Journal of Mathematical Chemistry, Vol. 42, No. 3, October 2007 (© 2006)
DOI: 10.1007/s10910-006-9132-7

Sharp bounds for the second Zagreb index of unicyclic graphs

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Received 17 March 2006; revised 5 April 2006

The second Zagreb index $M_2(G)$ of a (molecule) graph G is the sum of the weights $d(u)d(v)$ of all edges uv of G, where $d(u)$ denotes the degree of the vertex u. In this paper, we give sharp upper and lower bounds on the second Zagreb index of unicyclic graphs with n vertices and k pendant vertices. From which, U^n_{n-3} and C_n have the maximum and minimum the second Zagreb index among all unicyclic graphs with n vertices, respectively.

KEY WORDS: Zagreb index, unicyclic graph, pendant vertex

AMS subject classification: 05C35, 05C18

1. Introduction

For a molecular graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined in [1] as

$$M_1(G) = \sum_{u \in V(G)} (d(u))^2, \qquad M_2(G) = \sum_{uv \in E(G)} d(u)d(v),$$

where $d(u)$ denotes the degree of the vertex u of G. The research background of Zagreb index together with its generalization appears in chemistry or mathematical chemistry and can be found in the literature (see [2–8]).

Recently, finding bounds for the topological index of graphs, as well as related problem of finding the graphs with maximum or minimum value of the respective index, attracted the attention of many researchers and many results are obtained (see [9–13]). Zhou [12] presented sharp upper bounds for the Zagreb indices M_1 and M_2 of a graph, especially for triangle-free graphs, in terms of the number of vertices and the number of edges.

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Here, unicyclic graphs with n vertices and k pendant vertices are considered, and the upper and lower bounds of their the second Zagreb index are given, and the corresponding extremal graphs are characterized.

First we introduce some graph notations used in this paper. We only consider finite, undirected and simple graphs. Other undefined terminologies and notations may refer to [14]. Let $G = (V, E)$ be a simple undirected graph with n vertices. For $v \in V(G)$, the degree of v, written by $d_G(v)$ or $d(v)$, is the number of edges incident with v. The maximum degree of a graph G is denoted by $\Delta(G)$. A pendant vertex is a vertex of degree 1 and a pendant edge is an edge incident with a pendant vertex. Let $PV(G) = \{v\colon d_G(v) = 1\}$. For two vertices u and v $(u \neq v)$, the distance between u and v, denoted by $d(u, v)$, is the number of edges in a shortest path joining u and v. Let $P = v_0v_1 \cdots v_s$ $(s \geq 1)$ be a path of G with $d(v_1) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$). If $d(v_0), d(v_s) \geq 3$, then we call P an *internal path* of G; if $d(v_0) \geq 3$ and $d(v_s) = 1$, then we call P a *pendant path* of G. Let C_q a cycle of length q. We will use $G - x$ or $G - xy$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$ or the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from G by adding an edge $xy \notin E(G)$, where $x,\ y \in V(G)$.

Unicyclic graphs are connected graphs with n vertices and n edges. Let $\mathscr{U}_{n,k} = \{G : G$ is a unicyclic graph with n vertices and k pendant vertices, $0 \leq k \leq n-3\}$.

Let $C_q(p_1, p_2, \ldots, p_k)(k \geq 1)$ be a unicyclic graph with n vertices created from C_q by attaching paths of lengths $p_1, p_2, \ldots, p_k$ to one vertex of the cycle C_q, respectively, where $n = q + \sum_{i=1}^{k} p_i,\ p_i \geq 1,\ i = 1, 2, \ldots, k$. Denote

$$\mathscr{U}^*_{n,0} = \{C_n\},\ \ \mathscr{U}^*_{n,k} = \{C_q(p_1, p_2, \ldots, p_k)\colon p_i \geq 2, 1 \leq i \leq k, q \geq 3\} \quad (k \geq 1),$$

and $U^n_k = C_3(1, \ldots, 1, \overbrace{2, \cdots, 2}^{n-k-3})$ (see figure 1). Then $\mathscr{U}^*_{n,k} \subseteq \mathscr{U}_{n,k}$ and $U^n_k \in \mathscr{U}_{n,k}$.

Let $\mathscr{U}^+_{n,k} = \{G \in \mathscr{U}_{n,k} : \Delta(G) \leq 3$, each pendant vertex of G is adjacent to another vertex of degree 3 and every pair of vertices of degree 3 are nonadjacent$\}$. Clearly, $\mathscr{U}^+_{n,0} = \{C_n\}$. In figure 2, we have drawn $G_1,\ G_2,\ G_3,\ G_4 \in \mathscr{U}^+_{13,4}$.

The main results of this paper are stated in the following theorems.

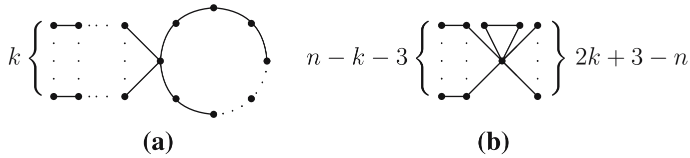

Figure 1. (a) an element of $\mathscr{U}^*_{n,k}$; (b) U^n_k.

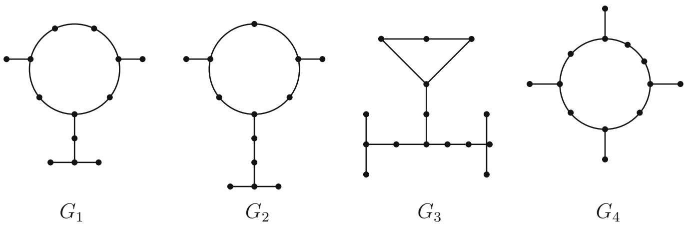

Figure 2.

Theorem 1. Let $G \in \mathscr{U}_{n,k}$, $0 \le k \le n-3$. Then

$$M_2(G) \le \begin{cases} 4n + 2k(k+1) & \text{if } n \ge 2k+3; \quad (1) \\ 4n + (n-1)k & \text{if } n \le 2k+2. \quad (2) \end{cases}$$

Equalities in (1) and (2) hold if and only if $G \in \mathscr{U}^*_{n,k}$ and $G \cong U^n_k$, respectively.

Theorem 2. Let $G \in \mathscr{U}_{n,k}$, $0 \le k \le n-3$. Then

$$M_2(G) \ge 4n + 3k. \quad (3)$$

Equality in (3) holds if and only if $n \ge 3k$ and $G \in \mathscr{U}^+_{n,k}$.

2. The upper bound

We first give some lemmas that will be used in the proof of our result. Denote $\overline{\mathscr{U}_{n,k}} = \{G \in \mathscr{U}_{n,k} : M_2(G) \text{ is maximum}\}$.

Lemma 1. Suppose that $G \in \overline{\mathscr{U}}_{n,k}$ with C being unique cycle in G. Then $d_G(v) \le 2$ for each vertex $v \in V(G) - V(C)$.

Proof. By contradiction. Assume that there is a vertex $v \in V(G) - V(C)$ such that $d_G(v) \ge 3$. We consider two cases.

Case 1. There is a vertex $w \in V(C)$ such that $vw \in E(G)$.

Denote $N_G(w) = \{w_1, w_2, v, y_1, \ldots, y_s\}$, $N_G(v) = \{w, x_1, \ldots, x_t\}$, $t \ge 2$, where $w_1, w_2 \in V(C)$. Then $d_G(w) = s + 3 \ge 3$, $d_G(v) = t + 1 \ge 3$. Let $u_1 \in PV(G)$ and

$$G^* = G - \{wv, vx_1, vx_2, \ldots, vx_t\} + \{wx_1, \ldots, wx_t, vu_1\}.$$

Denote $N_{G^*}(u_1) = \{u_2, v\}$. Then $G^* \in \mathscr{U}_{n,k}$ and $d_{G^*}(u_2) \geq 2$. But

$$\begin{aligned}
&M_2(G^*) - M_2(G) \\
&= (d_G(v) - 2)\left(d_G(w_1) + d_G(w_2) + \sum_{i=1}^{s} d_G(y_i)\right) + (d_G(w) - 2)\left(\sum_{i=1}^{t} d_G(x_i)\right) \\
&\quad + d_{G^*}(u_2) + 2 - d_G(w)d_G(v) \\
&\quad \geq (d_G(v) - 2)(4 + d_G(w) - 3) + (d_G(w) - 2)(d_G(v) - 1) \\
&\quad + d_{G^*}(u_2) + 2 - d_G(v)d_G(w) \\
&= d_G(v)d_G(w) - 3d_G(w) - d_G(v) + d_{G^*}(u_2) + 2 \\
&= (d_G(v) - 3)(d_G(w) - 1) + d_{G^*}(u_2) - 1 \\
&\quad \geq d_{G^*}(u_2) - 1 > 0,
\end{aligned}$$

a contradiction with the choice of G.

Case 2. There is a vertex $w \in V(C)$ such that $P = wv_0 \ldots v_{l-2}v$, $l \geq 2$ is an internal path.

Let $N_G(w) = \{w_1, w_2, v_0, y_1, \ldots, y_s\}$, $N_G(v) = \{v_{l-2}, x_1, \ldots, x_t\}$, $t \geq 2$, where $w_1, w_2 \in V(C)$. Then $d_G(w) = s + 3 \geq 3$, $d_G(v) = t + 1 \geq 3$. Let $u_1 \in PV(G)$ and

$$G^* = G - \{wv_0, vx_1, vx_2, \ldots, vx_t\} + \{wx_1, \ldots, wx_t, vu_1\}.$$

Denote $N_{G^*}(u_1) = \{u_2, v\}$. Then $G^* \in \mathscr{U}_{n,k}$ and $d_{G^*}(u_2) \geq 2$. But

$$\begin{aligned}
&M_2(G^*) - M_2(G) \\
&= (d_G(v) - 2)\left(d_G(w_1) + d_G(w_2) + \sum_{i=1}^{s} d_G(y_i)\right) + (d_G(w) - 2)\left(\sum_{i=1}^{t} d_G(x_i)\right) \\
&\quad + d_{G^*}(u_2) - 2d_G(w) - 2d_G(v) + 6 \\
&\quad \geq (d_G(v) - 2)(4 + d_G(w) - 3) + (d_G(w) - 2)(d_G(v) - 1) \\
&\quad + d_{G^*}(u_2) - 2d_G(w) - 2d_G(v) + 6 \\
&= 2(d_G(v) - 3)(d_G(w) - 2) + d_G(v) + d_G(w) + d_{G^*}(u_2) - 6 > 0,
\end{aligned}$$

a contradiction with the choice of G. □

Lemma 2. Suppose that $G \in \overline{\mathscr{U}_{n,k}}$ with C being unique cycle in G. If $n \geq 2k+3$, then there exists a vertex $v \in V(G) - V(C)$ such that $d_G(v) = 2$.

Proof. Assume that $d_G(v) \neq 2$ for all $v \in V(G) - V(C)$. Then by lemma 1, $d_G(v) = 1$ for all $v \in V(G) - V(C)$.

We first show that there is a vertex $w \in V(C)$ such that $d_G(w) = 2$. Otherwise, $d_G(w) > 2$ for all $w \in V(C)$, thus $|V(G)| \leq 2k$, a contradiction with the assumption $n \geq 2k+3$. Therefore we set $N_G(w) = \{w_1, w_2\}$, $vv_1 \in E(G)$ with $w_1, w_2, v_1 \in V(C)$, $v \in V(G) - V(C)$. Let $G^* = G - \{w_1w, ww_2\} + \{w_1w_2, vw\}$. Then $G^* \in \mathscr{U}_{n,k}$. But

$$\begin{aligned} M_2(G^*) - M_2(G) &= d_G(w_1)d_G(w_2) + d_G(v_1) + 2 - 2d_G(w_1) - 2d_G(w_2) \\ &= (d_G(w_1) - 2)(d_G(w_2) - 2) + d_G(v_1) - 2 \\ &> 0, \end{aligned}$$

a contradiction with the choice of G. □

Lemma 3. Suppose that $G \in \overline{\mathscr{U}_{n,k}}$ with C being unique cycle in G. If $n \leq 2k+2$, then there exists a vertex $v \in PV(G)$ such that $N_G(v) \cap V(C) \neq \emptyset$.

proof. By contradiction. Assume that $N_G(v) \cap V(C) = \emptyset$ for all $v \in PV(G)$. Then, by lemma 1, $d_G(u) = 2$ for $u \in V(G) - (V(C) \cup PV(G))$. Hence $|V(G) - (V(C) \cup PV(G))| \geq k$. Since $|V(C)| \geq 3$, we have

$$n = |V(G)| \geq k + k + 3 = 2k + 3,$$

a contradiction with the assumption $n \leq 2k+2$. □

Lemma 4. Suppose that $G \in \overline{\mathscr{U}_{n,k}}$ with C being unique cycle in G. Let $v \in V(C)$ and $d_G(v) = t \geq 3$. Let $|N_G(v) \cap PV(G)| = r$, $N_G(v) \setminus PV(G) = \{w_1, w_2, x_1, \cdots, x_{t-r-2}\}$ with $w_1, w_2 \in V(C)$. Then

(i) $d_G(w_1) + d_G(w_2) \leq k + 6 - t$;

(ii) $r \geq \max\{0,\ 2t - n - 1\}$.

Proof. (i) By lemma 1, we have $\sum_{v \in V(C)}(d_G(v) - 2) = k$. Thus

$$(d_G(w_1) - 2) + (d_G(w_2) - 2) + (d_G(v) - 2) \leq \sum_{v \in V(C)} (d_G(v) - 2) = k, \tag{4}$$

i.e., $d_G(w_1) + d_G(w_2) \leq k + 6 - t$.

(ii) Suppose that $n < 2t - 1$. Note that

$$\begin{aligned} 2n = 2|E(G)| &= \sum_{u \in V(G)} d_G(u) \\ &\geq \sum_{i=1}^{t-r-2} \left(d_G(x_i) + \sum_{w \in N(x_i) \setminus \{v\}} d_G(w) \right) + t + r + d_G(w_1) + d_G(w_2) \\ &\geq 2(t - r - 2) + (t - r - 2) + t + r + 4 \\ &= 4t - 2r - 2. \end{aligned}$$

Thus $4t - 2r - 2 \leq 2n$, that is, $r \geq 2t - n - 1$. □

Denote $\varphi_1(n,k) = 4n + 2k(k+1)$, $\varphi_2(n,k) = 4n + (n-1)k$, where n, k are integers with $0 \le k \le n-3$.

Proof of theorem 1. First we note that if $G \in \mathscr{U}^*_{n,k}$ (or $G \cong U^n_k$, resp.), then equality in (1) (or (2), resp.) holds.

Now we prove that if $G \in \mathscr{U}_{n,k}$, then (1) (or (2), resp.) holds and equality in (1) (or (2), resp.) holds only if $G \in \mathscr{U}^*_{n,k}$ (or $G \cong U^n_k$, resp.).

Applying induction on k.

If $k = 0$, then $G \cong C_n$. If $k = 1$, then $G \cong U^4_1$ if $n = 4$ and $G \in \mathscr{U}^*_{n,1}$ if $n \ge 5$. Hence the result holds obviously.

Therefore we assume that $k \ge 2$ and the result holds for small values of k. Assume that $G \in \overline{\mathscr{U}}_{n,k}$.

We consider the following two case.

Case 1. $n \ge 2k+3$.

In this case, by lemma 2, let $P = v_0v_1\cdots v_{s-1}v_s$ be a pendant path of G with $v_0 \in PV(G)$, $v_s \in V(C)$ and $d_G(v_s) = t \ge 3$. Then $t \le k+2$. Let $|N_G(v_s) \cap PV(G)| = r$ and $N_G(v_s) \setminus (PV(G) \cup \{v_{s-1}\}) = \{w_1, w_2, x_1, x_2, \ldots, x_{t-r-3}\}$ with $w_1, w_2 \in V(C)$. Then $r \ge 0$, $t - r \ge 3$ and all $d(x_i) = d_i \ge 2$. By lemma 1, $d_i \le 2$. Therefore $d_i = 2$.

Set $G^* = G - \{v_0, v_1, \ldots, v_{s-1}\}$. Then $G^* \in \mathscr{U}_{n-s,k-1}$ and

$$\begin{aligned} M_2(G) &= M_2(G^*) + 2 + 4(s-2) + 2t + d_G(w_1) + d_G(w_2) + r + \sum_{i=1}^{t-r-3} d_i \\ &= M_2(G^*) + 2 + 4(s-2) + 2t + d_G(w_1) + d_G(w_2) + r + 2(t-r-3). \end{aligned}$$

If $n - s \le 2(k-1)+2$, then $M_2(G^*) \le \varphi_2(n-s, k-1)$ by the induction hypothesis, and thus

$$\begin{aligned} M_2(G) &\le \varphi_2(n-s,k-1) + 2 + 4s - 8 + 2t + (k+6-t) + r + 2t - 2r - 6 \\ &\le \varphi_1(n,k) + (n-s-1)(k-1) - 2k^2 - 2k - 6 + 3t + k - r \\ &\le \varphi_1(n,k) + (2k-1)(k-1) - 2k^2 - 2k - 6 + 3t + k - r \\ &= \varphi_1(n,k) - 3(k+2-t) - (k-1) - r \\ &< \varphi_1(n,k). \end{aligned}$$

The last inequality follows by $k \ge 2$, $r \ge 0$ and $t \le k+2$.

If $n - s \ge 2(k-1)+3$, then $M_2(G^*) \le \varphi_1(n-s, k-1)$ by the induction hypothesis, and thus

$$\begin{aligned} M_2(G) &\le \varphi_1(n-s,k-1) + 2 + 4s - 8 + 2t + (k+6-t) + r + 2t - 2r - 6 \\ &= \varphi_1(n,k) - 3(k+2-t) - r \\ &\le \varphi_1(n,k). \end{aligned}$$

The last inequality follows by $r \geq 0$ and $t \leq k+2$.

In order for equality to hold, all inequalities in the above argument should be equalities. Thus, we have $M_2(G^*) = \varphi_1(n-s, k-1)$, $r = 0$, $t = k+2$. By the induction hypothesis, $G \in \mathscr{U}^*_{n-s,k-1}$. Note that G^* has a unique vertex of degree greater than 2, and hence $G \in \mathscr{U}^*_{n,k}$.

Case 2. $n \leq 2k+2$.

By lemma 3, we can set $v \in V(C)$ with $d(v) = t \geq 3$ and $N_G(v) \cap PV(G) \neq \emptyset$. Let $u_1 \in N_G(v) \cap PV(G)$, $|N_G(v) \cap PV(G)| = r (r \geq 1)$, $N_G(v) \backslash PV(G) = \{w_1, w_2, x_1, \cdots, x_{t-r-2}\}$ with $w_1, w_2 \in V(C)$ and all $d(x_i) = d_i \geq 2$. By lemma 1, $d_i \leq 2$. Therefore $d_i = 2$.

Set $G^* = G - u_1$. Then $G^* \in \mathscr{U}_{n-1,k-1}$. Thus

$$\begin{aligned} M_2(G) &= M_2(G^*) + d_G(w_1) + d_G(w_2) + t + r - 1 + \sum_{i=1}^{t-r-2} d_i \\ &= M_2(G^*) + d_G(w_1) + d_G(w_2) + t + r - 1 + 2(t-r-2) \\ &\leq M_2(G^*) + k - t + 6 + t + r + 2t - 2r - 5 \\ &= M_2(G^*) + k + 2t - r + 1. \end{aligned}$$

If $n = 2k+2$, then $n - 1 = 2(k-1) + 3$. So

$$\begin{aligned} M_2(G) &\leq M_2(G^*) + k + 2t - r + 1 \\ &\leq \varphi_1(n-1, k-1) + k + 2t - r + 1 \\ &= \varphi_2(n,k) - 4 - 3k + k + 2t - r + 1 \\ &= \varphi_2(n,k) - 2(k+2-t) - r + 1 \\ &\leq \varphi_2(n,k). \end{aligned}$$

and the equality holds only if $M_2(G^*) = \varphi_1(n-1, k-1)$, $r = 1$ and $t = k+2$. Since $G^* \cong U^{n-1}_{k-1}$ and U^{n-1}_{k-1} having a unique vertex of degree greater than 2, we have $G \cong U^n_k$.

If $n < 2k+2$, then $n - 1 \leq 2(k-1) + 2$. Thus

$$\begin{aligned} M_2(G) &\leq M_2(G^*) + k + 2t - r + 1 \\ &\leq \varphi_2(n-1, k-1) + k + 2t - r + 1 \\ &= \varphi_2(n,k) - n - k - 2 + k + 2t - r + 1 \\ &= \varphi_2(n,k) + 2t - n - 1 - r \\ &\leq \varphi_2(n,k). \end{aligned}$$

The last inequality follows by lemma 4(ii).

Equality $M_2(G) = \varphi_2(n,k)$ implies that the equalities hold in the above inequalities. In particular, $M_2(G^*) = \varphi_2(n-1, k-1)$. By the induction hypothesis,

$G^* \cong U_{k-1}^{n-1}$. Note that U_{k-1}^{n-1} has a unique vertex of degree than 2 and $d_G(v) \geq 3$, hence $G \cong U_k^n$.

The proof of the theorem 1 is completed. □

3. The lower bound

We give the following useful lemma that will be used in the proof of our another result. Denote $\underline{\mathscr{U}_{n,k}} = \{G \in \mathscr{U}_{n,k} : M_2(G) \text{ is minimum}\}$ and

$$PN(G) = \{u \in V(G) : uv \in E(G), v \in PV(G)\}.$$

Lemma 5. If $G \in \underline{\mathscr{U}_{n,k}}$, then $d_G(u) \geq 3$ for all $u \in PN(G)$.

Proof. Assume that $P = v_0v_1 \cdots v_s$ $(s \geq 2)$ is a pendant path of G with $v_0 \in PV(G)$ and $d_G(v_s) \geq 3$. Let $w_1w_2 \in E(G)$ with $d_G(w_i) \geq 2$, $i = 1, 2$.

Let $G^* = G - \{v_{s-2}v_{s-1}, w_1w_2\} + \{w_1v_{s-2}, w_2v_0\}$. Then $G^* \in \mathscr{U}_{n,k}$. But

$$\begin{aligned} M_2(G^*) - M_2(G) &= 2d_G(w_1) + 2d_G(w_2) + d_G(v_s) - d_G(w_1)d_G(w_2) - 2d_G(v_s) - 2 \\ &= -(d_G(w_1) - 2)(d_G(w_2) - 2) + (2 - d_G(v_s)) < 0, \end{aligned}$$

a contradiction with the choice of G. □

Denote $\phi(n, k) = 4n + 3k$, where $n,\ k$ are integers with $0 \leq k \leq n - 3$.

Proof of theorem 2. It is easy to check if $G \in \mathscr{U}_{n,k}^+$, then (3) holds. Thus we need to show that if $G \in \mathscr{U}_{n,k}$, then (3) holds and the equality holds only if $G \in \mathscr{U}_{n,k}^+$.

Applying induction on k. If $k = 0$, then $G \cong C_n$. If $k = 1$, then $G \in \mathscr{U}_{n,1}^+$. Hence the result holds clearly. Therefore we assume that $k \geq 2$ and the result holds for small values of k.

Suppose that $G \in \underline{\mathscr{U}_{n,k}}$. Let $v_1 \in PV(G)$ with $uv_1 \in E(G)$. Then $d_G(u) = t \geq 3$ by lemma 5. Let $N_G(u) \cap PV(G) = \{v_1, \ldots, v_r\}$, $N_G(u) \backslash PV(G) = \{x_1, \cdots, x_{t-r}\}$. Then $t - r \geq 1$ and all $d_G(x_i) = d_i \geq 2$.

We consider the following two case.

Case 1. $d_G(u) = t \geq 4$.

In this case, we set $G^* = G - v_1$. Then $G^* \in \mathscr{U}_{n-1,k-1}$. Thus

$$\begin{aligned} M_2(G) &= M_2(G^*) + t + r - 1 + \sum_{i=1}^{t-r} d_i \\ &\geq \phi(n-1, k-1) + t + r - 1 + 2(t - r) \end{aligned}$$

$$= \phi(n,k) + 2t + (t-r) - 8$$
$$> \phi(n,k).$$

Case 2. $d_G(u) = 3$.

If $r = 1$, then $N_G(u)\backslash\{v_1\} = \{x_1, x_2\}$. Set $G^* = G - v_1$. Then $G^* \in \mathscr{U}_{n-1,k-1}$. Thus

$$M_2(G) = M_2(G^*) + 3 + d_1 + d_2 \geq \phi(n-1, k-1) + 7 = \phi(n,k),$$

and the equality holds only if $d_1 = d_2 = 2$ and $M_2(G^*) = \phi(n-1, k-1)$. By the induction hypothesis, $G^* \in \mathscr{U}^+_{n-1,k-1}$. Since $d_1 = d_2 = 2$, there is an internal path of length at least 4 connecting x_1 and x_2 in G^* and $|V(G^*)| \geq 3(k-1)+2$. Thus $n = |V(G^*)| + 1 \geq 3k$ and $G \in \mathscr{U}^+_{n,k}$.

If $r = 2$, then $N_G(u)\backslash\{v_1, v_2\} = \{x_1\}$. Let $P = u_0u_1 \cdots u_l$ $(u = u_0, x_1 = u_1)$ be an internal path of G with $d_G(u) = 3$ and $d_G(u_l) = s \geq 3$, where $l \geq 1$. Let

$$G^* = \begin{cases} G - \{v_1, v_2\} & \text{if } l = 1 \\ G - \{v_1, v_2, u_0 \cdots u_{l-1}\} & \text{if } l \geq 2 \end{cases}$$

Then $G^* \in \mathscr{U}_{n-l-1,k-1}$. If $l = 1$, then $d_1 = d(x_1) \geq 3$ and

$$\begin{aligned} M_2(G) &= M_2(G^*) + 6 + 2d_1 \\ &\geq \phi(n-2, k-1) + 2d_1 + 6 \\ &= \phi(n,k) + 2d_1 - 5 \\ &> \phi(n,k). \end{aligned}$$

If $l \geq 2$, then

$$\begin{aligned} M_2(G) &= M_2(G^*) + 4l + 4 + s \\ &\geq \phi(n-l-1, k-1) + 4l + 4 + s \\ &= \phi(n,k) + s - 3 \\ &\geq \phi(n,k). \end{aligned}$$

In order for the equality to hold, all inequalities in the above argument should be equalities. Thus we have

$$M_2(G^*) = \phi(n-l-1, k-1), l \geq 2 \text{ and } s = 3.$$

By the induction hypothesis, $G^* \in \mathscr{U}^+_{n-l-1,k-1}$ and $|V(G^*)| \geq 3(k-1)$. Thus $n = |V(G^*)| + (l+1) \geq 3k$ and $G \in \mathscr{U}^+_{n,k}$.

Hence the proof of theorem 2 is completed. □

4. Remarks

It is easy to check that $\varphi_1(n,k)$ and $\phi(n,k)$ are strictly monotone increasing in $0 \le k \le n-3$, respectively. Note that the set of all unicyclic graphs with n vertices is $\bigcup_{k=0}^{n-3} \mathscr{U}_{n,k}$. Thus, by theorems 1 and 2, U_{n-3}^n and C_n have the maximum and minimum the second Zagreb index among all unicyclic graphs with n vertices, respectively.

5. Acknowledgements

Partially supported by NSFC (No. 10571105). Partially supported by NSFC (No. 10371032).

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