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The Greatest Hosoya Index of Bicyclic Graphs with Given Maximum Degree

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Abstract

The Hosoya index of a graph G is the total number of matchings of G, including the empty edge set. Let $\mathcal{B}(n,\Delta)$ be the set of connected n-vertex bicyclic graphs with maximum degree Δ. We determine the greatest Hosoya index in $\mathcal{B}(n,\Delta)$, and characterize the corresponding extremal graphs.

1 Introduction

The Hosoya index of a graph G, denoted by $Z(G)$, is one of well-known topological indices in mathematical chemistry [18, 20–22]. It is defined as the total number of the matchings (independent edge subsets), including the empty edge set. The Hosoya index was introduced by Hosoya in 1971 [18]. Since then it received much attention by mathematical chemists (see the book [14] and the recent papers [1, 3, 4, 6, 28, 37, 38, 40, 42]). It plays an important role in the study of the relation between molecular structure and a variety of physical and chemical properties of certain hydrocarbon compounds [11, 23–25, 30–32].

It is of some importance to determine the graphs having extremal (maximal or minimal) Hosoya indices. The first such result was obtained by one of the present authors [7], by demonstrating that in the class of trees with a fixed number of vertices, the star has minimum and the path maximum Z-value. By now, many results along these lines have been obtained, see e. g. [1, 3–6, 26, 28, 33–35, 37, 38, 40–43]. In particular, Xu and Xu [41] characterized the unicyclic graphs with given maximum degree Δ, maximizing the Hosoya index.

Much earlier [8], a relation $\succ$ between graphs was introduced, defined so that $G_1 \succ G_2$ holds if for all $k \geq 1$, the number of k-matchings of G_1 is greater than or equal to the number of k-matchings of G_2. Evidently, $G_1 \succ G_2$ implies $Z(G_1) \geq Z(G_2)$, with equality if and only if the numbers of k-matchings of G_1 and G_2 are equal for all k. Numerous relations for the Hosoya index were (implicitly) obtained by means of the relation $\succ$ [9, 10, 13, 16, 17]. In particular, in [9, 10, 13] the unicyclic, bicyclic, and tricyclic graphs with greatest Hosoya indices were (implicitly) determined. In [6] Deng et al. reproduced these results for unicyclic graphs, and in [4, 5] for bicyclic graphs (but see Remark 3.1).

All graphs considered in this paper are finite and simple. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, we denote by $N_G(v)$ the set of neighbors of v in G. The cardinality of $N_G(v)$ is called the degree of v and is denoted by $d_G(v)$ or, shorter, by $d(v)$. If a vertex x has degree k, then x is said to be a k-vertex. In the following we denote by P_n and C_n the path graph and the cycle graph with n vertices, respectively. For undefined notations and terminology, the readers are referred to [2].

A connected graph of order n is bicyclic if it has $n+1$ edges. Let $\mathcal{B}(n)$ be the set of connected bicyclic graphs of order n. Denote by $\mathcal{B}(n, \Delta)$ the set of connected bicyclic graphs of order n with maximum degree Δ. Any graph $G \in \mathcal{B}(n, \Delta)$ possesses at least two cycles. With regard to these cycles, we distinguish between the following three cases:

(1) The two cycles in G have only one common vertex.

(2) The two cycles in G are linked by a path of length $l > 0$.

(3) The two cycles in G have a common path of length $s > 0$.

In Fig. 1 are depicted the graphs $C_{p,q}$, $C_{p,l,q}$ and $\theta_{r,s,t}$. These correspond to the above cases (1), (2), and (3), and are called, respectively, the main subgraphs of $G \in \mathcal{B}(n)$ of type (1), (2), and (3). In Section 2 some basic lemmas are listed or proved. In Section 3 we characterize the graphs in $\mathcal{B}(n, \Delta)$ with the greatest Hosoya index, and determine the corresponding Z-values.

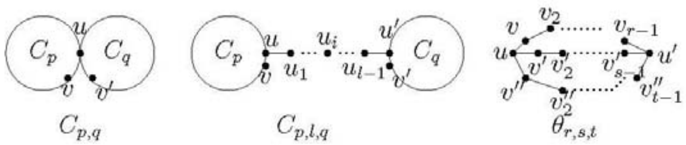


Fig. 1. The three main subgraphs of $G \in \mathcal{B}(n)$ of type (1), (2), and (3), and the labeling of their vertices.

2 Some lemmas

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

Lemma 2.1. ([14, 18]) *Let G be a graph.*

(1) *If $v \in V(G)$, then $Z(G) = Z(G - v) + \sum_{w \in N_G(v)} Z(G - \{w, v\})$.*

(2) *If $uv \in E(G)$, then $Z(G) = Z(G - uv) + Z(G - \{u, v\})$.*

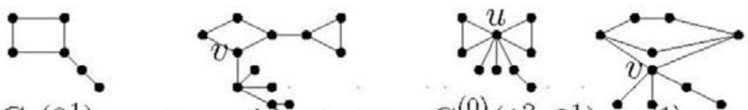
(3) *If $G_1, G_2, \ldots, G_t$ are the components of G, then $Z(G) = \prod_{k=1}^{t} Z(G_k)$.*

Lemma 2.2. ([14, 19]) *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 $Z(P_n) = F_{n+1}$ and $Z(C_n) = F_{n+1} + F_{n-1}$.*

A tree T is said to be *starlike* if it contains only one vertex v of degree greater than two [12, 15, 27, 36, 39, 44]. Then v is the *center* of T. If the degree of v is equal to d, then T is said to be d-starlike. Let c_i be the length of the i-th branch going out from the center of a d-starlike tree, $i = 1, 2, \ldots, d$. We denote by $R(c_1, c_2, \ldots, c_d)$ the d-starlike tree for which $\sum_{k=1}^{d} c_k = n - 1$. Then $R(c_1, c_2, \ldots, c_d) - v = \bigcup_{k=1}^{d} P_{c_k}$. If the number of branches of length c_k is l_k, then we write it as $c_k^{l_k}$ in the following. For example, $R(2, 2, 3, 3)$ will be written as $R(2^2, 3^2)$ for short. For convenience, $R(c_1, c_2, c_3)$ will be denoted by $T(c_1, c_2, c_3)$.

If G_1, G_2 are two graphs with $V(G_1) \bigcap V(G_2) = \{v\}$, then $G = G_1 v G_2$ is defined as a new graph with $V(G) = V(G_1) \bigcup V(G_2)$ and $E(G) = E(G_1) \bigcup E(G_2)$. For a starlike tree $T = R(k_1^{l_1}, k_2^{l_2}, \ldots, k_m^{l_m})$, the graph GvT (where v is the center of T) can be also denoted by $Gv(k_1^{l_1}, k_2^{l_2}, \ldots, k_m^{l_m})$. When $G \cong C_k$, then the latter graph will be written as $C_k(k_1^{l_1}, k_2^{l_2}, \ldots, k_m^{l_m})$ for short. For convenience, we let $C_k = C_k(0^1)$ and $P_{k-1} = C_k((-1)^1)$. Further, let $Gv^{[l]}(k_1^{l_1}, k_2^{l_2}, \ldots, k_m^{l_m})$ be the graph obtained by identifying the vertex v of G with a pendent vertex of P_{l+1} of the graph $R(k_1^{l_1}, k_2^{l_2}, \ldots, k_m^{l_m}, l^1)$ where $l \geq 1$.

In what follows any graph of one of three types (1), (2), and (3) will be always labeled as shown in Fig. 1. For a graph M of one of the three types (1), (2), and (3), $Mu(k_1^{l_1}, k_2^{l_2})$ and $Mv(k_1^{l_1}, k_2^{l_2})$ will be denoted by $M^{(0)}(k_1^{l_1}, k_2^{l_2})$ and $M^{(1)}(k_1^{l_1}, k_2^{l_2})$, respectively. For example, $C_4(2^1)$, $C_{4,1,3}v^{[1]}(1^2, 2^1)$, $C_{3,3}^{(0)}(1^2, 2^1)$, and $\theta_{2,2,3}^{(1)}(1^2, 2^1)$ are shown in Fig. 2.



$C_4(2^1)$ $C_{4,1,3}v^{[1]}(1^2, 2^1)$ $C_{3,3}^{(0)}(1^2, 2^1)$ $\theta_{2,2,3}^{(1)}(1^2, 2^1)$

Fig. 2. Examples of graphs of the type $M^{(0)}(k_1^{l_1}, k_2^{l_2})$ and $M^{(1)}(k_1^{l_1}, k_2^{l_2})$.

Lemma 2.3. ([38]) *Let $G \ncong K_1$ be a connected graph, and $v \in V(G)$. The graph $G(k, n-1-k)$ is obtained by 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 $l = \lfloor (j-1)/2 \rfloor$, and where $G(0, n-1)$ can be also viewed as a graph obtained by attaching at $v \in V(G)$ a path of length $n-1$.

By repeating Lemma 2.3, the following remark is easily obtained.

Remark 2.1. ([9,38]) *When a tree T of size t, attached to a graph G, is replaced by a path P_{t+1} (see Fig. 3), then the Hosoya index increases.*

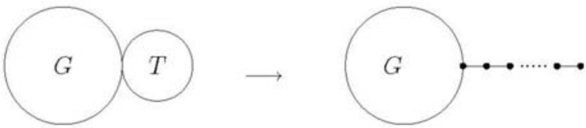


Fig. 3. The graphs in Remark 2.1.

Lemma 2.4. ([4,9]) *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 $u_1, u_2, \ldots u_t$ in G are 2, $t \geq 1$. By G_1 we denote the graph obtained by identifying u_r, $(0 \leq r \leq t)$ with the vertex v_k of a simple path $v_1v_2\cdots v_k$. Further, $G_2 = G_1 - u_ru_{r+1} + u_{r+1}v_1$ (see Fig. 4). Then, $Z(G_1) < Z(G_2)$.*

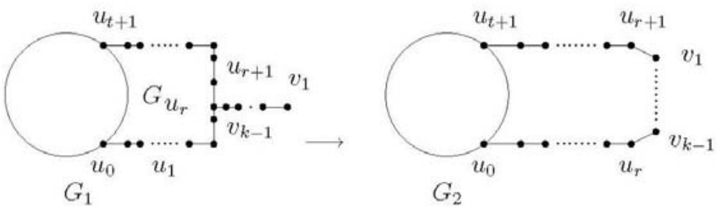


Fig. 4. The graphs in Lemma 2.4.

Lemma 2.5. ([6]) *$F_n = F_k F_{n-k+1} + F_{k-1} F_{n-k}$ for $1 \le k \le n$.*

Lemma 2.6. ([29]) *Let $n = 4s + r$, with $s > 0$ and $0 \le r \le 3$.*

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

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

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

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

From Lemma 2.6, the following corollary is obvious.

Corollary 2.1. *For a given positive integer $n \ge 4$, the maximal value of the sequence $\{F_k F_{n-k}\}$ is $F_1 F_{n-1}$, the second maximal value of this sequence is $F_3 F_{n-3}$.*

Lemma 2.7. *Let G_1 and G_2 be two graphs and v_i be a vertex of G_i for $i = 1, 2$. If either $Z(G_2) \ge Z(G_1)$ or $Z(G_2 - v_2) \ge Z(G_1 - v_1)$, then we have $Z(G_2 v_2 T_l) > Z(G_1 v_1 T_l)$, where T_l is a tree of order $l \ge 2$ and, in T_l, the vertex v_1 in G_1 is identified with v_2 in G_2.*

Proof. We prove this lemma by induction on l (the order of T_l).

For $l = 2$, the graph $G_i v_i T_l$ is just the graph obtained by attaching a pendent edge to vertex v_i of G_i for $i = 1, 2$. Applying Lemma 2.1 (1) to that pendent vertex, we get

$$\begin{aligned} Z(G_1 v_1 T_l) &= Z(G_1) + Z(G_1 - v_1) \\ Z(G_2 v_2 T_l) &= Z(G_2) + Z(G_2 - v_2) \ . \end{aligned}$$

Thus, considering the conditions in this lemma, we have

$$Z(G_2 v_2 T_l) - Z(G_1 v_1 T_l) = [Z(G_2) - Z(G_1)] + [Z(G_2 - v_2) - Z(G_1 - v_1)] > 0 \ .$$

Therefore $Z(G_2 v_2 T_l) > Z(G_1 v_1 T_l)$ for $l = 2$.

Now we assume that $Z(G_2v_2T_l) > Z(G_1v_1T_l)$ for $l < k$. In the next step we will show that $Z(G_2v_2T_l) > Z(G_1v_1T_l)$ for $l = k$. Note that there must be at least a pendent vertex in the tree T_k of graph $G_iv_iT_k$. Choose a pendent vertex u_1 with the greatest distance from v_1 (resp. v_2) in T_k, where the neighbor vertex u_1 is u_t of degree $t \geq 2$. Similarly, by applying Lemma 2.1 (2) to the pendent vertex u_1 in T_k of $G_iv_iT_k$, from Lemma 2.1 (3) and Lemma 2.2, we obtain

$$\begin{aligned} Z(G_1v_1T_k) &= Z(G_1v_1T_{k-1}) + F_2^{t-2} Z(G_1v_1T_{k-t}) \\ &= Z(G_1v_1T_{k-1}) + Z(G_1v_1T_{k-t}) \end{aligned}$$

$$\begin{aligned} Z(G_2v_2T_k) &= Z(G_2v_2T_{k-1}) + F_2^{t-2} Z(G_2v_2T_{k-t}) \\ &= Z(G_1v_1T_{k-1}) + Z(G_1v_1T_{k-t}) \ . \end{aligned}$$

By assumption, it is obvious that $Z(G_2v_2T_k) - Z(G_1v_1T_k) > 0$, which completes the proof of this lemma. ■

Remark 2.2. *Let G be a graph and v_1, v_2 be two vertices of G such that $Z(G - v_2) > Z(G - v_1)$. Suppose that T_l is a tree of order $l \geq 2$. Then $Z(Gv_2T_l) > Z(Gv_1T_l)$.*

From Lemmas 2.1, 2.2, and 2.5, the following result can be easily obtained. Note that a simple calculation shows the validity of the formula of $Z(C_a(b^1))$ for $b = 0$ or $b = -1$.

Lemma 2.8.

$$\begin{aligned} Z(T(a,b,c)) &= F_{a+c+2}F_{b+1} + F_{a+1}F_{c+1}F_b \\ Z(C_a(b^1)) &= F_{a+b+1} + F_{a-1}F_{b+1} \ . \end{aligned}$$

Lemma 2.9. ([4]) *Let $P = uu_1u_2 \cdots u_{t-1}v$ be a path in a graph G not isomorphic to path graph, where the degrees of $u_1, u_2, \ldots, u_{t-1}$ in G are 2. By $G^t(a,b)$ is denoted the graph obtained by identifying a pendent vertex of P_{a+1} with vertex u in G and a pendent vertex of P_{b+1} with vertex v in G. Then $Z(G^t(a,b)) < Z(Gu((a+b)^1))$ or $Z(G^t(a,b)) < Z(Gv((a+b)^1))$.*

Lemma 2.10. ([4]) *If $C_{p,l,q}$, $C_{p,l+q}$, and $C_{p+l,q}$ are three graphs defined as above, then $Z(C_{p,l+q}) > Z(C_{p,l,q})$ and $Z(C_{p+l,q}) > Z(C_{p,l,q})$.*

3 Main results

We now consider the greatest Hosoya index of graphs from the class $\mathcal{B}(n,\Delta)$. For $\Delta \leq 2$ there are no bicyclic graphs. In [4] and [10], the graphs from $\mathcal{B}(n)$ with greatest Hosoya index were characterized completely. All these graphs belong to $\mathcal{B}(n,3)$ (see Remark 3.1). Thus the case $\Delta = 3$ has been settled.

If $\Delta = n-1$, there exist only two connected bicyclic graphs $\theta^{(0)}_{2,1,2}(1^{n-4})$ and $C^{(0)}_{3,3}(1^{n-5})$. By a direct calculation we find that $C^{(0)}_{3,3}(1^{n-5})$ has greater Hosoya index, equal to $4n-8$. For $n=4$, only one graph $\theta_{2,1,2}$ belongs to $\mathcal{B}(n)$ and there is nothing to prove. For $n=5$ there are two cases, i. e., $\Delta = 3$ and $\Delta = 4$. From the above arguments it is easy to obtain the greatest Hosoya index of graphs from $\mathcal{B}(n,\Delta)$. Therefore, in what follows we assume that $3 < \Delta < n-1$ and $n > 5$.

Remark 3.1. *Deng* [4] *found that the greatest Hosoya index of graphs from $\mathcal{B}(n)$ is attained at $\theta_{3,1,n-3}$ if $n > 6$, or at $\theta_{3,1,2}$ or $\theta_{2,2,2}$ if $n=5$. But the result when $n > 7$ is false. By a simple calculation, we obtain that $Z(C_{4,1,n-4}) = 58 > 57 = Z(\theta_{3,1,n-3})$ for $n=8$, $Z(C_{4,1,n-4}) = Z(\theta_{3,1,n-3})$ for $n=9$ and $Z(C_{4,1,n-4}) - Z(\theta_{3,1,n-3}) = F_{n-9} > 0$ for $n > 9$. Therefore we conclude that the graph from $\mathcal{B}(n)$ with greatest Hosoya index is $\theta_{3,1,2}$ or $\theta_{2,2,2}$ if $n=5$, $\theta_{3,1,n-3}$ if $n = 6,7$, $C_{4,1,n-4}$ if $n=8$ or $n \geq 10$, $\theta_{3,1,n-3}$ or $C_{4,1,n-4}$ if $n=9$, as shown in* [10] *except that $\theta_{2,2,2}$ is missing if $n=5$.*

In order to continue our study, we introduce two subsets of of $\mathcal{B}(n,\Delta)$. Suppose that M is of one of the types (1), (2), and (3). Let $\mathcal{B}_1(n,\Delta)$ be the set of all graphs $Mv_i^{[l]}(k_1^{l_1}, k_2^{l_2})$ with $l_1 + l_2 = \Delta - 1$ where $k_1 = 1$ and $1 \leq k_2 \leq 2$, or $k_1 = 2$ and $k_2 \geq 2$ and $l_2 = 1$ when $k_2 > 2$. Denote by $\mathcal{B}_2(n,\Delta)$ the set of all graphs $Mv_i(k_1^{l_1}, k_2^{l_2})$ with $l_1 + l_2 = \Delta - 2$, where $k_1 = 1$ and $1 \leq k_2 \leq 2$, or $k_1 = 2$ and $k_2 \geq 2$ and $l_2 = 1$ when $k_2 > 2$. In the following we always assume that k_1 and k_2 are positive integers defined as above.

Lemma 3.1. *Suppose that G^* from $\mathcal{B}(n,\Delta)$ has maximal Hosoya index. Then we have either $G^* \in \mathcal{B}_1(n,\Delta)$ or $G^* \in \mathcal{B}_2(n,\Delta)$.*

Proof. Note that any bicyclic graph can be viewed as a graph obtained by attaching some trees to some vertices of a graph M of one of three types (1), (2) and (3).

If each Δ-vertex is not in $V(M)$ of the graph G^* from $\mathcal{B}(n,\Delta)$, then we assume that T_1 is a subtree such that $V(T_1)\setminus V(M)$ contains a Δ-vertex. By Remark 2.1, if we replace all subtrees attached to M by paths of the same order, then the Hosoya index will increase. Therefore, after removing the paths attached to M but not in T_1, and increasing the length of the corresponding cycle C_0 in M, the obtained graph is still in $\mathcal{B}(n,\Delta)$. Then, in view of Remark 2.1 and Lemma 2.4, the Hosoya index will increase again. By Lemma 2.3, all paths attached to the Δ-vertex of T_1 must be of the lengths 1 or 2 except, possibly, a unique path of length $k>2$. So G^* belongs to $\mathcal{B}_1(n,\Delta)$. If all the Δ-vertices have $\Delta-1$ neighbors of degree 1, then $k_1=k_2=1$.

If there exists a Δ-vertex belonging to the main subgraph M, by a similar argument we have that $G^*\in\mathcal{B}_2(n,\Delta)$. This completes the proof. ■

Lemma 3.2. *If M is a graph of one of the three types* (1), (2), *or* (3), *then $Z(M-v)$ reaches its maximum value when v is a vertex in a cycle of M which is adjacent to one vertex of maximum degree in M.*

Proof. Assume that $M\cong C_{p,q}$ with $p,q\geq 3$ when M is of type (1). From Lemmas 2.3 and 2.8, if $w\neq u$, it follows that $Z(C_{p,q}-w)$ reaches its maximum value

$$Z(C_p((q-2)^1))=Z(C_q((p-2)^1))=F_{p+q+1}+F_{p-1}F_{q-1}$$

where w is a vertex in $C_{p,q}$ adjacent to u, and $Z(C_{p,q}-u)=F_pF_q$. Clearly, by Lemma 2.5, we have $Z(C_{p,q}-v)>Z(C_{p,q}-u)$. Therefore this lemma follows immediately for the case when M is a graph of type (1).

We next deal with the case when M is of type (2). Assume that $M\cong C_{p,l,q}$. Set $i-1=l_1$ and $l-1-i=l_2$, i. e., $l_1+l_2=l-2$. In a similar manner as above,

$$\begin{aligned}
Z(C_{p,l,q}-u) &= Z(C_q((l-1)^1))F_p=F_p(F_{q+l}+F_{q-1}F_l)\\
Z(C_{p,l,q}-v) &= Z(C_q((p+l-2)^1))=F_{p+q+l-1}+F_{q-1}F_{p+l-1}\\
Z(C_{p,l,q}-v') &= Z(C_p((q+l-2)^1))=F_{p+q+l-1}+F_{p-1}F_{q+l-1}\\
Z(C_{p,l,q}-u_i) &= Z(C_p(l_1^1))Z(C_q(l_2^1))=(F_{p+l_1+1}+F_{p-1}F_{l_1+1})(F_{q+l_2+1}+F_{q-1}F_{l_2+1})\\
Z(C_{p,l,q}-v) &- Z(C_{p,l,q}-u)=F_{p-1}F_{q+l-1}+F_{q-1}F_{p-1}F_{l-1}>0\,. \qquad (1)
\end{aligned}$$

If $l=1$, then by inequality (1), this lemma holds immediately. If $l\geq 2$, set $A=Z(C_{p,l,q}-v)-Z(C_{p,l,q}-u_i)+Z(C_{p,l,q}-v')-Z(C_{p,l,q}-u_i)$. Then, by Lemma 2.5,

$$
\begin{aligned}
A &= Z(C_{p,l,q}-v)+Z(C_{p,l,q}-v')-2Z(C_{p,l,q}-u_i)\\
&= 2F_{p+q+l_1+l_2+1}+F_{p-1}F_{q+l_1+l_2+1}+F_{q-1}F_{p+l_1+l_2+1}-2(F_{p+l_1+1}F_{q+l_2+1}\\
&+ F_{p-1}F_{l_1+1}F_{q+l_2+1}+F_{q-1}F_{l_2+1}F_{p+l_1+1}+F_{p-1}F_{q-1}F_{l_1+1}F_{l_2+1})\\
&= 2F_{p+l_1}F_{q+l_2}+F_{q-1}F_{p+l_1+1}F_{l_2+1}+F_{q-1}F_{p+l_1}F_{l_2}+F_{p-1}F_{q+l_2+1}F_{l_1+1}\\
&+ F_{p-1}F_{q+l_2}F_{l_1}-2F_{q-1}F_{l_2+1}F_{p+l_1+1}-2F_{p-1}F_{l_1+1}F_{q+l_2+1}\\
&- 2F_{p-1}F_{q-1}F_{l_1+1}F_{l_2+1}\\
&= 2F_{p+l_1}F_{q+l_2}+F_{q-1}F_{p+l_1}F_{l_2}-F_{q-1}F_{p+l_1+1}F_{l_2+1}+F_{p-1}F_{q+l_2}F_{l_1}\\
&- F_{p-1}F_{q+l_2+1}F_{l_1+1}-2F_{p-1}F_{q-1}F_{l_1+1}F_{l_2+1}\\
&= (F_pF_{l_1+1}+2F_{p-1}F_{l_1})F_{q+l_2}+(F_qF_{l_2+1}+2F_{q-1}F_{l_2})F_{p+l_1}\\
&- F_{p-1}F_{l_1+1}F_{q+l_2+1}-F_{q-1}F_{l_2+1}F_{p+l_1+1}-2F_{p-1}F_{q-1}F_{l_1+1}F_{l_2+1}\\
&= (F_{p-1}F_{l_1+1}+F_{p-2}F_{l_1+1}+2F_{p-1}F_{l_1})F_{q+l_2}\\
&+ (F_{q-1}F_{l_2+1}+F_{q-2}F_{l_2+1}+2F_{q-1}F_{l_2})F_{p+l_1}\\
&- F_{p-1}F_{l_1+1}F_{q+l_2+1}-F_{q-1}F_{l_2+1}F_{p+l_1+1}-2F_{p-1}F_{q-1}F_{l_1+1}F_{l_2+1}\\
&= (F_{p-2}F_{l_1+1}+2F_{p-1}F_{l_1})F_{q+l_2}+(F_{q-2}F_{l_2+1}+2F_{q-1}F_{l_2})F_{p+l_1}\\
&- F_{p-1}F_{l_1+1}F_{q+l_2-1}-F_{q-1}F_{l_2+1}F_{p+l_1-1}-2F_{p-1}F_{q-1}F_{l_1+1}F_{l_2+1}\\
&= F_{p-2}F_{l_1+1}F_{q+l_2}+F_{q-2}F_{l_2+1}F_{p+l_1}-2F_{p-1}F_{q-1}F_{l_1+1}F_{l_2+1}\\
&+ F_{p-1}(2F_{l_1}F_{q+l_2}-F_{l_1+1}F_{q+l_2-1})+F_{q-1}(2F_{l_2}F_{p+l_1}-F_{l_2+1}F_{p+l_1-1})\\
&\geq F_{p-1}F_{l_1+1}F_{q+l_2-2}+F_{p-2}F_{l_1+1}F_{q+l_2}-F_{p-1}F_{q-1}F_{l_1+1}F_{l_2+1}\\
&+ F_{q-1}F_{l_2+1}F_{p+l_1-2}+F_{q-2}F_{l_2+1}F_{p+l_1}-F_{p-1}F_{q-1}F_{l_1+1}F_{l_2+1}\\
&= F_{l_1+1}[F_{p-2}F_{q+l_2}+F_{p-1}(F_{q-1}F_{l_2}+F_{q-2}F_{l_2-1})-F_{p-1}F_{q-1}F_{l_2+1}]\\
&+ F_{l_2+1}[F_{q-2}F_{p+l_1}+F_{q-1}(F_{p-1}F_{l_1}+F_{p-2}F_{l_1-1})-F_{p-1}F_{q-1}F_{l_1+1}]\\
&= F_{l_1+1}(F_{p-2}F_{q+l_2}-F_{p-1}F_{l_2-1}F_{q-3})+F_{l_2+1}(F_{q-2}F_{p+l_1}-F_{q-1}F_{l_1-1}F_{p-3})\\
&= F_{l_1+1}(F_{p-2}F_qF_{l_2+1}+F_{p-2}F_{q-1}F_{l_2}-F_{p-2}F_{l_2-1}F_{q-3}-F_{p-3}F_{l_2-1}F_{q-3})\\
&+ F_{l_2+1}(F_{q-2}F_pF_{l_1+1}+F_{q-2}F_{p-1}F_{l_1}-F_{q-2}F_{l_1-1}F_{p-3}-F_{q-3}F_{l_1-1}F_{p-3})>0\,.
\end{aligned}
$$

Note that if $l_1 = 0$ or $l_2 = 0$, then $A > 0$. Therefore, we have

$$Z(C_{p,l,q} - v) - Z(C_{p,l,q} - u_i) > 0 \quad \text{or} \quad Z(C_{p,l,q} - v') - Z(C_{p,l,q} - u_i) > 0 \; .$$

Thus the lemma follows when M is of type (2).

Finally, we prove this lemma for the case when M is of type (3). Assume that $M \cong \theta_{r,s,t}$. In view of Lemma 2.8,

$$Z(\theta_{r,s,t} - u) = Z(\theta_{r,s,t} - u') = Z(T(r-1, s-1, t-1)) = F_{r+s}F_t + F_r F_s F_{t-1} \; .$$

By Lemma 2.9, we claim that for a 2-vertex w in $\theta_{r,s,t}$, $Z(\theta_{r,s,t} - w)$ reaches its maximum value if $w \in \{v, v', v''\}$. This maximum value is one of the three values $Z(C_{s+t}((r-2)^1) = F_{r+s+t-1} + F_{s+t-1}F_{r-1}$, $Z(C_{r+t}((s-2)^1) = F_{r+s+t-1} + F_{r+t-1}F_{s-1}$ or $Z(C_{r+s}((t-2)^1) = F_{r+s+t-1} + F_{r+s-1}F_{t-1}$. By direct calculation we find that any one of these three values is greater than $Z(\theta_{r,s,t} - u) = Z(\theta_{r,s,t} - u')$, which implies that this lemma holds for the case when M is of type (3). Thus the proof is completed. ■

Lemma 3.3. *For any graph $G_1 \in \mathcal{B}_1(n, \Delta)$, there exists a graph $G_2 \in \mathcal{B}_2(n, \Delta)$ such that $Z(G_2) > Z(G_1)$.*

Proof. Suppose that $G_1^* \in \mathcal{B}_1(n, \Delta)$ has the maximal Hosoya index and the main subgraph of G_1^* is M. Then it suffices to show that there exists a graph $G_2 \in \mathcal{B}_2(n, \Delta)$ such that $Z(G_2) > Z(G_1^*)$. By Lemma 3.2, Remark 2.2, and the definition of $\mathcal{B}_1(n, \Delta)$, we claim that a graph G_1^* must be of the form $Mv^{[k]}(k_1^{l_1}, k_2^{l_2})$ with $l_1 + l_2 = \Delta - 1$, where v is a vertex in a cycle of M adjacent to one vertex of maximum degree in it. In the following we assume that $T_0 \cong R(k_1^{l_1 - 1}, k_2^{l_2})$.

We first consider the case when M is of type (1). Let $M \cong C_{p,q}$. Then we have $G_1^* = C_{p,q}v^{[k]}(k_1^{l_1}, k_2^{l_2}) \cong C_{p,q}v((k+k_1)^1)w_1T_0$ as shown in Fig. 5. Now we choose a graph $G_2^{(1)} \cong C_{p+k+k_1,q}w_1T_0 \in \mathcal{B}_2(n, \Delta)$, which is obtained from G_1^* by deleting the edge uv and adding an edge uv_0. Suppose that

$$G_0 = C_{p+k+k_1,q} - w_1 - uv_0 \cong C_{p,q}v((k+k_1)^1) - w_1 - uv \; .$$

From Lemma 2.4, we have $Z(C_{p+k+k_1,q}) > Z(C_{p,q}v((k+k_1)^1))$. Set

$$A_1 = Z(C_{p+k+k_1,q} - w_1) - Z(C_{p,q}v((k+k_1)^1) - w_1) \; .$$

By Lemmas 2.1 (2) and 2.5,

$$\begin{aligned} Z(C_{p+k+k_1,q} - w_1) &= Z(G_0) + F_q F_{p+k} F_{k_1} \\ Z(C_{p,q}v((k+k_1)^1) - w_1) &= Z(G_0) + F_q F_{p-1} F_{k-1} F_{k_1+1} \end{aligned}$$

$$\begin{aligned} A_1 &= F_q(F_{p+k}F_{k_1} - F_{p-1}F_{k-1}F_{k_1+1}) \\ &= F_q(F_pF_{k+1}F_{k_1} + F_{p-1}F_kF_{k_1} - F_{p-1}F_{k-1}F_{k_1} - F_{p-1}F_{k-1}F_{k_1-1}) > 0\ . \end{aligned}$$

From Lemma 2.7 it follows that $Z(G_2^{(1)}) > Z(G_1^*)$, as desired.

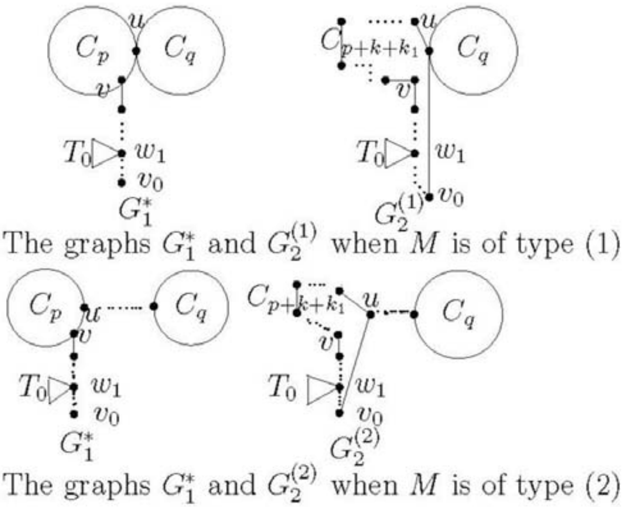


Fig. 5. Graphs used for proving Lemma 3.3.

Next we consider the case when M is of type (2). Suppose that $M \cong C_{p,l,q}$. Based on Lemma 3.2 and Remark 2.2, we claim that

$$G_1^* = C_{p,l,q}v^{[k]}(k_1^{l_1}, k_2^{l_2}) \cong C_{p,l,q}v((k+k_1)^1)w_1T_0$$

as shown in Fig. 5. Now we choose a graph

$$G_2^{(2)} \cong C_{p+k+k_1,l,q}w_1T_0 \in \mathcal{B}_2(n, \Delta)$$

that is obtained from G_1^* by deleting the edge uv and adding an edge uv_0. Let

$$G_0 = C_{p+k+k_1,l,q} - w_1 - uv_0 \cong C_{p,l,q}v((k+k_1)^1) - w_1 - uv \ .$$

Set

$$A_2 = Z(C_{p+k+k_1,l,q} - w_1) - Z(C_{p,l,q}v((k+k_1)^1) - w_1) \ .$$

We then have

$$\begin{aligned} Z(C_{p+k+k_1,l,q}) &> Z(C_{p,l,q}v((k+k_1)^1)) \\ Z(C_{p+k+k_1,l,q} - w_1) &= Z(G_0) + Z(C_q(k-1)^1)F_{p+k-1}F_{k_1} \\ Z(C_{p,l,q}v((k+k_1)^1) - w_1) &= Z(G_0) + Z(C_q(k-1)^1)F_{p-1}F_kF_{k_1+1} \end{aligned}$$

$$\begin{aligned} A_2 &= Z(C_q(k-1)^1)(F_pF_kF_{k_1} + F_{p-1}F_{k-1}F_{k_1} - F_{p-1}F_kF_{k_1} - F_{p-1}F_kF_{k_1-1}) \\ &> F_{p-2}F_kF_{k_1} + F_{p-1}F_{k-1}F_{k_1} - F_{p-1}F_kF_{k_1-1} \\ &= \frac{1}{2}(2F_{p-2}F_kF_{k_1} - F_{p-1}F_kF_{k_1-1} + F_{p-1}2F_{k-1}F_{k_1} - F_{p-1}F_kF_{k_1-1}) \geq 0 \end{aligned}$$

Thanks to Lemma 2.7, we have $Z(G_2^{(2)}) > Z(G_1^*)$, as desired.

Finally we turn to the case when M is of type (3). Suppose that $M \cong \theta_{r,s,t}$. In view of Lemma 3.2 and Remark 2.2, we claim that

$$G_1^* = \theta_{r,s,t}v^{[k]}(k_1^{l_1}, k_2^{l_2}) \cong \theta_{r,s,t}v((k+k_1)^1)w_1T_0$$

as shown in Fig. 6. By symmetry, we only need to consider the case when v is on the path P_{r+1} in $\theta_{r,s,t}$ and is adjacent to u. Choose the graph $G_2^{(3)} \cong \theta_{r+k+k_1,s,t}w_1T_0 \in \mathcal{B}_2(n,\Delta)$, obtained from $\theta_{r,s,t}v((k+k_1)^1)w_1T_0$ by deleting the edge uv and adding an edge uv_0. Let

$$G_0 = \theta_{r+k+k_1,s,t} - w_1 - uv_0 \cong \theta_{r,s,t}v((k+k_1)^1) - w_1 - uv \ .$$

First we consider the case when $r > 2$. Set

$$A_3 = Z(\theta_{r+k+k_1,s,t} - w_1) - Z(\theta_{r,s,t}v((k+k_1)^1) - w_1) \ .$$

Then,

$$\begin{aligned} Z(\theta_{r+k+k_1,s,t}) &> Z(\theta_{r,s,t}v((k+k_1)^1)) \\ Z(\theta_{r+k+k_1,s,t} - w_1) &= Z(G_0) + F_{k_1}Z(T(r+k-2,s-1,t-1)) \\ Z(\theta_{r,s,t}v((k+k_1)^1) - w_1) &= Z(G_0) + F_{k_1+1}F_kZ(T(r-2,s-1,t-1)) \end{aligned}$$

$$\begin{aligned}
A_3 &= F_{k_1}(F_{s+t}F_{r+k-1} + F_sF_tF_{r+k-2}) - F_{k_1+1}F_k(F_{s+t}F_{r-1} + F_sF_tF_{r-2}) \\
&= F_{s+t}(F_{k_1}F_{r+k-1} - F_{k_1+1}F_kF_{r-1}) + F_sF_t(F_{k_1}F_{r+k-2} - F_{k_1+1}F_kF_{r-2}) \\
&= F_{s+t}[F_{k_1}(F_rF_k + F_{r-1}F_{k-1}) - F_{k_1}F_kF_{r-1} - F_{k_1-1}F_kF_{r-1}] \\
&+ F_sF_t[F_{k_1}(F_{r-1}F_k + F_{r-2}F_{k-1}) - F_{k_1}F_kF_{r-2} - F_{k_1-1}F_kF_{r-2}] \\
&= F_{s+t}[F_{k_1}F_{r-2}F_k + F_{k_1}F_{r-1}F_{k-1} - F_{k_1-1}F_kF_{r-1}] \\
&+ F_sF_t[(F_{r-1} - F_{r-2})F_{k_1}F_k + F_{k_1}F_{r-2}F_{k-1} - F_{k_1-1}F_{r-2}F_k]\ .
\end{aligned}$$

Therefore, we have

$$\begin{aligned}
A_3 &= \frac{1}{2}F_{s+t}(F_{k_1}2F_{r-2}F_k - F_{k_1-1}F_{r-1}F_k + 2F_{k_1}F_{r-1}F_{k-1} - F_{k_1-1}F_kF_{r-1}) \\
&+ \frac{1}{2}F_sF_t(2F_{r-3}F_{k_1}F_k - F_{k_1-1}F_{r-2}F_k + 2F_{k_1}F_{r-2}F_{k-1} \\
&- F_{k_1-1}F_{r-2}F_k) \geq 0 \quad \text{if } r \geq 4
\end{aligned}$$

$$\begin{aligned}
A_3 &= F_{s+t}(F_{k_1}F_k + F_{k_1}F_{k-1} - F_{k_1-1}F_k) + F_sF_t(F_{k_1}F_{k-1} - F_{k_1-1}F_k) \\
&> F_sF_t(F_{k_1}F_{k+1} - F_{k_1-1}F_k + F_{k_1}F_{k-1} - F_{k_1-1}F_k) \\
&= F_sF_t(F_{k_1}F_k - F_{k_1-1}F_k + F_{k_1}2F_{k-1} - F_{k_1-1}F_k) \geq 0 \quad \text{if } r = 3\,.
\end{aligned}$$

Moreover it is easily checked that $A_3 > 0$ when $r = 2$ and $k_1 = 1$. Therefore, by Lemma 2.7, Lemma 3.3 holds immediately for the cases $r > 2$ as well as $r = 2$ and $k_1 = 1$.

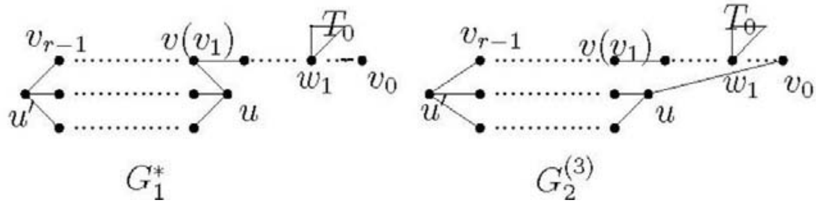


Fig. 6. Graphs used for proving Lemma 3.3.

Now we consider the case when $r = 2$ and $k_1 = 2$. In this case we find that $G_1^* = \theta_{2,s,t}v^{[k]}(2^{\Delta-2}, k_2^1) \cong \theta_{2,s,t}v((k+2)^1)w_1T_0'$ where $T_0' \cong R(2^{\Delta-3}, k_2^1)$. We construct a graph $C_{s+t,k+4}v_0T_0' \in \mathcal{B}_2(n,\Delta)$ which is obtained from $G_1^* \cong \theta_{2,s,t}v((k+2)^1)w_1T_0'$

by deleting the edge uv and adding an edge $u'v_0$ and moving the tree T_0' from w_1 to vertex v_0 as shown in Fig. 6. Let

$$G_0 = \theta_{2,s,t}v((k+2)^1) - uv \cong C_{s+t,k+4} - u'v_0$$

and

$$A_4 = Z(C_{s+t,k+4}) - v_0) - Z(\theta_{2,s,t}w_1((k+2)^1) - w_1)\ .$$

Then in a similar manner as before we have

$$\begin{aligned}
Z(C_{s+t,k+4}) &= Z(G_0) + F_{k+3}F_{s+t} = Z(\theta_{2,s,t}v((k+2)^1)) \\
Z(C_{s+t,k+4}) - v_0) &= Z(C_{s+t}(k+2)^1) = F_{s+t+k+3} + F_{s+t-1}F_{k+3} \\
Z(\theta_{2,s,t}w_1((k+2)^1) - w_1) &= 2Z(\theta_{2,s,t}w_1(k-1)^1) = 2(Z(C_{s+t}(k^1)) + F_{s+t}F_k) \\
&= 2(F_{s+t+k+1} + F_{s+t-1}F_{k+1} + F_{s+t}F_k)
\end{aligned}$$

$$\begin{aligned}
A_4 &= F_{s+t+k} + F_{s+t-1}F_k - 2F_{s+t}F_k \\
&= F_{s+t}F_{k+1} - F_{s+t}F_k + 2F_{s+t-1}F_k - F_{s+t}F_k \geq 0\ .
\end{aligned}$$

Moreover, $A_4 = 0$ holds if and only if $s+t=3$ and $k=1$. Thus by Lemma 2.7,

$$Z(C_{s+t,k+4}v_0T_0') > Z(\theta_{2,s,t}v((k+2)^1)w_1T_0')$$

except when $s+t=3$ and $k=1$.

As in the case when $s+t=3$ and $k=1$, note that $G_1^* = \theta_{2,1,2}v(3^1)v_1T_0'$ where v_1 is a vertex in a pendent path P_4 of $\theta_{2,1,2}v(3^1)$ which is adjacent to v. We consider a graph $C_{4,4}u_1T_0' \in \mathcal{B}_2(n,\Delta)$ where u_1 is a vertex in $C_{4,4}$ adjacent to the 4-vertex u of $C_{4,4}$. With a same method as above, we have $Z(C_{4,4}v_2T_0') > Z(\theta_{2,s,t}v(3^1)v_1T_0')$, which completes the proof of the lemma. ■

From Lemmas 3.1 and 3.3, the following result is obvious.

Lemma 3.4. *Suppose that G has maximal Hosoya index in $\mathcal{B}(n,\Delta)$. Then $G \in \mathcal{B}_2(n,\Delta)$.*

Let $\mathcal{B}_2^{(i)}(n,\Delta) = \{G : G \in \mathcal{B}_2(n,\Delta), \textit{the main subgraph of } G \textit{ is of type } (i)\}$ for $i = 1,2,3$. Now we state a lemma in which the possible forms of the graphs from $\mathcal{B}_2(n,\Delta)$ with greatest Hosoya index are specified.

Lemma 3.5. *For any graph* $G \in \mathcal{B}_2(n,\Delta)$, $Z(G)$ *reaches its maximum when* G *is of the form* $C_{p,q}^{(0)}(k_1^{l_1'}, k_2^{l_2'})$ *with* $l_1'+l_2' = \Delta-4$, *or of the form* $\theta_{r,s,t}^{(1)}(2^{\Delta-3}, k_2^1)$ *with* $k_2 \geq 2$.

Proof. From the definition of $\mathcal{B}_2^{(i)}(n,\Delta)$ for $i=1,2,3$, we have $\mathcal{B}_2(n,\Delta) = \bigcup_{i=1}^{3} \mathcal{B}_2^{(i)}(n,\Delta)$. Assume that $T \cong R(k_1^{l_1}, k_2^{l_2})$ with $l_1+l_2 = \Delta-2$. In order to obtain our result, we first need to prove the following three claims.

Claim 1. For any graph $G \in \mathcal{B}_2^{(2)}(n,\Delta)$ there exists a graph $G_1 \in \mathcal{B}_2^{(1)}(n,\Delta)$, such that $Z(G_1) > Z(G)$.

Proof of Claim 1. By Lemma 3.2 and Remark 2.2, we find that if $G \in \mathcal{B}_2^{(2)}(n,\Delta)$, then the maximum of $Z(G)$ is attained when G is of the form $C_{p,l,q}vT$ where v is a vertex on one cycle, say C_p, of $C_{p,l,q}$ adjacent to one of 3-vertices in $C_{p,l,q}$. Thus it suffices to show that there exists a graph $G_1 \in \mathcal{B}_1^{(2)}(n,\Delta)$, such that $Z(G_1) > Z(C_{p,l,q}vT)$.

Choose $G_1 \cong C_{p+l,q}v_1T$ where v_1 is a vertex of C_{p+l} in $C_{p+l,q}$ adjacent to the unique 4-vertex of $C_{p+l,q}$. By Lemma 2.10 and Lemma 2.1 (2),

$$\begin{aligned} Z(C_{p+l,q}) &> Z(C_{p,l,q}) \\ Z(C_{p+l,q}-v_1) = Z(C_q((p+l-2)^1)) &= F_{p+q+l-1} + F_{q-1}F_{p+l-1} = Z(C_{p,l,q}-v)\ . \end{aligned}$$

By Lemma 2.7 we have $Z(G_1) = Z(C_{p+l,q}v_1T) > Z(C_{p,l,q}vT) = Z(G)$, which completes the proof of this claim.

Claim 2. For any graph $G \in \mathcal{B}_2^{(1)}(n,\Delta)$, $Z(G)$ reaches its maximum value when G is of the form $C_{p,q}^{(0)}(k_1^{l_1'}, k_2^{l_2'})$ with $l_1'+l_2' = \Delta-4$.

Proof of Claim 2. By Lemma 3.2 and Remark 2.2, we find that if $G \in \mathcal{B}_1^{(1)}(n,\Delta)$, then the maximum value of $Z(G)$ is attained when G is of the form $C_{p,q}vT$, or of the form $C_{p',q'}uT'$ where $T' \cong R(k_1^{l_1'}, k_2^{l_2'})$ with $l_1'+l_2' = \Delta-4$. Therefore, it suffices to show that for any graph G of the form $C_{p,q}vT$, there exists a graph G_1 of the form $C_{p',q'}uT'$, such that $Z(G_1) > Z(G)$.

Let $G = C_{p,q}^{(1)}(k_1^{l_1}, k_2^{l_2}) \cong C_{p,q}vT$ and $G_1 = C_{p+k_1+k_2,q}^{(0)}(k_1^{l_1-1}, k_2^{l_2-1}) \cong C_{p+k_1+k_2,q}uT_0$ where $T_0 \cong R(k_1^{l_1-1}, k_2^{l_2-1})$. Note that $G \cong C_{p,q}v(k_1^1, k_2^1)vT_0$. From Lemma 2.4,

$$Z(C_{p+k_1+k_2,q}) > Z(C_{p,q}v(k_1^1, k_2^1))\ .$$

Set $A_1 = Z(C_{p+k_1+k_2,q} - u) - Z(C_{p,q}v(k_1^1, k_2^1) - v)$. Then we have

$$\begin{aligned} Z(C_{p+k_1+k_2,q} - u) &= F_{p+k_1+k_2}F_q \\ Z(C_{p,q}v(k_1^1, k_2^1) - v) &= F_{k_1+1}F_{k_2+1}Z(C_q((p-2)^1)) \\ &= F_{k_1+1}F_{k_2+1}(F_{p+q-1} + F_{p-1}F_{q-1}) \end{aligned}$$

$$\begin{aligned} A_1 &= F_{p+k_1+k_2}F_q - F_{p+q-1} - F_{k_1+1}F_{k_2+1}(F_{p+q-1} + F_{p-1}F_{q-1}) \\ &= (F_pF_{1+k_1+k_2} + F_{p-1}F_{k_1+k_2})F_q - F_{k_1+1}F_{k_2+1}(F_pF_q + 2F_{p-1}F_{q-1}) \\ &= F_pF_qF_{k_1}F_{k_2} + F_{p-1}F_qF_{k_1+k_2} - 2F_{k_1+1}F_{k_2+1}F_{p-1}F_{q-1} \ . \end{aligned}$$

Direct calculation shows that $A_1 > 0$ if $k_1 = k_2 = 1$, or $k_1 = 1$ and $k_2 = 2$.

Therefore, by Lemma 2.7, we have $Z(G_1) > Z(G)$ as desired, except when $k_1 = 2$.

If $k_1 = 2$, then

$$G = C_{p,q}^{(1)}(2^{\Delta-3}, (k+2)^1) \cong C_{p,q}v(2^2, (k+2)^1)vT_1$$

where $T_1 \cong R(2^{\Delta-5})$. We choose the graph

$$G_1 = C_{3,3}^{(0)}(2^{\Delta-5}, (p+q+k)^1) \cong C_{3,3}u((p+q+k)^1)uT_1$$

and set

$$A_2 = Z(C_{3,3}u((p+q+k)^1) - u) - Z(C_{p,q}v(2^2, (k+2)^1) - v)$$

and

$$B_2 = Z(C_{3,3}u((p+q+k)^1)) - Z(C_{p,q}v(2^2, (k+2)^1)) \ .$$

Similarly as before, we have

$$\begin{aligned} Z(C_{3,3}u((p+q+k)^1) - u) &= 4F_{p+q+k+1} \\ Z(C_{p,q}v(2^2, (k+2)^1) - v) &= 4F_{k+3}(F_{p+q-1} + F_{p-1}F_{q-1}) \\ Z(C_{3,3}u((p+q+k)^1)) &= 4F_{p+q+k+1} + 8F_{p+q+k+1} + 4F_{p+q+k} \\ &= 4(F_{p+q+k+3} + F_{p+q+k+1}) \end{aligned}$$

$$\begin{aligned} & Z(C_{p,q}v(2^2, (k+2)^1)) = 4F_{k+3}Z(C_q((p-2)^1)) + 4F_{k+2}Z(C_q((p-2)^1)) \\ + \ & 4F_{k+3}F_{p-1}F_q + 2F_3F_{k+3}Z(C_q((p-2)^1)) + 4F_{k+3}Z(C_q((p-3)^1)) \\ = \ & 4F_{k+5}(F_{p+q-1} + F_{p-1}F_{q-1}) + 4F_{k+3}(F_{p+q-2} + F_{p-2}F_{q-1} + F_{p-1}F_q) \\ = \ & 4F_{k+5}(F_{p+q-1} + F_{p-1}F_{q-1}) + 8F_{k+3}F_{p+q-2} \end{aligned}$$

$$\begin{aligned}
A_2 &= 4(F_{k+3}F_{p+q-1} - F_{k+3}F_{p+q-1} - F_{k+3}F_{p-1}F_{q-1} + F_{k+2}F_{p+q-2}) \\
&= 4(F_{k+2}F_{p-1}F_q + F_{k+2}F_{p-2}F_{q-1} - F_{k+2}F_{p-1}F_{q-1} - F_{k+1}F_{p-1}F_{q-1}) \\
&= 4(F_{k+2}F_{p-1}F_{q-2} + F_{k+2}F_{p-2}F_{q-1} - F_{k+1}F_{p-1}F_{q-1}) \\
&= 2(F_{k+2}F_{p-1}2F_{q-2} - F_{k+1}F_{p-1}F_{q-1} + F_{k+2}2F_{p-2}F_{q-1} - F_{k+1}F_{p-1}F_{q-1}) \geq 0
\end{aligned}$$

$$\begin{aligned}
B_2 &= 4[F_{p+q+k+3} - F_{k+5}(F_{p+q-1} + F_{p-1}F_{q-1})] \\
&+ 4(F_{k+3}F_{p+q-1} + F_{k+2}F_{p+q-2} - 2F_{k+3}F_{p+q-2}) \\
&= 4(F_{k+4}F_{p+q-2} - F_{k+4}F_{p-1}F_{q-1} - F_{k+3}F_{p-1}F_{q-1}) \\
&+ 4(F_{k+2}F_{p+q-2} - F_{k+3}F_{p+q-4}) \\
&= 4(F_{k+4}F_{p-1}F_q + F_{k+4}F_{p-2}F_{q-1} - F_{k+4}F_{p-1}F_{q-1} - F_{k+3}F_{p-1}F_{q-1}) \\
&+ 4(F_{k+2}F_{p+q-2} - F_{k+3}F_{p+q-4}) \\
&= 4(F_{k+4}F_{p-1}F_{q-2} + F_{k+4}F_{p-2}F_{q-1} - F_{k+3}F_{p-1}F_{q-1}) \\
&+ 4(F_{k+2}F_{p+q-2} - F_{k+3}F_{p+q-4}) \\
&= 2(F_{k+4}F_{p-1}2F_{q-2} - F_{k+3}F_{p-1}F_{q-1} + F_{k+4}2F_{p-2}F_{q-1} - F_{k+3}F_{p-1}F_{q-1}) \\
&+ 4(F_{k+2}F_{p+q-3} - F_{k+1}F_{p+q-4}) \\
&\geq 4F_{k+1}F_{p+q-5} > 0\ .
\end{aligned}$$

Note that the last inequality holds because of the fact that $p+q \geq 6$. Using Lemma 2.7, we have

$$Z(G_1) = Z(C_{3,3}u((p+q+k)^1)uT_1) > Z(C_{p,q}v(2^2,(k+2)^1)vT_1) = Z(G)$$

which completes the proof of Claim 2.

By Lemma 3.2 and Remark 2.2, we find that if $G \in \mathcal{B}_2^{(3)}(n,\Delta)$, then the maximum value of $Z(G)$ is attained when G is of the form $\theta_{r,s,t}^{(1)}(k_1^{l_1},k_2^{l_2})$ with $l_1+l_2=\Delta-2$ and $r \geq 2$. In order to obtain this lemma, it suffices to prove:

Claim 3. For any graph $G \in \mathcal{B}_2^{(3)}(n,\Delta)$ of the form $\theta_{r,s,t}^{(1)}(k_1^{l_1},k_2^{l_2})$ with $k_1=1$, there exists a graph $G_1 \in \mathcal{B}_2^{(1)}(n,\Delta)$, such that $Z(G_1) > Z(G)$.

Proof of Claim 3. Suppose that $G=\theta^{(1)}_{r,s,t}(k_1^{l_1},k_2^{l_2})$ with $k_1=1$ and $r\geq 2$. We now construct a graph

$$G_1=C^{(0)}_{r+s+t-1,k_2+2}(1^{l_1-1},k_2^{l_2-1})\cong C_{r+s+t-1,k_2+2}uT_2$$

where $T_2\cong R(1^{l_1-1},k_2^{l_2-1})$. Note that $G\cong\theta_{r,s,t}v(1^1,k_2^1)vT_2$. Setting

$$A_3=Z(C_{r+s+t-1,k_2+2}-u)-Z(\theta_{r,s,t}v(1^1,k_2^1)-v)$$

and

$$B_3=Z(C_{r+s+t-1,k_2+2})-Z(\theta_{r,s,t}v(1^1,k_2^1))$$

we arrive at

$$\begin{aligned}
Z(\theta_{r,s,t}v(1^1,k_2^1)) &= (F_{k_2}+2F_{k_2+1})Z(C_{s+t}((r-2)^1))\\
&+ F_{k_2+1}Z(T(r-2,s-1,t-1))+F_{k_2+1}Z(C_{s+t}((r-3)^1))\\
&= F_{k_2+2}(F_{r+s+t-1}+F_{r-1}F_{s+t-1})+F_{k_2+1}(F_{r+s+t-1}+F_{r-1}F_{s+t-1})\\
&+ F_{k_2+1}(F_{s+t}F_{r-1}+F_sF_tF_{r-2})+F_{k_2+1}(F_{r+s+t-2}+F_{r-2}F_{s+t-1})\\
&= F_{k_2+2}(F_{r+s+t-1}+F_{r-1}F_{s+t-1})\\
&+ F_{k_2+1}(F_{r+s+t}+F_{r+s+t-2}+F_{r-1}F_{s+t-1}+F_sF_tF_{r-2})
\end{aligned}$$

$$\begin{aligned}
Z(C_{r+s+t-1,k_2+2}) &= F_{k_2+2}F_{r+s+t-1}+2F_{k_2+1}F_{r+s+t-1}+2F_{k_2+2}F_{r+s+t-2}\\
&= F_{k_2+2}F_{r+s+t}+2F_{k_2+1}F_{r+s+t-1}+F_{k_2+2}F_{r+s+t-2}
\end{aligned}$$

$$\begin{aligned}
Z(\theta_{r,s,t}v(1^1,k_2^1)-v) &= F_{k_2+1}Z(C_{s+t}((r-2)^1))=F_{k_2+1}(F_{r+s+t-1}+F_{r-1}F_{s+t-1})\\
Z(C_{r+s+t-1,k_2+2}-u) &= F_{k_2+2}F_{r+s+t-1}
\end{aligned}$$

$$\begin{aligned}
A_3 &= F_{k_2}F_{r+s+t-1}-F_{k_2+1}F_{r-1}F_{s+t-1}\\
&= F_{k_2}F_rF_{s+t}+F_{k_2}F_{r-1}F_{s+t-1}-F_{k_2+1}F_{r-1}F_{s+t-1}\\
&= F_{k_2}F_rF_{s+t}-F_{k_2-1}F_{r-1}F_{s+t-1}>0
\end{aligned}$$

$$\begin{aligned}
B_3 &= F_{k_2+2}F_{r+s+t} + 2F_{k_2+1}F_{r+s+t-1} + F_{k_2+2}F_{r+s+t-2} \\
&- F_{k_2+2}(F_{r+s+t-1} + F_{r-1}F_{s+t-1}) - F_{k_2+1}(F_{r+s+t} + F_{r+s+t-2} \\
&+ F_{r-1}F_{s+t-1} + F_sF_tF_{r-2}) \\
&= F_{k_2}(F_{r+s+t} + F_{r+s+t-2}) + F_{k_2+1}(2F_{r-1}F_{s+t+1} \\
&+ 2F_{r-2}F_{s+t} - F_{r-1}F_{s+t-1} - F_sF_tF_{r-2}) - F_{k_2+2}(F_{r+s+t-1} + F_{r-1}F_{s+t-1}) \\
&= F_{k_2}(F_{r+s+t} + F_{r+s+t-2}) + F_{k_2+1}(F_rF_{s+t} + F_{r+s+t-1} - F_sF_tF_{r-2}) \\
&- F_{k_2+2}(F_{r+s+t-1} + F_{r-1}F_{s+t-1}) \\
&= F_{k_2}F_{r+s+t} - F_{k_2}F_{r+s+t-1} + F_{k_2}F_{r+s+t-2} + F_{k_2+1}(F_rF_{s+t} - F_sF_tF_{r-2}) \\
&- F_{k_2+2}F_{r-1}F_{s+t-1} \\
&= 2F_{k_2}F_{r+s+t-2} + F_{k_2+1}(F_rF_{s+t} - F_sF_tF_{r-2}) - F_{k_2+2}F_{r-1}F_{s+t-1} \\
&> 2F_{k_2}F_{r+s+t-2} + F_{k_2+1}F_{r-1}F_sF_t - F_{k_2+2}F_{r-1}F_{s+t-1}\ .
\end{aligned}$$

It is not difficult to check that

$$2F_{k_2}F_{r+s+t-2} + F_{k_2+1}F_{r-1}F_sF_t - F_{k_2+2}F_{r-1}F_{s+t-1} > 0$$

if $k_2 = 1$ or $k_2 = 2$, that is to say, $B_3 > 0$ when $k_2 = 1$ or $k_2 = 2$.

Thanks to Lemma 2.7 again, we have $Z(G_1) > Z(G)$, as desired. This completes the proof of Claim 3.

Combining Claims 1, 2 and 3, Lemma 3.5 follows immediately. ■

Lemma 3.6. *For any graph G of the form $\theta^{(1)}_{r,s,t}(2^{\Delta-3}, k_2^1)$ with $r > 2$ and $k_2 \geq 2$, there exists a graph $G_1 \in \mathcal{B}^{(1)}_2(n,\Delta)$, such that $Z(G_1) > Z(G)$.*

Proof. In order to obtain the result in this lemma, we have to prove the following two claims.

Claim 1. For a graph $G_0 = \theta^{(1)}_{r,s,t}(2^{\Delta-3}, (k+2)^1)$ with $k > 0$, there exists a graph $\theta^{(1)}_{r',s',t'}(2^{\Delta-2})$ of the same order as G_0, such that $Z(\theta^{(1)}_{r',s',t'}(2^{\Delta-2})) > Z(G_0)$.

Proof of Claim 1. Let $T_1 \cong R(2^{\Delta-3})$. Note that $G_0 \cong \theta^{(1)}_{r,s,t}v((k+2)^1)vT_1$. From the fact that $s+t \geq 3$ in $\theta^{(1)}_{r,s,t}v((k+2)^1)vT_1$, we find that one of the two positive integers s and t is greater than 1. Without loss of generality, we may assume that

$s \geq 2$. Let $r' = r$, $s' = s+k$, and $t' = t$. Choose the graph $G = \theta^{(1)}_{r,s+k,t}(2^{\Delta-2})$. Clearly, $G \cong \theta^{(1)}_{r,s+k,t}v(2^1)vT_0$. Now we only need to prove that

$$Z(\theta^{(1)}_{r,s+k,t}v(2^1)vT_0) > Z(\theta^{(1)}_{r,s,t}v((k+2)^1)vT_0) .$$

Set

$$A_1 = Z(\theta^{(1)}_{r,s+k,t}v(2^1) - v) - Z(\theta^{(1)}_{r,s,t}v((k+2)^1) - v)$$

and

$$B_1 = Z(\theta^{(1)}_{r,s+k,t}v(2^1)) - Z(\theta^{(1)}_{r,s,t}v((k+2)^1)) .$$

Then by Lemmas 2.1, 2.5, and 2.8,

$$\begin{aligned}
Z(\theta^{(1)}_{r,s+k,t}v(2^1) - v) &= F_3 Z(C_{s+t+k}((r-2)^1)) = F_3(F_{r+s+t+k-1} + F_{s+t+k-1}F_{r-1}) \\
Z(\theta^{(1)}_{r,s,t}v((k+2)^1) - v) &= F_{k+3} Z(C_{s+t}((r-2)^1)) = F_{k+3}(F_{r+s+t-1} + F_{s+t-1}F_{r-1})
\end{aligned}$$

$$\begin{aligned}
Z(\theta^{(1)}_{r,s+k,t}v(2^1)) &= (F_3+1)Z(C_{s+t+k}((r-2)^1)) + F_3 Z(T(r-2, s+k-1, t-1)) \\
&+ F_3 Z(C_{s+t+k}((r-3)^1)) \\
&= F_4(F_{r+s+t+k-1} + F_{s+t+k-1}F_{r-1}) + F_3(F_{r-1}F_{s+t+k} + F_{r-2}F_{s+k}F_t) \\
&+ F_3(F_{r+s+t+k-2} + F_{s+t+k-1}F_{r-2})
\end{aligned}$$

$$\begin{aligned}
Z(\theta^{(1)}_{r,s,t}v((k+2)^1)) &= F_{k+4}(F_{r+s+t-1} + F_{s+t-1}F_{r-1}) + F_{k+3}(F_{r-1}F_{s+t} + F_{r-2}F_sF_t) \\
&+ F_{k+3}(F_{r+s+t-2} + F_{s+t-1}F_{r-2})
\end{aligned}$$

$$\begin{aligned}
A_1 &= F_3F_{r+s+t+k-1} - F_{k+3}F_{r+s+t-1} + F_{r-1}(F_3F_{s+t+k-1} - F_{k+3}F_{s+t-1}) \\
&= F_3F_{k+1}F_{r+s+t-1} + F_3F_kF_{r+s+t-2} - F_3F_{k+1}F_{r+s+t-1} - F_2F_kF_{r+s+t-1} \\
&+ F_{r-1}(F_3F_{k+1}F_{s+t-1} + F_3F_kF_{s+t-2} - F_3F_{k+1}F_{s+t-1} - F_2F_kF_{s+t-1}) \\
&= F_kF_{r+s+t-4} + F_{r-1}(2F_{s+t-2} - F_{s+t-1}) > 0
\end{aligned}$$

$$\begin{aligned}
B_1 &= A_1 + F_{r+s+t+k-1} - F_{k+2}F_{r+s+t-1} + F_{r-1}(F_{s+t+k-1} - F_{k+2}F_{s+t-1}) \\
&+ F_{r-2}(F_3F_{s+t+k-1} - F_{k+3}F_{s+t-1}) + F_{r-1}(F_3F_{s+t+k} - F_{k+3}F_{s+t}) \\
&+ F_{r-2}F_t(F_3F_{s+k} - F_{k+3}F_s) + F_3F_{r+s+t+k-2} - F_{k+3}F_{r+s+t-2} \\
&= A_1 + F_k(F_{r+s+t-2} - F_{r+s+t-1}) + F_{r-1}F_k(F_{s+t-2} - F_{s+t-1}) \\
&+ F_{r-2}F_k(2F_{s+t-2} - F_{s+t-1}) + F_{r-1}F_k(2F_{s+t-1} - F_{s+t}) \\
&+ F_{r-2}F_tF_k(2F_{s-1} - F_s) + F_k(2F_{r+s+t-3} - F_{r+s+t-2})
\end{aligned}$$

$$
\begin{aligned}
&= F_kF_{r+s+t-4} + F_{r-1}(2F_{s+t-2} - F_{s+t-1}) - F_kF_{r+s+t-3} - F_{r-1}F_kF_{r+s+t-3} \\
&+ F_{r-2}F_k(2F_{s+t-2} - F_{s+t-1}) + F_{r-1}F_k(2F_{s+t-1} - F_{s+t}) \\
&+ F_{r-2}F_tF_k(2F_{s-1} - F_s) + F_k(2F_{r+s+t-3} - F_{r+s+t-2}) \\
&= F_kF_{r+s+t-4} + F_{r-1}(2F_{s+t-2} - F_{s+t-1}) - F_kF_{r+s+t-3} \\
&+ F_{r-2}F_k(2F_{s+t-2} - F_{s+t-1}) + F_{r-2}F_tF_k(2F_{s-1} - F_s) \\
&+ F_k(2F_{r+s+t-3} - F_{r+s+t-2}) \\
&= F_{r-1}(2F_{s+t-2} - F_{s+t-1}) + F_{r-2}F_k(2F_{s+t-2} - F_{s+t-1}) \\
&+ F_{r-2}F_tF_k(2F_{s-1} - F_s) \geq 0 \ .
\end{aligned}
$$

From Lemma 2.7 it follows that $Z(G) > Z(G_0)$, which completes the proof of Claim 1.

Claim 2. For a graph $G = \theta^{(1)}_{r,s,t}(2^{\Delta-2})$ with $r > 2$, there exists a graph $C^{(0)}_{p,q}(2^{\Delta-4})$ of the same order as G, such that $Z(C^{(0)}_{p,q}(2^{\Delta-4})) > Z(G)$.

Proof of Claim 2. Let $T_2 \cong R(2^{\Delta-4})$. Note that $G \cong \theta^{(1)}_{r,s,t}v(2^2)vT_2$. Let $p = 3$ and $q = r+s+t+1$. We choose a graph $G_1 = C^{(0)}_{3,r+s+t+1}(2^{\Delta-4})$. Clearly, $G \cong C_{5,r+s+t+1}uT_2$. Now we only need to prove that

$$Z(C_{3,r+s+t+1}uT_2) > Z(\theta^{(1)}_{r,s,t}v(2^2)vT_2) \ .$$

Set

$$A_2 = Z(C_{3,r+s+t+1} - u) - Z(\theta^{(1)}_{r,s,t}v(2^2) - v)$$

and

$$B_2 = Z(C_{3,r+s+t+1}) - Z(\theta^{(1)}_{r,s,t}v(2^2))$$

and then we have

$$
\begin{aligned}
Z(C_{3,r+s+t+1} - u) &= 2F_{r+s+t+1} \\
Z(\theta^{(1)}_{r,s,t}v(2^2) - v) &= 4Z(C_{s+t}((r-2)^1)) = 4(F_{r+s+t-1} + F_{r-1}F_{s+t-1}) \\
Z(C_{3,r+s+t+1}) &= 2F_{r+s+t+1} + 2F_{r+s+t+1} + 4F_{r+s+t} = 4F_{r+s+t+2}
\end{aligned}
$$

$$
\begin{aligned}
Z(\theta^{(1)}_{r,s,t}v(2^2)) &= (4+4)Z(C_{s+t}((r-2)^1)) + 4Z(C_{s+t}((r-3)^1)) \\
&+ 4Z(T(r-2, s-1, t-1)) \\
&= 8(F_{r+s+t-1} + F_{r-1}F_{s+t-1}) + 4(2F_{r+s+t-2} + F_sF_tF_{r-2})
\end{aligned}
$$

$$\begin{aligned} A_2 &= 2(F_{r+s+t-2} - 2F_{s+t-1}F_{r-1}) \\ &= 2(F_rF_{s+t-1} - F_{r-1}F_{s+t-1} + F_{r-1}F_{s+t-2} - F_{r-1}F_{s+t-1}) \\ &= 2(F_{r-2}F_{s+t-1} - F_{r-1}F_{s+t-3}) \\ &= 2(F_{r-2}F_{s+t-2} - F_{r-3}F_{s+t-3}) \geq 0 \quad \text{when } r \geq 3 \end{aligned}$$

$$\begin{aligned} B_2 &= 4(F_{r+s+t+2} - 2F_{r+s+t-1} - 2F_{r-1}F_{s+t-1} - 2F_{r+s+t-2} - F_sF_tF_{r-2}) \\ &= 4(F_rF_{s+t} + F_{r-1}F_{s+t-1} - 2F_{r-1}F_{s+t-1} - F_sF_tF_{r-2}) \\ &= 4(F_rF_{s+t} - F_{r-1}F_{s+t-1} - F_sF_tF_{r-2}) \\ &> 4(F_{r-1}F_{s+t} - F_{r-1}F_{s+t-1}) > 0\ . \end{aligned}$$

Again, by Lemma 2.7, $Z(G_1) > Z(G)$, and the proof of Claim 2 is complete.

Combining Claims 1 and 2, Lemma 3.6 follows immediately. ■

Let $\mathcal{G}_0 = \{\theta^{(1)}_{2,s,t}(2^{\Delta-2}) : s,t > 0 \ and\ s+t = n-2\Delta+3 > 3\}$. From Lemmas 3.4, 3.5, 3.6, and the proof of Claim 1 in Lemma 3.6, the following lemma holds immediately.

Lemma 3.7. *Suppose that $G \in \mathcal{B}(n,\Delta)$ has maximal Hosoya index. Then G must be either of the form $C^{(0)}_{p,q}(k_1^{l_1}, k_2^{l_2})$ with $l_1 + l_2 = \Delta - 4$, or must belong to the set $\mathcal{G}_0$.*

In the following two theorems the graphs from $\mathcal{B}(n,\Delta)$ with maximal Hosoya index are completely characterized.

Theorem 3.1. *If $\Delta > (n+3)/2$, then the graph $G \in \mathcal{B}(n,\Delta)$, maximizing the Hosoya index, is $C^{(0)}_{3,3}(1^{2\Delta-3-n}, 2^{n-1-\Delta})$ with $Z(C^{(0)}_{3,3}(1^{2\Delta-3-n}, 2^{n-1-\Delta})) = (3\Delta - n - 1)2^{n-\Delta}$.*

Proof. When $\Delta > (n+3)/2$, we claim that the graph G from $\mathcal{B}(n,\Delta)$ with maximal Hosoya index must be of the form $C^{(0)}_{p,q}(k_1^{l_1}, k_2^{l_2})$ with $l_1 + l_2 = \Delta - 4$. If not, then by Lemma 3.7, G must be $\theta^{(1)}_{2,s,t}(2^{\Delta-2})$ with $s+t \geq 3$. But the order of $\theta^{(1)}_{2,s,t}(2^{\Delta-2})$ is $2+s+t+2(\Delta-2) \geq 2\Delta+1 > n+4 > n$. This is impossible since G has n vertices.

Suppose that $G \cong C^{(0)}_{p,q}(k_1^{l_1}, k_2^{l_2})$ with $l_1 + l_2 = \Delta - 4$. We claim that $k_1 = 1$. The other option would be $k_1 = 2$. However, then the order of G would be at least $2(\Delta-4)+5 = 2\Delta+3 > n$, which again contradicts the fact that $G \in \mathcal{B}(n,\Delta)$.

If $k_2 = 2$, then we can assume that $G \cong C_{p,q}^{(0)}(1^x, 2^y)$ with $x, y > 0$ and $x + y = \Delta - 4$. If one of p and q is greater than 4, without loss of generality, we assume that $p > 4$. Set

$$A = Z(C_{p-1,q}^{(0)}(1^{x-1}, 2^{y+1})) - Z(C_{p,q}^{(0)}(1^x, 2^y)) .$$

By Lemmas 2.1 and 2.5, we have

$$\begin{aligned} Z(C_{p,q}^{(0)}(1^x, 2^y)) &= 2^y F_p F_q + 2F_{p-1}F_q 2^y + 2F_p F_{q-1} 2^y + y2^{y-1}F_p F_q + x2^y F_p F_q \\ &= 2^y(F_{p+q} + F_{p-1}F_q + F_p F_{q-1}) + (2x + y)2^{y-1}F_p F_q \\ Z(C_{p-1,q}^{(0)}(1^{x-1}, 2^{y+1})) &= 2^{y+1}(F_{p+q-1} + F_{p-2}F_q + F_{p-1}F_{q-1}) \\ &+ (2x + y - 1)2^y F_{p-1}F_q \end{aligned}$$

$$\begin{aligned} A &= 2^y(2F_{p+q-1} + 2F_{p-2}F_q + 2F_{p-1}F_{q-1} - F_{p+q} - F_{p-1}F_q - F_p F_{q-1}) \\ &+ (2x + y)2^{y-1}F_{p-1}F_q - (2x + y)2^y F_p F_q - 2^y F_{p-1}F_q \\ &= 2^y(F_{p+q-3} + F_{p-4}F_q + F_{p-3}F_{q-1}) + (2x + y)2^{y-1}(2F_{p-1}F_q - F_p F_q) - 2^y F_{p-1}F_q \\ &= 2^y(F_{p-2}F_q + 2F_{p-3}F_{q-1} + F_{p-4}F_q - F_{p-1}F_q) + (2x + y)2^{y-1}F_{p-3}F_q \\ &> 2^y(F_{p-3}2F_{q-1} - F_{p-3}F_q + F_{p-4}F_q) > 0 . \end{aligned}$$

Therefore, decreasing by one the length of one cycle of length greater than 4 in $C_{p,q}^{(0)}(1^x, 2^y)$ and replacing one pendent edge attached to the 4-vertex in it by a path P_3, the obtained graph has a greater Hosoya index than $C_{p,q}^{(0)}(1^x, 2^y)$. By repeating this transformation, we find that G must be $C_{3,3}^{(0)}(1^{2\Delta-3-n}, 2^{n-1-\Delta})$.

For the case of $k_2 = 1$, we claim that $p > 3$ or $q > 3$ in $G \cong C_{p,q}^{(0)}(1^{\Delta-4})$ since $\Delta < n-1$. Using a similar method as above, we can construct a new graph G' having a greater Hosoya index than G. This is a contradiction to the choice of G.

By Lemma 2.1 and by a simple calculation, we obtain

$$Z(C_{3,3}^{(0)}(1^{2\Delta-3-n}, 2^{n-1-\Delta})) = (3\Delta - n - 1)2^{n-\Delta}$$

which completes the proof of the theorem. ■

Theorem 3.2. *Suppose that* $4 \le \Delta \le (n+3)/2$ *and that the graph* G *has maximal Hosoya index in* $\mathcal{B}(n,\Delta)$ *. Then*
(a) if $n/2 \le \Delta \le (n+3)/2$ *, or* $4 \le \Delta \le 10$ *, then* $G \cong C^{(0)}_{3,n-2\Delta+6}(2^{\Delta-4})$ *;*

(b) if $11 \le \Delta < n/2$ *, then* G *is any graph from* $\{\theta^{(1)}_{2,s,t}(2^{\Delta-2}) : s,t > 0$ *and* $s+t = n-2\Delta+3\}$ *.*

Proof. From Lemma 3.7 and the proof of Theorem 3.1, we find that if $4 \le \Delta \le (n+3)/2$, then the graph G is either of the form $C^{(0)}_{p,q}(2^{\Delta-5}, k_2^1)$ with $k_2 \ge 2$, or belongs to the set $\mathcal{G}_0$. Now we prove:

Claim 1. For a graph $G_1 = C^{(0)}_{p,q}(2^{\Delta-5}, (k+2)^1)$ with $k > 0$, there exists a graph G_2 of the same order as G_1, such that $Z(G_2) > Z(G_1)$.

Proof of Claim 1. Let $T \cong R(2^{\Delta-5})$. Clearly, $G_1 = C^{(0)}_{p,q}((k+2)^1)uT$. Now we consider a graph $G_2 = C^{(0)}_{p+k,q}(2^{\Delta-4}) \cong C^{(0)}_{p+k,q}(2^1)uT$. Set

$$A_1 = Z(C^{(0)}_{p+k,q}(2^1) - u) - Z(C^{(0)}_{p,q}((k+2)^1) - u)$$

and

$$B_1 = Z(C^{(0)}_{p+k,q}(2^1)) - Z(C^{(0)}_{p,q}((k+2)^1))$$

which by Lemmas 2.1, 2.5, 2.8, and Corollary 2.1, yields

$$\begin{aligned}
Z(C^{(0)}_{p+k,q}(2^1) - u) &= F_3 F_{p+k} F_q \\
Z(C^{(0)}_{p,q}((k+2)^1) - u) &= F_{k+3} F_p F_q \\
Z(C^{(0)}_{p+k,q}(2^1)) &= (F_3+1) F_{p+k} F_q + 2F_3 F_{p+k-1} F_q + 2F_3 F_{p+k} F_{q-1} \\
Z(C^{(0)}_{p,q}((k+2)^1)) &= (F_{k+3} + F_{k+2}) F_p F_q + 2F_{k+3} F_{p-1} F_q + 2F_{k+3} F_p F_{q-1} \\
A_1 &= F_q (F_3 F_{p+k} - F_{k+3} F_p) \ge 0
\end{aligned}$$

$$\begin{aligned}
B_1 &= A_1 + F_{p+k}F_q - F_{k+2}F_pF_q + 2(F_3F_{p+k-1}F_q + F_3F_{p+k}F_{q-1}) \\
&- 2(F_{k+3}F_{p-1}F_q + F_{k+3}F_pF_{q-1}) \\
&= A_1 + 2F_kF_q(2F_{p-2} - F_{p-1}) + 2F_{q-1}F_k(2F_{p-1} - F_p) + F_{p+k}F_q - F_{k+2}F_pF_q \\
&= F_qF_kF_{p-3} + 2F_kF_q(2F_{p-2} - F_{p-1}) + 2F_{q-1}F_kF_{p-3} - F_qF_kF_{p-2} \\
&= F_qF_kF_{p-3} + 2F_{q-1}F_kF_{p-3} + F_kF_q(3F_{p-2} - 2F_{p-1}) \\
&= F_qF_k(2F_{p-2} - F_{p-1}) + 2F_{q-1}F_kF_{p-3} \\
&> F_qF_k(2F_{p-2} - F_{p-1} + F_{p-3}) = F_qF_kF_{p-2} > 0 \ .
\end{aligned}$$

Therefore, by Lemma 2.7, $Z(G_2) > Z(G_1)$, and Claim 1 follows.

Considering Claim 1, G is either of the form $C^{(0)}_{p,q}(2^{\Delta-4})$ with $p,q \geq 3$ and $p+q = n-2\Delta+9$, or belongs to $\mathcal{G}_0$. From Lemmas 2.1 and 2.5 it follows that $p+q = n-2\Delta+9$ and we have

$$\begin{aligned}
Z(C^{(0)}_{p,q}(2^{\Delta-4})) &= 2^{\Delta-4}F_pF_q + 2^{\Delta-4}2F_{p-1}F_q + 2^{\Delta-4}2F_{p-1}F_q + (\Delta-4)2^{\Delta-5}F_pF_q \\
&= 2^{\Delta-4}F_{p+q} + 2^{\Delta-4}(F_{p-1}F_q + F_{p-1}F_q) + (\Delta-4)2^{\Delta-5}F_pF_q \\
&= 2^{\Delta-4}(F_{p+q} + F_{p+q-2}) + 2^{\Delta-5}[(\Delta-4)F_pF_q + 2F_{p-1}F_{q-1}] \\
&= 2^{\Delta-4}(F_{p+q} + F_{p+q-2} + F_{p+q-1}) + 2^{\Delta-5}(\Delta-6)F_pF_q \\
&= 2^{\Delta-3}F_{n-2\Delta+9} + 2^{\Delta-5}(\Delta-6)F_pF_{n-2\Delta+9-p} \ .
\end{aligned}$$

From Lemma 2.6, we find that $Z(C^{(0)}_{p,q}(2^{\Delta-4}))$ reaches its maximum value at $p = 3$, and that

$$Z(C^{(0)}_{3,n-2\Delta+6}(2^{\Delta-4})) = 2^{\Delta-3}F_{n-2\Delta+9} + 2^{\Delta-4}(\Delta-6)F_{n-2\Delta+6} \ .$$

For any graph $G_0 = \theta^{(1)}_{2,s,t}(2^{\Delta-2}) \in \mathcal{G}_0$, from Lemmas 2.1 and 2.2, considering $s+t = n-2\Delta+3$, we have

$$\begin{aligned}
Z(G_0) &= 2^{\Delta-2}Z(C_{s+t}) + (\Delta-2)2^{\Delta-2}Z(C_{s+t}) + 2^{\Delta-2}2Z(P_{s+t-1}) \\
&= \Delta 2^{\Delta-3}(F_{n-2\Delta+4} + F_{n-2\Delta+2}) + 2^{\Delta-1}F_{n-2\Delta+3} \ .
\end{aligned}$$

If $n/2 < \Delta \leq (n+3)/2$, then we claim that G is not in $\mathcal{G}_0$. Otherwise the order of $G = \theta^{(1)}_{2,s,t}(2^{\Delta-2})$ would be $s+t+1+2(\Delta-2) = s+t+2\Delta-3 \geq 2\Delta > n$, which is impossible. From the above arguments, we conclude that $G \cong C^{(0)}_{3,n-2\Delta+6}(2^{\Delta-4})$ with $Z(C^{(0)}_{3,n-2\Delta+6}(2^{\Delta-4})) = 2^{\Delta-3}F_{n-2\Delta+9} + 2^{\Delta-4}(\Delta-6)F_{n-2\Delta+6}$.

Set $D = Z(C^{(0)}_{3,n-2\Delta+6}(2^{\Delta-4})) - Z(\theta^{(1)}_{2,s,t}(2^{\Delta-2}))$. For the case when $\Delta \leq n/2$, we have

$$\begin{aligned} D &= 2^{\Delta-4}[2F_{n-2\Delta+9} + (\Delta-6)F_{n-2\Delta+6} - 2\Delta(F_{n-2\Delta+4} + F_{n-2\Delta+2}) - 8F_{n-2\Delta+3}] \\ &= 2^{\Delta-4}[2(F_4F_{n-2\Delta+6} + F_3F_{n-2\Delta+5}) - 6F_{n-2\Delta+6} - 8F_{n-2\Delta+3} \\ &+ \Delta(F_{n-2\Delta+3} - 2F_{n-2\Delta+2})] \\ &= 2^{\Delta-4}[4F_{n-2\Delta+2} - \Delta F_{n-2\Delta}] . \end{aligned}$$

It is easy to see that $D > 0$ if $4 \leq \Delta < 11$ or $\Delta = n/2$, and $D < 0$ if $11 \leq \Delta < n/2$. Therefore our result in this theorem follows immediately. ■

* * * * *

As a concluding remark we note that the chemically interesting cases are $\Delta = 3$ and $\Delta = 4$. This is because the usual molecular graphs to which the Hosoya index is applied have maximum vertex degrees not greater than 4. The case $\Delta = 3$ was implicitly resolved long time ago [9, 10], see at the beginning of Section 3. The bicyclic molecular graphs with maximal Hosoya index and $\Delta = 4$ are determined within Theorem 3.2 (a).

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