Tricyclic Graphs With Minimum Modified Schultz Index And Maximum Zagreb Indices*

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Abstract

For a graph $G = (V, E)$, the modified Schultz index of G is defined as $S^*(G) = \sum_{\{u,v\}\subset V(G)} (d_G(u)\cdot d_G(v))d_G(u,v)$ where $d_G(u)$ (or $d(u)$) is the degree of the vertex u in G, and $d_G(u,v)$ is the distance between u and v. The first Zagreb index M_1 is equal to the sum of the squares of the degrees of the vertices, and the second Zagreb index M_2 is equal to the sum of the products of the degrees of pairs of adjacent vertices. In this paper, we present a unified approach to investigate the modified Schultz index and Zagreb indices of tricyclic graphs. The tricyclic graph with n vertices having minimum modified Schultz index and maximum Zagreb indices are determined.

1 Introduction

We use Bondy and Murty [1] for terminologies and notions not defined here. Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$, and $|V(G)| = n$, $|E(G)| = m$ are the number of vertices and edges of G, *resp.* For any $u, v \in V$, $d_G(u)$ (or simply by $d(u)$) and $d_G(u,v)$ denote the degree of u and the distance (i.e.,the number of edges on the shortest path) between u and v, *resp*, $N_G(v) = \{u|uv \in E(G)\}$ denotes the neighbors of v, and $d_G(v) = |N_G(v)|$. P_n, C_n and $K_{1,n-1}$(or S_n) be the path, cycle and the star on n vertices.

Schultz [2] in 1989 introduced a graph-theoretical descriptor for char-

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acterizing alkanes by an integer, namely the *Schultz index*, defined as

$$S(G) = \sum_{\{u,v\}\subset V(G)} (d_G(u) + d_G(v))d_G(u,v) \tag{1}$$

S. Klavžar and I. Gutman [3] introduced the modification of $S(G)$,

$$S^*(G) = \sum_{\{u,v\}\subset V(G)} (d_G(u) \cdot d_G(v))d_G(u,v) \tag{2}$$

which here we refer to as *the modified Schultz index.* In [4], the authors derived relations between $W(G)$ and $S(G)$, $S^*(G)$ for trees, i.e., $S(G) = 4W(G) - (n-1)(2n-1)$, $S^*(G) = 4W(G) - (n-1)(2n-1)$. In [5] the analogous results on (unbranched) hexagonal chain composed of n fused hexagons were derived as well, $S(G) = \frac{25}{4}W(G) - \frac{3}{4}(2n+1)(20n+7)$, $S^*(G) = 5W(G) - 3(2n+1)^2$. More results in this direction can be found in Refs. [6-10].

The Zagreb indices M_1 and M_2 were introduced in [11] and elaborated in [12], defined as

$$M_1(G) = \sum_{v\in V(G)} (d_G(v))^2, \quad M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v) \tag{3}$$

The main properties of M_1 and M_2 were summarized in [13]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [14]. Recently, finding the extremal values or bounds for the topological indices of graphs, as well as related problems of characterizing the extremal graphs, attracted the attention of many researchers and many results are obtained. [15] showed that the trees with the smallest and largest M_1 are the path and the star, respectively. In [16], the authors gave the the unicyclic graphs with the first three smallest and largest M_1. In [17], the authors ordered the unicyclic graphs with respect to Zagreb indices. [18] gave the bicyclic graph with the largest M_1. [19] presented a unified approach to the extremal

Zagreb indices for trees, unicyclic graphs and bicyclic graphs. In [20], the authors presented expressions for the first and second Zagreb indices of graph operations containing the cartesian product, composition, join, disjunction and symmetric difference of graphs. In [21], the authors studied the Zagreb indices of graphs with order n and $\kappa(G) \leq k$(resp., $\kappa'(G) \leq k$), the sharp lower and upper bounds were obtained with $M_i (i = 1, 2)$ for the set of graphs with $\kappa(G) \leq k \leq n-1$. In [22], the authors showed that $M_1/n \leq M_2/m$ for graphs with small difference between the maximum and minimum degree, the extremal graphs were characterized as well.

The cyclomatic number of a connected graph G is defined as $c(G) = m - n + 1$. A graph G with $c(G) = k$ is called a $k-$ cyclic graph, for $c(G) = 3$, we named G as a tricyclic graph. Let $\mathcal{T}_n$ be the set of all tricyclic graphs with n vertices. We know, by Li *et al.*[23-27], that a tricyclic graph G contains at least 3 cycles and at most 7 cycles, furthermore, there do not exist 5 cycles in G. G. Guo and Y. Wang in [28] investigated the laplacian radius of tricyclic graphs. Let $\mathscr{T}_n = \mathscr{T}_n^3 \cup \mathscr{T}_n^4 \cup \mathscr{T}_n^6 \cup \mathscr{T}_n^7$, where $\mathscr{T}_n^i$ denotes the set of tricyclic graph on n vertices with exact i cycles for $i = 3, 4, 6, 7$. Note that the induced subgraph of vertices on the cycles of $G \in \mathscr{T}_n^i (i = 3, 4, 6, 7)$ are depicted in Figure 1.

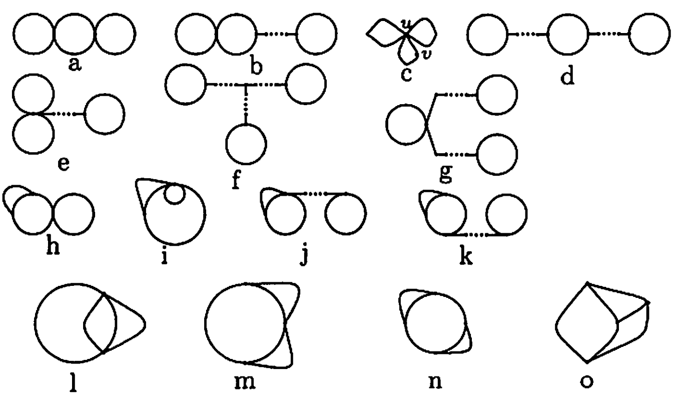


Figure 1. The arrangement of cycles of a tricyclic graph in $\mathscr{T}_n^i (i = 3, 4, 6, 7)$

For any graph $G \in \mathcal{T}_n$, G can be obtained from some graphs showed in Figure 1 by attaching trees to some vertices.

In this paper, we shall investigate the lower bounds and upper bounds for the modified Schultz index and Zagreb indices of tricyclic graphs by introducing some grafting transformations, and characterize the corresponding extremal graphs.

2 Preliminaries

Let $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. $W \subseteq V(G)$, $G - W$ denotes the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Let (G_1, v_1) and (G_2, v_2) be two graphs rooted at v_1 and v_2 respectively, then $G = (G_1, v_1)v(G_1, v_2)$ denote the graph obtained by identifying v_1 with v_2 as one common vertex v.

Lemma 1. Let C_p be the cycle of order p, v is a vertex on C_p. Then

$$\sum_{x \in V(C_p)} d_{C_p}(x, v) = \begin{cases} \frac{p^2}{4}, & \text{if } p \text{ is even;} \\ \frac{p^2 - 1}{4}, & \text{if } p \text{ is odd.} \end{cases}$$

$$W(C_p) = \begin{cases} \frac{1}{8}p^3, & \text{if } p \text{ is even;} \\ \frac{1}{8}(p^3 - p), & \text{if } p \text{ is odd.} \end{cases}$$

Similar to the Lemma 1, we have

Theorem 1. Let C_p be the cycle of order p, then

$$S^*(C_p) = 4W(C_p) = \begin{cases} \frac{1}{2}p^3, & \text{if } p \text{ is even;} \\ \frac{1}{2}(p^3 - p), & \text{if } p \text{ is odd.} \end{cases}$$

For convenience, we provide some grafting transformations, which will decrease the modified Schultz index and increase Zagreb indices of graphs as follows:

Transformations A. Let uv be an edge G, $d_G(v) \geq 2$, $N_G(v) = \{u, w_1, w_2, \cdots, w_t\}$, and $w_1, w_2, \cdots, w_t$ are leaves adjacent to v. $G' = G - \{vw_1, vw_2, \cdots, vw_t\} + \{uw_1, uw_2, \cdots, uw_t\}$, as shown in Figure 2.

Lemma 2. Let G' be obtained from G by transformation A, then

(i)[10] $S^*(G') < S^*(G)$; (ii)[19] $M_1(G') > M_1(G)$ and $M_2(G') > M_2(G)$.

Remark 1. Repeating Transformation A, any tree can changed into a star, any cyclic graph can be changed into a cyclic such that all the edges not on the cycles are pendant edges.

Transformations B. Let u and v be two vertices in G. $u_1, u_2, \cdots, u_s$ are the leaves adjacent to u, $v_1, v_2, \cdots, v_t$ are the leaves adjacent to v. $G' = G - \{vv_1, vv_2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$, $G'' = G - \{uu_1, uu_2, \cdots, uu_s\} + \{vu_1, vu_2, \cdots, vu_s\}$, as shown in Figure 3.

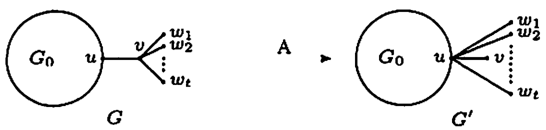


Figure 2. Transformation A.

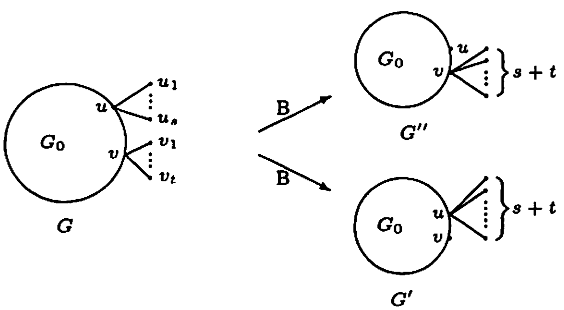


Figure 3. Transformation B.

Lemma 3. Let G', G'' are graphs obtained from G by transformation B. Then, (i)[10] $S^*(G') < S^*(G)$, or $S^*(G'') < S^*(G)$;

(ii)[19] $M_i(G') > M_i(G)$ or $M_i(G'') > M_i(G)$, $i = 1, 2$.

Remark 2. Repeating Transformation B, any cyclic graph can be changed into a cyclic graph such that all the pendant edges are attached to the same vertex.

Lemma 4. Let G' and G'' be the graphs depicted in transformation B, $G_0^* = G_0 - \{u, v\}$. Then

(i)[10] $S^*(G') > S^*(G'')$ if $d_{G_0}(u) > d_{G_0}(v)$ and $\sum_{x \in G_0^*} d_{G_0^*}(x) d_{G_0^*}(x, u) < \sum_{x \in G_0^*} d_{G_0^*}(x) d_{G_0^*}(x, v)$; otherwise $S^*(G') < S^*(G'')$.

(ii)$M_i(G') > M_i(G'')$, if $d_{G_0}(u) > d_{G_0}(v)$ and $\sum_{x \in N_{G_0}(u)} d_{G_0}(x) > \sum_{x \in N_{G_0}(v)} d_{G_0}(x)$; otherwise $M_i(G') < M_i(G'')$ for $i = 1, 2$.

Proof. We only prove the second case here.

Let $d_{G_0}(u) = p$ and $d_{G_0}(v) = q$. By the definition of Zagreb indices, we arrive at

$$M_1(G') - M_1(G'') = (p + s + t)^2 + q^2 - (q + s + t)^2 - p^2 = 2(s + t)(p - q)$$

(i) If u, v are not adjacent in G, then, by the definition of M_2, we have

$$M_2(G') - M_2(G'') = (s + t)[(\sum_{x \in N_{G_0}(u)} d_{G_0}(x) - \sum_{x \in N_{G_0}(v)} d_{G_0}(x)) + (p - q)]$$

(ii) u, v are adjacent in G, then

$$M_2(G') - M_2(G'') = (s + t)[(\sum_{x \in N_{G_0}(u)} d_{G_0}(x) - \sum_{x \in N_{G_0}(v)} d_{G_0}(x)) + 2(p - q)]$$

Therefore, if $d_{G_0}(u) > d_{G_0}(v)$ and $\sum_{x \in N_{G_0}(u)} d_{G_0}(x) > \sum_{x \in N_{G_0}(v)} d_{G_0}(x)$, then $M_i(G') > M_i(G'')(i = 1, 2)$; otherwise $M_i(G') < M_i(G'')(i = 1, 2)$. ■

Lemma 5. Suppose that G is a graph of order $n \geq 7$ obtained from a connected graph $G_0 \ncong P_1$ and a cycle $C_p = v_0 v_1 \cdots v_{p-1} v_0 (p \geq 4$ for p is even; otherwise $p \geq 5)$ by identifying v_0 with a vertex v of the graph G_0 (see Figure 4), i.e., $G = G_0 v C_p$. Let $G' = G - v_{p-1} v_{p-2} + v v_{p-2}$, i.e., $G' = G_0 v C_{p-1} v K_1$. We name above operation as grafting transformation

C. Then, we have (i) $S^*(G') < S^*(G)$; (ii) $M_i(G') > M_i(G) (i = 1, 2)$.

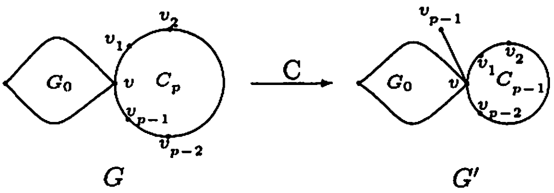


Figure 4. Transformation C

Proof. Let $G_0' = G_0 - v$, $C_p' = C_p - \{v, v_{p-1}\}$, $C_{p-1}' = C_{p-1} - v$.

(i) By the definition of modified Schultz index, we have

Case (1). p is even.

$$
\begin{aligned}
& S^*(G) \\
= & \sum_{x,y \in G_0'} d_{G_0'}(x) d_{G_0'}(y) d_{G_0'}(x,y) + \sum_{x \in G_0'} d_{G_0'}(x) d_G(v) d_{G_0'}(x,v) \\
& + 4 \sum_{x,y \in C_p'} d_{C_p'}(x,y) + 2 d_G(v) \sum_{x \in C_p'} d_{C_p'}(x,v) + 4 \sum_{x \in C_p'} d_{C_p'}(x,v) + 2 d_G(v) \\
& + 2 \sum_{x \in G_0'} d_{G_0'}(x) \sum_{y \in C_p'} [d_{G_0'}(x,v) + 2 \sum_{x \in G_0'} d_{G_0'}(x)(d_{G_0'}(x,v) + 1)] \\
= & \sum_{x,y \in G_0'} d_{G_0'}(x) d_{G_0'}(y) d_{G_0'}(x,y) + d_G(v) \sum_{x \in G_0'} d_{G_0'}(x) d_{G_0'}(x,v) + \frac{p^3 - 4p^2 + 8}{2} \\
& + 2 d_G(v)(\frac{1}{4}p^2 - 1) + p^2 - 4 + 2 d_G(v) + 2 \sum_{x \in G_0'} d_{G_0'}(x)[(p-2) d_{G_0'}(x,v) \\
& + \frac{1}{4}p^2 - 1] + 2 \sum_{x \in G_0'} d_{G_0'}(x)[d_{G_0'}(x,v) + 1] \\
= & \sum_{x,y \in G_0'} d_{G_0'}(x) d_{G_0'}(y) d_{G_0'}(x,y) + [d_G(v) + 2p - 2] \sum_{x \in G_0'} d_{G_0'}(x) d_{G_0'}(x,v) \\
& + \frac{1}{2}p^2 \sum_{x \in G_0'} d_{G_0'}(x) + \frac{1}{2}p^3 - p^2 + \frac{1}{2}p^2 d_G(v)
\end{aligned}
$$

Similarly, we have

$$
\begin{aligned}
&S^*(G') \\
&= \sum_{x,y\in G'_0} d_{G'_0}(x)d_{G'_0}(y)d_{G'_0}(x,y) + [d_G(v)+2p-2]\sum_{x\in G'_0} d_{G'_0}(x)d_{G'_0}(x,v) \\
&\quad + \frac{p^2-2p+2}{2}\sum_{x\in G'_0} d_{G'_0}(x) + \frac{p^3-3p^2+6p-6}{2} + \frac{p^2-2p+2}{2}d_G(v)
\end{aligned}
$$

Thus,

$$
\begin{aligned}
&S^*(G') - S^*(G) \\
&= (1-p)\sum_{x\in G'_0} d_{G'_0}(x) + (1-p)d_G(v) - \frac{1}{2}(p-3)^2 + \frac{3}{2} < 0 \text{ (since } p \geq 4)
\end{aligned}
$$

Case (2). p is odd.

Similar to case (1), we have

$$
\begin{aligned}
&S^*(G) \\
&= \sum_{x,y\in G'_0} d_{G'_0}(x)d_{G'_0}(y)d_{G'_0}(x,y) + [d_G(v)+2p-2]\sum_{x\in G'_0} d_{G'_0}(x)d_{G'_0}(x,v) \\
&\quad + \frac{1}{2}(p^2-1)\sum_{x\in G'_0} d_{G'_0}(x) + \frac{1}{2}p^3 - p^2 - \frac{1}{2}p + 1 + \frac{1}{2}(p^2-1)d_G(v)
\end{aligned}
$$

and

$$
\begin{aligned}
&S^*(G') \\
&= \sum_{x,y\in G'_0} d_{G'_0}(x)d_{G'_0}(y)d_{G'_0}(x,y) + [d_G(v)+2p-2]\sum_{x\in G'_0} d_{G'_0}(x)d_{G'_0}(x,v) \\
&\quad + \frac{p^2-2p+3}{2}\sum_{x\in G'_0} d_{G'_0}(x) + \frac{1}{2}p^3 - \frac{3p^2+7p-7}{2} + \frac{p^2-2p+3}{2}d_G(v)
\end{aligned}
$$

Thus,

$$
\begin{aligned}
&S^*(G') - S^*(G) \\
&= (2-p)\sum_{x\in G'_0} d_{G'_0}(x) + (2-p)d_G(v) - \frac{1}{2}(p-4)^2 + \frac{7}{2} < 0 \quad \text{(since } p \geq 5)
\end{aligned}
$$

(ii) By the definition of Zagreb indices, we have

$$M_1(G) - M_1(G') = d_G^2(v) + 4 - (d_G(v) + 1)^2 - 1 = 2(1 - d_G(v)) < 0$$

Similarly, we have

$$\begin{aligned} & M_2(G) - M_2(G') \\ = & \sum_{x \in N_{G_0'}(v)} d_{G_0}(x) d_G(v) + 4 d_G(v) + 4 - \sum_{x \in N_{G_0'}(v)} d_{G_0}(x)(d_G(v) + 1) \\ & - 5(d_G(v) + 1) \\ = & - \sum_{x \in N_{G_0'}(v)} d_{G_0}(x) - (d_G(v) + 1) < 0 \end{aligned}$$

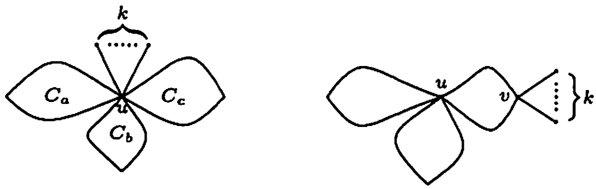
■

3 The smallest modified Schultz index and largest Zagreb indices of $\mathscr{T}_n^i$

In this section we shall determine the graphs achieve the smallest modified Schultz index and largest Zagreb indices in $\mathscr{T}_n^i (i = 3, 4, 6, 7)$, respectively.

3.1 The smallest modified Schultz index and largest Zagreb indices in $\mathscr{T}_n^3$

Let H be a graph formed by attaching three cycles C_a, C_b, C_c to a common vertex u; see Figure 1.(c). Then let $G_{a,b,c}^k$ is the graph on n vertices obtained from H by attaching k pendent edges to the vertex u. We also set $\mathcal{G} = \{G \in \mathscr{T}_n$: G is a graph obtained from H by attaching k pendent vertices to the vertex v of H except $u\}$, where $a + b + c + k = n + 2$, and let $\widetilde{G}_{a,b,c}^k$ is one of the resulted graph. See Figure 5.



$G^k_{a,b,c}$ $\widetilde{G}^k_{a,b,c}$

Figure 5. The graphs $G^k_{a,b,c}$ and $\widetilde{G}^k_{a,b,c}$

Immediately, by Lemma 4, the following result is obvious.

Lemma 6. Let $G^k_{a,b,c}$, $\widetilde{G}^k_{a,b,c}$ are graphs depicted above, then

(i) $S^*(G^k_{a,b,c}) < S^*(\widetilde{G}^k_{a,b,c})$;

(ii) $M_i(G^k_{a,b,c}) > M_i(\widetilde{G}^k_{a,b,c})(i = 1, 2)$.

Lemma 7. Let G is a n vertices tricyclic graph with exactly three cycles C_a, C_b and C_c, then $S^*(G) \geq S^*(G^k_{a,b,c})$ and $M_i(G) \leq M_i(G^k_{a,b,c})(i = 1, 2)$ with the equalities if and only if $G \cong G^k_{a,b,c}$.

Proof. Let G is a n vertices tricyclic graph with exactly three cycles C_a, C_b and C_c, then the arrangement of the three cycles contained in G are depicted in Figure 1. a,b,c,d,e,f,g, respectively. Repeating transformation A and B on G, and by Lemma 2 and Lemma 3, we have

(i) $S^*(G) \geq S^*(G^k_{a,b,c})$ or $S^*(G) \geq S^*(\widetilde{G}^k_{a,b,c})$;

(ii)$M_i(G) \leq M_i(G^k_{a,b,c})$ or $M_i(G) \leq M_i(\widetilde{G}^k_{a,b,c})$ for $i = 1, 2$.

Hence, by Lemma 6, we have

(i)$S^*(G^k_{a,b,c}) < S^*(\widetilde{G}^k_{a,b,c})$; (ii)$M_i(G^k_{a,b,c}) > M_i(\widetilde{G}^k_{a,b,c})$ for $i = 1, 2$.

Lemma 8. For any given positive integers a, b, c and k, then

(i) $S^*(G^k_{a,b,c}) > S^*(G^{k+1}_{a-1,b,c})$ and $M_i(G^k_{a,b,c}) < M_i(G^{k+1}_{a-1,b,c})(i = 1, 2)$, if $a \geq 4$, $b, c \geq 3$;

(ii) $S^*(G^k_{a,b,c}) > S^*(G^{k+1}_{a,b-1,c})$ and $M_i(G^k_{a,b,c}) < M_i(G^{k+1}_{a,b-1,c})(i = 1, 2)$, if $a, c \geq 3$, $b \geq 4$;

(iii) $S^*(G^k_{a,b,c}) > S^*(G^{k+1}_{a,b,c-1})$ and $M_i(G^k_{a,b,c}) < M_i(G^{k+1}_{a,b,c-1})(i = 1, 2)$, if $c \geq 4$, $a, b \geq 3$.

Proof. By the symmetry of three cycles C_a, C_b and C_c contained in G, here we only show that (i) holds. We omit the proofs for (ii) and (iii). Let $G_0 = C_b u C_c u k K_1$, $G_0' = C_b u C_c u (k+1) K_1$, then $G^k_{a,b,c} = C_a u G_0$ and $G^{k+1}_{a-1,b,c} = C_{a-1} u G_0'$. Applying transformation C on $G^k_{a,b,c}$ and we get $G^{k+1}_{a-1,b,c}$, by Lemma 5, the results hold.

Combing Lemma 6, Lemma 7 with Lemma 8, we have

Theorem 2. Let $G \in \mathscr{T}_n^3$, then

(i) $S^*(G) \geq 2n^2 + 13n - 9$;

(ii)$M_1(G) \leq n^2 - n + 18$ and $M_2(G) \leq n^2 + n + 7$.

The equalities hold if and only if $G \cong G^{n-7}_{3,3,3}$.

Proof. Follows Lemmas 6, 7 and 8, for any graph $G \in \mathscr{T}_n^3$,

$$S^*(G) \geq S^*(G^{n-7}_{3,3,3}).$$

It is ease to calculate out that the modified Schultz index and Zagreb indices of $G^{n-7}_{3,3,3}$ are $S^*(G^{n-7}_{3,3,3}) = 2n^2 + 13n - 9$; $M_1(G^{n-7}_{3,3,3}) = n^2 - n + 18$, $M_2(G^{n-7}_{3,3,3}) = n^2 + 4n + 7$. ■

3.2 The smallest modified Schultz index and largest Zagreb indices in $\mathscr{T}_n^4$

Let P_{a+1}, P_{b+1}, P_{c+1} be three vertex disjoint paths with $a, b, c \geq 1$, and at most one of them is 1. Identifying the three initial vertices and terminal vertices of them, *resp.* The resulting graph, denote as Θ−graph $\Theta(a, b, c)$. Connecting the cycle C_d and $\Theta(a, b, c)$ by a path P_k, where $k \geq 1$, naming the resulting graph as $\widetilde{\Theta}$−graph. From [23-27], we know that the are exactly four types of $\widetilde{\Theta}$−graph, see Figure 1. h,i,j,k. $\mathscr{T}_n^4$ is the set of graphs each of which is a $\widetilde{\Theta}$−graph, has some trees attached, if possible. Let $\mathcal{H}_0 = \Theta(a, b, c) v C_d$, and $H^k_{a,b,c,d}$ is a n vertex graph formed from $\mathcal{H}_0$ by attaching $k (k = n + 5 - a - b - c - d)$ pendent vertices to v, see Figure 6.

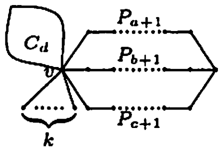


Figure 6. The graph $H^k_{a,b,c,d}$

Similar to the discussion way of section 3.1, we have

Lemma 9. Let $G \in \mathscr{T}_n^4$ such that G contains the $\Theta(a,b,c)$ and the cycle C_d with $E(\Theta(a,b,c)) \cap E(C_d) = \emptyset$. Then

(i) $S^*(G) \geq S^*(H^k_{a,b,c,d})$;

(ii) $M_i(G) \leq M_i(G)(H^k_{a,b,c,d})$ for $i = 1, 2$.

The equalities hold if and only if $G \cong H^k_{a,b,c,d}$.

Similarly, we have

Lemma 10. For any given positive integers a, b, c, d and k, then

(i) $S^*(H^k_{a,b,c,d}) > S^*(H^{k+1}_{a-1,b,c,d})$ and $M_i(H^k_{a,b,c,d}) < M_i(H^{k+1}_{a-1,b,c,d})$ ($i = 1, 2$), for either $a \geq 4$, $b, c \geq 2$ and $bc \geq 6$, $d \geq 3$ or $a = 3$, $b, c, d \geq 3$;

(ii) $S^*(H^k_{a,b,c,d}) > S^*(H^{k+1}_{a,b-1,c,d})$ and $M_i(H^k_{a,b,c,d}) < M_i(H^{k+1}_{a,b-1,c,d})$ ($i = 1, 2$), for either $b \geq 4$, $a, c \geq 2$ and $ac \geq 6$, $d \geq 3$ or $b = 3$, $a, c, d \geq 3$;

(iii) $S^*(H^k_{a,b,c,d}) > S^*(H^{k+1}_{a,b,c-1,d})$ and $M_i(H^k_{a,b,c,d}) < M_i(H^{k+1}_{a,b,c-1,d})$ ($i = 1, 2$), for either $c \geq 4$, $a, b \geq 2$ and $ab \geq 6$, $d \geq 3$ or $c = 3$, $a, b, d \geq 3$;

(iv) $S^*(H^k_{a,b,c,d}) > S^*(H^{k+1}_{a,b,c,d-1})$ and $M_i(H^k_{a,b,c,d}) < M_i(H^{k+1}_{a,b,c,d-1})$ ($i = 1, 2$), for $d \geq 4$, $a, b, c \geq 2$ and $abc \geq 18$.

And

Theorem 3. Let $G \in \mathscr{T}_n^4$, then

(i) $S^*(G) \geq 2n^2 + 13n - 15$;

(ii)$M_1(G) \leq n^2 - n + 20$ and $M_2(G) \leq n^2 + 4n + 11$.

The equalities hold if and only if $G \cong H^{n-6}_{2,3,3,3}$ (or $H^{n-6}_{3,2,3,3}$, $H^{n-6}_{3,3,2,3}$).

Proof. Note that $H^{n-6}_{2,3,3,3} \cong H^{n-6}_{3,2,3,3} \cong H^{n-6}_{3,3,2,3}$. By Lemma 10, for any graph $G \in \mathscr{T}_n^4$, $S^*(G) \geq S^*(H^{n-6}_{2,3,3,3})$; $M_i(G) \leq M_i(H^{n-6}_{2,3,3,3})$ for $i = 1, 2$, Note that the modified Schultz index and the Zagreb indices of $H^{n-6}_{2,3,3,3}$ are

$S^*(H^{n-6}_{2,3,3,3}) = 2n^2+13n-15$; $M_1(H^{n-6}_{2,3,3,3}) = n^2-n+20$, $M_2(H^{n-6}_{2,3,3,3}) = n^2+4n+11$.

3.3 The smallest modified Schultz index and largest Zagreb indices in $\mathscr{T}_n^6$

Let $I^k_{a,b,c,d}$ is a tricyclic graph with exact 6 cycles on n vertices obtained from Figure 1(l) by attaching k pendent vertices to v showed in Figure 7(i);

$J^k_{a,b,c}$ is a tricyclic graph with exact 6 cycles on m vertices obtained from Figure 1(m) by attaching k pendent vertices to v showed in Figure 7(ii);

$K^k_{a,b,c}$ is a tricyclic graph with exact 6 cycles on n vertices obtained from Figure 1(n) by attaching k pendent vertices to v showed in Figure 7(iii).

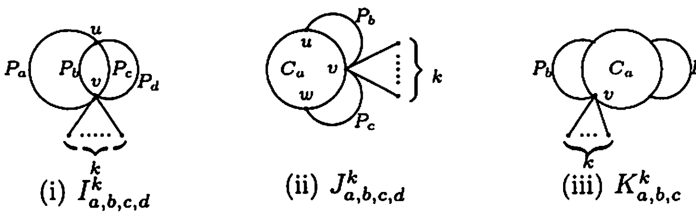


Figure 7. The graphs $I^k_{a,b,c,d}$, $J^k_{a,b,c}$, $K^k_{a,b,c}$

Lemma 11. Let $G \in \mathscr{T}_n^6$. Then

(i) $S^*(G) \geq S^*(I^k_{a,b,c,d})$ and $M_i(G) \leq M_i(I^k_{a,b,c,d})$ $(i = 1, 2)$, if the six cycles in G are arranged the same way with the graphs depicted in Figure 1(l);

(ii) $S^*(G) \geq S^*(J^k_{a,b,c})$ and $M_i(G) \leq M_i(J^k_{a,b,c})$ $(i = 1, 2)$, if the six cycles in G are arranged the same way with the graphs depicted in Figure 1(m);

(iii) $S^*(G) \geq S^*(K^k_{a,b,c})$ and $M_i(G) \leq M_i(K^k_{a,b,c})$ $(i = 1, 2)$, if the six cycles in G are arranged the same way with the graphs depicted in Figure 1(n);

Similarly, we have

Theorem 4. Let $G \in \mathscr{T}_n^6$,

(i) If the arrangement of the six cycles is the same as Fig 1(l), then $S^*(G) \geq S^*(I_{3,3,3,2}^{n-5})$ and $M_i(G) \leq M_i(I_{3,3,3,2}^{n-5})$ $(i = 1,2)$. The equalities hold if and only if $G \cong I_{3,3,3,2}^{n-5}$;

(ii) If the arrangement of the six cycles is the same as Fig 1(m), then $S^*(G) \geq S^*(J_{3,3,3}^{n-5})$ and $M_i(G) \leq M_i(J_{3,3,3}^{n-5})$ $(i = 1,2)$. The equalities hold if and only if $G \cong J_{3,3,3}^{n-5}$;

(iii) If the arrangement of the six cycles is the same as Fig 1(n), then $S^*(G) \geq S^*(K_{4,3,3}^{n-6})$ and $M_i(G) \leq M_i(K_{4,3,3}^{n-6})$ $(i = 1,2)$. The equalities hold if and only if $G \cong K_{4,3,3}^{n-6}$.

Moreover, It is easily to compute out that

$S^*(I_{3,3,3,2}^{n-5}) = 2n^2 + 13n - 27$, $S^*(J_{3,3,3}^{n-5}) = 2n^2 + 13n - 22$;

$S^*(K_{4,3,3}^{n-6}) = 2n^2 + 27n - 78$, and

$M_1(I_{3,3,3,2}^{n-5}) = n^2 - n + 24$, $M_2(I_{3,3,3,2}^{n-5}) = n^2 + 4n + 19$,

$M_1(J_{3,3,3}^{n-5}) = n^2 - n + 22$, $M_2(J_{3,3,3}^{n-5}) = n^2 + 4n + 16$;

$M_1(K_{4,3,3}^{n-6}) = n^2 - 5n + 37$, $M_2(K_{4,3,3}^{n-6}) = n^2 - n + 30$.

Combining above results, we arrive at:

Theorem 5. Let $G \in \mathscr{T}_n^6$, then

(i) $S^*(G) \geq 2n^2 + 13n - 27$;

(ii)$M_1(G) \leq n^2 - n + 24$, $M_2(G) \leq n^2 + 4n + 19$.

The equalities hold if and only if $G \cong I_{3,3,3,2}^{n-5}$.

3.4 The smallest modified Schultz index and largest Zagreb indices in $\mathscr{T}_n^7$

Let $R^k(a,b,c,d,e,f)$ is a tricyclic graph with exact seven cycles on n vertices obtained from Figure 1(o) by attaching k pendent vertices to v showed in Figure 8, where $a+b+c+d+e+f+k=n+8$.

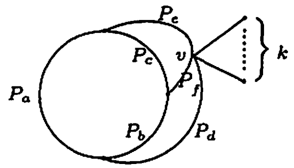


Figure 8. The graph $R^{k}_{a,b,c,d,e,f}$

Applying the similar methods above, we can obtain the following results, and we omit the proof here.

Theorem 6. Let $G \in \mathscr{T}_n^7$, then

(i) $S^*(G) \geq S^*(R^{n-4}_{2,2,2,2,2,2})$;

(ii) $M_i(G) \leq M_i(R^{n-4}_{2,2,2,2,2,2})$ $(i=1,2)$.

The equalities hold if and only if $G \cong R^{n-4}_{2,2,2,2,2,2}$.

Note that $S^*(R^{n-4}_{2,2,2,2,2,2}) = 2n^2+13n-30$; $M_1(R^{n-4}_{2,2,2,2,2,2}) = n^2-n+24$, $M_2(R^{n-4}_{2,2,2,2,2,2}) = n^2+4n+22$.

4 The smallest modified Schultz index and largest Zagreb indices of $\mathscr{T}_n$

Combining all the results above, we arrive at our main result:

Theorem 7. Let $G \in \mathscr{T}_n$, then

(i) $S^*(G) \geq 2n^2+13n-30$;

(ii) $M_1(G) \leq n^2-n+24$ and $M_2(G) \leq n^2+4n+22$.

The equalities hold if and only if $G \cong R^{n-4}_{2,2,2,2,2,2}$.

Proof. By Theorem 2, 3, 5 and 6, for any graph $G \in \mathscr{T}_n$.

$$\begin{aligned} S^*(G) &\geq \max\{S^*(G^{n-7}_{3,3,3}), S^*(H^{n-6}_{2,3,3,3}), S^*(I^{n-5}_{3,3,3,2}), S^*(R^{n-4}_{2,2,2,2,2,2})\} \\ &= S^*(R^{n-4}_{2,2,2,2,2,2}) = 2n^2+13n-30 \end{aligned}$$

and

$$M_i(G) \leq \min\{M_i(G^{n-7}_{3,3,3}), M_i(H^{n-6}_{2,3,3,3}), M_i(I^{n-5}_{3,3,3,2}), S^*(R^{n-4}_{2,2,2,2,2,2})\}$$
$$= M_i(R^{n-4}_{2,2,2,2,2,2}) \ (i = 1, 2)$$

■

Therefore, $R^{n-4}_{2,2,2,2,2,2}$ has the smallest modified Schultz index and largest Zagreb indices among all tricyclic graphs with n vertices.

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