MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **68** (2012) 855-870

ISSN 0340 - 6253

Minimizing the $(2n, q)$-Graphs with Perfect Matchings in Terms of the Hosoya Index

Wen-Huan Wang*

Department of Mathematics, Shanghai University, Shanghai 200444, China

(Received December 12, 2011)

The Hosoya index of a graph is defined as the total number of matchings of the graph. Ordering of the graphs with perfect matchings having $2n$ vertices and q edges according to their minimal Hosoya indices is investigated. We characterize the first two graphs for $q = 2n-1, 2n$ and obtain the first three graphs for $q = 2n+1$. For $2n+2 \leq q \leq 3n-3$, we deduce the first two graphs.

1. INTRODUCTION

The Hosoya index for a graph was introduced by Hosoya in 1971 [1] and was subsequently named as the Hosoya index [2]. The Hosoya index of G, denoted by $Z(G)$, is defined as follows:

$$Z(G) = \sum_{k=0}^{[n/2]} m(G, k), \tag{1}$$

where n is the number of vertices of G and $m(G, k)$ is the number of k-matchings in G, k is a positive integer and $0 \leq k \leq [n/2]$. Obviously, $m(G, 1) = n$. In addition, it is consistent to define $m(G, 0) = 1$.

As is well known, the Hosoya index is closely related with various thermodynamic indicators for the corresponding hydrocarbon, for example, the boiling point, the absolute entropy, calculated bond orders, coding of chemical structures, and the total π-electron energy [2]. It was recently shown that the Hosoya index can be employed to determine the molecular structure in the so-called inverse structure-property problem [3]. Therefore,

* Email: whwang@shu.edu.cn

the ordering of molecular graphs in terms of their Hosoya indices is of interest in chemical thermodynamics. Several authors dealt with the characterization of the extremal Hosoya indices for various classes of graphs, for example, acyclic [4–11], unicyclic [3, 12–14], bicyclic [15–17] graphs, double hexagonal chains [18], and hexagonal spiders [19]. In 2010, Pan et al. [20] characterized the graphs with the minimal Hosoya index among all graphs of n vertices and q edges, where $n+2 \leq q \leq 2n-3$. The characterization of graphs having perfect matchings with the minimal Hosoya indices, however, has not been fully elucidated.

In this paper, we will investigate the ordering of the graphs with perfect matchings according to their minimal Hosoya indices. For simplicity, we refer to the connected graphs having n vertices and q edges as the (n, q)-graphs. Let $\mathcal{Z}_{2n,q}$ be set of the $(2n, q)$-graphs with perfect matchings. In particular, as $q = 2n-1, 2n, 2n+1$, $\mathcal{Z}_{2n,q}$ is the set of trees, unicyclic graphs, and bicyclic graphs, with perfect matchings, respectively.

As a starting point, we introduce a quasi-ordering relation which has important applications in comparing the Hosoya indices for molecular graphs [21]. Let G_1 and G_2 be two graphs. If $m(G_1, k) \leqslant m(G_2, k)$ holds for all $k \geqslant 0$, we denote $G_1 \preccurlyeq G_2$. Furthermore, if $G_1 \preccurlyeq G_2$ and $m(G_1, k) < m(G_2, k)$ for an arbitrary k, we have $G_1 \prec G_2$. If neither $G_1 \prec G_2$ nor $G_1 \succ G_2$ holds, then G_1 and G_2 are m-incomparable. By the definition of the Hosoya index, we have

$$G_1 \preccurlyeq G_2 \implies Z(G_1) \leqslant Z(G_2), \quad G_1 \prec G_2 \implies Z(G_1) < Z(G_2). \tag{2}$$

It should be noted that the ordering in terms of energy for acyclic graphs investigated by means of the quasi-ordering relation is the same as that in terms of the Hosoya index [4, 5, 9]. For the cyclic graphs, the two orderings are not the same [12]. For a survey of the mathematical properties of the energy one can refer to Ref. [2]. Other recent results can be found in Refs. [4, 5, 8, 9, 11, 12, 22, 23]

2. PRELIMINARIES

Let $G \in \mathcal{Z}_{2n,q}$ and $Q(G) = L(G) - M(G)$, where $L(G)$ is the edge set of G and $M(G)$ the perfect matching of G. Let $|M(G)|$ and $|Q(G)|$ denote the numbers of edges in $M(G)$ and $Q(G)$ respectively. It is evident that $|M(G)| = n$ and $|Q(G)| = q - n$. Let $\widehat{G} = G - M(G) - S_0$, where $M(G)$ is a perfect matching of G and S_0 is the set of isolated vertices in $G - M(G)$. We call $\widehat{G}$ the capped graph of G and G the original graph of $\widehat{G}$. Each k-matching Ω of G can be partitioned into two parts: $\Omega = \Phi \bigcup \Psi$, where Φ is a matching in $\widehat{G}$ and $\Psi \subseteq M(G)$. On the other hand, any i-matching Φ of $\widehat{G}$ and $k-i$ edges Ψ of $M(G)$ that are not adjacent to Φ form a k-matching Ω of G with a partition $\Omega = \Phi \bigcup \Psi$ [5].

We denote by j the number of the edges in $M(G)$ which are adjacent to an i-matching Φ of $\widehat{G}$. Obviously, $j = 0$ for $i = 0$ while $j = 2$ for $i = 1$. Next we assume $2 \leqslant i \leqslant k$ and denote $m_{2i-c}(\widehat{G}, i)$ the number of the i-matchings of $\widehat{G}$ for $j = 2i - c$ with $0 \leqslant c \leqslant i$. Then we have

$$m(\widehat{G}, i) = m_{2i}(\widehat{G}, i) + \sum_{c=1}^{i} m_{2i-c}(\widehat{G}, i). \tag{3}$$

It follows from (3) that

$$m(G, k) - p = \sum_{i=2}^{k} \left[m_{2i}(\widehat{G}, i) \cdot \binom{n-2i}{k-i} + \sum_{c=1}^{i} m_{2i-c}(\widehat{G}, i) \cdot \binom{n-2i+c}{k-i} \right] \tag{4}$$

$$= \sum_{i=2}^{k} \left\{ m(\widehat{G}, i) \cdot \binom{n-2i}{k-i} + \sum_{c=1}^{i} m_{2i-c}(\widehat{G}, i) \cdot \left[\binom{n-2i+c}{k-i} - \binom{n-2i}{k-i} \right] \right\}, \tag{5}$$

where

$$p = \binom{n}{k} + (q - n) \cdot \binom{n-2}{k-1}.$$

To obtain the final results of this paper, we introduce some notations and simply quote Lemmas 1 and 2.

For $n \geq 3$, P_n is a path with n vertices, and the vertices of P_n are labelled consecutively by $v_1, v_2, \cdots, v_n$.

For $n \geq 3$, X_n is the star $K_{1,n-1}$.

For $n \geq 5$, Y_n is the graph obtained from P_4 by attaching $n - 4$ pendant edges to v_2.

For $n \geq 5$, Z_n is the graph obtained from P_4 by attaching $n - 5$ and one pendant edges to v_2 and v_3, respectively.

For $n \geq 5$, W_n is the graph obtained from P_5 by attaching $n - 5$ pendant edges to v_2.

Lemma 1 *[4] Let T be a tree with n vertices, where $n \geq 5$. Then $X_n \prec Y_n \prec Z_n \prec W_n \prec T$, where $T \neq X_n, Y_n, Z_n, W_n$.*

Lemma 2 *[2] Let $e = uv$ be an edge of G and k a positive integer. Then we have*

$$m(G,k) = m(G-e,k) + m(G-u-v,k-1). \tag{6}$$

3. MAIN RESULTS

The main results are organized as follows. As $q = 2n-1$, we use a new method to get the first two trees with the minimal Hosoya indices in Subsection 3.1. The results are the same as those obtained by Zhang and Li [5]. But the method here is very simple. Next we derive some new results for the cases with $q \neq 2n-1$. As $q = 2n$ and $q = 2n+1$, we will characterize the first two and three graphs with the minimal Hosoya indices in Subsections 3.2 and 3.3, respectively. As $2n+2 \leq q \leq 3n-3$, we will characterize the first two graphs with the minimal Hosoya indices in Subsection 3.4.

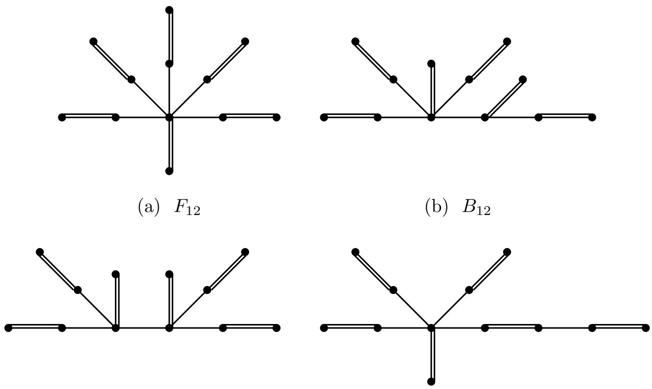
3.1. $(2n, 2n-1)$-graphs with a perfect matching

As $q = 2n-1$, we denote $\mathcal{Z}_{2n,q}$ by $\mathcal{T}_{2n}$. Namely $\mathcal{T}_{2n}$ is the set of trees with a perfect matching having $2n$ vertices. It is evident that $|M(T)| = n$ and $|Q(T)| = n-1$ for $T \in \mathcal{T}_{2n}$.

Let F_{2n}, B_{2n}, and L_{2n} be respectively the trees obtained from X_n, Y_n, and Z_n by attaching a pendant edge to every vertex. Let M_{2n} be the tree obtained from P_7 by attaching $n-4$ paths of length 2 and P_2 to v_3. Obviously, $\widehat{F}_{2n} = X_n$, $\widehat{B}_{2n} = Y_n$, $\widehat{L}_{2n} = Z_n$, and $\widehat{M}_{2n} = X_{n-1} \cup P_2$. For example, F_{12}, B_{12}, L_{12}, and M_{12} are shown in Figs. 1.

Zhang and Li [5] had obtained $F_{2n} \prec B_{2n} \prec L_{2n} \prec T$ for $|c(\widehat{T})| = 1$ and $F_{2n} \prec B_{2n} \prec M_{2n} \prec T$ for $|c(\widehat{T})| \geq 2$, where $T \in \mathcal{T}_{2n}$ and T is a tree that does not occur in the list that precedes T. In this subsection, we obtain the same results. But the method is much simpler than that of Zhang and Li [5]. To give our proof, we first introduce a tree $\widetilde{T}$ and Lemma 3, which play a key role.

Let $\widetilde{T}$ be the tree obtained from $\widehat{T}$ by coalescing the two vertices in T which are incident with a common edge in $M(T)$. Obviously, $\widetilde{T}$ is a tree with n vertex and the edges of $\widetilde{T}$ are those of $\widehat{T}$. For an i-matching Φ of $\widehat{T}$, if $j = 2i$, then there do not exist two edges in the i-matching of $\widehat{T}$ which are adjacent to a common edge in $M(T)$. Thus, we obtain $m_{2i}(\widehat{T}, i) = m(\widetilde{T}, i)$. Furthermore, by (4) and (5), Wang and Kang [9] obtained the following Lemma 3.



(a) F_{12} (b) B_{12}

(c) L_{12} (d) M_{12}

Fig. 1:

Lemma 3 *[9] Let $T_1, T_2 \in \mathcal{T}_{2n}$ and $1 \le c \le i$.*
(i) If $\widetilde{T}_1 \preceq \widetilde{T}_2$ and $m_{2i-c}(\widehat{T}_1, i) \le m_{2i-c}(\widehat{T}_2, i)$, then $T_1 \preceq T_2$.
(ii) If $m(\widehat{T}_1, i) \le m(\widehat{T}_2, i)$ and $m_{2i-c}(\widehat{T}_1, i) \le m_{2i-c}(\widehat{T}_2, i)$, then $T_1 \preceq T_2$.
$m(T_1, k) = m(T_2, k)$ holds for all $0 \le k \le n$ if and only if (iff) the equalities in the two conditions hold simultaneously.

Lemma 3 provides us a straightforward method to deduce the first two trees with the minimal Hosoya indices in $\mathcal{T}_{2n}$, as shown in Theorem 1.

Theorem 1 *Let $T \in \mathcal{T}_{2n}$ and $n \ge 5$. We have $Z(F_{2n}) < Z(B_{2n}) < Z(T)$ for $T \ne F_{2n}, B_{2n}$.*

Proof. Let $T \in \mathcal{T}_{2n}$ and $n \ge 5$. Let $c(\widehat{T})$ be the component number of $\widehat{T}$. We consider two cases as follows.

Case (i). $|c(\widehat{T})| = 1$.

Since $c(\widehat{T}) = 1$, any i-matching of $\widehat{T}$ is adjacent to $2i$ edges of $M(T)$. Hence we have $m_{2i-c}(\widehat{T}, i) = 0$ for $2 \le i \le n$ and $1 \le c \le i$. It follows from Lemma 3(ii) that $m(T, k)$ is a strictly monotonously increasing function of $m(\widehat{T}, i)$. Since $\widehat{F}_{2n} = X_n$, $\widehat{B}_{2n} = Y_n$, and $\widehat{L}_{2n} = Z_n$, $F_{2n} \prec B_{2n} \prec L_{2n} \prec T$ follows from Lemmas 1 and 3(ii) for $T \ne F_{2n}, B_{2n}, L_{2n}$. By (2), we have $Z(F_{2n}) < Z(B_{2n}) < Z(L_{2n}) < Z(T)$ for $|c(\widehat{T})| = 1$ and $T \ne F_{2n}, B_{2n}, L_{2n}$.

Case (ii). $|c(\widehat{T})| \ge 2$.

Since $\widehat{B}_{2n} = Y_n$ and $\widehat{M}_{2n} = X_{n-1} \cup P_2$, we have $m(\widehat{B}_{2n}, 2) = n-3 < n-2 = m(\widehat{M}_{2n}, 2)$ and $m(\widehat{B}_{2n}, i) = m(\widehat{M}_{2n}, i) = 0$ for $3 \leq i \leq n$. In $\widehat{B}_{2n}$, any 2-matching is adjacent to 4 edges of $M(B_{2n})$. In $\widehat{M}_{2n}$, there are $(n-3)$ 2-matchings which are adjacent to 4 edges of $M(M_{2n})$ and one 2-matching which is adjacent to 3 edges of $M(M_{2n})$. Namely, we have $m_4(\widehat{B}_{2n}, 2) = m_4(\widehat{M}_{2n}, 2) = n-3$ and $m_3(\widehat{B}_{2n}, 2) = 0 < 1 = m_3(\widehat{M}_{2n}, 2)$. By Lemma 3(ii), we have $B_{2n} \prec M_{2n}$. By (2), we get $Z(B_{2n}) < Z(M_{2n})$.

Next we prove $Z(M_{2n}) < Z(T)$ according to the type of $\widetilde{T}$, where $|c(\widehat{T})| \geq 2$ and $T \neq M_{2n}$. Two subcases are considered.

Subcase (ii.i) $\widetilde{T} = X_n$.

If $\widetilde{T} = X_n$ and $T \neq F_{2n}$, in view of the definition of $\widetilde{T}$, we have $\widehat{T} = X_{y+1} \cup X_{z+1}$, where y and z are positive integers, $y + z = n - 1$ and $1 \leq y \leq [(n-1)/2]$. Hence T is the tree obtained from X_{y+1} and X_{z+1} by adding an edge between the central vertices of X_{y+1} and X_{z+1} and then attaching a pendant edge to each other vertex of X_{y+1} and X_{z+1}, respectively. We denote this kind of tree T by $H_{y,z}$.

Obviously, we get $m(\widehat{H}_{y,z}, 2) = m(X_{y+1} \cup X_{z+1}, 2) = y \cdot z = y \cdot (n-1-y)$ and $m(\widehat{H}_{y,z}, i) = 0$ for $3 \leq i \leq n$. Hence, $m(\widehat{H}_{y,z}, 2)$ is a strictly monotonously increasing function of y for $1 \leq y \leq [(n-1)/2]$. Since $\widetilde{H}_{y,z} = X_n$ and each 2-matching of $\widehat{H}_{y,z}$ is adjacent to 3 edges of $M(H_{y,z})$, by Lemma 3(i), we obtain $H_{1,n-2} \prec H_{y,z}$ for $2 \leq y \leq [(n-1)/2]$.

We have $m(\widehat{M}_{2n}, 2) = m(\widehat{H}_{1,n-2}, 2) = n-2$ and $m_3(\widehat{M}_{2n}, 2) = 1 < n-2 = m_3(\widehat{H}_{1,n-2}, 2)$. By Lemma 3(ii), we have $M_{2n} \prec H_{1,n-2}$.

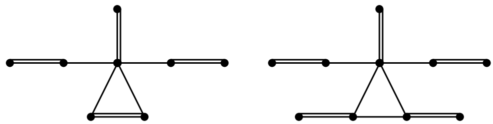
In conclusion, we have $M_{2n} \prec H_{y,z}$ for $1 \leq y \leq [(n-1)/2]$. By (2), we get $Z(M_{2n}) < Z(T)$ for $\widetilde{T} = X_n$.

Subcase (ii.ii) $\widetilde{T} \neq X_n$.

Since $\widetilde{T} \neq X_n$, by Lemma 1, we get $\widehat{M}_{2n} = \widetilde{M}_{2n} = Y_n \preceq \widetilde{T}$. Since $|c(\widehat{T})| \geq 2$, there is at least one 2-matching of $\widehat{T}$ which is adjacent to 3 edges in $M(T)$, namely we have $m_3(\widehat{M}_{2n}, 2) = 1 \leq m_3(\widehat{T}, 2)$. Furthermore, we have $m_{2i-c}(\widehat{M}_{2n}, i) = 0 \leq m_{2i-c}(\widehat{T}, i)$ for $3 \leq i \leq n$ and $1 \leq c \leq i$. The equal signs in all the inequalities in Subcase (ii.ii) hold iff $T = M_{2n}$. Thus, by Lemma 3(i), we have $M_{2n} \prec T$ for $\widetilde{T} \neq X_n$ and $T \neq M_{2n}$. Hence, by (2), we have $Z(M_{2n}) < Z(T)$ for $\widetilde{T} \neq X_n$ and $T \neq M_{2n}$.

For Case (ii), we obtain $Z(B_{2n}) < Z(M_{2n}) < Z(T)$ for $|c(\widehat{T})| \geq 2$ and $T \neq B_{2n}, M_{2n}$.

■



(a) S_8^3 (b) R_{10}^3

Fig. 2:

Remark: By direct calculation on (5), we have $m(L_{2n}, 2) - m(M_{2n}, 2) = n - 6 > 0$ for $n \geq 7$ and $m(L_{2n}, n-1) - m(M_{2n}, n-1) = -1 < 0$. Thus, L_{2n} and M_{2n} are m-incomparable. We can see from Theorem 1 that the candidate tree with the third minimal Hosoya index in $\mathcal{T}_{2n}$ is either L_{2n} or M_{2n}. It is noted that Guo [22] and Wang and Kang [9] proved that the tree with the third minimal energy in $\mathcal{T}_{2n}$ is M_{2n}. However, a further determination for the tree with the third minimal Hosoya index in $\mathcal{T}_{2n}$ remains a task for the future.

3.2. $(2n, 2n)$-graphs with perfect matchings

As $q = 2n$, we denote $\mathcal{Z}_{2n,q}$ by $\mathcal{K}_{2n}$. Namely $\mathcal{K}_{2n}$ is the set of unicyclic graphs with perfect matchings having $2n$ vertices. It is evident that $|M(G)| = n$ and $|Q(G)| = n$ for $G \in \mathcal{K}_{2n}$.

We introduce some notations and the first two graphs with the minimal Hosoya indices in $\mathcal{K}_{2n}$.

For $l \geq 3$, C_l is a cycle with l vertices, and the vertices of C_l are labelled consecutively by $u_1, u_2, \cdots, u_l$.

Let S_{2n}^3 be a graph obtained by attaching one pendant edge and $n-2$ paths of length 2 to one vertex of C_3.

Let R_{2n}^3 be a graph obtained by attaching one pendant edge to every vertex of C_3 and then by attaching $n-3$ paths of length 2 to a vertex of C_3.

For example, S_8^3 and R_{10}^3 are shown in Figs. 2(a) and 2(b), respectively.

We introduce Lemma 4, from which Theorem 2 can be obtained.

Lemma 4 *[23] Let $G \in \mathcal{K}_{2n}$ with $n \geq 4$. If $G \neq S_{2n}^3, R_{2n}^3$, then $m(\widehat{G}, 2) > n - 3$.*

Theorem 2 *Let $G \in \mathcal{K}_{2n}$ with $n \geq 4$. We have $Z(S_{2n}^3) < Z(R_{2n}^3) < Z(G)$ for $G \neq S_{2n}^3, R_{2n}^3$.*

Proof. Since $\widehat{S}^3_{2n} = X_{n+1}$, we have $m(\widehat{S}^3_{2n}, i) = 0$ for $2 \le i \le n$. Thus,

$$m(S^3_{2n}, k) = \binom{n}{k} + n \cdot \binom{n-2}{k-1} \triangleq p_a. \tag{7}$$

Obviously, we have $m(\widehat{R}^3_{2n}, 2) = n - 3$ and $m(\widehat{R}^3_{2n}, i) = 0$ for $3 \le i \le n$. Since each 2-matching of $\widehat{R}^3_{2n}$ is adjacent to 4 edges of $M(R^3_{2n})$, we get

$$m(R^3_{2n}, k) = p_a + (n-3) \cdot \binom{n-4}{k-2}. \tag{8}$$

Thus, $Z(S^3_{2n}) < Z(R^3_{2n})$ follows from (7), (8), and (2).

By (5) and Lemma 4, we have

$$m(G, k) > p_a + (n-3) \cdot \binom{n-4}{k-2}. \tag{9}$$

It follows from (8), (9), and (2) that $Z(R^3_{2n}) < Z(G)$, where $G \in \mathcal{K}_{2n}$ and $G \neq S^3_{2n}, R^3_{2n}$. ■

From Theorem 2 and the results obtained by Wang et al. [23], one can confirm that for the unicyclic graphs with perfect matchings, the ordering in terms of their minimal Hosoya index is not the same as that in terms of their minimal energy.

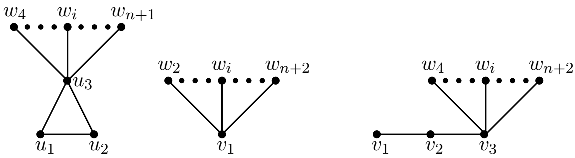
3.3. $(2n, 2n+1)$-graphs with perfect matchings

As $q = 2n+1$, we denote $\mathcal{Z}_{2n,q}$ by $\mathcal{B}_{2n}$. Namely $\mathcal{B}_{2n}$ is the set of bicyclic graphs with perfect matchings having $2n$ vertices. It is evident that $|M(G)| = n$ and $|Q(G)| = n+1$ for $G \in \mathcal{B}_{2n}$.

In 2008, Deng [15, 16] characterized the graphs with the maximal and minimal Hosoya indices among the $(n, n+1)$-graphs. In Subsection 3.3, we will derive the first three graphs with the minimal Hosoya indices in $\mathcal{B}_{2n}$. The graph A^3_{n+1} and the first three graphs are introduced as follows.

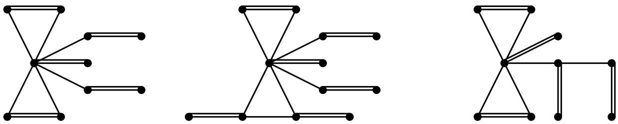
Let A^3_{n+1} be the unicyclic graph obtained from C_3 by attaching $n-2$ pendant edges to u_3. The $n-2$ pendant vertices of A^3_{n+1} are labeled by $w_4, \cdots, w_{n+1}$, as shown in Fig. 3(a).

Let $S^{3,3}_{2n}$ be the graph obtained from X_{n+2} (see Fig. 3(b)) by adding an edge between w_i and w_{i+1} for $i = 2, 4$ and then attaching a pendant edge to each of the other $(n-2)$ vertices in $\{w_6, w_7, \cdots, w_{n+2}, v_1\}$. Obviously, $S^{3,3}_{2n} \in \mathcal{B}_{2n}$ and $\widehat{S}^{3,3}_{2n} = X_{n+2}$.



(a) A^3_{n+1} (b) X_{n+2} (c) Y_{n+2}

Fig. 3:



(a) $S^{3,3}_{10}$ (b) $R^{3,3}_{12}$ (c) $Y^{3,3}_{10}$

Fig. 4:

Let $R^{3,3}_{2n}$ be the graph obtained from A^3_{n+1} (see Fig. 3(a)) by adding an edge between w_4 and w_5, and then attaching a pendant edge to each of the other $n-1$ vertices in $\{w_6, w_7, \cdots, w_{n+1}, u_1, u_2, u_3\}$. Obviously, $R^{3,3}_{2n} \in \mathcal{B}_{2n}$ and $\widehat{R}^{3,3}_{2n} = A^3_{n+1}$.

Let $Y^{3,3}_{2n}$ be the graph obtained from Y_{n+2} (see Fig. 3(c)) by adding an edge between w_i and w_{i+1} for $i = 4, 6$ and then attaching a pendant edge to each of the other $(n-2)$ vertices in $\{w_8, w_9, \cdots, w_{n+2}, v_1, v_2, v_3\}$. Obviously, $Y^{3,3}_{2n} \in \mathcal{B}_{2n}$ and $\widehat{Y}^{3,3}_{2n} = Y_{n+2}$.

For example, $S^{3,3}_{10}$, $R^{3,3}_{12}$, and $Y^{3,3}_{10}$ are shown in Figs. 4(a), 4(b), and 4(c), respectively.

To obtain the first three graphs with the minimal Hosoya indices in $\mathcal{B}_{2n}$, we introduce Lemmas 5–8 at first.

Lemma 5 *For $n \geqslant 5$, we have $Z(S^{3,3}_{2n}) < Z(R^{3,3}_{2n}) < Z(Y^{3,3}_{2n})$.*

Proof. Since $\widehat{S}^{3,3}_{2n} = X_{n+2}$, we have $m(\widehat{S}^{3,3}_{2n}, i) = 0$ for $2 \le i \le n$. Thus, we get

$$m(S^{3,3}_{2n}, k) = \begin{pmatrix} n \\ k \end{pmatrix} + (n+1) \cdot \begin{pmatrix} n-2 \\ k-1 \end{pmatrix} \triangleq p_b. \tag{10}$$

Since $\widehat{R}^{3,3}_{2n} = A^3_{n+1}$, we have $m(\widehat{R}^{3,3}_{2n}, 2) = n-2$ and $m(\widehat{R}^{3,3}_{2n}, i) = 0$ for $3 \le i \le n$. Since each 2-matching of $\widehat{R}^{3,3}_{2n}$ is adjacent to 4 edges of $M(R^{3,3}_{2n})$, we have

$$m(R^{3,3}_{2n}, k) = p_b + (n-2) \cdot \begin{pmatrix} n-4 \\ k-2 \end{pmatrix}. \tag{11}$$

Since $\widehat{Y}_{2n}^{3,3} = Y_{n+2}$, we have $m(\widehat{Y}_{2n}^{3,3}, 2) = n - 1$ and $m(\widehat{Y}_{2n}^{3,3}, i) = 0$ for $3 \le i \le n$. Since each 2-matching of $\widehat{Y}_{2n}^{3,3}$ is adjacent to 4 edges of $M(Y_{2n}^{3,3})$, we get

$$m(Y_{2n}^{3,3}, k) = p_b + (n-1) \cdot \binom{n-4}{k-2}. \tag{12}$$

It follows from (10), (11), (12), and (2) that $Z(S_{2n}^{3,3}) < Z(R_{2n}^{3,3}) < Z(Y_{2n}^{3,3})$ for $n \geqslant 5$. ■

Lemma 6 *Let $G \in \mathcal{B}_{2n}$ and $n \ge 5$. If $\widehat{G} = Y_{n+2}$ and $G \ne Y_{2n}^{3,3}$, we have $Z(Y_{2n}^{3,3}) < Z(G)$.*

Proof. Let $G \in \mathcal{B}_{2n}$ and $n \ge 5$. If $\widehat{G} = Y_{n+2}$, then we can see from Fig. 3(c) that $m(\widehat{G}, 2) = n - 1$ and the $(n-1)$ 2-matchings of $\widehat{G}$ are v_1v_2 and v_3w_i, where $4 \le i \le n+2$. If v_1v_2 and v_3w_i $(4 \le i \le n+2)$ are not adjacent to a common edge in $M(G)$, then $j = 4$. Otherwise, $j = 3$ or $j = 2$. We consider two cases as follows.

Case (i). All the 2-matchings v_1v_2 and v_3w_i $(4 \le i \le n+2)$ are not adjacent to a common edge in $M(G)$.

In G, either v_1 or v_2 cannot be linked with any of v_3 and w_i, where $4 \le i \le n+2$. Since $G \in \mathcal{B}_{2n}$ and $\widehat{G} = Y_{n+2}$, we can readily verify that $G = Y_{2n}^{3,3}$.

Case (ii). At least one 2-matching of v_1v_2 and v_3w_i $(4 \le i \le n+2)$ is adjacent to a common edge in $M(G)$.

In this case, we have $m_3(\widehat{G}, 2) \ge 1$ or $m_2(\widehat{G}, 2) \ge 1$. Furthermore, since $m(\widehat{G}, 2) = n - 1$ and $m(\widehat{G}, i) = 0$ for $3 \le i \le n$, by (5), we get

$$\begin{aligned} m(G,k) &= p_b \\ &+ (n-1) \cdot \binom{n-4}{k-2} + \sum_{c=1}^{2} m_{4-c}(\widehat{G}, 2) \cdot \left[\binom{n-4+c}{k-2} - \binom{n-4}{k-2} \right]. \end{aligned} \tag{13}$$

It follows from (12), (13) and (2) that $Z(Y_{2n}^{3,3}) < Z(G)$ for $\widehat{G} = Y_{n+2}$ and $G \ne Y_{2n}^{3,3}$. ■

Lemma 7 *Let $G \in \mathcal{B}_{2n}$ and $n \ge 5$. If $\widehat{G} = A_{n+1}^3$ and $G \ne R_{2n}^{3,3}$, then $Z(Y_{2n}^{3,3}) < Z(G)$.*

Proof. As $G \in \mathcal{B}_{2n}$ and $\widehat{G} = A_{n+1}^3$, we can verify that there are only two graphs for this kind of G. One graph is $R_{2n}^{3,3}$, the other graph is $Q_{2n}^{3,3}$, where $Q_{2n}^{3,3}$ is the graph obtained from A_{n+1}^3 (see Fig. 3(a)) by adding an edge between u_1 and w_4 and then attaching a pendant edge to each of the other $n-1$ vertices in $\{w_5, w_6, \cdots, w_{n+1}, u_2, u_3\}$. Next we shall prove $Z(Y_{2n}^{3,3}) < Z(Q_{2n}^{3,3})$.

We have $m(\widehat{Q}_{2n}^{3,3}, 2) = m(A_{n+1}^3, 2) = n-2$ and $m(\widehat{Q}_{2n}^{3,3}, i) = m(A_{n+1}^3, i) = 0$ for $3 \le i \le n$. In $\widehat{Q}_{2n}^{3,3}$, there are $(n-3)$ 2-matchings which are adjacent to 4 edges of $M(Q_{2n}^{3,3})$ and one 2-matching which is adjacent to 3 edges of $M(Q_{2n}^{3,3})$. Namely, $m_4(\widehat{Q}_{2n}^{3,3}, 2) = n-3$ and $m_3(\widehat{Q}_{2n}^{3,3}, 2) = 1$. Thus, we get

$$m(Q_{2n}^{3,3}, k) = p_b + (n-3) \cdot \binom{n-4}{k-2} + \binom{n-3}{k-2}. \tag{14}$$

It is well known that

$$\binom{n-3}{k-2} = \binom{n-4}{k-2} + \binom{n-4}{k-3}. \tag{15}$$

Substitution (15) into (14) yields

$$m(Q_{2n}^{3,3}, k) = p_b + (n-2) \cdot \binom{n-4}{k-2} + \binom{n-4}{k-3}. \tag{16}$$

Since

$$\binom{n-4}{k-3} > \binom{n-4}{k-2}, \tag{17}$$

by comparing (12) and (16), we get $Y_{2n}^{3,3} \prec Q_{2n}^{3,3}$. By (2), we have Lemma 7. ■

Lemma 8 *Let $G \in \mathcal{B}_{2n}$ and $n \ge 7$. If $\widehat{G} \ne X_{n+2}, Y_{n+2}, A_{n+1}^3$, then $m(\widehat{G}, 2) > n-1$.*

Proof. Let $G \in \mathcal{B}_{2n}$ and $n \ge 7$. $\widehat{G}$ is classified into two cases as follows.

Case (i). $\widehat{G}$ is a connected graph with $n+1$ edges.

Subcase (i.i). $\widehat{G}$ is a tree with $n+2$ vertices.

As $\widehat{G} \ne X_{n+2}, Y_{n+2}$, by Lemma 1, we have $m(\widehat{G}, 2) \ge m(Z_{n+2}, 2) = 2n-4 > n-1$.

Subcase (i.ii). $\widehat{G}$ is a unicyclic graph with $n+1$ vertices.

Let C_l be the cycle contained in $\widehat{G}$. As $l \ge 4$ or $l = 3$ and $\widehat{G} \ne A_{n+1}^3$, we can choose an edge e on C_l such that $\widehat{G} - e$ is a tree on $n+1$ vertices with diameter at least 4. Therefore, $\widehat{G} - e \ne X_{n+1}, Y_{n+1}, Z_{n+1}$ since the diameter of X_{n+1}, Y_{n+1}, and Z_{n+1} is 3. By Lemma 1, we have $m(\widehat{G}, 2) \ge m(\widehat{G} - e, 2) \ge m(W_{n+1}, 2) = 2n-5 > n-1$.

Subcase (i.iii). $\widehat{G}$ is a bicyclic graph with n vertices.

Obviously, $\widehat{G}$ has either two or three distinct cycles.

If $\widehat{G}$ has two distinct cycles, then let the two cycles be C_a and C_b. Obviously, C_a and C_b are connected by a unique path P or C_a and C_b have exactly one common vertex. We can choose an edge e_1 on C_a and an edge e_2 on C_b such that $\widehat{G} - e_1 - e_2$ is a tree on n vertices with diameter at least 4. By Lemma 1, we have $m(\widehat{G}, 2) \geq m(\widehat{G} - e_1 - e_2, 2) \geq m(W_n, 2) = 2n - 7 > n - 1$.

If $\widehat{G}$ has three cycles, then any two cycles must have at least one common edge. We can choose an edge e which is a common edge of C_a and C_b in such a way that $\widehat{G} - e$ is a connected unicyclic graph with n vertices and $\widehat{G} - e \neq A_n^3$. By the approach similar to that for Subcase (i.ii), we have $m(\widehat{G}, 2) \geq m(\widehat{G} - e, 2) \geq m(W_n, 2) = 2n - 7 > n - 1$.

Case (ii). $\widehat{G}$ is an unconnected graph with $n + 1$ edges.

Let the components of $\widehat{G}$ be H_1, H_2, $\cdots$, H_k, where $k \geq 2$. Without loss of generality, we can concatenate H_2, $\cdots$, H_k into a connected graph H_c. Suppose that the number of edges in H_1 is a, where $1 \leq a \leq n$. Then the number of edges in H_c is $n + 1 - a$. We have $m(\widehat{G}, 2) \geq a \cdot (n + 1 - a) \geq n > n - 1$. ∎

By Lemmas 5–8, we have the first three graphs with the minimal Hosoya indices in $\mathcal{B}_{2n}$.

Theorem 3 *Let $G \in \mathcal{B}_{2n}$ and $n \geqslant 7$. We get $Z(S_{2n}^{3,3}) < Z(R_{2n}^{3,3}) < Z(Y_{2n}^{3,3}) < Z(G)$, where $G \neq S_{2n}^{3,3}, R_{2n}^{3,3}, Y_{2n}^{3,3}$.*

Proof. By Lemma 5, we have $Z(S_{2n}^{3,3}) < Z(R_{2n}^{3,3}) < Z(Y_{2n}^{3,3})$. Next, we prove $Z(Y_{2n}^{3,3}) < Z(G)$ for $G \neq S_{2n}^{3,3}, R_{2n}^{3,3}, Y_{2n}^{3,3}$.

If $\widehat{G} = X_{n+2}$, then $G = S_{2n}^{3,3}$. If $\widehat{G} = Y_{n+2}$ and $G \neq Y_{2n}^{3,3}$, then by Lemma 6, we have $Z(Y_{2n}^{3,3}) < Z(G)$. If $\widehat{G} = A_{n+1}^3$ and $G \neq R_{2n}^{3,3}$, then by Lemma 7, we have $Z(Y_{2n}^{3,3}) < Z(G)$.

If $\widehat{G} \neq X_{n+2}, Y_{n+2}, A_{n+1}^3$, then by Lemma 8 and (5), we have

$$m(G, k) > p_b + (n - 1) \cdot \begin{pmatrix} n - 4 \\ k - 2 \end{pmatrix}. \tag{18}$$

It follows from (12), (18), and (2) that $Z(Y_{2n}^{3,3}) < Z(G)$ for $\widehat{G} \neq X_{n+2}, Y_{n+2}, A_{n+1}^3$. ∎

In Theorems 1–3, we have obtained the first two, two, and three graphs with the minimal Hosoya indices in $\mathcal{Z}_{2n,q}$ for $q = 2n - 1$, $q = 2n$, and $q = 2n + 1$, respectively. Next, for $2n + 2 \leq q \leq 3n - 3$, we will further consider the same ordering for graphs in $\mathcal{Z}_{2n,q}$.

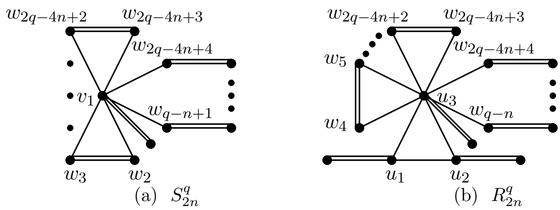


Fig. 5:

3.4. $(2n, q)$-graphs with perfect matchings for $2n+2 \leq q \leq 3n-3$

In 2010, Pan et al. [20] characterized the graphs with the minimal Hosoya index among the (n, q)-graphs for $n+2 \leq q \leq 2n-3$. In this subsection, we will characterize the first two graphs with the minimal Hosoya indices among $\mathcal{Z}_{2n,q}$ for $2n+2 \leq q \leq 3n-3$. The first two graphs are introduced as follows.

Let S_{2n}^q be the graph obtained from X_{q-n+1} (see Fig. 3(b)) by adding an edge between w_i and w_{i+1} for $i = 2, 4, \cdots, 2q-4n+2$ and then attaching a pendant edge to each of the other $(3n-1-q)$ vertices in $\{w_{2q-4n+4}, w_{2q-4n+5}, \cdots, w_{q-n+1}, v_1\}$, where $2n+2 \leq q \leq 3n-3$. Obviously, $S_{2n}^q \in \mathcal{Z}_{2n,q}$ and $\widehat{S}_{2n}^q = X_{q-n+1}$. S_{2n}^q is shown in Figs. 5(a).

Let R_{2n}^q be the graph obtained from A_{q-n}^3 (see Fig. 3(a)) by adding an edge between w_i and w_{i+1} for $i = 4, 6, \cdots, 2q-4n+2$ and then attaching a pendant edge to each of the other $(3n-q)$ vertices in $\{w_{2q-4n+4}, w_{2q-4n+5}, \cdots, w_{q-n}, u_1, u_2, u_3\}$, where $2n+2 \leq q \leq 3n-3$. Obviously, $R_{2n}^q \in \mathcal{Z}_{2n,q}$ and $\widehat{R}_{2n}^q = A_{q-n}^3$. R_{2n}^q is shown in Figs. 5(b).

Lemma 9 is introduced, from which Theorem 4 can be obtained.

Lemma 9 *Let H be a graph (connected or unconnected) with b edges and $H \neq X_{b+1}$, then $m(H, 2) \geq b-3$, the equality holds iff $H = A_b^3$, where $b \geq 9$.*

Proof. As $H = A_b^3$, we have $m(H, 2) = b-3$. Next, we assume that $H \neq A_b^3$ and $b \geq 9$.

If H is an unconnected graph with b edges, then by the approach similar to that for Case (ii) in Lemma 8, we have $m(H, 2) > b-3$. Next, we assume that H is a connected graph with b edges and $b \geq 8$.

As H is a tree or a unicyclic graph or a bicyclic graph with b edges, by the approach similar to that for Case (i) in Lemma 8, we have $m(H, 2) > b-3$.

As H is a tricyclic graph with b edges, we can choose an edge $e = uv$ on a cycle in H such that $H - e$ is a connected bicyclic graph with $b-1$ edges and $H - u - v$ contains at least one edge as its subgraph. We have $m(H-e,2) > b-4$ and $m(H-u-v,1) \geq 1$. Thus, by Lemma 2, we have $m(H,2) = m(H-e,2) + m(H-u-v,1) > b-3$.

As H is a graph not being included in the afore-mentioned cases, the minimal number of distinct cycles contained in H is not less than 4. Then we can repeat the procedure similar to that for H being a tricyclic graph and employ a recursive algorithm to get $m(H,2) > b-3$. ■

Theorem 4 *Let $G \in \mathcal{Z}_{2n,q}$ with $2n+2 \leq q \leq 3n-3$ and $n \geq 7$. We have $Z(S_{2n}^q) < Z(R_{2n}^q) < Z(G)$ for $G \neq S_{2n}^q, R_{2n}^q$.*

Proof. Since $\widehat{S}_{2n}^q = X_{q-n+1}$, we have $m(\widehat{S}_{2n}^q, i) = 0$ for $2 \leq i \leq n$. We obtain

$$m(S_{2n}^q, k) = \binom{n}{k} + (q-n) \cdot \binom{n-2}{k-1} \triangleq p_c. \tag{19}$$

Since $\widehat{R}_{2n}^q = A_{q-n}^3$, we have $m(\widehat{R}_{2n}^q, 2) = q-n-3$ and $m(\widehat{R}_{2n}^q, i) = 0$ for $3 \leq i \leq n$. Since each 2-matching of $\widehat{R}_{2n}^q$ is adjacent to 4 edges of $M(R_{2n}^q)$, we obtain

$$m(R_{2n}^q, k) = p_c + (q-n-3) \cdot \binom{n-4}{k-2}. \tag{20}$$

It follows from (19), (20), and (2) that $Z(S_{2n}^q) < Z(R_{2n}^q)$.

Next we prove $Z(R_{2n}^q) < Z(G)$, where $G \in \mathcal{Z}_{2n,q}$ and $G \neq S_{2n}^q, R_{2n}^q$.

If $\widehat{G} = X_{q-n+1}$, it can readily be verified that $G = S_{2n}^q$.

If $\widehat{G} = A_{q-n}^3$, then we have $m(\widehat{G}, 2) = q-n-3$ and $m(\widehat{G}, i) = 0$ for $3 \leq i \leq n$. By (5), we get

$$\begin{aligned} m(G,k) &= p_c \\ &+ (q-n-3) \cdot \binom{n-4}{k-2} + \sum_{c=1}^{2} m_{4-c}(\widehat{G},2) \cdot \left[\binom{n-4+c}{k-2} - \binom{n-4}{k-2} \right]. \end{aligned} \tag{21}$$

Furthermore, as $\widehat{G} = A_{q-n}^3$ and $G \neq R_{2n}^q$, it can readily be verified that there is at least one 2-matching of $\widehat{G}$ which is adjacent to 3 edges of $M(G)$. Namely, $m_3(\widehat{G}, 2) \geq 1$. It follows from (20), (21), and (2) that $Z(R_{2n}^q) < Z(G)$ for $\widehat{G} = A_{q-n}^3$ and $G \neq R_{2n}^q$.

Next, we assume $\widehat{G} \neq X_{q-n+1}, A_{q-n}^3$. As $2n+2 \leq q \leq 3n-3$ and $n \geq 7$, we have $q-n \geq n+2 \geq 9$. By Lemma 9, we have $m(\widehat{G}, 2) > q-n-3$ since $G \in \mathcal{Z}_{2n,q}$ and $\widehat{G}$ has

$q-n$ edges. Furthermore, by (5), we have

$$m(G,k) > p_c + (q-n-3) \cdot \binom{n-4}{k-2}. \tag{22}$$

It follows from (20), (22), and (2) that $Z(R_{2n}^q) < Z(G)$, where $G \in \mathcal{Z}_{2n,q}$ and $\widehat{G} \neq X_{q-n+1}, A_{q-n}^3$. ■

Remark: The first two graphs with the minimal Hosoya indices in $\mathcal{Z}_{2n,q}$ were characterized in Theorem 4, where $2n+2 \leq q \leq 3n-3$. The ordering in $\mathcal{Z}_{2n,q}$ for $q \geq 3n-2$ remains a task for the future.

Acknowledgments

The work was supported by the National Natural Science Foundation of China under Grant No. 11001166 and the Shanghai Leading Academic Discipline Project under Project No. S30104.

[1] H. Hosoya, Topological index, a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* **44** (1971) 2332–2339.

[2] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Berlin, Springer–Verlag, 1986.

[3] J. P. Ou, On extremal unicyclic molecular graphs with prescribed girth and minimal Hosoya index, *J. Math. Chem.* **42** (2007) 423–432.

[4] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.

[5] F. J. Zhang, H. Li, On acyclic conjugated molecules with minimal energies, *Discr. Appl. Math.* **92** (1999) 71–84.

[6] Y. P. Hou, On acyclic systems with minimal Hosoya index, *Discr. Appl. Math.* **119** (2002) 251–257.

[7] S. G. Wagner, Extremal trees with respect to Hosoya index and Merrifield–Simmons index, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 221–233.

[8] C. Heuberger, S. G. Wagner, Chemical trees minimizing energy and Hosoya index, *J. Math. Chem.* **46** (2009) 214–230.

[9] W. H. Wang, Ordering of the trees with a perfect matching by minimal energies, *Lin. Algebra Appl.* **431** (2009) 946–961.

[10] S. C. Li, X. C. Li, W. Jing, On the extremal Merrifield–Simmons index and Hosoya index of quasi–tree graphs, *Discr. Appl. Math.* **157** (2009) 2877-2885.

[11] H. B. Hua, On maximal energy and Hosoya index of trees without perfect matching, *Bull. Austral. Math. Soc.* **81** (2010) 47–57.

[12] S. C. Li, X. C. Li, Z. X. Zhu, On minimal energy and Hosoya index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 325–339.

[13] L. X. Xu, The second largest Hosoya index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 621–628.

[14] J. P. Ou, On extremal unicyclic molecular graphs with maximal Hosoya index, *Discr. Appl. Math.* **157** (2009) 391–397.

[15] H. Y. Deng, The largest Hosoya index of $(n, n+1)$-graphs, *Comput. Math. Appl.* **56** (2008) 2499–2506.

[16] H. Y. Deng, The smallest Hosoya index in $(n, n + 1)$-graphs, *J. Math. Chem.* **43** (2008) 119–133.

[17] K. Xu, I. Gutman, The greatest Hosoya index of bicyclic graphs with given maximum degree, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 795–824.

[18] H. Ren, F. Zhang, Double hexagonal chains with maximal Hosoya index and minimal Merrifield–Simmons index, *J. Math. Chem.* **42** (2007) 679–690.

[19] W. C. Shiu, Extremal Hosoya index and Merrifield–Simmons index of hexagonal spiders, *Discr. Appl. Math.* **156** (2008) 2978–298.

[20] X. F. Pan, Z. R. Sun, The (n, m)-graphs of minimal Hosoya index, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 811–820.

[21] A. T. Balaban, *Chemical Application of Graph Theory*, Academic Press, London, 1976, p. 3.

[22] J. M. Guo, On the minimal energy ordering of trees with perfect matchings, *Discr. Appl. Math.* **156** (2008) 2598–2605.

[23] W. H. Wang, A. Chang, L. Z. Zhang, D. Q. Lu, Unicyclic Hückel molecular graphs with minimal energy, *J. Math. Chem.* **39** (2006) 231–241.