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# On minimal energy and Hosoya index of unicyclic graphs*

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**Abstract.** The energy of a graph is defined as the sum of the absolute values of all the eigenvalues of the graph and the Hosoya index of a graph is defined as the total number of the matchings of the graph. Let $\mathscr{G}_n$ be the set of all unicyclic graphs with $n$ vertices. Y. Hou [J. Math. Chem. 29 (2001), no. 3, 163–168] obtained the minimal value on the energies of the graphs in $\mathscr{G}_n$ and determined the corresponding graph. A. Chen et al. [MATCH Commun. Math. Comput. Chem. 55 (2006), no. 1, 95–102] obtained the second- and third-minimal values of the energies of graphs in $\mathscr{G}_n$ and determine their corresponding graphs. In this paper, we not only give the fourth-, fifth- and sixth-minimal energies of graphs in $\mathscr{G}_n$ and characterize their corresponding graphs, but also determine the graphs in $\mathscr{G}_n$ with minimal, second-minimal, third-minimal, fourth-minimal, fifth-minimal and sixth-minimal Hosoya index.

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## 1. Introduction

Let $G$ be a simple connected graph with $n$ vertices. Let $A(G)$ be the *adjacency matrix* of $G$. The *characteristic polynomial* of $G$ is

$$\phi(G,\lambda) = \det(\lambda I - A) = \sum_{i=0}^{n} a_i \lambda^{n-i},$$

Sachs theorem states that [11] for $i \geqslant 1$,

$$a_i = \sum_{S \in L_i} (-1)^{p(S)} 2^{c(S)},$$

where $L_i$ denotes the set of *Sachs graphs* of $G$ with $i$ vertices, that is, the graphs in which every component is either a $K_2$ or a cycle, $p(S)$ is the number of components of $S$ and $c(S)$ is the number of cycles contained in $S$. In addition, $a_0 = 1$. The roots $\lambda_1, \ldots, \lambda_n$ of $\phi(G,\lambda)$ are called the *eigenvalues* of $G$. Since $A(G)$ is symmetric, all eigenvalues of $G$ are real. Let $C_n$ denote the cycle of length $n$. A connected graph with $n$ vertices and $n$ edges is called a *unicyclic graph*. Let $\mathscr{G}_n$ be the set of unicyclic graph $G$ with $n$ vertices.

In chemistry the experimental heats from the formation of conjugated hydrocarbons are closely related to the total $\pi$-electron energy. And the calculation of the total energy of all $\pi$-electrons in conjugated hydrocarbons can be reduced to (within the framework of HMO approximation) (see [9, 11]) that

$$E(G) = \sum_{i=1}^{n} |\lambda_i|,$$

where $\lambda_1, \ldots, \lambda_n$ are eigenvalues of the corresponding molecular graph $G$. Thus there are numerous results on $E(G)$ (e.g., see [1,4,8,9,12,15,17-26,30-39]).

It is known that [11] $E(G)$ can be expressed as the Coulson integral formula

$$E(G) = \frac{1}{\pi} \int_0^{+\infty} \frac{dx}{x^2} \ln \left[ \left( \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i a_{2i} x^{2i} \right)^2 + \left( \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i a_{2i+1} x^{2i+1} \right)^2 \right]. \quad (1.1)$$

Let $b_{2i}(G) = (-1)^i a_{2i}$ and $b_{2i+1}(G) = (-1)^i a_{2i+1}$ for $0 \leqslant i \leqslant \lfloor \frac{n}{2} \rfloor$. Clearly, $b_0(G) = 1$ and $b_2(G)$ equals the number of edges of $G$. Thus, by (1.1), $E(G)$ is a strictly monotonically increasing function of $b_i(G), i = 1, \ldots, \lfloor n/2 \rfloor$. A *quasi-order* is introduced (see [11]): if $G_1$ and $G_2$ are two graphs, then

$$G_1 \succeq G_2 \Leftrightarrow b_i(G_1) \geqslant b_i(G_2) \text{ for all } i \geqslant 0.$$

If $G_1 \succeq G_2$, and there exists one $j$ such that $b_j(G_1) > b_j(G_2)$, then we write $G_1 \succ G_2$. Therefore,

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2).$$

Many results on the minimal energy have been obtained for various classes of graphs; see [15,19,21,24,26,28,30,31,33-37]. In [1], Caporossi et al. gave the following conjecture.

**Conjecture 1.** *Connected graphs $G$ with $n \geqslant 6$ vertices, $n-1 \leqslant e \leqslant 2(n-2)$ edges and minimum energy are star with $e-n+1$ additional edges all connected to the same vertex for $e \leqslant n + \lfloor \frac{n-7}{2} \rfloor$, and bipartite graphs with two vertices on one side, one of which is connected to all vertices on the other side otherwise.*

This conjecture is true when $e = n-1, 2(n-2)$ [3, Theorem 1], and when $e = n$ [15], $e = n+1$ [33], $e = n+2$ [22].

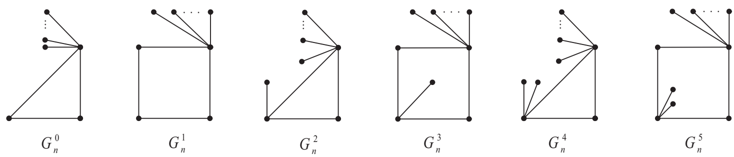


Figure 1: Graphs $G_n^0, G_n^1, G_n^2, G_n^3, G_n^4$ and $G_n^5$.

Let $G_n^0$ be the graph formed by joining 2 pendent vertices of the $K_{1,n-1}$, and $G_n^1$ be the graph formed by joining $n-4$ pendent vertices to a vertex of degree 2 of the complete bipartite graph $K_{2,2}$. Let $G_n^2$, $G_n^3$ be, respectively, the graph formed from $G_n^0$, $G_n^1$ by moving a pendant edge to the vertex of degree two. Let $G_n^4, G_n^5$ be, respectively, the graph formed from $G_n^2$, $G_n^3$ by moving a pendant edge to the vertex of degree three. all of these graphs are exhibited in Figure 1. For the structure of $G_n^5$, we assume that $n \geqslant 8$ in the whole paper. In [17], Hou determined that $G_n^0$ has minimal energy in $\mathscr{G}_n$. In [4], Chen et al., obtains that $G_n^1, G_n^2$, respectively, is the unique graph in $\mathscr{G}_n$ with the second-minimal, third-minimal energies. In this paper, we show that $G_n^3$ ($G_n^4, G_n^5$, respectively), is the unique graph in $\mathscr{G}_n$ with the fourth- (fifth-, sixth-, respectively) minimal energy.

*Hosoya index* of a graph $G$ with $n$ vertices, denoted by $Z(G)$, is defined as

$$Z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G,k), \tag{1.2}$$

where $m(G,k)$ is the number of matchings with $k$ edges in $G$. This topological index was introduced by Hosoya [14] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures [27]. Since then, many authors have investigated the Hosoya index (e.g., see [2,6,7,10,11,14]). An important direction is to determine the graphs with maximal or minimal Hosoya indices in a given class of graphs. In [13], Gutman showed that linear hexagonal chain is the unique chain with minimal Hosoya index among all hexagonal chains. In [29], Zhang determined the graph with the second minimal Hosoya index among all hexagonal chains. In [20], Zhang and Tian determined the graphs with minimal and second minimal Hosoya indices among catacondensed systems. As for $n$-vertex trees, Gutman [8] determined the graphs with the maximal, second-maximal, minimal, second-minimal, third-minimal and fourth-minimal Hoyosa indices. Recently, Hou [16] characterized the trees with a given size of matching and having minimal and second-minimal Hosoya index, respectively. Li and one of the authors in the present paper determined the trees on $n$ vertices having third-maximal, fifth-minimal, six-minimal and seven-minimal Hoyosa indices [20]. In this paper, we determine the graphs in $\mathscr{G}_n$ with minimal, second-minimal, third-minimal, fourth-minimal, fifth-minimal and sixth-minimal Hosoya index.

The following lemmas are needed in this paper.

**Lemma 1.1** ([33])**.** *Let $G$ be a graph with $n$ vertices and let $uv$ be a pendent edge of $G$ with pendent vertex $v$. Then for $2 \leqslant i \leqslant n$, $b_i(G) = b_i(G-v) + b_{i-2}(G-u-v)$.*

**Lemma 1.2** ([33])**.** *Let $G$ be any graph. Then $b_4(G) = m(G,2) - 2s$, where $m(G,2)$ is the number of 2-matchings of $G$ and $s$ is the number of quadrangles in $G$.*

**Lemma 1.3** ([15]). *Let $G$ be a unicyclic graph with $n \geqslant 6$ vertices, $G \ncong G_n^0$. Then $E(G_n^0) < E(G)$.*

**Lemma 1.4** ([4]). *$G_n^1$, $G_n^2$, respectively, has the second-minimal and third-minimal energy in the unicyclic graphs on $n$ vertices.*

## 2. Minimal energies

In this section, we shall determine the unicyclic graphs in $\mathscr{G}_n$ having the fourth-minimal, fifth-minimal, and sixth-minimal energies.

Let $m(G,2)$ denote the number of 2-matchings of a graph $G$. Obviously, $m(P_n,2) = (n-2)(n-3)/2$ and $m(C_n,2) = n(n-3)/2$.

**Lemma 2.1.** *If $G \in \mathscr{G}_n$, then $b_{2i} \geqslant 0$ for $0 \leqslant i \leqslant \lfloor \frac{n}{2} \rfloor$.*

*Proof.* Since $\mathscr{G}_n$ is the class of unicyclic graph $G$ with $n$ vertices, then

$$\begin{aligned} b_{2i}(G) &= \sum_{S \in L_{2i}} (-1)^{p(S)+i} 2^{c(S)} = \sum_{S \in L_{2i}^1} (-1)^{p(S)+i} + \sum_{S \in L_{2i}^2} (-1)^{p(S)+i} 2^{c(S)} \\ &= \sum_{S \in L_{2i}^1} 1 + 2 \sum_{S \in L_{2i}^2} (-1)^{p(S)+i}, \end{aligned} \tag{2.3}$$

where $L_{2i}^1$ is the set of graphs with no cycles in $L_{2i}$, and $L_{2i}^2 = L_{2i} \setminus L_{2i}^1$. Since there is only one cycle, say $C$, in $\mathscr{G}_n$, then $C$ (contained in $S \in L_{2i}$) must be even. Its corresponding term in $b_{2i}$ is $(-1)^{p(S)+i}2^1$. On the other hand, $C$ has two perfect matchings $M_1, M_2$, hence there exist two Sachs graphs $S'$ and $S''$ in $L_{2i}^1$ such that $S' := (S \setminus C) \cup M_1, S'' := (S \setminus C) \cup M_2$. Their corresponding terms in $b_{2i}$ are the following

$$(-1)^{p(S')+i} + (-1)^{p(S'')+i} = 2,$$

where $p(S') + i = p(S'') + i = 2i$. It is easy to see $|L_{2i}^1| \geqslant 2|L_{2i}^2|$, together with (2.3),

$$b_{2i} \geqslant \sum_{M_1, M_2 \subseteq C}^{C \subseteq S \in L_{2i}^2} \left[ (-1)^{p((S \setminus C) \cup M_1)+i} + (-1)^{p((S \setminus C) \cup M_2)+i} + (-1)^{p(S)+i} \cdot 2 \right] \geq 0.$$

□

**Lemma 2.2.** *$E(G_n^2) < E(G_n^3)$ for $n \geqslant 8$.*

*Proof.* By Sachs theorem $a_0(G_n^3) = 1, a_1(G_n^3) = 0, a_2(G_n^3) = -n, a_3(G_n^3) = 0$, $a_4(G_n^3) = 3n - 13$ and $a_i(G_n^3) = 0$ for $i \geqslant 5$, and so

$$\phi(G_n^3, \lambda) = \lambda^n - n\lambda^{n-2} + (3n-13)\lambda^{n-4}.$$

Similarly,

$$\phi(G_n^2, \lambda) = \lambda^n - n\lambda^{n-2} - 2\lambda^{n-3} + (2n-7)\lambda^{n-4}.$$

By (1.1),

$$E(G_n^3) - E(G_n^2) = \frac{1}{\pi}\int_0^{\infty} \frac{1}{x^2} \ln \frac{\left[1 + nx^2 + (3n-13)x^4\right]^2}{\left[1 + nx^2 + (2n-7)x^4\right]^2 + 4x^6} dx.$$

Let

$$\begin{aligned} f(x) &= \left[1 + nx^2 + (3n-13)x^4\right]^2 - \left[1 + nx^2 + (2n-7)x^4\right]^2 - 4x^6 \\ &= 2(n-6)x^4 + 2[(n-3)^2 - 11)x^8 + (n-6)(5n-20)x^8. \end{aligned}$$

It follows that $f(x) > 0$ for $n \geqslant 8$. Hence $E(G_n^2) < E(G_n^3)$ for $n \geqslant 8$. □

**Lemma 2.3.** *$E(G_n^3) < E(G_n^4)$ for $n \geqslant 8$.*

*Proof.* From Lemma 2.2, we know that

$$\phi(G_n^3, \lambda) = \lambda^n - n\lambda^{n-2} + (3n-13)\lambda^{n-4}.$$

By Sachs theorem, $a_0(G_n^4) = 1, a_1(G_n^4) = 0, a_2(G_n^4) = -n$, $a_3(G_n^4) = -2, a_4(G_n^4) = 3n - 13$ and $a_i(G_n^4) = 0$ for $i \geqslant 5$, and so

$$\phi(G_n^4, \lambda) = \lambda^n - n\lambda^{n-2} - 2\lambda^{n-3} + (3n-13)\lambda^{n-4}.$$

By (1.1),

$$E(G_n^4) - E(G_n^3) = \frac{1}{\pi}\int_0^{\infty} \frac{1}{x^2} \ln \frac{\left[1 + nx^2 + (3n-13)x^4\right]^2 + 4x^6}{\left[1 + nx^2 + (3n-13)x^4\right]^2} dx.$$

Obviously, $E(G_n^3) < E(G_n^4)$ for $n \geqslant 8$. □

**Lemma 2.4.** *$E(G_n^4) < E(G_n^5)$ for $n \geqslant 8$.*

*Proof.* By Sachs theorem, $a_0(G_n^5) = 1, a_1(G_n^5) = 0, a_2(G_n^5) = -n, a_3(G_n^5) = 0, a_4(G_n^5) = 4n - 20$ and $a_i(G_n^5) = 0$ for $i \geqslant 5$, and so

$$\phi(G_n^5, \lambda) = \lambda^n - n\lambda^{n-2} + (4n-20)\lambda^{n-4}.$$

By (1.1),

$$E(G_n^5) - E(G_n^4) = \frac{1}{\pi}\int_0^{\infty} \frac{1}{x^2} \ln \frac{\left[1 + nx^2 + (4n-20)x^4\right]^2}{\left[1 + nx^2 + (3n-13)x^4\right]^2 + 4x^6} dx.$$

Let

$$\begin{aligned} f(x) &= \left[1 + nx^2 + (4n-20)x^4\right]^2 - \left[1 + nx^2 + (3n-13)x^4\right]^2 - 4x^6 \\ &= 2(n-7)x^4 + (n-7)(7n-33)x^8 + 2\left[\left(n - \frac{7}{2}\right)^2 - \frac{57}{4}\right] x^6. \end{aligned}$$

It follows that $f(x) > 0$ for $n \geqslant 8$. Hence $E(G_n^4) < E(G_n^5)$ for $n \geqslant 8$. □

Let $\mathscr{G} := \{U_n^0, U_n^1, U_n^2, U_n^3, U_n^4, U_n^5, U_n^6\}$, where $U_n^0, U_n^1, U_n^2, U_n^3, U_n^4, U_n^5, U_n^6$ are graphs exhibited as in Figure 2.

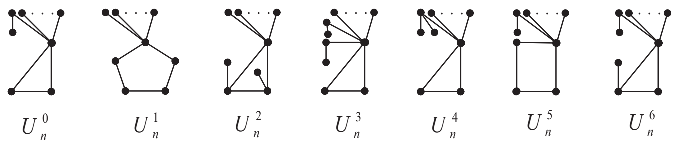


Figure 2: Graphs $U_n^0, U_n^1, U_n^2, U_n^3, U_n^4, U_n^5$ and $U_n^6$.

**Lemma 2.5.** *$E(G_n^4) < E(U_n^i)$ for $n \geqslant 8$, where $i = 1, 2, \ldots, 6$.*

*Proof.* By Sachs theorem,

$$\begin{aligned} \phi(U_n^1, \lambda) &= \lambda^n - n\lambda^{n-2} + (3n-10)\lambda^{n-4} - 2\lambda^{n-5} - (n-5)\lambda^{n-6}, \\ \phi(U_n^2, \lambda) &= \lambda^n - n\lambda^{n-2} - 2\lambda^{n-3} + (3n-12)\lambda^{n-4} - (n-5)\lambda^{n-6}, \\ \phi(U_n^3, \lambda) &= \lambda^n - n\lambda^{n-2} - 2\lambda^{n-3} + (3n-13)\lambda^{n-4} + 4\lambda^{n-5} - (2n-13)\lambda^{n-6}, \\ \phi(U_n^4, \lambda) &= \lambda^n - n\lambda^{n-2} - 2\lambda^{n-3} + (3n-11)\lambda^{n-4} + 4\lambda^{n-5} - (2n-12)\lambda^{n-6}, \\ \phi(U_n^5, \lambda) &= \lambda^n - n\lambda^{n-2} + (3n-12)\lambda^{n-4} - (2n-12)\lambda^{n-6}, \\ \phi(U_n^6, \lambda) &= \lambda^n - n\lambda^{n-2} - 2\lambda^{n-3} + (3n-11)\lambda^{n-4} + 2\lambda^{n-5} - (2n-11)\lambda^{n-6}. \end{aligned}$$

By (1.1),

$$E(U_n^1) - E(G_n^4) = \frac{1}{\pi}\int_0^{\infty} \frac{1}{x^2} \ln \frac{\left[1 + nx^2 + (3n-10)x^4 + (n-5)x^6\right]^2 + 4x^{10}}{\left[1 + nx^2 + (3n-13)x^4\right]^2 + 4x^6} dx.$$

Let

$$\begin{aligned} f(x) &= \left[1 + nx^2 + (3n-10)x^4 + (n-5)x^6\right]^2 + 4x^{10} \\ &\quad -\left[1 + nx^2 + (3n-13)x^4\right]^2 - 4x^6 \\ &= 6x^4 + (8n-14)x^6 + (n+2-\frac{\sqrt{154}}{2})(n+2+\frac{\sqrt{154}}{2})x^8 \\ &\quad +(n-\frac{13}{3})(n-4)x^{10} + (n-5)x^{12}. \end{aligned}$$

It follows that $f(x) > 0$ for $n \geqslant 8$. Hence, $E(G_n^4) < E(U_n^1)$ for $n \geqslant 8$.

Similarly, we can show that $E(G_n^4) < E(U_n^i)$ for $n \geqslant 8$, where $i = 2, 3, \ldots, 6$. □

**Lemma 2.6.** *If* $G \in \mathscr{G}_n$, $G \ncong G_n^0$, $G_n^1$, $G_n^2$, $G_n^3$, $G_n^4$, $G_n^5$, $U_n^0, U_n^1$, $U_n^2, U_n^3, U_n^4, U_n^5, U_n^6$, *then* $b_4(G) > b_4(G_n^5)$ *for* $n \geqslant 8$.

*Proof.* Since $G \in \mathscr{G}_n$ contains exactly one cycle, say $C_c$, then $n-c \geq 0$. By induction on $n-c$. If $n-c=0$, by Lemma 1.2, we have

$$b_4(G) = m(G,2) - 2s \geqslant m(G,2) - 2 = \frac{n(n-3)}{2} - 2,$$

and so

$$b_4(G) - b_4(G_n^5) \geqslant \frac{n^2}{2} - \frac{3n}{2} - 2 - (4n-20) = \frac{n^2}{2} - \frac{11n}{2} + 18,$$

hence $b_4(G) > b_4(G_n^5)$ for $n \geqslant 8$.

Suppose it is true for all graphs in this case with $n-c < p$ $(p \geqslant 1)$, and suppose $n-c = p$. Then these must be pendent edges, let $uv$ be a pendent edge of $G$ with pendent vertex $v$. By Lemma 1.1,

$$b_4(G) = b_4(G-v) + b_2(G-u-v), \quad b_4(G_n^4) = b_4(G_{n-1}^5) + b_2(K_{1,4}),$$

by induction hypothesis, $b_4(G-v) > b_4(G_{n-1}^5)$. Since $G \in \mathscr{G}_n$, $G \ncong G_n^0$, $G_n^1$, $G_n^2$, $G_n^3$, $G_n^4, G_n^5$, $U_n^0, U_n^1$, $U_n^2, U_n^3, U_n^4, U_n^5, U_n^6$, we have $b_2(G-u-v) \geqslant b_2(K_{1,4}) = 4$. It is immediate that $b_4(G) > b_4(G_n^5)$. □

**Lemma 2.7.** *If $G \in \mathscr{G}_n$ and $G \ncong G_n^0$, $G_n^1$, $G_n^2$, $G_n^3$, $G_n^4$, $G_n^5, U_n^0, U_n^1$, $U_n^2, U_n^3, U_n^4, U_n^5, U_n^6$, then $E(G) > E(G_n^5)$ for $n \geqslant 8$.*

*Proof.* By Sachs theorem, $b_0(G) = b_0(G_n^5) = 1$, $b_1(G) = b_1(G_n^5) = 0$, $b_2(G) = b_2(G_n^5) = n$, $b_3(G_n^5) = 0, b_i(G_n^5) = 0$ for $i \geqslant 5$. By Lemmas 2.7, $b_4(G) > b_4(G_n^5)$ for $n \geqslant 8$. By Lemma 2.1, $b_{2i}(G) \geqslant 0$ for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$. Hence by Coulson integral formula (1.1)

$$\begin{aligned} E(G) &= \frac{1}{\pi}\int_0^{+\infty}\frac{dx}{x^2}\ln\left[\left(\sum_{i=0}^{\lfloor \frac{n}{2}\rfloor} b_{2i}(G)x^{2i}\right)^2 + \left(\sum_{i=0}^{\lfloor \frac{n}{2}\rfloor} b_{2i+1}(G)x^{2i+1}\right)^2\right], \\ E(G_n^5) &= \frac{1}{\pi}\int_0^{+\infty}\frac{dx}{x^2}\ln\left[\left(\sum_{i=0}^{\lfloor \frac{n}{2}\rfloor} b_{2i}(G_n^5)x^{2i}\right)^2\right]. \end{aligned}$$

From these formulas it is immediate that $E(G) > E(G_n^5)$ for $n \geqslant 8$. □

Combining with Lemmas 1.3-1.4, 2.2-2.5 and 2.7, we have the main results in this section.

**Theorem 2.8.** *Let $G \in \mathscr{G}_n$, and $G \ncong G_n^0$, $G_n^1$, $G_n^2$, $G_n^3$, $G_n^4, U_n^0$, then for $n \geqslant 8$*

$$E(G_n^0) < E(G_n^1) < E(G_n^2) < E(G_n^3) < E(G_n^4) < E(G).$$

*Furthermore, let $G \in \mathscr{G}_n$, and $G \ncong G_n^0$, $G_n^1$, $G_n^2$, $G_n^3$, $G_n^4$, $G_n^5$, $U_n^0, U_n^1$, $U_n^2, U_n^3, U_n^4$, $U_n^5, U_n^6$, then for $n \geqslant 8$*

$$E(G_n^0) < E(G_n^1) < E(G_n^2) < E(G_n^3) < E(G_n^4) < E(G_n^5) < E(G).$$

*That is to say, under the isomorphism relation, $G_n^3$, $G_n^4$, respectively, has the fourth-minimal, fifth-minimal energy among $\mathscr{G}_n - \{U_n^0\}$ and $G_n^5$ has the sixth-minimal energy in $\mathscr{G}_n - \{U_n^0, U_n^1, U_n^2, U_n^3, U_n^4, U_n^5, U_n^6\}$.*

## 3. Inequalities for Hosoya index of unicyclic graphs

In this section, we determine the graphs in $\mathscr{G}_n$ with minimal, second-minimal, third-minimal, fourth-minimal, fifth-minimal and sixth-minimal Hosoya index.

It is straightforward to enumerate the $k$-matchings of $G_n^0, G_n^1, G_n^2, G_n^3, G_n^4, G_n^5$ and $R_n$ for $k \geqslant 0$.

$$\begin{aligned}
&m(G_n^0,0)=1, m(G_n^0,1)=n, m(G_n^0,2)=n-3, m(G_n^0,k)=0 \text{ for } k\geq 3,\\
&m(G_n^1,0)=1, m(G_n^1,1)=n, m(G_n^1,2)=2n-6, m(G_n^1,k)=0 \text{ for } k\geq 3,\\
&m(G_n^2,0)=1, m(G_n^2,1)=n, m(G_n^2,2)=2n-7, m(G_n^2,k)=0 \text{ for } k\geq 3,\\
&m(G_n^3,0)=1, m(G_n^3,1)=n, m(G_n^3,2)=3n-11, m(G_n^3,k)=0 \text{ for } k\geq 3,\\
&m(G_n^4,0)=1, m(G_n^4,1)=n, m(G_n^4,2)=3n-13, m(G_n^4,k)=0 \text{ for } k\geq 3,\\
&m(G_n^5,0)=1, m(G_n^5,1)=n, m(G_n^5,2)=4n-18, m(G_n^5,k)=0 \text{ for } k\geq 3.
\end{aligned} \tag{3.1}$$

Note that

$$m(U_n^i,0)=1, m(U_n^i,1)=n \text{ for } i\in\{0,1,\ldots,6\} \tag{3.2}$$

and

$$\begin{array}{llll}
m(U_n^0,2)=2n-6, & m(U_n^0,3)=n-5, & m(U_n^0,k)=0 & \text{for } k\geq 4,\\
m(U_n^1,2)=3n-10, & m(U_n^1,3)=n-5, & m(U_n^1,k)=0 & \text{for } k\geq 4,\\
m(U_n^2,2)=3n-12, & m(U_n^2,3)=n-5, & m(U_n^2,k)=0 & \text{for } k\geq 4,\\
m(U_n^3,2)=3n-13, & m(G_n^3,3)=3n-16, & m(U_n^3,k)=0 & \text{for } k\geq 4,\\
m(U_n^4,2)=3n-11, & m(U_n^4,3)=2n-12, & m(U_n^4,k)=0 & \text{for } k\geq 4,\\
m(U_n^5,2)=3n-10, & m(U_n^5,3)=2n-10, & m(U_n^5,k)=0 & \text{for } k\geq 4,\\
m(U_n^6,2)=3n-11, & m(U_n^6,3)=2n-11, & m(U_n^6,k)=0 & \text{for } k\geq 4.
\end{array} \tag{3.3}$$

By (3.1)-(3.3) and (1.2), it is immediate that for $n \geqslant 8$

$$Z(G_n^0)<Z(G_n^2)<Z(G_n^1)<Z(G_n^4)<Z(G_n^3)=Z(U_n^0)<Z(G_n^5)<Z(G), \tag{3.4}$$

where $G \in \{U_n^1, U_n^2, \ldots, U_n^6\}$.

For any $G \in \mathscr{G}_n$ with $G \ncong G_n^0, G_n^1, G_n^2, G_n^3, G_n^4, G_n^5, U_n^0, U_n^1, U_n^2, U_n^3, U_n^4, U_n^5, U_n^6$, by Lemma 2.6, $b_4(G) > b_4(G_n^5)$. Together with Lemma 1.2, we obtain

$$m(G,2)-2s > m(G_n^5,2)-2, \tag{3.5}$$

where $s$ is the number of quadrangles in $G$.

*Case* 1. If $G$ contains a cycle of length 4, then by (3.5) $m(G,2) > m(G_n^5,2)$. It is immediate that

$$\begin{aligned}
Z(G) &= 1+n+m(G,2)+m(G,3)+\cdots\\
&> 1+n+m(G_n^5,2)=Z(G_n^5).
\end{aligned}$$

*Case* 2. $G$ does not contain a cycle of length 4. Then by (3.5) $m(G,2)+2 > m(G_n^5,2)$.

At first, assume that $G$ contains a triangle. If the minimal valence of vertices on this triangle in $G$ is no less than 3, it is straightforward to check that $m(G,3) > 2$, then

$$\begin{aligned} Z(G) &= 1+n+m(G,2)+m(G,3)+m(G,4)+\cdots \\ &> 1+n+m(G,2)+2 > 1+n+m(G_n^5,2) = Z(G_n^5). \end{aligned} \tag{3.6}$$

Otherwise, there exists a vertex of valence 2 on this triangle of $G$. Furthermore, if the longest path in $G$ is no less than 5, then there exist at least two 3-matchings in $G$, similarly as above, we obtain $Z(G) > Z(G_n^3)$. Hence assume that the longest path in $G$ is less than 5. Together with $G \ncong G_n^0, G_n^1, G_n^2, G_n^3, G_n^4, G_n^5, U_n^1, U_n^5$, $G$ must be the following form in Figure 3. Denote the valence of the three vertices on the triangle

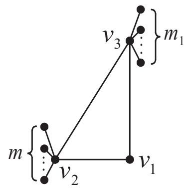


Figure 3: Graph $G$ with a vertex of valence two on the cycle.

of $G$ in increasing order as $d_1, d_2, d_3$, then $d_1 = 2 \leqslant d_2 \leqslant d_3$. Since $G \ncong G_n^0, G_n^2, G_n^4$, we assume $d_2 = m+2 \geqslant 5$, where $m$ is number of pendent edges attached to $v_2$. Thus, $m(G,2) = mm_1 + m + m_1 = (m+1)(n-m-3)+m$, and hence

$$\begin{aligned} m(G,2) - m(G_n^5,2) > 0 \ &\Leftrightarrow mn + n - m^2 + 2m - (4n-20) > 0 \\ &\Leftrightarrow (m-3)n > m^2 + 3m - 17. \end{aligned}$$

(i) $m > 3$. Then $m(G,2) - m(G_n^5,2) > 0 \Leftrightarrow n > \frac{m^2+3m-17}{m-3} = m+6+\frac{1}{m-3}$. Notice that $d_2 \leqslant d_3$, so we get $m \leqslant n-(m+3)$, namely that $m \leqslant \frac{n-3}{2}$. Thus

$$m + 6 + \frac{1}{m-3} \leqslant \frac{n+9}{2} + 1 = \frac{n+11}{2}.$$

Therefore, if $n > \frac{n+11}{2}$, i.e., $n > 11$, then $n > \frac{m^2+3m-11}{m-3}$, namely $m(G,2) - m(G_n^5,2) > 0$. When $n = 11$, then $m(G,2) = m(G_n^5,2) = 24$, therefore $Z(G) = Z(G_n^5)$ for $n = 11$.

(ii) $m = 3$. Denote the graph by $S_n$, then $m(S_n,2) = 4(n-6)+3 = 4n-21$. It is easy to see $Z(S_n) < Z(G_n^5)$. Note that $m(G_n^3,2) = 3n-11$, so $Z(G_n^3) < Z(S_n)$ if and only if $n > 10$. Furthermore, if $n = 9$, then $Z(G_n^4) < Z(S_n) < Z(G_n^3)$ and $Z(S_n) = Z(G_n^3)$ if $n = 10$.

Next, if $G$ contains a cycle of length no less than 5, then it is straightforward to check that $m(G,3) > 2$. Therefore, it is easy to see $Z(G) > Z(G_n^5)$ in this case.

Combining with (3.4), Cases 1 and 2, we get our main results in this section.

**Theorem 3.1.** *$G \in \mathscr{G}_n$ with $G \ncong G_n^0, G_n^1, G_n^2, G_n^3, G_n^4, G_n^5, U_0$,*

(i) *if $G$ does not contain a cycle of length 3, then*

$$Z(G_n^0) < Z(G_n^2) < Z(G_n^1) < Z(G_n^4) < Z(G_n^3) = Z(U_n^0) < Z(G_n^5) < Z(G)$$

*for $n \geqslant 8$.*

(ii) *if $G \ncong S_n$ contains a cycle of length 3 and does not have a vertex of valence 2 on this triangle, then*

$$Z(G_n^0) < Z(G_n^2) < Z(G_n^1) < Z(G_n^4) < Z(G_n^3) = Z(U_n^0) < Z(G_n^5) < Z(G)$$

*for $n \geqslant 8$.*

(iii) *if $G \ncong S_n$ contains a cycle of length 3 and has a vertex of valence 2 on this triangle, then $n \geqslant 11$ and either*

$$Z(G_n^0) < Z(G_n^2) < Z(G_n^1) < Z(G_n^4) < Z(G_n^3) = Z(U_n^0) < Z(G_n^5) < Z(G)$$

*for $n > 11$, or*

$$Z(G_n^0) < Z(G_n^2) < Z(G_n^1) < Z(G_n^4) < Z(G_n^3) = Z(U_n^0) < Z(G) < Z(G_n^5)$$

*for $n = 11$.*

(iv) *if $G \cong S_n$, then $n \geqslant 9$ and either*

$$Z(G_n^0) < Z(G_n^2) < Z(G_n^1) < Z(G_n^4) < Z(G_n^3) = Z(U_n^0) < Z(S_n) < Z(G_n^5)$$

*for $n > 10$, or*

$$Z(G_{10}^0) < Z(G_{10}^2) < Z(G_{10}^1) < Z(G_{10}^4) < Z(G_{10}^3) = Z(U_{10}^0) = Z(S_{10}) < Z(G_{10}^5),$$

*or*

$$Z(G_9^0) < Z(G_9^2) < Z(G_9^1) < Z(G_9^4) < Z(S_9) < Z(G_9^3) = Z(U_9^0) < Z(G_9^5).$$

## 4. Discussion

From this paper and [35], we can see the ordering of a class of cyclic graphs ordered by energy is not the same as the ordering of this class of graphs ordered by Hoyosa index. However, the latter has relation to the former. That is to say, if we know the ordering of a class of cyclic graphs ordered by energy, it may help us to determine the Hoyosa index ordering of this class of graphs. For acyclic graphs, this relation also holds, one may refer to [8] and [20].

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