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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 $\Delta$ 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.*

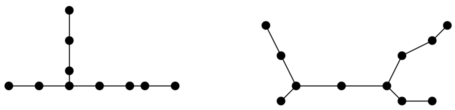
(1) *If $v \in V(G)$, then we have $z(G)=z(G-v)+\sum\limits_{w \in N_G(v)} z(G-\{w,v\})$ ;*

(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 $z(G)=\prod\limits_{k=1}^{t} z(G_k)$.*

**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 $z(S_n) = n$.*

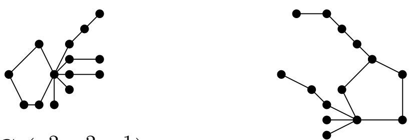
A tree is called a $d$-pode (see [15]) if it contains only one vertex $v$ of degree $d > 2$. $v$ is called the *center*. Denote by $R(c_1, c_2, \cdots, c_d)$ the $d$-pode where $\sum_{k=1}^{d} c_k = n-1$, $c_i$ is the length of the $i-$th "ray" going out from the center. That is to say, $R(c_1, c_2, \cdots, c_d) - v = \bigcup_{k=1}^{d} P_{c_k}$. 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* $P = u_0 u_1 u_2 \cdots u_t u_{t+1}$ *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* $v_1 v_2 \cdots v_k$*,* $G_2 = G_1 - u_r u_{r+1} + u_{r+1} v_1$ *(see Fig. 3). Then we have* $z(G_1) < z(G_2)$*.*

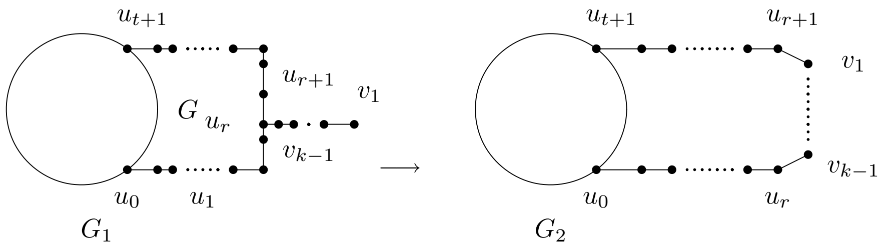



Figure 3: *Graphs in Lemma 4*

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

$$\begin{aligned} F_1 F_{n+1} &> F_3 F_{n-1} > F_5 F_{n-3} > \cdots F_{2s+1} F_{2s+r+1} > F_{2s} F_{2s+r+2} \\ &> F_{2s-2} F_{2s+r+4} > \cdots > F_4 F_{n-2} > F_2 F_n; \end{aligned}$$

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

$$\begin{aligned} F_1 F_{n+1} &> F_3 F_{n-1} > F_5 F_{n-3} > \cdots F_{2s+1} F_{2s+r+1} > F_{2s+2} F_{2s+r} \\ &> F_{2s} F_{2s+r+2} > \cdots > F_4 F_{n-2} > F_2 F_n. \end{aligned}$$

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

**Corollary 1.** *The sequence* $\{F_k F_{n-k}\}$ *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*

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

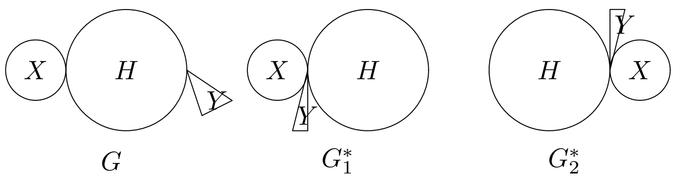



Figure 4: *Graphs $G$, $G_1^*$ and $G_2^*$ in Lemma 9*

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

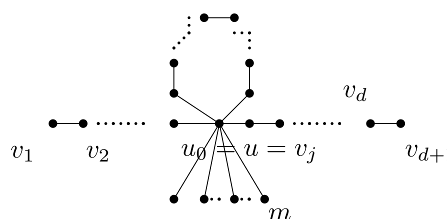



Figure 5: *Main path and unique cycle in graph $G'$*

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

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

and

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

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

**Theorem 1.** *For any graph $G \in \mathcal{U}_{n,d}^{(1)}$, 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 $G_0 \in \mathcal{U}_{n,d}^{(1)}$ has the smallest Hosoya index. By the definition of $\mathcal{U}_{n,d}^{(1)}$, 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 $G_0 \cong G_M v_j S_x$, or $G_0 \cong G_M u_t S_x$, 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 $G_0 \cong G_M v_j S_x$, 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 $G_0 \cong G_M u_t S_x$, 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 $G_0 \in \{G_C v_j S_y, G_C v_i S_y, G_C u_t S_y\}$, where $j, i$ are defined as above and $t \in \{1, 2\}$. Graphs $G_C v_j S_y, G_C v_i S_y, G_C u_1 S_y$ are shown as three examples in Fig. 6. By Lemma 9, we claim that $G_C v_i S_y$ and $G_C u_t S_y$ with $t = 1, 2$ cannot have the smallest Hosoya index. Thus we find that $G_0$ must be of the form $G_C v_j S_y$.

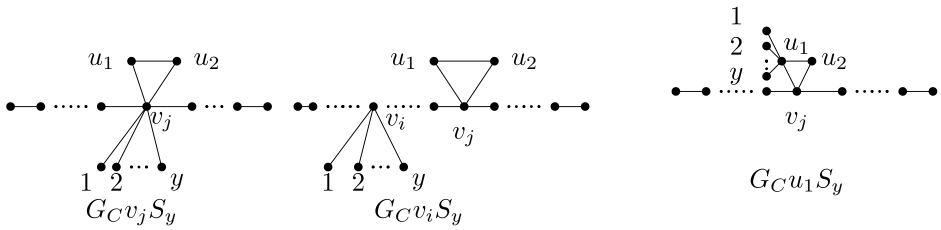



Figure 6: *Graphs $G_C v_j S_y$, $G_C v_i S_y$ and $G_C u_1 S_y$*

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. $\square$

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 $G_Cv_0S_y$, or of the form $G_Cv_tS_y$, where $t \in \{j, j+1\}$, or of the form $G_Cv_iS_y$, where $i \in \{2, 3, \cdots, d-1\} \setminus \{j, j+1\}$.

Now we claim that $G_0$ is of the form $G_Cv_tS_y$, where $t \in \{j, j+1\}$ or $G_Cv_2S_y$ with $j > 2$. If not, $G_0$ must be of the form $G_Cv_0S_y$, or of the form $G_Cv_iS_y$, where $i \in \{2, 3, \cdots, d-1\} \setminus \{j, j+1\}$. If $G_0$ is of the form $G_Cv_0S_y$, 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 $G_0' \cong G_Cv_jS_y$, by Lemma 9, we have

$$z(G_0') = z(G_Cv_jS_y) < z(G_Cv_0S_y),$$

this is impossible because of the minimality of $z(G_Cv_0S_y)$. If $G_0$ is of the form $G_Cv_iS_y$, 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

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

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

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

By Lemma 11, we have $z(G_Cv_jS_y) < z(G_Cv_iS_y)$ when $i > 2$. Therefore this claim holds immediately.

Denote by $G_2^{(j)}$ the graph $G_Cv_2S_y$ with $j \geq 3$. Let $G_j$ be the graph $G_Cv_jS_y$ 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

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

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

$$\begin{aligned} z(G_2^{(j)}) - (y+3)F_{d+1} &= (y+2)F_{j-2}F_{d-j+1} + F_d + F_{j-3}F_{d-j+1} - F_{d+1} \\ &= (n-d)F_{j-2}F_{d-j+1} + F_{j-3}F_{d-j+1} - F_{d-1} \\ &\geq 2F_{j-2}F_{d-j+1} + F_{j-3}F_{d-j+1} - F_{d-1} \\ &= F_jF_{d-j+1} - F_{d-1} > F_2F_{d-1} - F_{d-1} = 0. \end{aligned}$$

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

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

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 $j \in \{1, 2, \cdots, k-1\}$.

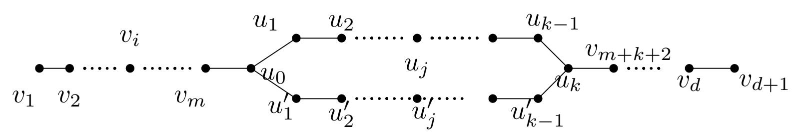



Figure 7: *The graph $C_{2k}^{(k)}(m^1; h^1)$ in $G_0$*

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

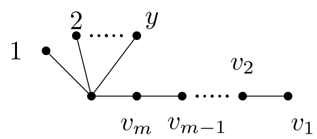



Figure 8: *The tree* $T_{m+y}^{(0)}$

$z(G'_C u_j T_{m+y}^{(0)})$. 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 $z(G_C - u_j) = z_{k+1}$, $z(G_C - u_0) = z^{(0)}_C$, $z(G_C - u_k) = z^{(k)}_C$, and $B = z_{k+1} - z^{(0)}_C + z_{k+1} - z^{(k)}_C$. Note that $k_1 + k_2 = k - 2$, by Lemmas 1, 2, 5 and Corollary 3, we have

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

and

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

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

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

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 $z(G_Cu_0S_y) < z(G_Cu_jS_y)$ or $z(G_Cu_kS_y) < z(G_Cu_jS_y)$, which finishes the proof for this case since $G_Cu_0S_y$ and $G_Cu_kS_y$ 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

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

and

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

Set

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

and

$$\begin{aligned}E = &(F_{h+1}F_{2k-1} - F_{h+2}F_{2k-3}) + (F_hF_kF_{k-1} - F_{h+1}F_{k-1}F_{k-2})\\&-(F_{h+2}F_{2k-2} + F_{h+1}(F_{k-1})^2).\end{aligned}$$

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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