_j^t)$ ($1 \leq s \leq m_i, 1 \leq t \leq m_j$). If $i = j$ and $m_i = 2$, by the construction of the graph $(H \circ m)^U$, we have $y \in N_{(H \circ m)^U}(v_i^1)$ and $y \notin N_{(H \circ m)^U}(v_i^2)$; $x \in N_{(H \circ m)^U}(y)$ and $x \notin N_{(H \circ m)^U}(v)$ for all $v(\neq y) \in V((H \circ m)^U)$; $N_{(H \circ m)^U}(x) = \{y\}$ and $N_{(H \circ m)^U}(v) \neq \{y\}$ for all $v(\neq x) \in V((H \circ m)^U)$ (this is because H has no isolated vertex). In a word, any two vertices in $(H \circ m)^U$ don't have the same neighborhoods. Therefore, $(H \circ m)^U$ is a basic graph. This proves the lemma.

Let $\Gamma(H) = \{(H \circ m)^U \mid U \in V_1, m = (m_1, m_2, \dots, m_n), m_i = 1 \text{ or } 2\}$ be the collection of all graphs $(H \circ m)^U$. For the convenience of drawing, when $m_i = 2$, we use a hollow circle to indicate two vertices v_i^1 and v_i^2 , which have the same neighborhoods in $H \circ m$, the vertex y is adjacent to v_i^1 and not adjacent to v_i^2 , and we use a black dot to indicate exactly one vertex. For example, the graph $(H \circ m)^U$ is depicted in Figure 6, where $H = C_5$, $V(H) = \{v_1, v_2, v_3, v_4, v_5\}$, $m = (2, 2, 1, 1, 1)$ and $U = \{v_3, v_4\}$.

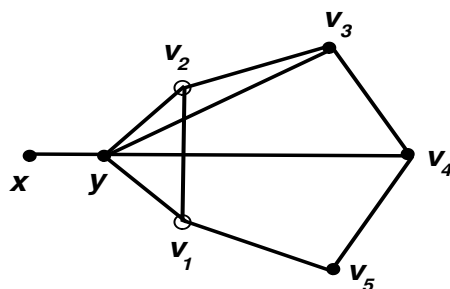


Figure 5: the graph $(C_5 \circ m)^U$ where $m = (2, 2, 1, 1, 1)$, $U = \{v_3, v_4\}$

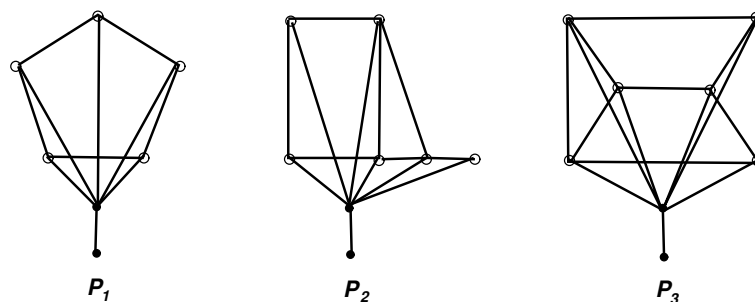


Figure 6: The graphs $P_1 = (C_5 \circ m_1)^\emptyset$, $P_2 = (H_6 \circ m_2)^\emptyset$, $P_3 = (H_7 \circ m_2)^\emptyset$.

Lemma 4.2 Let G be a connected graph with pendent vertices and $n(G) = 3$. Then $G \in \mathcal{M}(\Omega_5)$, where $\Omega_5 = \Gamma(2K_2) \cup \Gamma(K_3) \cup \Gamma(C_5) \cup \bigcup_{i=1}^7 \Gamma(H_i)$ and H_i ($i = 1, 2, \dots, 7$) are depicted in Figure 1.

Proof Without loss of generality, assume that G is a basic graph. Let H be the induced subgraph of G obtained by deleting the pendant vertex x together with the vertex y adjacent to it. By Lemma 2.7, we have $n(H) = 2$. Furthermore, H does not have isolated vertices (if not, then the G contains at least an isolated vertex or two pendant vertices all adjacent to y , so G is not a connected graph, or G is not a basic graph, a contradiction). If the graph H is not connected, then by Lemma 3.1, $H \in \mathcal{M}(\{2K_2\})$. If the graph H is connected, then by Lemma 3.2, $H \in \mathcal{M}(\{K_3, C_5, H_1, H_2, \dots, H_7\})$, where graphs H_i ($i = 1, 2, \dots, 7$) are depicted in Figure 1. We present the proof for the case when $H = K_3 \circ m$, where $m = (m_1, m_2, \dots, m_n)$ be a vector of positive integers, as the proofs for other cases are similar and will be omitted. If $m_i \geq 3$, then there exist $s, t \in \{1, 2, \dots, m_i\}$ such that $N_G(v_i^s) = N_G(v_i^t)$. If $m_i = 2$, v_i^1 and v_i^2 are all adjacent to y or none is adjacent to y , then $N_G(v_i^1) = N_G(v_i^2)$. However, G is a basic graph, this is a contradiction. So $m_i \leq 2$, furthermore, one and only one of the two vertices v_i^1 and v_i^2 is adjacent to y when $m_i = 2$. Therefore, we conclude that $G \in \Gamma(2K_2) \cup \Gamma(K_3) \cup \Gamma(C_5) \cup \bigcup_{i=1}^7 \Gamma(H_i)$.

For vectors $m_1 = (2, 2, 2, 2, 2)$ and $m_2 = (2, 2, 2, 2, 2, 2)$, define $P_1 = (C_5 \circ m_1)^\emptyset$, $P_2 = (H_6 \circ m_2)^\emptyset$, $P_3 = (H_7 \circ m_2)^\emptyset$, as depicted in Figure 6. If

$$G \in \Gamma(2K_2) \cup \Gamma(K_3) \cup \Gamma(C_5) \cup \bigcup_{i=1}^7 \Gamma(H_i),$$

it is straightforward to verify that graphs G are a vertex-induced subgraph of P_1 , P_2 , or P_3 . Hence Theorem 4.1 below follows from Lemma 4.2.

Theorem 4.1 Let G be a graph with pendent vertices and $n(G) \leq 3$. Then $G \in \mathcal{M}(\Omega_6)$, where Ω_6 is the set of all vertex-induced subgraph of each graph in $\Theta_2 = \{P_1 \cup K_1, P_2 \cup K_1, P_3 \cup K_1\}$, where P_i ($i = 1, 2, 3$) are depicted in Figure 6.

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具有小的负惯性指数的图

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摘要: 设 G 是有 n 个点的图, 在 G 的所有特征根中, 正特征根的个数和负特征根的个数分别称为图 G 的正惯性指数和负惯性指数, 分别记为 $p(G)$ 和 $n(G)$. 这两个参数密切联系与图 G 的零度, 而图的零度是具有重要化学应用的图参数, 特别是对分子图, 它已经被大量的研究. 这篇文章的主要目的是刻画具有小的负惯性指数的图. 利用图的点繁殖运算, 刻画了具有 $n(G) \leq 2$ 的所有图, 也刻画了具有 $n(G) \leq 3$ 的带有悬挂点的所有图.

关键词: 正惯性指数; 负惯性指数; 点繁殖.

MR(2010)主题分类号: 05C50 中图分类号: O157.5