

# On extremal unicyclic molecular graphs with prescribed girth and minimal Hosoya index

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Let  $G$  be an  $n$ -vertex unicyclic molecular graph and  $Z(G)$  be its Hosoya index, let  $F_n$  be the  $n$ th Fibonacci number. It is proved in this paper that if  $G$  has girth  $l$  then  $Z(G) \geq F_{l+1} + (n-l)F_l + F_{l-1}$ , with the equality holding if and only if  $G$  is isomorphic to  $S_n^l$ , the unicyclic graph obtained by pasting the unique non-1-valent vertex of the complete bipartite graph  $K_{1,n-l}$  to a vertex of an  $l$ -vertex cycle  $C_l$ . A direct consequence of this observation is that the minimum Hosoya index of  $n$ -vertex unicyclic graphs is  $2n - 2$  and the unique extremal unicyclic graph is  $S_n^3$ . The second minimal Hosoya index and the corresponding extremal unicyclic graphs are also determined.

**KEY WORDS:** Hosoya index, unicyclic molecular graph, Fibonacci number, matching

**AMS Subject Classification:** 05C90

## 1. Introduction

Hosoya index of a graph  $G$  is the total number of its matchings, where a matching of graph  $G$  is a subset of its edge-set that consists of edges without common ends [1]. If denote by  $m(G, k)$  the number of the  $k$ -matchings, matching with  $k$  edges, of graph  $G$ , then its Hosoya index  $Z(G)$  can be expressed as

$$Z(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G, k),$$

where  $n$  stands for the order, the number of vertices, of  $G$  and  $\lfloor n/2 \rfloor$  is the integer part of  $n/2$ . As a chemical descriptor of molecular structures, Hosoya index has received much attention since its first introduction by Hosoya, the readers are suggested to refer to Refs. [2–5]. Recent researches show that Hosoya index can be employed to determine the molecular structure in the so-called inverse structure-property problem [6]. In this case, molecular graphs with extremal Hosoya index are of their own importance (we remark here that for acyclic molecular graphs those that have extremal Hosoya index are one and the same

as have extremal total  $\pi$ -electron energy [4], but this is not true for cyclic graphs since  $C_n$  is the unique unicyclic graph that has maximal Hosoya index [7] but it does not has maximal total  $\pi$ -electron energy when  $n \geq 13$  [8]).

For acyclic conjugated graphs (graphs containing perfect matching), those that have extremal Hosoya index are characterized in [9,10]. Some results on the ordering of acyclic conjugated molecular graphs according to their Hosoya indices (or according to their total  $\pi$ -electron energies) are presented in [11]. Recently we characterize the acyclic graphs with maximal Hosoya index that contains no perfect matchings [12]. But for cyclic graphs, the advances on this subject are fairly few. Extremal unicyclic graphs of girth  $l$  that have minimal and second minimal Hosoya indices are characterized in this paper, where  $l \geq 3$  is any given integer. The explicit expressions of these Hosoya indices are also presented herein.

To state the main results, we define two classes of graphs at first. Let  $S_n^l$  be the unicyclic graph obtained by pasting the center of an  $(n - l + 1)$ -vertex complete bipartite graph  $K_{1,n-l}$  (or an  $(n-l+1)$ -vertex star) to an  $l$ -cycle  $C_l$  and,  $R_n^l$  can be obtained by joining an isolated vertex with an edge to the vertex labelled with number 2 of an  $S_{n-1}^l$ , refer to figure 1.

Let  $F_n$  indicate the  $n$ th Fibonacci number. Denote by  $g(G)$  the girth of graph  $G$ , namely the length of its shortest cycle. Our main results are

**Theorem 1.** Let  $G$  be a connected  $n$ -vertex unicyclic graph. If  $g(G) = l$  then  $Z(G) \geq F_{l+1} + (n - l)F_l + F_{l-1}$ , with the equality holding if and only if  $G$  is isomorphic to  $S_n^l$ .

**Theorem 2.** Let  $G$  be a connected  $n$ -vertex unicyclic graph. Then  $Z(G) \geq 2n - 2$ , with the equality holding if and only if  $G = S_n^3$ .

To our surprising, these extremal graphs are just the same as those that have minimal energy, the sum of the absolute values of the eigenvalues of the corresponding graphs.

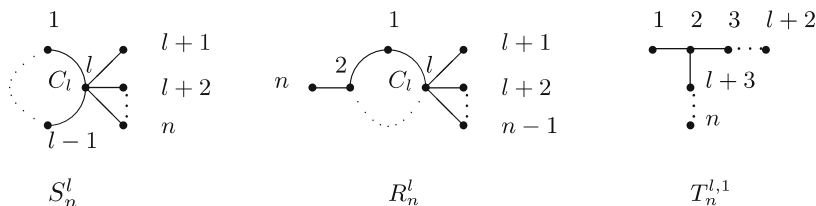


Figure 1. Three special graphs.

**Theorem 3.** Let  $G$  be a connected  $n$ -vertex unicyclic graph of girth  $l \geq 4$ . If  $G \neq S_n^l$ , then  $Z(G) \geq 2F_{l+1} + (n - l + 1)(F_l + F_{l-2})$  with equality holding if and only if  $G = R_n^l$ .

**Theorem 4.** Let  $G$  be a connected  $n$ -vertex unicyclic graph. If  $G \neq S_n^3$ , then  $Z(G) \geq 3n - 6$  with equality holding if and only if  $G = R_n^3$ .

Let  $G$  be an  $n$ -vertex graph with vertices being labeled with  $1, 2, \dots, n$  respectively, and let  $A(G)$  stand for its adjacency matrix,  $(1, 0)$ -matrix of order  $n$  with the  $(i, j)$ -entry equal to 1 if and only if vertex  $i$  is adjacent to vertex  $j$ . Name  $B(G) = A(G) + I$  the neighbor matrix of graph  $G$ , where  $I$  is the unit matrix of order  $n$ . For graph-theoretical symbols and terminologies not explicitly stated, we follow that of Ref. [13].

## 2. Minimal Hosoya index

In this section, we shall determine the minimal Hosoya indices of unicyclic graphs and characterize the corresponding extremal graphs. Before proceeding, we need some preliminaries. Denote by  $P_n$  the  $n$ -vertex path and  $S_n$  the  $n$ -vertex star (complete bipartite graph  $K_{1,n-1}$ ).

**Lemma 1** (2,9). Let  $T$  be an  $n$ -vertex tree. Then  $n = Z(S_n) \leq Z(T) \leq Z(P_n) = F_{n+1}$ ,  $Z(S_n) < Z(T)$  if and only if  $T \neq S_n$  and,  $Z(T) < Z(P_n)$  if and only if  $T \neq P_n$ .

**Lemma 2.** If  $l \geq 3$ , then  $Z(S_n^l) = F_{l+1} + (n - l)F_l + F_{l-1}$ .

*Proof.* Label the vertices of  $S_n^l$  as in figure 1. Then the neighbor matrix of  $S_n^l$  is

$$\begin{pmatrix} 1 & 1 & 0 & 0 & \dots & 0 & 0 & 0 & 1 & 0 & 0 & \dots & 0 & 0 \\ 1 & 1 & 1 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 1 & 1 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 & 1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & 1 & 1 & 0 & 0 & \dots & 0 & 0 \\ 1 & 0 & 0 & 0 & \dots & 0 & 0 & 1 & 1 & 1 & 1 & \dots & 1 & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 & 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 & 0 & 0 & \dots & 0 & 1 \end{pmatrix}_n,$$

where the  $(\overset{1,2,\dots,l}{1,2,\dots,l})$ -minor is a cyclic matrix with the first row vector equal to  $(1, 1, 0, \dots, 0, 1)$ . Expanding  $\text{Per}(B(S_n^l))$ , the permanent of  $B(S_n^l)$ , along the first  $l$  rows, we get

$$\text{Per}(B(S_n^l)) = \text{Per}(B(C_l)) \times \text{Per}(I_{n-l}) + \sum_{j=1}^{n-l} \text{Per}(M_l) \times \text{Per}(Q_{n-l}^j),$$

where  $M_l$  is the minor of  $B(S_n^l)$  formed by the first  $l$  rows, the first  $l-1$  columns and the  $(l+j)$ th column, namely

$$M_l = \begin{pmatrix} 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 \end{pmatrix}_l$$

and  $Q_{n-l}^j$  is an  $(n-l)$ -order matrix obtained by deleting the  $(j+1)$ th column of the following  $(n-l) \times (n-l+1)$  matrix.

$$\begin{pmatrix} 1 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & 1 & 0 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}.$$

Noticing that  $\text{Per}(I_{n-l}) = 1 = \text{Per}(Q_{n-l}^j)$ , we have

$$\text{Per}(B(S_n^l)) = \text{Per}(B(C_l)) + \sum_{j=l+1}^n \text{Per}(M_l). \tag{1}$$

If expanding  $\text{Per}(M_l)$  along its  $l$ th column, one gets

$$\text{Per}(M_l) = \text{Per}(B(P_{l-1})) = F_l. \tag{2}$$

On the other hand, if expanding  $\text{Per}(B(S_n^l))$  according to its definition, one can get

$$\text{Per}(B(S_n^l)) = \sum_{\sigma} b_{1,\sigma(1)} \cdots b_{n,\sigma(n)},$$

where  $\sigma$  goes over the symmetric group of order  $n$ . In above formula, term  $b_{1,\sigma(1)} \dots b_{n,\sigma(n)} = 0$  if and only if either vertex  $i$  is not adjacent to vertex  $\sigma(i)$  for some  $i \neq \sigma(i)$  or,  $\sigma$  contains a cycle with length more than 2 but not equal to  $l$  since graph  $S_n^l$  contains unique cycle which has length  $l$ . And so every term of  $\text{Per}(B(S_n^l))$  corresponds to a matching of  $S_n^l$  and vice versa, with only two exceptions in which  $\sigma$  has a cycle of length  $l$ . Consequently,

$$Z(S_n^l) = \text{Per}(B(S_n^l)) - 2. \tag{3}$$

Similarly,

$$Z(C_l) = \text{Per}(B(C_l)) - 2. \tag{4}$$

Let  $e = uv$  be an edge of  $C_l$ . Then  $m(C_l, k) = m(C_l - e, k) + m(C_l - \{u, v\}, k - 1)$  when  $k \geq 1$ , it follows from lemma 1 that

$$Z(C_l) = Z(P_l) + Z(P_{l-2}) = F_{l+1} + F_{l-1}. \tag{5}$$

Now, lemma 2 follows from the combination of formulas (1)–(5). □

**Lemma 3.** Let  $T$  be an  $n$ -vertex unicyclic graph of girth  $l$ . Then  $Z(T) \geq Z(S_n^l)$ , the equality holds if and only if  $T$  is isomorphic to  $S_n^l$ .

*proof.* The lemma is evidently true when  $l = n$ , so we assume  $l < n$  in what follows and let  $x$  be a one-degree (one-valent) vertex of  $S_n^l$  and  $y$  its maximum degree vertex. When  $k \geq 1$ , we have

$$m(S_n^l, k) = m(S_n^l - xy, k) + m(S_n^l - \{x, y\}, k - 1) = m(S_{n-1}^l, k) + m(P_{l-1}, k - 1).$$

And so,

$$Z(S_n^l) = Z(S_{n-1}^l) + F_l. \tag{6}$$

Let  $C_l$  be the unique cycle of  $T$ . If  $T$  contains a one-degree vertex  $u$  at distance at least 2 from its nearest vertex in  $C_l$ , let  $v$  be the unique neighbor of  $u$ , then  $m(T, k) = m(T - uv, k) + m(T - \{u, v\}, k - 1)$  when  $k \geq 1$ , and so  $Z(T) = Z(T - uv) + Z(T - \{u, v\})$ . Since  $P_{l-1}$  is a proper subgraph of  $T - \{u, v\}$  and  $T - \{u, v\}$  has more edges than  $P_{l-1}$ , it follows that  $Z(T - \{u, v\}) > F_l$ , and that  $Z(T - uv) \geq Z(S_{n-1}^l)$  by induction on  $n$ . Lemma 3 follows from (6) in this case. On the other hand, if every one-degree vertex of  $T$  is at distance 1 from their nearest vertex of  $C_l$  but  $C_l$  contains at least two vertices  $u$  and  $w$  of degree at least 3, let  $v$  be a one-degree vertex of  $T$  and  $u$  be its neighbor, then the last two equalities hold still. Consequently, lemma 3 follows in either case. □

*Proof of theorems 1 and 2.* Theorem 1 follows directly from the combination of lemmas 2 and 3. When  $l \geq 4$ , by lemma 2 we have,

$$\begin{aligned} Z(S_n^l) &= F_{l+1} + (n - l)F_l + F_{l-1} = F_l + F_{l-1} + (n - l)F_l + F_{l-1} \\ &> F_l + (n - l + 1)F_{l-1} + F_{l-2} = Z(S_n^{l-1}) > \dots > Z(S_n^3) \\ &= F_4 + (n - 3)F_3 + F_2 = 2n - 2. \end{aligned}$$

Theorem 2 follows. □

### 3. Second minimal Hosoya index

Let  $G$  and  $T$  be two graphs of the same order. If  $m(G, k) \leq m(T, k)$  for every nonnegative integer  $k$ , graph  $G$  is called  $m$ -smaller than  $T$ , written as  $G \preceq T$  or  $T \succeq G$  [11,14].

**Lemma 4** [15]. Let  $P_n$  be a path of order  $n = 4s + r$ , where  $s$  and  $r$  are two integers with  $0 \leq r \leq 3$ . Then

$$\begin{aligned} P_n &\succeq P_2 \cup P_{n-2} \succeq P_4 \cup P_{n-4} \succeq \dots \succeq P_{2s} \cup P_{2s+r} \succeq P_{2s+1} \cup P_{2s+r-1} \\ &\succeq P_{2s-1} \cup P_{2s+r+1} \succeq \dots \succeq P_3 \cup P_{n-3} \succeq P_1 \cup P_{n-1}. \end{aligned}$$

Let  $T_n^{1,l}$  be a tree obtained by joining an isolated vertex with an edge to the  $(l + 1)$ th vertex (according to its natural labeling) of an  $(n - 1)$ -vertex path, where  $l \leq n/2 - 1$ , refer to figure 1. It is worth noting that  $T_n^{1,0}$  is the  $n$ -vertex path  $P_n$ .

**Lemma 5.** If  $l \neq 1$ , then  $Z(T_n^{1,l}) > Z(T_n^{1,1})$ .

*Proof.* Let  $u$  be the vertex of  $T_n^{1,l}$  labeled with number 1 in figure 1 and  $v$  be its neighbor. Then  $l$ -matchings of  $T_n^{1,l}$  are partitioned into two different classes according to whether it covers vertex  $u$  or not, and so

$$m(T_n^{1,l}, k) = m(P_{n-1}, k) + m(P_l \cup P_{n-l-2}, k - 1).$$

When  $l = 0$ , we have  $m(P_{n-l-2}, 1) - m(P_{n-3}, 1) = (n - 3) - (n - 4) = 1 > 0$ , and so  $m(T_n^{1,0}, 2) > m(T_n^{1,1}, 2)$ . From lemma 4 it follows that  $Z(T_n^{1,0}) > Z(T_n^{1,1})$ . To confirm the lemma, since  $m(P_1 \cup P_{n-3}, 2) = m(P_{n-3}, 2)$ , by lemma 4 it suffices to show that  $m(P_l \cup P_{n-l-2}, 2) > m(P_{n-3}, 2)$  when  $l \geq 2$ . When  $l = 2$ , with a well-known result [16, p. 2] that  $m(P_n, k) = \binom{n-k}{k}$  we have

$$\begin{aligned} m(P_l \cup P_{n-l-2}, 2) - m(P_{n-3}, 2) &= m(P_2 \cup P_{n-4}, 2) - m(P_{n-3}, 2) \\ &= \binom{n-5}{1} + \binom{n-6}{2} - \binom{n-5}{2} = 1 > 0, \end{aligned} \tag{7}$$

when  $3 \leq l \leq n - 3$ , we have

$$\begin{aligned}
 & m(P_l \cup P_{n-l-2}, 2) - m(P_{n-3}, 2) \\
 &= \binom{l-2}{2} + \binom{l-1}{1} \binom{n-l-3}{1} + \binom{n-l-4}{2} - \binom{n-5}{2} \\
 &= 1 > 0.
 \end{aligned}
 \tag{8}$$

Lemma 5 follows from the combination of (7) and (8). □

Let  $R_n^l$  stand for the unicyclic graph obtained by joining an isolated vertex with an edge to the vertex of  $S_{n-1}^l$  labeled with number 2, refer to figure 1. In what follows we shall prove that among unicyclic graphs of girth  $l \geq 4$ ,  $R_n^l$  is the unique extremal graph that has second minimal Hosoya index.

**Lemma 6.** Let  $G$  be an  $n$ -vertex unicyclic graph of girth  $l \geq 4$ . If  $G \neq S_n^l$ , then  $Z(G) \geq Z(R_n^l)$ , with the equality holding if and only if  $G = R_n^l$ .

*Proof.* The lemma is evidently true when  $l \geq n - 1$  since  $R_n^l = S_n^l$  in this case, and so we assume  $l \leq n - 2$  in what follows. Now  $G$  contains  $n - l \geq 2$  vertices outside its unique cycle  $C_l$ . For two vertices  $a$  and  $b$  of  $G$ , we define the distance  $d(a, b)$  between  $a$  and  $b$  to be the length of a shortest path of  $G$  from  $a$  to  $b$  and, the distance  $d(a, C_l)$  between a vertex  $a \notin V(C_l)$  and  $C_l$  to be  $\min\{d(a, c) : c \in V(C_l)\}$ . Let  $u$  be a one-degree vertex of  $G$  that is at furthest distance from  $C_l$  and  $v$  be its unique neighbor.

If the distance  $d(u, C_l) \geq 2$ , then  $G - \{u, v\}$  contains  $C_l$  as its subgraph. On the one hand, since  $C_l$  contains  $P_l$  as its proper subgraph and  $C_l$  contains more edge than  $P_l$ , it follows that  $Z(C_l) > Z(P_l)$ . On the other hand, when  $k \geq 1$  we have  $m(S_{n-1}^l, k) + m(P_l, k - 1) = m(R_n^l, k)$ , and so  $Z(R_n^l) = Z(S_{n-1}^l) + Z(P_l)$ . Therefore

$$\begin{aligned}
 Z(G) &= \sum_{k=1}^{\lfloor n/2 \rfloor} m(G, k) + 1 = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G - u, k) + \sum_{k=1}^{\lfloor n/2 \rfloor} m(G - \{u, v\}, k - 1) \\
 &\geq Z(S_{n-1}^l) + Z(C_l) > Z(S_{n-1}^l) + Z(P_l) = Z(R_n^l).
 \end{aligned}$$

If  $d(u, C_l) = 1$ , then  $v \in V(C_l)$  and  $C_l$  contains another vertex  $x$  of degree at least 3 ( this vertex  $x$  is different from vertex  $v$  ) since  $G \neq S_n^l$ . Assume that  $v$  has maximal degree in  $G$ . In this case,  $G - \{u, v\}$  contains a  $T_l^{1,s}$  as its subgraph and, if  $G \neq R_n^l$  then the component  $M$  of  $G - \{u, v\}$  that contains at least two vertices is not isomorphic to  $T_l^{1,1}$ . It follows from lemma 5 that  $Z(M) > Z(T_l^{1,1})$ .

And so,

$$\begin{aligned} Z(G) &= \sum_{k=1}^{\lfloor n/2 \rfloor} m(G, k) + 1 = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G - u, k) + \sum_{k=1}^{\lfloor n/2 \rfloor} m(G - \{u, v\}, k - 1) \\ &\geq \sum_{k=0}^{\lfloor n/2 \rfloor} m(R_{n-1}^l, k) + \sum_{k=1}^{\lfloor n/2 \rfloor} m(M, k - 1) = Z(R_{n-1}^l) + Z(M) \\ &> Z(R_{n-1}^l) + Z(T_l^{1,1}) = Z(R_n^l). \end{aligned}$$

Consequently, lemma 6 follows in either case. □

**Lemma 7.** If  $n \geq 4$ , then  $Z(R_n^l) = 2F_{l+1} + (n - l + 1)(F_l + F_{l-2})$ .

*Proof.* Labeling  $R_n^l$  just as in figure 1 and expanding  $\text{Per}(B(R_n^l))$  along its first  $l$  rows, we get

$$\text{Per}(B(S_n^l)) = \text{Per}(B(C_l)) + \sum_{j=1}^{n-l-1} \text{Per}(M_j) + \text{Per}(L_l) + (n - l - 1)\text{Per}(N_l), \tag{9}$$

where  $M_l$  is the same  $l$ -order matrix as stated in proof of lemma 2;  $L_l$  is the  $\binom{1,2,\dots,l-1,l}{1,3,4,\dots,l,n}$ -minor of  $B(R_n^l)$ ;  $N_l$  is the  $\binom{1,2,3,\dots,l-1,l}{1,3,4,\dots,l-1,l+1,n}$ -minor of  $B(R_n^l)$ . If expand  $\text{Per}(L_l)$  along its  $l$ th column, one gets

$$\text{Per}(L_l) = F_{l-1} + F_{l-2}, \tag{10}$$

similarly, if expand  $\text{Per}(N_l)$  along its first,  $(l - 1)$ th and  $l$ th columns, one gets

$$\text{Per}(N_l) = \text{Per}(B(P_{l-3})) = F_{l-2}. \tag{11}$$

Combining formula (2), (4), (5), (9) – (11) and recalling that  $Z(G) = \text{Per}(B(G)) - 2$  holds for every unicyclic graph, we finish our proof of lemma 7. □

*Proof of theorem 3.* The theorem follows directly from the combination of lemmas 6 and 7. □

*Proof of theorem 4.* It is not difficult to show that  $Z(R_n^3) = 3n - 6$ . By theorem 3, it suffices to show that  $Z(R_n^l) > Z(R_n^3)$  when  $l \geq 4$  and that  $Z(G) > Z(R_n^3)$  when  $G$  has girth 3 but it is not isomorphic to  $R_n^3$ . Let  $u_i$  stand for the vertex of  $R_n^l$  labeled with number  $i$ . When  $k \geq 1$ , since

$$\begin{aligned} m(R_n^l, k) &= m(R_n^l - u_n, k) + m(R_n^l - \{u_n, u_2\}, k - 1) \\ &= m(S_{n-1}^l, k) + m(R_n^l - \{u_n, u_2\}, k - 1) \end{aligned}$$



and further by lemma 1  $Z(R_n^l - \{u_n, u_2\}) > Z(S_{n-2})$  when  $l \geq 4$ , according to theorem 2 we have

$$\begin{aligned} Z(R_n^l) &= \sum_{k=1}^{\lfloor n/2 \rfloor} m(R_n^l, k) + 1 = \sum_{k=0}^{\lfloor n/2 \rfloor} m(S_{n-1}^l, k) + \sum_{k=1}^{\lfloor n/2 \rfloor} m(R_n^l - \{u_n, u_2\}, k - 1) \\ &= Z(S_{n-1}^l) + Z(R_n^l - \{u_n, u_2\}) > Z(S_{n-1}^3) + Z(S_{n-2}) = Z(R_n^3). \end{aligned}$$

When  $G$  has girth 3 but it is not isomorphic to  $R_n^3$ , let  $u$  be a vertex of  $G$  that is at farthest distance from  $C$ , we discuss this case in two different subcases:  $d(u, C) \geq 2$  and  $d(u, C) = 1$ .

Subcase 1  $d(u, C) \geq 2$ . Clearly,  $u$  has unique neighbor in  $G$ , denote it by  $v$ . Noting that  $Z(R_n^3) = \sum_{k=1}^{\lfloor n/2 \rfloor} m(R_n^3, k) + 1 = \sum_{k=0}^{\lfloor n/2 \rfloor} m(R_n^3 - u_{n-1}, k) + \sum_{k=1}^{\lfloor n/2 \rfloor} m(R_n^3 - \{u_3, u_{n-1}\}, k - 1) = Z(R_{n-1}^3) + Z(P_3)$  and that  $G - \{u, v\}$  contains  $C_3 \supset P_3$ , we have

$$\begin{aligned} Z(G) &= \sum_{k=1}^{\lfloor n/2 \rfloor} m(G, k) + 1 = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G - u, k) + \sum_{k=1}^{\lfloor n/2 \rfloor} m(G - \{u, v\}, k - 1) \\ &> Z(R_{n-1}^3) + Z(P_3) = Z(R_n^3). \end{aligned}$$

Subcase 2  $d(u, C) = 1$ . Let  $v$  be a vertex of  $C$  and  $u$  be one of its neighbor with degree 1. Since  $G \neq S_n^3$ , either every vertex of  $C$  has degree at least 3 or  $C$  contains exactly two vertices of degree more than 2 and each of these two vertices has degree at least 4, it follows that  $G - \{u, v\}$  contains  $P_4$  as its subgraph in the first case and  $K_{1,3}$  in the second case. Therefore,

$$\begin{aligned} Z(G) &= \sum_{k=1}^{\lfloor n/2 \rfloor} m(G, k) + 1 = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G - u, k) + \sum_{k=1}^{\lfloor n/2 \rfloor} m(G - \{u, v\}, k - 1) \\ &\geq Z(R_{n-1}^3) + \min\{Z(P_4), Z(K_{1,3})\} > Z(R_{n-1}^3) + Z(P_3) = Z(R_n^3). \end{aligned}$$

Theorem 4 follows. □

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