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The smallest Hosoya index of unicyclic graphs with given diameter*

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Abstract. The Hosoya index of a (molecular) graph is defined as the total number of the matchings, including the empty edge set, of this graph. Let $\mathcal{U}_{n,d}$ be the set of connected unicyclic (molecular) graphs of order n with diameter d. In this paper we completely characterize the graphs from $\mathcal{U}_{n,d}$ minimizing the Hosoya index and determine the values of corresponding indices. Moreover, the third smallest Hosoya index of unicyclic graphs is determined.

AMS subject classifications: 05C90

Key words: Hosoya index, unicyclic (molecular) graph, diameter

1. Introduction

The Hosoya index of a graph G, denoted by $z(G)$, is a well-known topological index in combinatorial chemistry. For a graph G, $z(G)$ is defined as the total number of the matchings (independent edge subsets), including the empty edge set, of the graph. If we denote by $m(G,k)$ the number of $k-$matchings, matching with k edges, of the graph G, then $z(G)$ can also be written as

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

where n is the order of G and $\lfloor \frac{n}{2} \rfloor$ is the integer part of $\frac{n}{2}$. Other topological indices of graphs can be seen in [6, 5].

The Hosoya index was introduced by Hosoya [8] in 1971. It has received much attention since its first introduction (see [2, 15, 4, 12]). Moreover, it plays an important role in studying the relation between a molecular structure and physical and chemical properties of certain hydrocarbon compounds. For example, it was shown [6] that a nearly linear correlation exists between the logarithm of $z(G)$ and the boiling points of saturated hydrocarbon represented by the graph G. More precisely, a better reproduction of boiling points was given in [6] by the formula $(a \ln z + b)n^{-\frac{1}{2}} + c$, where a, b, c are empirical parameters.

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It is significant to determine the extremal (maximal or minimal) graphs with respect to the Hosoya index. By now, many nice results can be found in [2, 15, 4, 12, 11, 6, 10, 3, 13, 18, 16, 17] concerning the extremal graphs with respect to the Hosoya index. For example, trees [15], unicyclic graphs [4, 13, 18], bicyclic graphs [2, 3, 17] and so on, are of major interest. Especially, Wagner [15] characterizes the trees with the given maximum degree maximizing the Hosoya index. Deng et al. [4] determine all the extremal (maximal and minimal) unicyclic graphs with respect to the Hosoya index. Deng [2, 3] characterizes the extremal (maximal and minimal) bicyclic graphs with respect to Hosoya index. Xu and Xu [18] characterize all the unicyclic graphs of order n and with given maximum degree Δ maximizing the Hosoya index. Very recently, the present author [16] has determined the smallest and the largest Hosoya indices of graphs with a given clique number.

All graphs considered in this paper are finite and simple. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For a subset W of $V(G)$, let $G-W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, for a subset E' of $E(G)$, by $G-E'$ we denote the subgraph of G obtained by deleting the edges of E'. If $W=\{v\}$ and $E'=\{xy\}$, the subgraphs $G-W$ and $G-E'$ will be written as $G-v$ and $G-xy$ for short, respectively. For any two nonadjacent vertices x and y of a graph G, $G+xy$ denotes the graph obtained from G by adding an edge xy. For a vertex $v \in V(G)$, we denote by $N_G(v)$ the neighbors of v in G. $d_G(v)=|N_G(v)|$ is called the degree of v in G. For a vertex v of graph G, if $d_G(v)=1$ and $uv \in E(G)$, then v is called a pendant vertex, and $e=uv$ is called a pendant edge. In the following, by P_n, C_n and S_n we always denote the path, the cycle and the star with n vertices, respectively. For undefined notations and terminology from graph theory, the readers are referred to [1].

Let $\mathcal{U}_{n,d}$ be the set of connected unicyclic graphs of order n with diameter d. Denote by $\mathcal{U}(n)$ the set of connected unicyclic graphs of order n. In Section 2, we list or prove some lemmas which will be used in the proofs. In Section 3, we characterize the graphs $\mathcal{U}_{n,d}$ with the smallest Hosoya index and determine the corresponding Hosoya indices. The graph from $\mathcal{U}(n)$ with the third smallest Hosoya index is also determined in this section.

2. Some lemmas

To obtain our main results, we first introduce some new definitions and list or prove some lemmas as necessary preliminaries.

Lemma 1 (see [12, 6]). *Let G be a graph.*

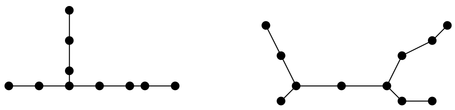
(1) *If $v \in V(G)$, then we have $z(G)=z(G-v)+\sum_{w\in N_G(v)} z(G-\{w,v\})$;*

(2) *If $uv \in E(G)$, then we have $z(G)=z(G-uv)+z(G-\{u,v\})$;*

(3) *If $G_1, G_2, \cdots, G_t$ are all the components of G, then we have $z(G)=\prod_{k=1}^{t} z(G_k)$.*

Lemma 2 (see [12, 6]). *Let F_n be the $n-th$ Fibonacci number, that is, $F_0 = 0$, $F_1 = F_2 = 1$, and $F_n = F_{n-1} + F_{n-2}$ for $n \geq 3$. Then we have $z(P_n) = F_{n+1}$ and $z(S_n) = n$.*

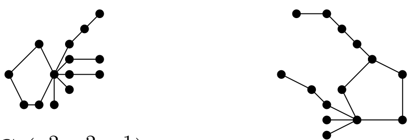
A tree is called a d-pode (see [15]) if it contains only one vertex v of degree $d > 2$. v is called the *center*. Denote by $R(c_1, c_2, \cdots, c_d)$ the d-pode where $\sum_{k=1}^{d} c_k = n-1$, c_i is the length of the $i-$th "ray" going out from the center. That is to say, $R(c_1, c_2, \cdots, c_d) - v = \bigcup_{k=1}^{d} P_{c_k}$. Especially, the tree $R(c_1, c_2, c_3)$ will be written as $T(c_1, c_2, c_3)$ in the following. If we attach two paths of length b_3 and b_4 to one pendant vertex of the path P_{a+1} in $T(a, b_1, b_2)$, the obtained tree will be denoted by $H(a+1; b_1, b_2; b_3, b_4)$. Graphs $T(2, 3, 4)$ and $H(3; 2, 1; 2, 3)$ are shown as two examples in Fig. 1.



$T(2,3,4)$ $H(3;2,1;2,3)$

Figure 1: *Graphs $T(2, 3, 4)$ and $H(3; 2, 1; 2, 3)$*

For some positive integers $k_1 \leq k_2 \leq \cdots \leq k_m$ we denote by $C_k(k_1^{l_1}, k_2^{l_2}, \cdots, k_m^{l_m})$ a graph obtained by attaching $l_1, l_2, \cdots, l_m$ paths of length $k_1, k_2, \cdots, k_m$, respectively, to one vertex of C_k. Let $C_k^{(l)}(k_1^{l_1}, k_2^{l_2}, \cdots, k_m^{l_m}; p_1^{q_1}, p_2^{q_2}, \cdots, p_t^{q_t})$ be a graph obtained by attaching l_1 paths of length k_1, l_2 paths of length k_2, $\cdots$, l_m paths of length k_m to a vertex, say v_0, of C_k and attaching q_1 paths of length p_1, q_2 paths of length p_2, $\cdots$, q_t paths of length p_t to another vertex in C_k at distance l from v_0. For example, the graphs $C_5(1^2, 2^2, 3^1)$ and $C_5^{(2)}(1^2, 3^1; 4^1)$ are shown in Fig. 2.



$C_5(1^2, 2^2, 3^1)$ $C_5^{(2)}(1^2, 3^1; 4^1)$

Figure 2: *The graphs $C_5(1^2, 2^2, 3^1)$ and $C_5^{(2)}(1^2, 3^1; 4^1)$*

Lemma 3 (see [15]). *Let $G \neq K_1$ be a connected graph, $v \in V(G)$. $G(k, n-1-k)$ is the graph resulting from attaching at v two paths of length k and $n-1-k$,* *respectively. Let* $n = 4m + j$*, where* $j \in \{1, 2, 3, 4\}$ *and* $m \geq 0$*. Then*

$$\begin{aligned} z(G(1, n-2)) &< z(G(3, n-4)) < \cdots < z(G(2m+2l-1, n-2m-2l)) \\ &< z(G(2m, n-1-2m)) < \cdots < z(G(2, n-3)) \\ &< z(G(0, n-1)), \end{aligned}$$

where $l = \lfloor \frac{j-1}{2} \rfloor$*, and* $G(0, n-1)$ *can also be viewed as a graph obtained by attaching at* $v \in V(G)$ *a path of length* $n-1$*.*

Lemma 4 (see [2])**.** *Let* $P = u_0u_1u_2\cdots u_tu_{t+1}$ *be a path or a cycle (if* $u_0 = u_{t+1}$*) in a graph* G*, where the degrees of* $u_1, u_2, \cdots u_t$ *in* G *are 2,* $t \geq 1$*.* G_1 *denotes the graph that results from identifying* $u_r (0 \leq r \leq t)$ *with the vertex* v_k *of a simple path* $v_1v_2\cdots v_k$*,* $G_2 = G_1 - u_ru_{r+1} + u_{r+1}v_1$ *(see Fig. 3). Then we have* $z(G_1) < z(G_2)$*.*

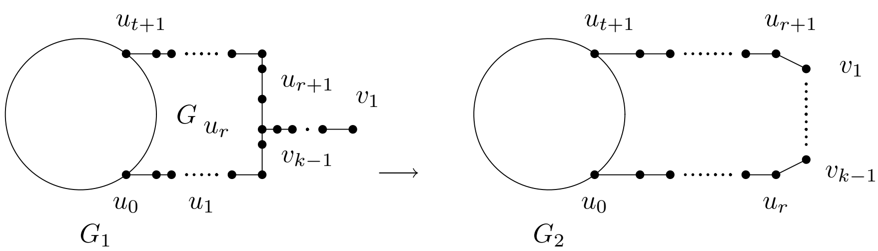


Figure 3: *Graphs in Lemma 4*

Lemma 5 (see [4])**.** $F_n = F_kF_{n-k+1} + F_{k-1}F_{n-k}$ *for* $1 \leq k \leq n$*.*

The following lemma is important and useful to continue the next proofs.

Lemma 6 (see [9])**.** *Let* $n = 4s + r$*, where* n, s *and* r *are nonnegative integers with* $0 \leq r \leq 3$*.*

(1) If $r \in \{0, 1\}$*, then*

$$\begin{aligned} F_1F_{n+1} &> F_3F_{n-1} > F_5F_{n-3} > \cdots F_{2s+1}F_{2s+r+1} > F_{2s}F_{2s+r+2} \\ &> F_{2s-2}F_{2s+r+4} > \cdots > F_4F_{n-2} > F_2F_n; \end{aligned}$$

(2) If $r \in \{2, 3\}$*, then*

$$\begin{aligned} F_1F_{n+1} &> F_3F_{n-1} > F_5F_{n-3} > \cdots F_{2s+1}F_{2s+r+1} > F_{2s+2}F_{2s+r} \\ &> F_{2s}F_{2s+r+2} > \cdots > F_4F_{n-2} > F_2F_n. \end{aligned}$$

From Lemma 6, it is not difficult to deduce the following result.

Corollary 1. *The sequence* $\{F_kF_{n-k}\}$ *reaches its minimum at* $k = 2$ *or* $k = n - 2$*.*

Lemma 7 (see [18]). *For two positive integers k and m, we have*

$$F_kF_m - F_{k-1}F_{m+1} = \begin{cases} (-1)^{k-1}F_{m-k+1} & if \quad k \le m; \\ (-1)^{m-1}F_{k-m-1} & if \quad k > m. \end{cases}$$

Corollary 2. *For a positive integer k, we have $F_k^2 - F_{k-1}F_{k+1} = (-1)^{k-1}$.*

If positive integers b_1, b_2, b_3, b_4 are fixed and $a > 2$ is an integer, the Hosoya index $z(H(a; b_1, b_2; b_3, b_4))$ will be written as z_a for short.

Lemma 8 (see [15]). *For four given positive integers b_1, b_2, b_3, b_4 and an integer $a > 2$, we have $z_a = z_{a-1} + z_{a-2}$.*

Corollary 3. *For every integer $n > 2$, we have $z_n = F_{n-1}z_2 + F_{n-2}z_1$.*

Proof. First we prove an equality below analogously to that in Lemma 6.

$$z_n = F_kz_{n-k+1} + F_{k-1}z_{n-k} \quad (*)$$

We prove equality $(*)$ by induction on k.

From Lemma 8, we have $z_n = F_2z_{n-1} + F_1z_{n-2}$, which means that equality $(*)$ holds for $k = 2$.

Assume that $z_n = F_{k-1}z_{n-k+2} + F_{k-2}z_{n-k+1}$. Then, by Lemma 8, we have

$$\begin{aligned} z_n &= F_{k-1}(z_{n-k+1} + z_{n-k}) + F_{k-2}z_{n-k+1} \\ &= (F_{k-1} + F_{k-2})z_{n-k+1} + F_{k-1}z_{n-k} \\ &= F_kz_{n-k+1} + F_{k-1}z_{n-k}. \end{aligned}$$

Thus equality $(*)$ holds immediately. By choosing $k = n - 1$ in equality $(*)$, the result in this lemma is obtained. □

Lemma 9 (see [10]). *Let H, X, Y be three connected, pairwise disjoint graphs. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u', and G_2^* be the graph obtained from H, X, Y by identifying vertices u, u', v' as shown in Fig. 4. Then we have*

$$z(G_1^*) < z(G) \quad or \quad z(G_2^*) < z(G).$$

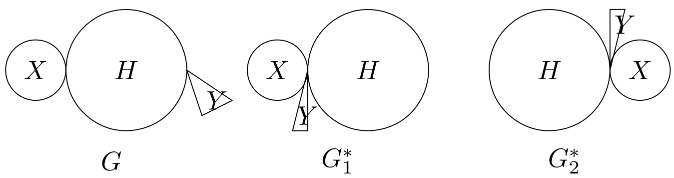


Figure 4: *Graphs G, G_1^* and G_2^* in Lemma 9*

If H_1, H_2 are two graphs with $V(H_1) \bigcap V(H_2) = \{v\}$, then $G = H_1vH_2$ is defined as a new graph with $V(G) = V(H_1) \bigcup V(H_2)$ and $E(G) = E(H_1) \bigcup E(H_2)$.

Lemma 10 (see [11]). *Let H be a graph and T_l a tree of order $l \geq 2$ with $V(H) \bigcap V(T_l) = \{v\}$. Then we have $z(HvT_l) \geq z(HvS_l)$. And the equality holds if and only if $HvT_l \cong HvS_l$, where v is identified with the center of the star S_l in HvS_l.*

Lemma 11 (see [17]). *Let G_1 and G_2 be two graphs and v_i a vertex of G_i for $i = 1, 2$. If both $z(G_1) \leq z(G_2)$ and $z(G_1 - v_1) \leq z(G_2 - v_2)$, and at least one of the inequalities is strict, then we have $z(G_1v_1T_l) < z(G_2v_2T_l)$, where T_l is a tree of order $l \geq 2$ and there is a vertex v in T_l such that v is identified with the vertex v_1 in G_1 when $G_1v_1T_l$ is formed, and with v_2 in G_2 when $G_2v_2T_l$ is formed.*

Corollary 4. *Let G be a graph and v_1, v_2 two vertices of G such that $z(G - v_1) < z(G - v_2)$. Suppose that T_l is a tree of order $l \geq 2$ and v_1, v_2 in T_l represent the same vertex in it. Then we have $z(Gv_1T_l) < z(Gv_2T_l)$.*

In the following lemma the values of the Hosoya indices of the two graphs defined above are determined.

Lemma 12.

$$\begin{aligned} z(T(a,b,c)) &= F_{a+c+2}F_{b+1} + F_{a+1}F_{c+1}F_b, \\ z(C_{2k}^{(k)}(1^l, m^1; h^1)) &= F_{h+1}F_{2k+m+1} + F_hF_kF_{k+m+1} \\ &\quad + F_{m+1}[F_{h+1}(lF_{2k} + F_{2k-1}) + F_hF_k(lF_k + F_{k-1})]. \end{aligned}$$

Proof. Using Lemma 1 (1) to the unique vertex of degree 3 in graph $T(a,b,c)$, and from Lemma 1 (3) and Lemmas 2, 5, we have

$$\begin{aligned} z(T(a,b,c)) &= F_{a+1}F_{b+1}F_{c+1} + F_aF_{b+1}F_{c+1} + F_{a+1}F_bF_{c+1} + F_{a+1}F_{b+1}F_c \\ &= F_{a+2}F_{b+1}F_{c+1} + F_{a+1}F_bF_{c+1} + F_{a+1}F_{b+1}F_c \\ &= F_{a+c+2}F_{b+1} + F_{a+1}F_{c+1}F_b. \end{aligned}$$

Now we start to determine the value of $z(C_{2k}^{(k)}(1^l, m^1; h^1))$. Set

$$A = z(C_{2k}^{(k)}(1^l, m^1; h^1)).$$

Considering the formula of $z(T(a,b,c))$, applying Lemma 1 (1) to the vertex of degree 1+l+2=l+3 in graph $C_{2k}^{(k)}(1^l, m^1; h^1)$, similarly we get

$$\begin{aligned} A &= z(P_m)z(T(k-1,k-1,h)) + lz(P_m)z(T(k-1,k-1,h)) \\ &\quad + z(P_{m-1})z(T(k-1,k-1,h)) + 2z(P_m)z(T(k-2,k-1,h)) \\ &= [(l+1)F_{m+1} + F_m](F_{h+1}F_{2k} + F_hF_k^2) + 2F_{m+1}(F_{h+1}F_{2k-1} + F_hF_kF_{k-1}) \\ &= F_{h+1}F_{m+1}(lF_{2k} + F_{2k+1} + F_{2k-1}) + F_mF_{h+1}F_{2k} \\ &\quad + F_hF_k[F_{m+1}((l+1)F_k + 2F_{k-1}) + F_mF_k] \\ &= F_{h+1}F_{2k+m+1} + F_{m+1}F_{h+1}(lF_{2k} + F_{2k-1}) \\ &\quad + F_hF_k[F_{m+1}(lF_k + F_{k+1} + F_{k-1}) + F_mF_k] \\ &= F_{h+1}F_{2k+m+1} + F_{m+1}F_{h+1}(lF_{2k} + F_{2k-1}) + F_hF_k[F_{m+k+1} + F_{m+1}(lF_k + F_{k-1})] \\ &= F_{h+1}F_{2k+m+1} + F_hF_kF_{k+m+1} + F_{m+1}[F_{h+1}(lF_{2k} + F_{2k-1}) + F_hF_k(lF_k + F_{k-1})]. \end{aligned}$$

Therefore the proof of this lemma is completed. □

Lemma 13 (see [14]). *Let G be a connected graph with $v_1v_2 \in E(G)$ such that $G - v_1v_2 = G_1 \bigcup G_2$ and $v_i \in V(G_i)$ for $i = 1, 2$. Denote by G' the graph obtained from G by deleting the edge v_1v_2 and identifying v_1 with v_2 to form a new vertex v and attaching a pendent vertex w to v. Then we have $z(G') < z(G)$.*

3. Main results

In this section we will determine the graphs from $\mathcal{U}_{n,d}$ minimizing the Hosoya index for all the possible values of d. If $n = 3$, there is only one unicyclic graph C_3, and so there is nothing to prove. When $n = 4$, there are exactly two connected unicyclic graphs C_4 and $C_3(1^1)$. From Lemmas 1 and 2, it is easy to find that $z(C_3(1^1)) < z(C_4)$, which finishes our proof for $n = 4$. If $d = n - 1$, there exists only one graph, i.e. a path P_n, but it does not belong to $\mathcal{U}_{n,d}$. For $d = 1$, any two vertices in a graph of this form are all adjacent, so it is the complete graph K_n, but it is not a unicyclic graph when $n > 4$. Therefore, we always assume that $n > 4$ and $1 < d < n - 1$ in the following.

For any graph $G \in \mathcal{U}_{n,d}$, a path with length d of G is called the *main path* of G, the only cycle of G is called a *unique cycle* of G. Note that the number of main paths in $G \in \mathcal{U}_{n,d}$ is possibly more than one. The following lemma presents a property of graphs from $\mathcal{U}_{n,d}$ with the smallest Hosoya index.

Lemma 14. *Suppose that $G \in \mathcal{U}_{n,d}$ has the smallest Hosoya index. Let C be a unique cycle of G. Then there exists a main path P of G such that $V(P) \bigcap V(C) \neq \Phi$.*

Proof. Let $P = v_1v_2 \cdots v_dv_{d+1}$. To the contrary, there exists a vertex $u_0 \in V(C)$ such that the vertices u_0 and v_j (where $j \in \{2, 3, \cdots, d\}$) are linked by a unique path $P_0 = u_0u_1u_2 \cdots u_{l-1}u_l$, where $u_l = v_j$. Assume that in G a subtree $T^i_{m_i}$ (with the vertex u_i included) of order m_i is attached at u_i for $i \in \{0, 1, \cdots, l-1, l\}$, and

$$\sum_{i=0}^{l} m_i = m + l.$$

Now we construct a new graph G' as shown in Fig. 5, which is obtained from G by

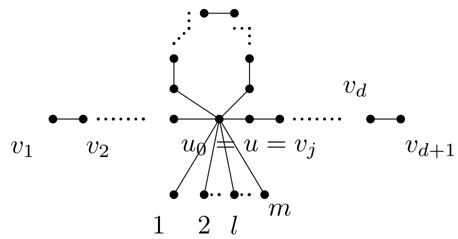


Figure 5: *Main path and unique cycle in graph G'*

replacing all subtrees $T^i_{m_i}$ by stars S_{m_i} with u_i as its center for $i \in \{0, 1, \cdots, l-1, l\}$, and then deleting all the edges $u_0u_1, \cdots, u_iu_{i+1}, \cdots, u_{l-1}u_l$ and identifying these vertices $u_0, u_1, \cdots, u_{l-1}, u_l$ to form a new vertex $u(= u_0)$ and attaching l pendant vertices to the vertex $u(= u_0)$. Note that $G' \in \mathcal{U}_{n,d}$. Applying repeatedly Lemma 13 and considering Lemma 10, we have $z(G') < z(G)$. This is a contradiction to the choice of G, which completes the proof of this lemma. □

Next we will look for the graph from $\mathcal{U}_{n,d}$ with the smallest Hosoya index. To do it, we first introduce two subsets of $\mathcal{U}_{n,d}$. Let

$$\mathcal{U}^{(1)}_{n,d} = \{G : G \in \mathcal{U}_{n,d}, \text{the main path of G and the unique cycle of G have exactly one vertex in common}\}$$

and

$$\mathcal{U}^{(2)}_{n,d} = \{G : G \in \mathcal{U}_{n,d}, \text{the main path of G and the unique cycle of G have at least two vertices in common}\}.$$

From Lemma 14, to determine the graph from $\mathcal{U}_{n,d}$ with the smallest Hosoya index, it suffices to find the graph from $\mathcal{U}^{(i)}_{n,d}$ with minimal the Hosoya index for $i = 1, 2$, respectively.

Theorem 1. *For any graph $G \in \mathcal{U}^{(1)}_{n,d}$, we have $z(G) \geq 2(n-d)F_d + 2F_{d+1}$. The equality holds if and only if $G \cong C_3(1^{n-d-2}, (d-1)^1)$.*

Proof. Suppose that $G_0 \in \mathcal{U}^{(1)}_{n,d}$ has the smallest Hosoya index. By the definition of $\mathcal{U}^{(1)}_{n,d}$, we assume that $P = v_1v_2\cdots v_dv_{d+1}$ and C_k is the main path and the unique cycle of G, respectively, and $V(P)\bigcap V(C_k) = \{v_j\}$, where $j \in \{2, 3, \cdots, d\}$.

Note that the subgraph of G_0 induced by $V(P)\bigcup V(C_k)$ is just

$$C_k((j-1)^1, (d+1-j)^1) \cong G_M.$$

Set $x = n - |V(P)\bigcup V(C_k)|$, by Lemmas 9, 10, we find that either $G_0 \cong G_Mv_jS_x$, or $G_0 \cong G_Mu_tS_x$, where $u_t \in V(C_k) \setminus \{v_j\}$.

Now we claim that $k = 3$, that is, the length of C_k in G_M is 3. Otherwise, we have $k \geq 4$. If $G_0 \cong G_Mv_jS_x$, after decreasing the length of C_k by 1 and attaching a pendant edge to vertex v_j in G_0, by Lemma 4, the obtained graph has a smaller Hosoya index than G_0. If $G_0 \cong G_Mu_tS_x$, then, similarly, G_0 can be changed into G'_0 with $z(G'_0) < z(G_0)$ by decreasing the length of C_k by 1 and attaching a pendant edge to u_t in G_0. These are two contradictions to the choice of G_0, which complete the proof of this claim.

Let

$$G_C \cong C_3((j-1)^1, (d+1-j)^1)$$

and $y = n - d - 3$. By now we have found that $G_0 \in \{G_Cv_jS_y, G_Cv_iS_y, G_Cu_tS_y\}$, where j, i are defined as above and $t \in \{1, 2\}$. Graphs $G_Cv_jS_y, G_Cv_iS_y, G_Cu_1S_y$ are shown as three examples in Fig. 6. By Lemma 9, we claim that $G_Cv_iS_y$ and $G_Cu_tS_y$ with $t = 1, 2$ cannot have the smallest Hosoya index. Thus we find that G_0 must be of the form $G_Cv_jS_y$.

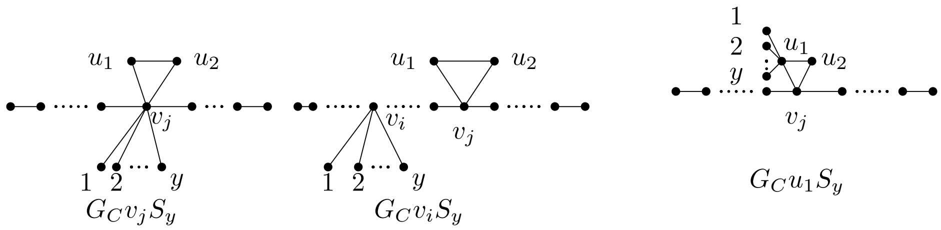


Figure 6: *Graphs $G_C v_j S_y$, $G_C v_i S_y$ and $G_C u_1 S_y$*

Note that

$$G_C v_j S_y \cong C_3(1^y, (j-1)^1, (d+1-j)^1).$$

From Lemma 3, we have

$$z(G_C v_j S_y) \geq z(C_3(1^{n-d-2}, (d-1)^1))$$

with equality holding if and only $G_C v_j S_y \cong C_3(1^{n-d-2}, (d-1)^1)$. By Lemmas 1, 2, it is not difficult to obtain

$$z(C_3(1^{n-d-2}, (d-1)^1)) = 2(n-d)F_d + 2F_{d+1},$$

which completes the proof of this theorem. □

To determine the graph from $\mathcal{U}_{n,d}^{(2)}$ with the smallest Hosoya index, we divide this set into two subsets:

$$\mathcal{U}_{n,d}^{(2)} = \mathcal{U}_{n,d}^{(2)1} \bigcup \mathcal{U}_{n,d}^{(2)2},$$

where

$$\mathcal{U}_{n,d}^{(2)1} = \{G : G \in \mathcal{U}_{n,d}^{(2)}, g(G) = 3\}$$

and

$$\mathcal{U}_{n,d}^{(2)2} = \{G : G \in \mathcal{U}_{n,d}^{(2)}, g(G) > 3\}.$$

The following theorem presents the graph from $\mathcal{U}_{n,d}^{(2)1}$ with the minimal Hosoya index.

Theorem 2. *For any graph $G \in \mathcal{U}_{n,d}^{(2)1}$, we have*

$$z(G) \geq (n-d+1)F_{d+1}.$$

The equality holds if and only if $G \cong C_3^{(1)}(1^{n-d-1}; (d-2)^1)$.

Proof. Suppose that $G_0 \in \mathcal{U}_{n,d}^{(2)1}$ has the minimal Hosoya index. Let $P = v_1 v_2 \cdots v_d v_{d+1}$ and C_k be the main path and the unique cycle of G, respectively. From the definition of the set $\mathcal{U}_{n,d}^{(2)1}$, it is easy to see that $C_k = C_3$, and there exist two vertices v_j, v_{j+1}, where $j \in \{2, 3, \cdots, d-1\}$ from $V(P)$ and another vertex, say v_0, such that $C_3 = v_j v_{j+1} v_0 v_j$. Denote by G_C the subgraph of G_0 induced by $V(P) \bigcup \{v_0\}$, that is to say,

$$G_C \cong C_3^{(1)}((j-1)^1; (d-j)^1).$$

Let $y = n - d - 2$. In a similar way to that in the proof of Theorem 1, we claim that G_0 must be of the form $G_C v_0 S_y$, or of the form $G_C v_t S_y$, where $t \in \{j, j+1\}$, or of the form $G_C v_i S_y$, where $i \in \{2, 3, \cdots, d-1\} \setminus \{j, j+1\}$.

Now we claim that G_0 is of the form $G_C v_t S_y$, where $t \in \{j, j+1\}$ or $G_C v_2 S_y$ with $j > 2$. If not, G_0 must be of the form $G_C v_0 S_y$, or of the form $G_C v_i S_y$, where $i \in \{2, 3, \cdots, d-1\} \setminus \{j, j+1\}$. If G_0 is of the form $G_C v_0 S_y$, we construct a graph G_0' by deleting the path P_j attached at v_j of G_C and attaching a path P_j to the vertex v_0. Note that $G_0' \cong G_C v_j S_y$, by Lemma 9, we have

$$z(G_0') = z(G_C v_j S_y) < z(G_C v_0 S_y),$$

this is impossible because of the minimality of $z(G_C v_0 S_y)$. If G_0 is of the form $G_C v_i S_y$, where $i \in \{2, 3, \cdots, d-1\} \setminus \{j, j+1\}$, without loss of generality, we assume that $i \in \{2, 3, \cdots, j-1\}$. From Lemmas 1, 2 and 5, we have

$$\begin{aligned} z(G_C - v_j) &= F_j F_{d+3-j}, \\ z(G_C - v_i) &= F_i z(C_3^{(1)}((j-i-1)^1, \\ (d-j)^1)) &= F_i (F_{d-i+3} + F_{j-i} F_{d-j+1}). \end{aligned}$$

When j is fixed, from Corollary 1, $z(G_C - v_i)$ reaches its minimum at $i = 2$, and its minimum is $F_{d+1} + F_{j-2} F_{d-j+1}$. Thus we have

$$\begin{aligned} z(G_C - v_i) - z(G_C - v_j) &\geq F_{d+1} + F_{j-2} F_{d-j+1} - F_j F_{d+3-j} \\ &= F_j F_{d+2-j} + F_{j-1} F_{d+1-j} + F_{j-2} F_{d-j+1} - F_j F_{d+3-j} = 0. \end{aligned}$$

By Lemma 11, we have $z(G_C v_j S_y) < z(G_C v_i S_y)$ when $i > 2$. Therefore this claim holds immediately.

Denote by $G_2^{(j)}$ the graph $G_C v_2 S_y$ with $j \geq 3$. Let G_j be the graph $G_C v_j S_y$ with $j \in \{2, 3, \cdots, d-1\}$. Applying Lemma 1 (1) to the vertex of maximum degree in G_j and $G_2^{(j)}$, respectively, by Lemmas 2, 5, we have

$$\begin{aligned} z(G_j) &= (y+1) F_j F_{d+3-j} + F_{j-1} F_{d+3-j} + F_j F_{d+2-j} + F_j F_{d+1-j} \\ &= y F_j F_{d+3-j} + 2 F_j F_{d+3-j} + F_{j-1} F_{d+3-j} \\ &= y F_j F_{d+3-j} + F_{j+2} F_{d+3-j}, \\ z(G_2^{(j)}) &= (y+2)(F_{d+1} + F_{j-2} F_{d-j+1}) + z(C_3^{(1)}((j-4)^1; (d-j)^1) \\ &= (y+2)(F_{d+1} + F_{j-2} F_{d-j+1}) + F_d + F_{j-3} F_{d-j+1}. \end{aligned}$$

Note that a simple calculation shows the validity of $z(G_2^{(j)})$ for $j = 3$ or 4. In view of Corollary 1, the minimum of $z(G_j)$ is attained at $j = 2$, and its minimum is $(y+3) F_{d+1}$. Moreover, considering $y = n - d - 2$ and $d < n - 1$, we have

$$\begin{aligned} z(G_2^{(j)}) - (y+3) F_{d+1} &= (y+2) F_{j-2} F_{d-j+1} + F_d + F_{j-3} F_{d-j+1} - F_{d+1} \\ &= (n-d) F_{j-2} F_{d-j+1} + F_{j-3} F_{d-j+1} - F_{d-1} \\ &\geq 2 F_{j-2} F_{d-j+1} + F_{j-3} F_{d-j+1} - F_{d-1} \\ &= F_j F_{d-j+1} - F_{d-1} > F_2 F_{d-1} - F_{d-1} = 0. \end{aligned}$$

Note that the last inequality holds since in $G_2^{(j)}$, $j \geq 3$. Therefore we find that each graph $G_2^{(j)}$ for $j \geq 3$ has a larger Hosoya index than G_j (which is just $G_C v_j S_y$) with $j = 2$, which has the smallest Hosoya index in the set $\{G_C v_j S_y : j = 2, 3, \cdots, d-1\}$. We have now proven that $C_3^{(1)}(1^{n-d-1}; (d-2)^1)$ from $\mathcal{U}_{n,d}^{(2)1}$ has the minimal Hosoya index $(n-d+1)F_{d+1}$, which completes the proof of this theorem. □

Let

$$\mathcal{G}_0 = \{C_{2k}^{(k)}(m^1, 1^y; h^1) : y = n-d-k, k \geq 2, m \geq 0, h \geq 0, \ and\ m+h \geq 1\}.$$

Before determining the minimal Hosoya index of graphs from $\mathcal{U}_{n,d}^{(2)2}$, we first prove the following lemma.

Lemma 15. *Suppose that $G_0 \in \mathcal{U}_{n,d}^{(2)2}$ has the minimal Hosoya index. Then $G_0 \in \mathcal{G}_0$.*

Proof. From the definition of $\mathcal{U}_{n,d}^{(2)2}$, by Lemmas 9, 10, we find that G_0 must be a graph obtained by attaching $x = n-m-l-h$ pendant edges to one of the non-pendant vertices of $C_l^{(k)}(m^1; h^1)$ with $l \geq 2k$ and $k+m+h = d$, that is, $G_0 \cong C_l^{(k)}(m^1; h^1)v_0 S_x$, where v_0 is a non-pendant vertex of $C_l^{(k)}(m^1; h^1)$.

Now we claim that in $C_l^{(k)}(m^1; h^1)v_0 S_x$, $l = 2k$. Assume that, to the contrary, $l-k+1 > k$. Considering the structure of $C_l^{(k)}(m^1, ; h^1)v_0 S_x$, after decreasing the length of path P_{l-k+1} (which is on the cycle C_l in G_0, but not on the main path of G_0) by 1 and attaching a pendant edge to one vertex of resulting path P_{l-k}, by Lemma 4, the obtained graph has a smaller Hosoya index. This is a contradiction to the choice of G_0, which completes the proof of this claim. Let $y = n-d-k$. Note that $C_{2k}^{(k)}(m^1; h^1)$ in G_0 is a graph as shown in Fig. 7. Therefore G_0 must be in the set $\mathcal{G}_0$ of the type $C_{2k}^{(k)}(m^1; h^1)v_i S_y$, where $i \in \{2, 3, \cdots, m, m+k+2, m+k+3, \cdots, d\}$, or of the type $C_{2k}^{(k)}(m^1; h^1)u_j S_y$, where $j \in \{1, 2, \cdots, k-1\}$.

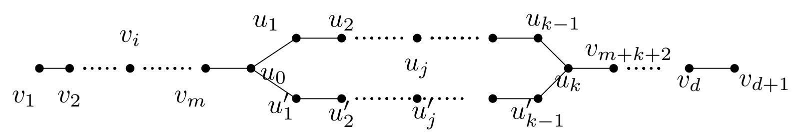


Figure 7: *The graph $C_{2k}^{(k)}(m^1; h^1)$ in G_0*

If G_0 is in the set $\mathcal{G}_0$, we are done. In the following we use G_C to denote $C_{2k}^{(k)}(m^1; h^1)$. If G_0 is of the type $C_{2k}^{(k)}(m^1; h^1)v_i S_y$, where $i \in \{2, 3, \cdots, m, m+k+2, m+k+3, \cdots, d+1\}$, without loss of generality, we assume that $G_0 \cong C_{2k}^{(k)}(m^1; h^1)v_i S_y$ with $i \in \{2, 3, \cdots, m\}$. Set $A = z(G_C - v_i) - z(G_C - u_0)$, by Lemmas 1, 2, 5 and 12, we have

$$z(G_C - u_0) = F_{m+1}(F_{2k}F_{h+1} + (F_k)^2 F_h),$$

$$\begin{aligned} z(G_C - v_i) &= F_i z(C_{2k}^{(k)}((m-i)^1; h^1)) \\ &= F_i[(F_{m-i+1} + F_{m-i})z(T(h, k-1, k-1)) \\ &\quad +2F_{m-i+1}z(T(h, k-1, k-2))] \\ &= F_i[F_{m-i+2}(F_{2k}F_{h+1} + (F_k)^2 F_h) \\ &\quad +2F_{m-i+1}(F_{2k-1}F_{h+1} + F_k F_{k-1} F_h)], \end{aligned}$$

and

$$\begin{aligned} A &= (F_i F_{m-i+2} - F_{m+1})(F_{2k}F_{h+1} + (F_k)^2 F_h) + 2F_i F_{m-i+1}(F_{2k-1}F_{h+1} + F_k F_{k-1} F_h) \\ &= 2F_i F_{m-i+1}(F_{2k-1}F_{h+1} + F_k F_{k-1} F_h) - F_{i-1}F_{m-i+1}(F_{2k}F_{h+1} + (F_k)^2 F_h) \\ &= F_{h+1}F_{m-i+1}(F_i 2F_{2k-1} - F_{i-1}F_{2k}) + F_k F_h F_{m-i+1}(F_i 2F_{k-1} - F_{i-1}F_k) > 0. \end{aligned}$$

Note that the last inequality holds since $2F_{2k-1} > F_{2k}$ and $2F_{k-1} \geq F_k$ if $k \geq 2$. By Lemma 11, we have $z(G_C u_0 S_y) < z(G_C v_i S_y)$ for $i \in \{2, 3, \cdots, m\}$. This is impossible because of the minimality of $z(G_0) = z(G_C v_i S_y)$.

Next we will prove that for any graph G' of the type $C_{2k}^{(k)}(m^1; h^1)u_j S_y$ with $j \in \{1, 2, \cdots, k-1\}$, there exists a graph $G'' \in \mathcal{G}_0$ such that $z(G'') < z(G')$. Set $j = k_1 + 1$ and $k - j = k_2 + 1$, i.e., $k_1 + k_2 = k - 2$. To do this, we distinguish the following two cases.

Case 1. k is odd.

Let $G'_C = G_C - \{v_1, v_2, \cdots, v_m\}$ and $T_{m+y}^{(0)}$ be a tree as shown in Fig. 8. Note that $G_C u_0 S_y \cong G'_C u_0 T_{m+y}^{(0)}$. By Lemma 9, we have $z(G_C u_0 S_y) < z(G_C u_j S_y)$ or $z(G'_C u_j T_{m+y}^{(0)}) < z(G_C u_j S_y)$, where $G'_C u_j T_{m+y}^{(0)}$ is a graph obtained by identifying u_j of G'_C with the vertex of maximum degree in $T_{m+y}^{(0)}$. If the former holds, we are done for this case. If not, we will compare the values of $z(G'_C u_0 T_{m+y}^{(0)})$ and

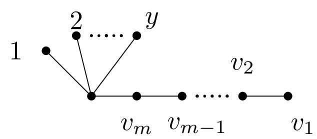


Figure 8: *The tree* $T_{m+y}^{(0)}$

$z(G'_C u_j T_{m+y}^{(0)})$. From Lemma 12, we have

$$\begin{aligned} z(G'_C - u_0) &= F_{2k}F_{h+1} + (F_k)^2 F_h, \\ z(G'_C - u_j) &= F_{h+1}F_{k+k_1+1+k_2+1} + F_h F_{k+k_1+1} F_{k_2+1} \\ &= F_{h+1}F_{2k} + F_h F_{k+k_1+1} F_{k_2+1}, \end{aligned}$$

and

$$z(G'_C - u_0) - z(G'_C - u_j) = F_h((F_k)^2 - F_{k+k_1+1}F_{k_2+1}).$$

Since k is odd and $k_1 + k_2 = k - 2$, one of k_1 and k_2 is even. If k_2 is even, From Lemma 6, we have $F_{k+k_1+1}F_{k_2+1} > (F_k)^2$, that is to say, $z(G'_C - u_0) <$

$z(G'_C - u_j)$. By Lemma 11, we have $z(G'_C u_0 T^{(0)}_{m+y}) = z(G_C u_0 S_y) < z(G'_C u_j T_{m+y})$. Therefore $z(G_C u_0 S_y) < z(G'_C u_j T^{(0)}_{m+y}) < z(G_C u_j S_y)$. When k_1 is even, similarly, $z(G_C u_k S_y) < z(G_C u_j S_y)$, which finishes the proof for this case.

Case 2. k is even.

If k_1 and k_2 are both even, we can obtain the result as desired in a way similar to that in the proof of Case 1.

So it suffices to deal with the case when k is even and k_1, k_2 are both odd. Note that $G_C - u_j$ is just $H(k+1; m, k_1; h, k_2)$. Set $z(G_C - u_j) = z_{k+1}$, $z(G_C - u_0) = z_C^{(0)}$, $z(G_C - u_k) = z_C^{(k)}$, and $B = z_{k+1} - z_C^{(0)} + z_{k+1} - z_C^{(k)}$. Note that $k_1 + k_2 = k - 2$, by Lemmas 1, 2, 5 and Corollary 3, we have

$$
\begin{aligned}
z_{k+1} &= F_k z_2 + F_{k-1} z_1 \\
&= F_k(F_{m+k_1+2}F_{h+k_2+2} + F_{m+1}F_{h+1}F_{k_1+1}F_{k_2+1}) \\
&\quad + F_{k-1}[F_{m+1}F_{h+1}F_{k_1+1}F_{k_2+1} + F_{m+1}F_{h+1}F_{k_1}F_{k_2+1} + F_{m+1}F_{h+1}F_{k_1+1}F_{k_2} \\
&\quad + (F_mF_{h+1} + F_{m+1}F_h)F_{k_1+1}F_{k_2+1}] \\
&= F_k[(F_{m+1}F_{k_1+2} + F_mF_{k_1+1})(F_{h+1}F_{k_2+2} + F_hF_{k_2+1}) + F_{m+1}F_{h+1}F_{k_1+1}F_{k_2+1}] \\
&\quad + F_{k-1}[F_{m+1}F_{h+1}F_{k_1+k_2+2} + (F_mF_{h+1} + F_{m+1}F_h)F_{k_1+1}F_{k_2+1}] \\
&= F_k[F_{m+1}F_{h+1}F_{k_1+k_2+3} + F_mF_{h+1}F_{k_1+1}F_{k_2+2} + F_{m+1}F_hF_{k_1+2}F_{k_2+1} \\
&\quad + F_mF_hF_{k_1+1}F_{k_2+1}] \\
&\quad + F_{k-1}[F_{m+1}F_{h+1}F_{k_1+k_2+2} + (F_mF_{h+1} + F_{m+1}F_h)F_{k_1+1}F_{k_2+1}] \\
&= F_{m+1}F_{h+1}F_k(F_{k+1} + F_{k-1}) + F_mF_{h+1}F_{k_1+1}(F_kF_{k_2+2} + F_{k-1}F_{k_2+1}) \\
&\quad + F_{m+1}F_hF_{k_2+1}(F_kF_{k_1+2} + F_{k-1}F_{k_1+1}) + F_mF_hF_kF_{k_1+1}F_{k_2+1} \\
&= F_{m+1}F_{h+1}F_k(F_{k+1} + F_{k-1}) + F_mF_{h+1}F_{k_1+1}F_{k+k_2+1} + F_{m+1}F_hF_{k_2+1}F_{k+k_1+1} \\
&\quad + F_mF_hF_kF_{k_1+1}F_{k_2+1}, \\
z_C^{(0)} &= F_{m+1}(F_{2k}F_{h+1} + (F_k)^2F_h), \\
z_C^{(k)} &= F_{h+1}(F_{2k}F_{m+1} + (F_k)^2F_m),
\end{aligned}
$$

and

$$
\begin{aligned}
B &= 2z_{k+1} - z_C^{(0)} - z_C^{(k)} \\
&= 2F_{m+1}F_{h+1}[F_k(F_{k+1} + F_{k-1}) - F_{2k}] + 2F_mF_{h+1}F_{k_1+1}(F_{k+1}F_{k_2+1} + F_kF_{k_2}) \\
&\quad + 2F_{m+1}F_hF_{k_2+1}(F_{k+1}F_{k_1+1} + F_kF_{k_1}) + 2F_mF_hF_kF_{k_1+1}F_{k_2+1} \\
&\quad - (F_k)^2(F_mF_{h+1} + F_{m+1}F_h) \\
&= (2F_{k+1}F_{k_1+1}F_{k_2+1} - (F_k)^2)(F_mF_{h+1} + F_{m+1}F_h) \\
&\quad + 2F_k(F_mF_{h+1}F_{k_1+1}F_{k_2} + F_{m+1}F_hF_{k_2+1}F_{k_1} + F_mF_hF_{k_1+1}F_{k_2+1}) \\
&> (2F_{k+1}F_{k_1+1}F_{k_2+1} - (F_k)^2)(F_mF_{h+1} + F_{m+1}F_h).
\end{aligned}
$$

Considering $k_1 + k_2 = k - 2$, and k_1, k_2 are both odd, and k is even (clearly, $k \geq 4$), by Lemma 6 and Corollary 2, we have

$$\begin{aligned} B &> (2F_{k-2}F_{k+1} - (F_k)^2)(F_m F_{h+1} + F_{m+1}F_h) \\ &> (F_{k-1}F_{k+1} - (F_k)^2)(F_m F_{h+1} + F_{m+1}F_h) \\ &= F_m F_{h+1} + F_{m+1}F_h > 0. \end{aligned}$$

So we have $z_{k+1} > z_C^{(0)}$, or $z_{k+1} > z_C^{(k)}$, that is, $z_C^{(0)} < z_{k+1}$, or $z_C^{(k)} < z_{k+1}$. By Lemma 11, we have $z(G_C u_0 S_y) < z(G_C u_j S_y)$ or $z(G_C u_k S_y) < z(G_C u_j S_y)$, which finishes the proof for this case since $G_C u_0 S_y$ and $G_C u_k S_y$ all belong to $\mathcal{G}_0$.

By now the proof of this lemma is completed. □

Theorem 3. *For any graph $G \in \mathcal{U}_{n,d}^{(2)2}$, we have*

$$z(G) \geq F_{d+2} + (n-d-1)F_d + (n-d+1)F_{d-2}.$$

The equality holds if and only if $G \cong C_4^{(2)}(1^{n-d-1}, (d-3)^1)$.

Proof. Suppose that $G_0 \in \mathcal{U}_{n,d}^{(2)2}$ has the minimal Hosoya index. From Lemma 15, we find that G_0 is of the form $C_{2k}^{(k)}(m^1, 1^y; h^1)$ with $y = n-d-k, k \geq 2, m \geq 0, h \geq 0$, and $m+h \geq 1$. Set $z(C_{2k}^{(k)}(m^1, 1^y; h^1)) = z^{(k)}$, $z(C_{2k-2}^{(k-1)}(m^1, 1^{y+1}; (h+1)^1)) = z^{(k-1)}$ and $\Delta = z^{(k)} - z^{(k-1)}$. From Lemma 12, for $k \geq 3$, we have

$$\begin{aligned} z^{(k)} &= F_{h+1}F_{2k+m+1} + F_h F_k F_{k+m+1} + F_{m+1}[F_{h+1}(yF_{2k} + F_{2k-1}) \\ &\quad + F_h F_k (yF_k + F_{k-1})], \\ z^{(k-1)} &= F_{h+2}F_{2k+m-1} + F_{h+1}F_{k-1}F_{k+m} \\ &\quad + F_{m+1}[F_{h+2}((y+1)F_{2k-2} + F_{2k-3}) + F_{h+1}F_{k-1}((y+1)F_{k-1} + F_{k-2})], \end{aligned}$$

and

$$\begin{aligned} \Delta &= F_{h+1}F_{2k+m+1} + F_h F_k F_{k+m+1} + F_{m+1}[F_{h+1}(yF_{2k} + F_{2k-1}) \\ &\quad + F_h F_k (yF_k + F_{k-1})] \\ &\quad - F_{h+2}F_{2k+m-1} - F_{h+1}F_{k-1}F_{k+m} \\ &\quad - F_{m+1}[F_{h+2}((y+1)F_{2k-2} + F_{2k-3}) + F_{h+1}F_{k-1}((y+1)F_{k-1} + F_{k-2})] \\ &= (F_{h+1}F_{2k+m+1} - F_{h+2}F_{2k+m-1}) + (F_h F_k F_{k+m+1} - F_{h+1}F_{k-1}F_{k+m}) \\ &\quad + F_{m+1}[y(F_{h+1}F_{2k} - F_{h+2}F_{2k-2}) + y(F_h(F_k)^2 - F_{h+1}(F_{k-1})^2) \\ &\quad + (F_{h+1}F_{2k-1} - F_{h+2}F_{2k-3}) + (F_h F_k F_{k-1} - F_{h+1}F_{k-1}F_{k-2}) \\ &\quad - (F_{h+2}F_{2k-2} + F_{h+1}(F_{k-1})^2)]. \end{aligned}$$

Set

$$\begin{aligned} A &= F_{h+1}F_{2k+m+1} - F_{h+2}F_{2k+m-1}, \\ B &= F_h F_k F_{k+m+1} - F_{h+1}F_{k-1}F_{k+m}, \\ D &= F_{h+1}F_{2k} - F_{h+2}F_{2k-2} + F_h(F_k)^2 - F_{h+1}(F_{k-1})^2, \end{aligned}$$

and

$$E = (F_{h+1}F_{2k-1} - F_{h+2}F_{2k-3}) + (F_hF_kF_{k-1} - F_{h+1}F_{k-1}F_{k-2})$$
$$-(F_{h+2}F_{2k-2} + F_{h+1}(F_{k-1})^2).$$

Then, by Lemma 5, we have

$$\begin{aligned}
D &= F_{h+1}F_{2k} - F_{h+1}F_{2k-2} - F_hF_{2k-2} + F_h(F_k)^2 - F_h(F_{k-1})^2 - F_{h-1}(F_{k-1})^2 \\
&= F_{h+1}F_{2k-1} - F_hF_{2k-2} + F_hF_{k+1}F_{k-2} - F_{h-1}(F_{k-1})^2 \\
&= F_{h+1}F_{2k-1} - F_hF_kF_{k-3} - F_{h-1}(F_{k-1})^2 \\
&= F_{h+1}F_kF_{k-2} - F_hF_kF_{k-3} + F_{h+1}F_{k+1}F_{k-1} - F_{h-1}(F_{k-1})^2 > 0, \\
B &= F_h(F_{k-1} + F_{k-2})(F_{k+m} + F_{k+m-1}) - (F_h + F_{h-1})F_{k-1}F_{k+m} \\
&= F_hF_{k-2}F_{k+m+1} + F_hF_{k-1}F_{k+m-1} - F_{h-1}F_{k-1}F_{k+m} \\
&= \frac{1}{2}(F_h2F_{k-2}F_{k+m+1} - F_{h-1}F_{k-1}F_{k+m} + F_hF_{k-1}2F_{k+m-1} - F_{h-1}F_{k-1}F_{k+m}) \\
&> 0, \\
E &= (F_{h+1}F_{2k-2} + F_{h+1}F_{2k-3} - F_{h+1}F_{2k-3} - F_hF_{2k-3}) \\
&\quad +(F_hF_kF_{k-1} - F_hF_{k-1}F_{k-2} - F_{h-1}F_{k-1}F_{k-2}) - (F_{h+2}F_{2k-2} + F_{h+1}(F_{k-1})^2) \\
&= F_{h+1}F_{2k-2} - F_hF_{2k-3} + F_h(F_{k-1})^2 - F_{h-1}F_{k-1}F_{k-2} \\
&\quad -(F_{h+2}F_{2k-2} + F_{h+1}(F_{k-1})^2) \\
&= -F_hF_{2k-2} - F_{h-1}(F_{k-1})^2 - F_hF_{2k-3} - F_{h-1}F_{k-1}F_{k-2} \\
&= -F_hF_{2k-1} - F_{h-1}F_kF_{k-1}, \\
A &= F_{h+1}F_{2k+m} + F_{h+1}F_{2k+m-1} - F_{h+1}F_{2k+m-1} - F_hF_{2k+m-1} \\
&= F_{h+1}F_{2k+m} - F_hF_{2k+m-1}.
\end{aligned}$$

So we have

$$\begin{aligned}
\Delta &= A + B + yF_{m+1}D + F_{m+1}E \\
&> A + F_{m+1}E + B \\
&= F_{h+1}F_{2k+m} - F_hF_{2k+m-1} - F_{m+1}(F_hF_{2k-1} + F_{h-1}F_kF_{k-1}) + B \\
&= F_hF_{2k+m} + F_{h-1}F_{2k+m} - F_hF_{2k+m-1} - F_{m+1}F_hF_{2k-1} \\
&\quad -F_{m+1}F_{h-1}F_kF_{k-1} + B \\
&= F_hF_{2k+m-2} + F_{h-1}F_{2k+m} - F_{m+1}F_hF_{2k-1} - F_{m+1}F_{h-1}F_kF_{k-1} + B \\
&= F_h(F_{2k+m-2} - F_{m+1}F_{2k-1}) + F_{h-1}(F_{2k+m} - F_{m+1}F_kF_{k-1}) + B \\
&= F_h(F_{m+1}F_{2k-2} + F_mF_{2k-3} - F_{m+1}F_{2k-1}) \\
&\quad +F_{h-1}(F_mF_{2k-1} + F_{m+1}F_{2k} - F_{m+1}F_kF_{k-1}) + B \\
&= F_h(F_mF_{2k-3} - F_{m+1}F_{2k-3}) + F_{h-1}(F_mF_{2k-1} + F_{m+1}F_kF_{k+1}) + B \\
&= F_{h-1}(F_mF_{2k-1} + F_{m+1}F_kF_{k+1}) - F_hF_{m-1}F_{2k-3} + B.
\end{aligned}$$

Then we have

$$\begin{aligned}
\Delta &> A + F_{m+1}E \\
&= F_{h-1}F_mF_{2k-1} - F_{h-1}F_{m-1}F_{2k-3} + F_{h-1}F_{m+1}F_kF_{k+1} - F_{h-2}F_{m-1}F_{2k-3} \\
&\geq F_{h-1}F_{m-1}F_{2k-2} + F_{h-2}F_{m-1}(F_kF_{k+1} - F_{2k-3}) \\
&= F_{h-1}F_{m-1}F_{2k-2} + F_{h-2}F_{m-1}(F_kF_{k+1} - F_kF_{k-2} - F_{k-1}F_{k-3}) \\
&= F_{h-1}F_{m-1}F_{2k-2} + F_{h-2}F_{m-1}F_{k-1}(2F_k - F_{k-3}) \geq 0, \text{ if } h \geq 2; \\
\Delta &> A + F_{m+1}E + B \\
&= F_{k-2}F_{k+m+1} + F_{k-1}F_{k+m-1} - F_{m-1}F_{2k-3} \\
&> F_kF_{k+m-1} - F_{m-1}F_{2k-3} \\
&= F_k(F_kF_m + F_{k-1}F_{m-1}) - F_{m-1}(F_{k-1}F_{k-1} + F_{k-2}F_{k-2}) \\
&= F_m(F_k)^2 - F_{m-1}(F_{k-1})^2 + F_{m-1}(F_kF_{k-1} - (F_{k-2})^2) > 0, \text{ if } h = 1.
\end{aligned}$$

Thus we have $\Delta = z(C_{2k}^{(k)}(m^1, 1^y; h^1)) - z(C_{2k-2}^{(k-1)}(m^1, 1^{y+1}; (h+1)^1)) > 0$, which means that after identifying vertex u_{k-1} with u_k, u'_{k-1} with u_k, and attaching a pendant edge to u_k, and the other pendant edge to pendant vertex v_{d+1} as shown in Fig. 7, the obtained graph has a smaller Hosoya index. After repeating the above operation, we find that for given positive integer m, the minimal Hosoya index of graphs of the form $C_{2k}^{(k)}(m^1, 1^y; h^1)$ with $y = n - d - k$ is attained at $C_4^{(2)}(m^1, 1^{n-d-2}; (d-m-2)^1)$.

Set $x = n - d - 2$ and $h = d - m - 2$. Now we start to determine the value of k at which $z(C_4^{(2)}(m^1, 1^x; h^1))$ reaches its minimum. Note that $h + m = d - 2$. From Lemmas 5, 12, we have

$$\begin{aligned}
z(C_4^{(2)}(m^1, 1^x; h^1)) &= F_{h+1}F_{m+5} + F_hF_{m+3} + F_{m+1}[F_{h+1}(xF_4 + F_3) + F_h(xF_2 + F_1)] \\
&= F_{h+m+4} + F_{h+1}F_{m+3} + (x+1)F_{m+1}(3F_{h+1} + F_h) - F_{m+1}F_{h+1} \\
&= F_{h+m+4} + F_{h+1}F_{m+3} + (x+1)F_{m+1}F_{h+3} + xF_{m+1}F_{h+1} \\
&= F_{h+m+4} + F_{h+1}F_{m+3} + F_{m+1}F_{h+3} + xF_{m+1}(F_{h+3} + F_{h+1}) \\
&= F_{h+m+4} + F_{h+1}F_{m+1} + F_{h+1}F_{m+2} + F_{m+1}(F_h + 2F_{h+1}) \\
&\quad + xF_{m+1}(F_{h+3} + F_{h+1}) \\
&= F_{h+m+4} + F_{m+h+2} + 3F_{m+1}F_{h+1} + xF_{m+1}(F_{h+3} + F_{h+1}) \\
&= F_{d+2} + F_d + 3F_{m+1}F_{h+1} + xF_{m+1}(F_{h+3} + F_{h+1}).
\end{aligned}$$

From Corollary 1, $z(C_4^{(2)}(m^1, 1^x; h^1))$ reaches its minimum at $m = 1$, and its minimum is

$$F_{d+2} + F_d + 3F_{d-2} + (n-d-2)(F_d + F_{d-2}) = F_{d+2} + (n-d-1)F_d + (n-d+1)F_{d-2}.$$

Therefore this theorem follows immediately. □

Note that the set $\mathcal{U}_{n,2}$ contains only one graph which is just $C_3(1^{n-3})$ with $z(C_3(1^{n-3})) = 2n - 2$. Next, we will prove our main theorem, in which all the graphs from $\mathcal{U}_{n,d}$ with the smallest Hosoya index are fully characterized.

Theorem 4. *Let* $G \in \mathcal{U}_{n,d}$.

(1) If $d = 3$*, then* $z(G) \geq 3n - 6$ *with the equality holding if and only if* $G \cong C_3^{(1)}(1^{n-4}; 1^1)$*;*

(2) If $4 \leq d < n-1$*, then* $z(G) \geq F_{d+2} + (n-d-1)F_d + (n-d+1)F_{d-2}$ *with the equality holding if and only if* $G \cong C_4^{(2)}(1^{n-d-1}; (d-3)^1)$*.*

Proof. By Theorems 1, 2 and 3, we find that the graph from $\mathcal{U}_{n,d}^{(1)}$ minimizing the Hosoya index is $C_3(1^{n-d-2}, (d-1)^1)$ with

$$z(C_3(1^{n-d-2}, (d-1)^1)) = 2(n-d)F_d + 2F_{d+1},$$

the graph from $\mathcal{U}_{n,d}^{(2)1}$ minimizing the Hosoya index is $C_3^{(1)}(1^{n-d-1}; (d-2)^1)$ with

$$z(C_3^{(1)}(1^{n-d-1}; (d-2)^1)) = (n-d+1)F_{d+1},$$

the graph from $\mathcal{U}_{n,d}^{(2)2}$ minimizing the Hosoya index is $C_4^{(2)}(1^{n-d-1}; (d-3)^1)$ with

$$z(C_4^{(2)}(1^{n-d-1}; (d-3)^1)) = F_{d+2} + (n-d-1)F_d + (n-d+1)F_{d-2}.$$

Moreover, we have

$$2(n-d)F_d + 2F_{d+1} - (n-d+1)F_{d+1} = (n-d-1)(2F_d - F_{d+1}) > 0, \text{ for } d > 2, \quad (**)$$

$$\begin{aligned}(n-d+1)&F_{d+1} - [F_{d+2} + (n-d-1)F_d + (n-d+1)F_{d-2}] \\ &= (n-d-1)F_{d-3} + F_{d-1} - 2F_{d-2} \\ &= (n-d)F_{d-3} - F_{d-2}.\end{aligned}$$

Set $A = (n-d)F_{d-3} - F_{d-2}$. Obviously, $A = -1 < 0$ if $d = 3$, and $A \geq 2F_{d-3} - F_{d-2} > 0$ if $d > 3$. Note that $n > 4$. Combining inequality $(**)$ and all the cases of the value of A, the results in (1) and (2) follow immediately. The proof of this theorem is completed. □

Note that $\mathcal{U}(n) = \bigcup_{d=2}^{n-2} \mathcal{U}_{n,d}$. From Theorem 4 the following corollary is easily obtained.

Corollary 5 (see [4, 13])**.** *The smallest Hosoya index of graphs from* $\mathcal{U}(n)$ *is attained at* $C_3(1^{n-3})$ *with* $z(C_3(1^{n-3})) = 2n-2$*; the second smallest Hosoya index of graphs from* $\mathcal{U}(n)$ *is attained at* $C_3^{(1)}(1^{n-4}; 1^1)$ *with* $z(C_3(C_3^{(1)}(1^{n-4}; 1^1))) = 3n - 6$.

Denote by $P_k(k_1; k_2)$ the tree obtained by attaching k_1, k_2 pendant edges to two pendant vertices of a path P_k. Now we end this paper with the theorem below, in which the graph from $\mathcal{U}(n)$ with the third smallest Hosoya index is determined.

Theorem 5. *Let* $n > 7$ *and* $G \in \mathcal{U}(n) \setminus \{C_3(1^{n-3}), C_3^{(1)}(1^{n-4}; 1^1)\}$*. Then we have* $z(G) \geq 3n - 5$ *with the equality holding if and only if* $G \cong C_4(1^{n-4})$*.*

Proof. Suppose that $G_0 \in \mathcal{U}(n)\backslash\{C_3(1^{n-3}), C_3^{(1)}(1^{n-4};1^1)\}$ has the smallest Hosoya index. First we claim that G_0 must be of the form $C_3^{(1)}(1^{n_1};1^{n_2})$ with $n_1+n_2=n-3$ and $(n_1,n_2)\neq(1,n-4)$, or $C_4(1^{n-4})$. From Theorem 4 and Lemma 10, any unicyclic graph with $d>3$ has a larger Hosoya index than $C_4^{(2)}(1^{n-d-1};1^{d-3})$, by Lemma 4, we have

$$z(C_4^{(2)}(1^{n-d-1};1^{d-3})) > z(C_3^{(1)}(1^{n-d-1};1^{d-2})).$$

Therefore any unicyclic graph with $d>3$ has a larger Hosoya index than $C_3^{(1)}(1^{n-d-1};1^{d-2})$. In fact, any unicyclic graph with $d=3$ is either $C_4(1^{n-4})$, or of the form $C_4^{(1)}(1^{k_1};1^{k_2})$ with $k_1+k_2=n-4$, or of the form $C_3^{(1)}(1^{n_1};1^{n_2})$ with $n_1+n_2=n-3$. In view of Lemma 4, we have

$$z(C_4^{(1)}(1^{k_1};1^{k_2})) > z(C_3^{(1)}(1^{k_1+1};1^{k_2})),$$

which finishes the proof of this claim.

Note that $n_1+n_2=n-3$, by Lemmas 1 and 2, we have

$$z(C_4(1^{n-4})) = (n-3)F_4 + 2F_3 = 3n-5,$$

$$\begin{aligned} z(C_3^{(1)}(1^{n_1};1^{n_2})) &= z(P_3(n_1;n_2))+1 \\ &= z(S_{n_1+1})z(S_{n_2+1}) + z(S_{n_1+1}) + z(S_{n_2+1}) + 1 \\ &= (n_1+1)(n_2+1) + n_1 + n_2 + 3 = 2n-2+n_1n_2. \end{aligned}$$

It is easy to see that $z(C_3^{(1)}(1^{n_1};1^{n_2}))$ reaches its minimum $2n-2+2(n-5)=4n-12$ at $(n_1,n_2)=(2,n-5)$ if $(n_1,n_2)\neq(1,n-4)$. Clearly, $4n-12-(3n-5)=n-7>0$. Therefore the result of this theorem follows immediately. □

By a simple calculation, we find that $C_4(1^3)$ or $C_3^{(1)}(1^2;1^2)$ has the third smallest Hosoya index in $\mathcal{U}(n)$ if $n=7$. It is not difficult to determine the graph from $\mathcal{U}(n)$ (which is still $C_4(1^{n-4})$) with the third smallest Hosoya index when $n=5$ or 6.

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