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The Lower Bound of Revised Szeged Index with Respect to Tricyclic Graphs

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Abstract

The revised Szeged index of a graph is defined as $Sz^*(G) = \sum_{e=uv\in E}(n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2})$, where $n_u(e)$ and $n_v(e)$ are, respectively, the number of vertices of G lying closer to vertex u than to vertex v and the number of vertices of G lying closer to vertex v than to vertex u, and $n_0(e)$ is the number of vertices equidistant to u and v. In the paper, we acquired the lower bound of revised Szeged index among all tricyclic graphs, and the extremal graphs that attain the lower bound are determined.

1 Introduction

A map taking graphs as arguments is referred to as a graph invariant if it assigns equal values to isomorphic graphs. These invariants have been used for modeling some properties of chemical compounds and capturing the structural essence of compounds with respect to a molecule, which, (in chemical) graph theory, are also called the topological indices.

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They include graph energy, various of graph like-energies, Randić index, Zagreb index, PI index and graph entropies, etc, see literatures [2, 5, 9, 13, 14, 17, 18, 22, 23, 25, 26, 33, 34] and cited in them for properties and applications of the variants.

For a simple connected graph G, Wiener gives the definition of Wiener index as follows:

$$W(G) = \sum_{\{u,v\} \subseteq V} d(u, v). \tag{1}$$

This topological index has been extensively studied, see [12, 13, 15, 34]. Let $e = uv$ be an edge of G, and define three subsets of $V(G)$ below.

$$N_u(e) = \{w \in V : d(u, w) < d(v, w)\},$$

$$N_v(e) = \{w \in V : d(u, w) > d(v, w)\},$$

$$N_0(e) = \{w \in V : d(u, w) = d(v, w)\}.$$

By the way $\{N_u(e), N_v(e), N_0(e)\}$ consists of a partition of vertices set V with respect to e. The number of vertices of $N_u(e), N_v(e), N_0(e)$ are denoted by $n_u(e), n_w(e), n_0(e)$, respectively. As we known, Wiener index has the following formula:

$$W(G) = \sum_{e=uv \in E} n_u(e) n_v(e), \tag{2}$$

which is applicable for trees. Using the above formula, Gutman [11] introduced a graph invariant named the *Szeged index*(Sz) as extension of the Wiener index and defined it by

$$Sz(G) = \sum_{e=uv \in E} n_u(e) n_v(e).$$

The two invariants have a simple and interesting relation [32]

$$Sz(G) \geq W(G), \tag{3}$$

with equality if and only if all blocks of G are complete graphs. Short later, Randić [31] observed that the Szeged index does not take into account the contributions of the vertices at equal distances from the endpoints of an edge, and so he conceived a modified version of the Szeged index which is named the *revised Szeged index*(Sz^*). The revised Szedged index of a connected graph G is defined as

$$Sz^*(G) = \sum_{e=uv \in E} (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2}).$$

Note that $Sz^*(G) \geq Sz(G)$, and equality holds if and only if G is a bipartite graph. Since Inequality (3), the differences $Sz(G) - W(G)$ and $Sz^*(G) - W(G)$ are interesting and has attracted many mathematicians to focus, see [3, 6, 8, 20, 27, 28, 35] for details.

In addition, some properties and applications of these two topological indices have been reported in [21,22,29,30,32]. Aouchiche and Hansen [1] showed that for a connected graph G of order n and m, an upper bound of the revised Szeged index of G is $\frac{n^2m}{4}$. In [36], Xing and Zhou acquired the unicyclic graphs of order n with the smallest and largest revised Szeged indices for $n \geq 5$.

Theorem 1.1 *Among unicyclic graphs with $n \geq 3$, $S_{n,3}$ for $12 \geq n \geq 3$ and $S_{n,4}$ for $n \geq 13$ are the unique graphs with the smallest revised Szeged index, where $Sz^*(S_{n,3}) = \frac{1}{4}(5n^2 - 4n - 6)$ and $Sz^*(S_{n,4}) = n^2 + 3n - 12$.*

Hansen et al. [16], utilizing the Autographix, proposed the upper bound of bicyclic graphs as a conjecture. One of present authors with Li [24] completely approved the conjecture. Short recently, the lower bound of bicyclic graphs and the graphs attached the bound are determined in [19].

Theorem 1.2 *Let G be a connected bicyclic graph G of order $n(n \geq 6)$. Then*

$$Sz^*(G) \geq \begin{cases} n^2 + 8n - 29, & \textit{if } n \geq 17, \textit{ and `=' holds iff } G \cong A_1, \\ 355, & \textit{if } n = 16, \textit{ and `=' holds iff } G \cong A_1, A_2, \\ \frac{5}{4}n^2 + 3n - 13, & \textit{if } 9 \leq n \leq 15, \textit{ and `=' holds iff } G \cong A_2, \\ 91, & \textit{if } n = 8, \textit{ and `=' holds iff } G \cong A_2, A_3. \\ \frac{3}{2}n^2 - 5, & \textit{if } n = 6, 7, \textit{ and `='holds iff } G \cong A_3. \end{cases}$$

These graphs A_1, A_2 and A_3 are presented in Fig.2.

In addition, Li et al. [7] got the upper bound for the topological index among all tricyclic graphs. It is natural to think about the dual problem. In the paper, for tricyclic graphs, the lower bound of Sz^* are obtained and these graphs for which the bound are attained are characterized completely.

Theorem 1.3 *Let G be a connected tricyclic graph G of order $n(\geq 8)$. Then*

$$Sz^*(G) \geq \begin{cases} n^2 + 13n - 50, & \textit{if } n \geq 20, \textit{ and `=' holds iff } G \cong C_1, \\ \frac{5}{4}n^2 + 7n - \frac{114}{4}, & \textit{if } 19 \geq n \geq 8, \textit{ and `=' holds iff } G \cong C_4. \end{cases}$$

Where, C_1 and C_4 are shown in Fig. 6.

We now introduce some graph-theoretical notations and terminology. For other undefined ones, see the book [4]. All graph considered in the paper are finite, undirected and simple. Let S_n and C_n be the star and cycle on n vertices, respectively. $G_1 \cdot G_2$ denote the graph obtained from G_1 and G_2 by fusing one vertex of the two graphs. Let w be the common vertex of G_1 and G_2. Obviously, w is a cut vertex of G. Especially, if the vertex w of $S_{n-r+1} \cdot C_r$ is the center of S_{n-r} and a vertex in C_{r+1}, we mark the graph as $S_{n,r}$ for short.

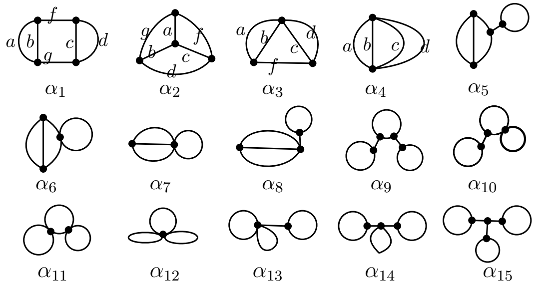

Figure 1. The all braces in tricyclic graphs $\mathscr{G}_n$.

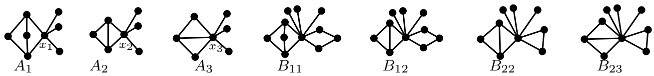

Figure 2. The graphs using in the Theorem 1.2 and Theorem 3.8.

If a graph H is gotten by removing repeatedly all pendants (If any) of G. Then we say H is the *brace* of G. That is to say, H doesn't contain any pendent vertex. Obviously, for all connected tricyclic graphs, their braces are shown in Fig. 1. Let $\mathscr{G}_n$ be the set of tricyclic graphs on order n, and $\mathscr{C}_n^i$ be the collection whose element contains α_i as its brace for $i = 1, 2, \cdots, 15$, respectively. Clearly, $\mathscr{G}_n = \cup_{i=1}^{15} \mathscr{C}_n^i$. For convenience, let $\mathscr{A} = \cup_{i=5}^{15} \mathscr{C}_n^i$. For the sake of brevity, let $P(i)$ denote the path with the length i, e.g., the length of $P(a)$ is a. Based on the lengths of the paths(they are shown in Fig.1) in some brace, we mark $\alpha_1 = \alpha_1(a, b, c, d, f, g)$, $\alpha_2 = \alpha_2(a, b, c, d, f, g)$, $\alpha_3 = \alpha_3(a, b, c, d, f)$ and $\alpha_4 = \alpha_4(a, b, c, d)$.

2 Preliminary

From the fact that $n_u(e) + n_v(e) + n_0(e) = n$ for every edge $e = uv \in E$, we have

$$\begin{aligned} Sz^*(G) &= \sum_{e=uv\in E} \big(n_u(e) + \frac{n_0(e)}{2}\big)\big(n_v(e) + \frac{n_0(e)}{2}\big) \\ &= \frac{mn^2}{4} - \frac{1}{4}\sum_{e=uv\in E} (n_u(e) - n_v(e))^2. \end{aligned}$$

Especially, set $m = n + 2$, we deduce

$$Sz^*(G) = \frac{n^3 + 2n^2}{4} - \frac{1}{4}\sum_{e=uv\in E} (n_u(e) - n_v(e))^2. \tag{1}$$

Moreover, $n^2 + 13n - 50 = \frac{n^3+2n^2}{4} - \frac{1}{4}(n^3 - 2n^2 - 52n + 200)$.

For short, let $\delta(e) = |n_u(e) - n_v(e)|$. Eq. (1) is rewritten as

$$Sz^*(G) = \frac{n^3 + 2n^2}{4} - \frac{1}{4}\sum_{e\in E}\delta(e)^2. \tag{2}$$

We now provide some results which will be used in the next Section.

Lemma 2.1 *Let $e \in E(G)$. Then*

$$\delta(e) \leq n - 2.$$

with equality if and only if e is a pendant edge.

We now consider the graph $G \cong G_1 \cdot G_2$. For every $e = uv \in E(G_1)$, w belongs to one of the three sets $N_u(e), N_v(e), N_0(e)$. Since every path connecting $u(v)$ and each vertex in $V(G_2)$ is via w, all vertices of G_2 must contained in one of the three sets $N_u(e), N_v(e), N_0(e)$ (the same with w). Therefore, the contribution of G_2 to the item $\sum\limits_{e\in E(G_1)} \big(n_u(e)+\frac{n_0(e)}{2}\big)\big(n_v(e)+\frac{n_0(e)}{2}\big)$ completely relies on the order of G_2, that is, changing the structure of G_2 and keeping the order $|G_2|$ cannot alter the value $\sum\limits_{e\in E(G_1)} \big(n_u(e)+\frac{n_0(e)}{2}\big)\big(n_v(e)+\frac{n_0(e)}{2}\big)$. Due to the contribution of the pendant edge to $(n_u(e)+\frac{n_0(e)}{2})(n_v(e)+\frac{n_0(e)}{2})$ is the smallest, we have the following lemmas.

Lemma 2.2 *Let G_2 be a connected graph of order n. Then*

$$Sz^*(G_1 \cdot S_n) \leq Sz^*(G_1 \cdot G_2),$$

where the common vertex of $G_1 \cdot S_n$ is the center vertex of S_n, and equality holds if and only if $G_1 \cdot S_n \cong G_1 \cdot G_2$.

Before exhibiting the key result in the proof of the Theorem 3.8, we represent the result in [19] as follows.

Lemma 2.3 *Let H_1 be a graph, and H_2, H_3 be the two unicyclic graphs with $|H_1| = n_1$ and $|H_2| = |H_3| = n_2$. If $H_3 \cong S_{n_2,3}(or\, S_{n_2,4})$. Then $Sz^*(H_1 \cdot H_2) \geq Sz^*(H_1 \cdot H_3)$. Especially, $Sz^*(H_1 \cdot H_2) \geq Sz^*(H_1 \cdot S_{n_2,3})$ for $n = n_1 + n_2 - 1 \leq 12$ and $Sz^*(H_1 \cdot H_2) \geq Sz^*(H_1 \cdot S_{n_2,4})$ for $n = n_1 + n_2 - 1 \geq 13$, where the common vertex of $H_1 \cdot S_{n_2,3}(H_1 \cdot S_{n_2,4})$ is the center vertex of $S_{n_2,3}(S_{n_2,4})$.*

By means of Theorem 1.2 and the above result, the next two conclusions are gotten. Note that the common vertex of $H \cdot S_{n_2,4}$(or $S_{n_2,3}$) is the center of $S_{n_2,4}$(or $S_{n_2,3}$).

Lemma 2.4 *Let G be a tricyclic graph on order $n(\geq 13)$ and H be a bicyclic graph on order n_1 with $n_1 \leq n-2$. If $G = H \cdot S_{n_2,4}$. Then $Sz^*(G) \geq Sz^*(A_1 \cdot S_{n_2,4})$ for $n \geq 17$ and equality holds if and only if $H \cong A_1$, $Sz^*(G) \geq Sz^*(A_2 \cdot S_{n_2,4})$ for $15 \geq n \geq 13$ and equality holds if and only if $H \cong A_2$. Especially, $Sz^*(G) \geq Sz^*(A_i \cdot S_{n_2,4})$ for $n = 16$ with equality if and only if $G \cong A_i$ for $i = 1, 2$.*

Lemma 2.5 *Let G be a tricyclic graph on order $n(\leq 12)$ and H be a bicyclic graph on order n_1 with $n_1 \leq n-2$. If $G = H \cdot S_{n_2,3}$. Then $Sz^*(H \cdot S_{n_2,3}) \geq Sz^*(A_2 \cdot S_{n_2,3})$ for $12 \geq n \geq 9$, and equality holds if and only if $H \cong A_2$. Especially, $Sz^*(G) \geq Sz^*(A_i \cdot S_{n_2,3})$ for $n = 8$ with equality if and only if $H \cong A_i$ for $i = 2, 3$, $Sz^*(G) \geq Sz^*(A_3 \cdot S_{n_2,3})$ for $n \leq 7$ with equality if and only if $H \cong A_3$.*

Proof of Lemma 2.4: Assume firstly that $n = n_1 + n_2 - 1 \geq 17$. $Sz^*(A_1) \leq Sz^*(H)$ from Theorem 1.2. The common vertex of $A_1 \cdot S_{n_2,4}$ is the center of $S_{n_2,4}$ and the vertex x_1 in A_1, see Fig.2. we deduce, from Lemma 2.2, that

$$\begin{aligned}
&Sz^*(H \cdot S_{n_2,4}) \\
&= \sum_{e=uv \in E(H \cdot S_{n_2,4})} (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2}) \\
&= \sum_{e \in E(H)} (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2}) + \sum_{e \in E(S_{n_2,4})} (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2}) \\
&= Sz^*(H \cdot S_{n_2}) - (|n_2| - 1)(n-1) + \sum_{e \in E(S_{n_2,4})} (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2}) \\
&\geq Sz^*(A_1 \cdot S_{n_2}) - (|n_2| - 1)(n-1) + \sum_{e \in E(S_{n_2,4})} (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2}) \\
&= \sum_{e \in E(A_1)} (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2}) + \sum_{e \in E(S_{n_2,4})} (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2}) \\
&= Sz^*(A_1 \cdot S_{n_2,4}).
\end{aligned}$$

With the same way, when $15 \geq n \geq 13$, we arrive at $Sz^*(G) \geq Sz^*(A_2 \cdot S_{n_2,4})$, when $n = 16$, we get $Sz^*(G) \geq Sz^*(A_i \cdot S_{n_2,4})$ for $i = 1, 2$. Therefore, the proof is complete. ■

We may use the same line of the proof of Lemma 2.4 to show Lemma 2.5. So the process is omitted here.

3 Proof of Theorem 1.3

In the section, we will verify the main result of the paper. In order to show Theorem 1.3, in view of Eq. (2), we need to choose the graph G for which $\sum_{e \in E(G)} \delta(e)^2$ is as large as possible. We thus assume that the all vertices of G outside its brace are pendent vertices through Lemma 2.1 and Lemma 2.2. For the sake of brevity, let $t_{i,j} = \sum_{e\in E_i}\delta(e)^2 - \sum_{e\in E_j}\delta(e)^2$ for $i,j\in\mathbb{N}$, especially, set $E_0 = E$. In terms of the categories of brace among all tricyclic graphs, we divide five steps to obtain the lower bound. Before listing the proof of these steps, some preparation are necessary.

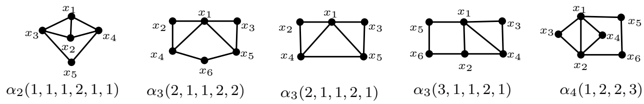

Figure 3. Labeling the vertices of some braces.

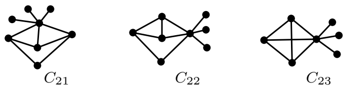

Figure 4. Using for the proof of Lemma 3.1 and Theorem 3.10.

Lemma 3.1 *Let G be a tricyclic graph and contain $\alpha_2(1,1,1,2,1,1)$ as its brace. Then $Sz^*(G)\geq Sz^*(C_{21})$ for $n\leq 8$, $Sz^*(G)\geq Sz^*(C_{22})$ for $n\geq 10$ and $Sz^*(G)=Sz^*(C_{2i})(i=1,2)$ for $n=5,9$. Particularly, $Sz^*(G)>n^2+13n-50$.*

Proof. Let x_1,x_2,x_3,x_4,x_5 be the five vertices of α_2 as shown in Fig. 3, and ℓ_i be the number of pendants of connecting to x_i. For $\ell_1+\ell_3\geq\ell_2+\ell_4\geq 1$ and $\ell_1\ell_2\neq 0$ (or $\ell_3\ell_4\neq 0$), let G_1 denote the graph which is obtained from G by deleting the pendants of x_2 and x_4 and adding to x_1 and x_3, respectively. Observe that, for $\ell_1\neq 0,\ell_3=0$ and $\ell_2=0,\ell_4\neq 0$(or $\ell_1=0,\ell_3\neq 0$ and $\ell_2\neq 0,\ell_4=0$), $G\cong G_1$ by the symmetry of α_2. We deduce, from direct computing, that

$$\begin{aligned}
t_{1,0} &= (\ell_1+\ell_2-\ell_3-\ell_4-\ell_5)^2+(\ell_1+\ell_2+\ell_3+\ell_4-\ell_5+1)^2\\
&\quad+(\ell_3+\ell_4-\ell_5)^2+(\ell_3+\ell_4+\ell_5)^2+(\ell_1+\ell_2)^2\\
&\quad+(\ell_1+\ell_2+\ell_3+\ell_4-\ell_5+1)^2+(\ell_1+\ell_2-\ell_3-\ell_4-\ell_5+1)^2\\
&\quad-(\ell_1+\ell_2+\ell_4-\ell_3-\ell_5+1)^2-(\ell_1+\ell_2+\ell_3-\ell_4-\ell_5+1)^2\\
&\quad-(\ell_1+\ell_4-\ell_3-\ell_5)^2-(\ell_1+\ell_3-\ell_4-\ell_5)^2-(x_1-x_2)^2\\
&\quad-(\ell_2+\ell_4-\ell_3-\ell_5)^2-(\ell_2+\ell_3-\ell_4-\ell_5)^2\\
&\quad=8\ell_1\ell_2+24\ell_3\ell_4>0.
\end{aligned}$$

For $\ell_5\geq 1$, let G_2 be the graph obtained from G_1 by deleting the all pendants of x_5 and adding to x_3. We have that

$$\begin{aligned} t_{2,1} = &(\ell_1-\ell_3-\ell_5)^2+2(\ell_3+\ell_5)^2+(\ell_1+\ell_3+\ell_5)^2+\ell_1^2 \\ &+(\ell_1+\ell_3+\ell_5+1)^2+(\ell_1-\ell_3-\ell_5+1)^2-(\ell_1+\ell_3)^2 \\ &-(\ell_1-\ell_3-\ell_5)^2-(\ell_1+\ell_3-\ell_5)^2-(\ell_3-\ell_5)^2 \\ &-\ell_1^2-(\ell_1+\ell_3-\ell_5+1)^2-(\ell_1-\ell_3-\ell_5+1)^2 \\ &=8\ell_1\ell_5+12\ell_3\ell_5+4\ell_5>0, \end{aligned}$$

For $x_1, x_3 \geq 1$, let G_3 be the graph obtained from G_2 by shifting ℓ_1 pendants from x_1 to x_3. Observe that $G_3 \cong C_{22}$. We get that

$$\begin{aligned} t_{3,2} = &4(\ell_1+\ell_3)^2+(\ell_1+\ell_3+1)^2+(\ell_1+\ell_3-1)^2 \\ &-(\ell_1-\ell_3)^2-(\ell_1+\ell_3)^2-(\ell_3-\ell_5)^2 \\ &-2\ell_3^2-\ell_1^2-(\ell_1+\ell_3+1)^2-(\ell_1-\ell_3+1)^2 \\ &=\ell_1^2+12\ell_1\ell_3-4\ell_1>0. \end{aligned}$$

Together with Eq. (2) and the above relation, it follows that $Sz^*(G) > Sz^*(G_1) > Sz^*(G_2) > Sz^*(C_{22})$. Clearly, $G_2 \cong C_{21}$ for $\ell_3 = 0$ and $G_2 \cong C_{22}$ for $\ell_1 = 0$. By direct comparing, we deduce that

$$\begin{aligned} Sz^*(C_{21}) &= \frac{3}{2}n^2+\frac{11}{2}n-\frac{87}{4} > n^2+13n-50, \\ Sz^*(C_{22}) &= \frac{5}{4}n^2+9n-33 > n^2+13n-50, \\ Sz^*(C_{21})-Sz^*(C_{22}) &= \frac{1}{4}(n-9)(n-5). \end{aligned} \tag{1}$$

We hence finish the proof. ■

Lemma 3.2 *If G includes $\alpha_3(3,1,1,2,1)$ as its brace. Then $Sz^*(G) \geq Sz^*(C_{15})$ for $7 \leq n \leq 12$ and $Sz^*(G) \geq Sz^*(C_{14})$ for $n \geq 13$. Especially, $Sz^*(G) \geq n^2+13n-50$.*

Proof. Label the six vertices α_3 as $x_1, x_2, \ldots, x_6$ shown in Fig. 4. Let ℓ_i is the number of pendants connecting to x_i. We first claim that $\ell_5 = \ell_6 = 1$. If not, it is easy to construct a new graph G' from G by switching all pendants from x_5 and x_6 to x_1 and x_2, respectively, and satisfying $Sz^*(G') < Sz^*(G)$ through direct calculation. For $\ell_3 \geq 1$, let G_1 denote the graph formed from G by deleting all pendants of x_2 and x_4 and adding to x_3, otherwise, denote G_2 the graph obtained from G by shifting ℓ_4 pendants from x_4 to x_2. For $\ell_1, \ell_2 \geq 1$, by G_3 denote the graph obtained from G_2 by shifting ℓ_1 pendants from

x_1 to x_2, where $G_3 \cong C_{14}$. We have the following relation:

$$\begin{aligned} t_{1,0} &= 2(\ell_1+\ell_2+\ell_3+\ell_4+2)^2 + 2(\ell_1+\ell_2+\ell_3+\ell_4+1)^2 + (\ell_1+1)^2 \\ &+ (\ell_2+\ell_3+\ell_4-\ell_1-3)^2 + (\ell_2+\ell_3+\ell_4-2)^2 + (\ell_2+\ell_3+\ell_4)^2 \\ &- 2(\ell_1+\ell_2+\ell_3+\ell_4+2)^2 - 2(\ell_1+\ell_3-\ell_2+1)^2 - (\ell_1-\ell_4+1)^2 \\ &- (\ell_3-\ell_1-\ell_2-3)^2 - (\ell_3-\ell_2-\ell_4-2)^2 - (\ell_2-\ell_3-\ell_4)^2 \\ &= 4\ell_1\ell_2 + 4\ell_1\ell_4 + 20\ell_2\ell_3 + 10\ell_2\ell_4 + 10\ell_3\ell_2 + 4\ell_1\ell_4 + 2\ell_4^2 - 12\ell_2 - 8\ell_4 \\ &\geq \ell_2(20\ell_3-12) + \ell_4(10\ell_3-8) + 2\ell_4^2 > 0, \end{aligned}$$

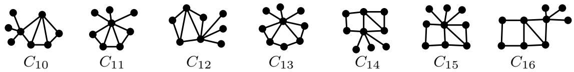

Figure 5. Using for the proof of Lemmas 3.2, 3.3, 3.4 and Theorem 3.11.

$$\begin{aligned} t_{2,0} &= 2(\ell_1+\ell_2+\ell_4+2)^2 + 2(\ell_1-\ell_2-\ell_4+1)^2 + (\ell_1+1)^2 \\ &+ (\ell_1+\ell_2+\ell_4+3)^2 + (\ell_2+\ell_4+2)^2 + (\ell_2+\ell_4)^2 \\ &- 2(\ell_1+\ell_2+\ell_4+2)^2 - 2(\ell_1-\ell_2+1)^2 - (\ell_1-\ell_4+1)^2 \\ &- (\ell_1+\ell_2+3)^2 - (\ell_2+\ell_4+2)^2 - (\ell_2-\ell_4)^2 \\ &= 10\ell_2\ell_4 + 2\ell_4^2 + 4\ell_4 > 0, \\ t_{3,2} &= 3(\ell_1+\ell_2+2)^2 + 2(\ell_1+\ell_2-1)^2 + (\ell_1+\ell_2+3)^2 + 1 \\ &+ (\ell_1+\ell_2)^2 - 2(\ell_1+\ell_2+2)^2 - 2(\ell_1-\ell_2+1)^2 - (\ell_2)^2 \\ &- (\ell_1+\ell_2+3)^2 - (\ell_2+2)^2 - (\ell_1+1)^2 \\ &= \ell_1^2 + 12\ell_1\ell_2 - 6\ell_1 > 0. \end{aligned}$$

Together with Eq. (2) and the above relation, we have that $Sz^*(G) > Sz^*(G_1)$ and $Sz^*(G) > Sz^*(G_2) > Sz^*(C_{14})$. Notice that, if $\ell_1, \ell_3 \geq 1$, it is easy to show that $\sum_{e\in E(G_1)} \delta(e)^2 \leq 3(n-4)^2 + 2(n-5)^2 + 2(n-7)^2 + 1 < \sum_{e\in E(C_{14})} \delta(e)^2$, otherwise, $G_1 \cong C_{15}$ for $\ell_3 = 0$ and $G_1 \cong C_{16}$ for $\ell_1 = 0$. Moreover, we arrive at

$$\begin{aligned} Sz^*(C_{14}) &= \frac{1}{4}(5n^2+42n-168) > n^2+13n-50, \\ Sz^*(C_{15}) &= \frac{1}{2}((3n^2+12n-48) > n^2+13n-50, \\ Sz^*(C_{16}) &= \frac{1}{4}(5n^2+54n-240) > n^2+13n-50, \qquad (2) \\ Sz^*(C_{15}) - Sz^*(C_{14}) &= \frac{1}{4}(n-12)(n-6), \\ Sz^*(C_{16}) - Sz^*(C_{14}) &= 12(n-6). \end{aligned}$$

Therefore, $Sz^*(G) \geq Sz^*(C_{15})$ for $n \leq 12$ and $Sz^*(G) \geq Sz^*(C_{14})$ for $n \geq 13$. ■

Lemma 3.3 *If G has the brace $\alpha_3(2,1,1,2,2)$. Then $Sz^*(G) \geq Sz^*(C_{13})$ with equality if and only if $G \cong C_{13}$.*

Proof. The six vertices of $\alpha_3(2,1,1,2,2)$ are labeling as $x_1, \ldots, x_6$, see Fig. 4. Let ℓ_i denote the number of pendants connecting to x_i. For $\ell_6 > 0$ we obtain a new graph G_1 by adding ℓ_6 attaching to x_1 of G from x_6.

$$\begin{aligned} t_{1,0} &= (\ell_1+\ell_3+\ell_5+\ell_6-\ell_2+2)^2 + (\ell_2-\ell_4-1)^2 + 2(\ell_1+\ell_3+\ell_5+\ell_6-\ell_4+1)^2 \\ &+ (\ell_1+\ell_2+\ell_4+\ell_6-\ell_3+2)^2 + (\ell_3-\ell_5-1)^2 + 2(\ell_1+\ell_2+\ell_4-\ell_5-\ell_6+1)^2 \\ &- (\ell_1+\ell_3+\ell_5-\ell_2+2)^2 - (\ell_2-\ell_4-\ell_6-1)^2 - 2(\ell_1+\ell_3+\ell_5-\ell_4-\ell_6+1)^2 \\ &- (\ell_1+\ell_2+\ell_4-\ell_3+2)^2 - (\ell_3-\ell_5-\ell_6-1)^2 - 2(\ell_1+\ell_2+\ell_4-\ell_5-\ell_6+1)^2 \\ &= 20\ell_1\ell_6 + 10\ell_2\ell_6 + 10\ell_3\ell_6 + 20\ell_6 > 0. \end{aligned}$$

G_2 denote the graph from G_1 by deleting ℓ_3 and ℓ_5 of x_3 and x_5 and adding to x_2 and x_4, respectively.

$$\begin{aligned} t_{2,1} &= (\ell_1+\ell_2+\ell_3+\ell_4+\ell_5+2)^2 + 2(\ell_1+\ell_2+\ell_3+\ell_4+\ell_5+1)^2 + 1 \\ &+ (\ell_1-\ell_2-\ell_3+3-1)^2 + (\ell_2+\ell_3-\ell_4-\ell_5-1)^2 + 2(\ell_1-\ell_4-\ell_5+1)^2 \\ &- (\ell_1+\ell_3+\ell_5-\ell_2+2)^2 - (\ell_1+\ell_2+\ell_4-\ell_3+2)^2 - (\ell_2-\ell_4-1)^2 \\ &- (\ell_3-\ell_5-1)^2 - 2(\ell_4-\ell_1-\ell_3-\ell_5-1)^2 - 2(\ell_5-\ell_1-\ell_2-\ell_4-1)^2 \\ &= 14\ell_2\ell_3 + 10(\ell_2\ell_5+\ell_3\ell_4) + 20\ell_4\ell_5 \geq 10(\ell_3+\ell_5)^2 > 0. \end{aligned}$$

Without lost of generality, assume that $\ell_2+\ell_4 \geq \ell_3+\ell_5 (\geq 1)$. Let G_3 be the graph obtained from G_2 by deleting all pendants of x_2 and x_4 and adding these to x_1. Obviously, $G_3 \cong C_{13}$. We have

$$\begin{aligned} t_{3,2} &= 2(\ell_1+\ell_2+\ell_4+2)^2 + 4(\ell_1+\ell_2+\ell_4+1)^2 + 2 \\ &- (\ell_1-\ell_2+2)^2 - (\ell_1+\ell_2+\ell_4+2)^2 - 2(2-\ell_4-1)^2 \\ &- 2(\ell_1-\ell_4+1)^2 - 2(\ell_1+\ell_2+\ell_4+1)^2 - 1 \\ &= (\ell_2)^2 + 8\ell_1\ell_2 + 10\ell_1\ell_4 + 8\ell_2\ell_4 + 14\ell_2 + 10\ell_4 \\ &\geq 10(\ell_2+\ell_4) > 0. \end{aligned}$$

Combining with Eq. (2) and the above three relation, we have $Sz^*(G) \geq Sz^*(C_{13}) = \frac{1}{2}(3n^2+14n-55) > n^2+13n-50$. ■

Lemma 3.4 *Let G be a tricyclic graph and not be C_{11}, C_{12}. If G includes $\alpha_3(2,1,1,2,1)$ as its brace. Then $Sz^*(G) > Sz^*(C_{12})$ for $n \geq 12$, $Sz^*(G) > Sz^*(C_{11})$ for $n \leq 10$ and $Sz^*(G) > Sz^*(C_{1i})$ with $i = 1,2$ for $n = 11$.*

Note that $G \cong \alpha_3(2,1,1,2,1)$. Label the six vertices of α_3 as shown in Fig. Let ℓ_i denote the number of pendants connecting to x_i. For $\ell_2+\ell_4 \geq \ell_3+\ell_5$, graph G_1 is formed from G by deleting all pendants of x_3 and x_5 and adding to x_2 and x_4, respectively. For $\ell_4, \ell_1 \geq 1$, The graph G_2 is formed from G_1 by deleting ℓ_1 pendent vertices of x_1 and adding to x_4. G_3 denote the graph obtained from G_2 by switching ℓ_2 pendants from x_2 to x_4. Clearly, $G_3 \cong C_{12}$. We have

$$\begin{aligned}
t_{1,0} =\ & (\ell_1-\ell_2-\ell_3+2)^2 + (\ell_1+\ell_2+\ell_3+\ell_4+\ell_5+2)^2 + (\ell_2+\ell_3-\ell_4-\ell_5-1)^2 \\
& + (\ell_4+\ell_5+1)^2 + (\ell_1-\ell_4-\ell_5+1)^2 + (\ell_1+\ell_2+\ell_3+1)^2 + (\ell_2+\ell_3+\ell_4+\ell_5)^2 \\
& - (\ell_1+\ell_3+\ell_5-\ell_2+2)^2 - (\ell_1+\ell_2+\ell_4-\ell_3+2)^2 - (\ell_2+\ell_4-\ell_3-\ell_5)^2 \\
& - (\ell_2-\ell_4-\ell_5-1)^2 - (\ell_3-\ell_4-\ell_5-1)^2 - (\ell_1+\ell_3-\ell_4+1)^2 - (\ell_1+\ell_2-\ell_5+1)^2 \\
& = 16\ell_2(\ell_3+\ell_5) + 10\ell_3\ell_4 + 8\ell_4\ell_5 \geq 8(\ell_3+\ell_5)^2 > 0
\end{aligned}$$

$$\begin{aligned}
t_{2,1} =\ & (\ell_2-2)^2 + (\ell_2-\ell_1-\ell_4-1)^2 + (\ell_1+\ell_4-1)^2 + (\ell_2+1)^2 \\
& + (\ell_1+\ell_2+\ell_4+2)^2 + (\ell_1+\ell_4+1)^2 + (\ell_1+\ell_2+\ell_4)^2 \\
& - (\ell_1-\ell_2+2)^2 - (\ell_2-\ell_4-1)^2 - (\ell_1+\ell_2+1)^2 - (\ell_4+1)^2 \\
& - (\ell_1-\ell_4+1)^2 - (\ell_2+\ell_4)^2 - (\ell_1+\ell_2+\ell_4+2)^2 \\
=\ & (\ell_1)^2 + 10\ell_1\ell_4 - 6\ell_1 \geq (\ell_1)^2 + 6\ell_1\ell_4 > 0. \\
t_{3,2} =\ & (2)^2 + (\ell_2+\ell_4+2)^2 + (1+\ell_2+\ell_4)^2 + (\ell_2+\ell_4+1)^2 \\
& + (1-\ell_2-\ell_4)^2 + 1 + (\ell_2+\ell_4)^2 - (\ell_2-2)^2 \\
& - (\ell_2+\ell_4)^2 - (\ell_2-\ell_4-1)^2 - 2(\ell_4+1)^2 \\
& - (1-\ell_4)^2 - (\ell_2+1)^2 - (\ell_2+\ell_4)^2 \\
=\ & 8\ell_2\ell_4 + 6\ell_2 > 0.
\end{aligned}$$

Combining with Eq. (2), $Sz^*(G) \geq Sz^*(G_1) > Sz^*(G_2) > Sz^*(G_3) = Sz^*(C_{12})$.

Note that $\ell_1, \ell_4 \geq 1$ is required from G_1 to G_2. Hence, the condition with $\ell_1 = 0$ or $\ell_4 = 0$ will be discussed. For $\ell_1 = 0$, $G_1 \cong G_2$. Hence $Sz^*(G_1) = Sz^*(G_2) > Sz^*(C_{12})$. For $\ell_4 = 0$, $G_1 \cong C_{11}$ with $\ell_2 = 0$. For $\ell_4 = 0$ and and $\ell_2 \neq 0$, let G_4 be the graph obtained from G_1 by shifting ℓ_1 pendants of x_1 to x_2 with $\ell_2 \geq 2$, and G_5 be the graph obtain from G_1 by shifting all pendants of x_2 to x_1 with $\ell_2 = 1$. Using the same way, it is easy to deduce that

$$t_{41} = \ell_1^2 + 4\ell_1(2\ell_2 - 4\ell_1) \geq \ell_1^2 > 0$$

$$t_{51} = 6\ell_1\ell_2 + 12\ell_2 - \ell_2^2 \geq 11 > 0.$$

Together with Eq. (2), $Sz^*(G_1) \geq Sz^*(C_{11})$ or $Sz^*(G_1) \geq Sz^*(C_{10})$. In addition,

$$\begin{aligned}
Sz^*(C_{10}) &= \frac{3}{2}n^2 + \frac{13}{2}n - \frac{117}{4} > n^2 + 13n - 50, \text{ for } n \geq 8,\\
Sz^*(C_{11}) &= \frac{7}{4}n^2 + n - 8 > n^2 + 13n - 50, \text{ for } n \geq 11,\\
Sz^*(C_{12}) &= \frac{3}{2}n^2 + 5n - \frac{87}{4} > n^2 + 13n - 50, \text{ for all } n,\\
Sz^*(C_{10}) - Sz^*(C_{12}) &= \frac{1}{4}(6n - 30) > 0, \text{ for } n \geq 6,\\
Sz^*(C_{11}) - Sz^*(C_{12}) &= \frac{1}{4}[(n-8)^2 - 9] > 0, \text{ for } n \geq 12.
\end{aligned} \tag{3}$$

Therefore, we complete the proof. ■

Lemma 3.5 *If G contains $\alpha_4(2,2,2,2)$ as its brace. Then $Sz^*(G) \geq n^2 + 13n - 50$ and equality holds if and only if $G \cong C_1$.*

Proof. The six vertices of $\alpha_4(2,2,2,2)$ are labeled as $x_1, x_2, \ldots, x_6$ with $d(x_1) = d(x_2) = 4$ and $d(x_i) = 2$ for $i \geq 6$. Let $\ell_i(\geq 0)$ be the number of pendants connecting to x_i.

Let G_1 be the graph formed from G by deleting the ℓ_i pendants of $x_i (i \geq 4)$ and adding to x_3. By direct calculation, we have

$$\begin{aligned}
t_{1,0} = {} & (\ell_1 - \ell_2 - \ell_3 - \ell_4 - \ell_5 - \ell_6 + 2)^2 + (\ell_2 - \ell_1 - \ell_3 - \ell_4 - \ell_5 - \ell_6 + 2)^2\\
& + 3(\ell_2 - \ell_1 - \ell_3 - \ell_4 - \ell_5 - \ell_6 - 2)^2 + 3(\ell_1 - \ell_2 - \ell_3 - \ell_4 - \ell_5 - \ell_6 - 2)^2\\
& - (\ell_1 + \ell_4 + \ell_5 + \ell_6 - \ell_2 - \ell_3 + 2)^2 - (\ell_2 + \ell_4 + \ell_5 + \ell_6 - \ell_1 - \ell_3 + 2)^2\\
& - (\ell_1 + \ell_3 + \ell_5 + \ell_6 - \ell_2 - \ell_4 + 2)^2 - (\ell_2 + \ell_3 + \ell_5 + \ell_6 - \ell_1 - \ell_4 + 2)^2\\
& - (\ell_1 + \ell_3 + \ell_4 + \ell_6 - \ell_2 - \ell_5 + 2)^2 - (\ell_2 + \ell_3 + \ell_4 + \ell_6 - \ell_1 - \ell_5 + 2)^2\\
& - (\ell_1 + \ell_3 + \ell_4 + \ell_5 - \ell_2 - \ell_6 + 2)^2 - (\ell_2 + \ell_3 + \ell_4 + \ell_5 - \ell_1 - \ell_6 + 2)^2\\
= {} & 16(\ell_3\ell_4 + \ell_3\ell_5 + \ell_4\ell_5 + \ell_4\ell_6 + \ell_5\ell_6) > 0
\end{aligned}$$

Let G_2 be the graph which is obtained from G_1 by shifting all pendants of x_1 and x_2 to x_3. clearly, $G_2 \cong C_1$. For $\ell_1 + \ell_2 \geq 1$ we have

$$\begin{aligned}
t_{2,1} = {} & 2(\ell_1 + \ell_2 + \ell_3 - 2)^2 + 6(\ell_1 + \ell_2 + \ell_3 + 2)^2 - (\ell_1 - \ell_2 - \ell_3 + 2)^2\\
& - (\ell_2 - \ell_1 - \ell_3 + 2)^2 - 3(\ell_2 - \ell_1 - \ell_3 - 2)^2 - 3(\ell_1 - \ell_2 - \ell_3 - 2)^2\\
= {} & 32\ell_1\ell_2 + 16\ell_1\ell_3 + 16\ell_2\ell_3 + 16\ell_1 + 16\ell_2 > 0.
\end{aligned}$$

Combining with Eq. (2), we hence get $Sz^*(G) > Sz^*(G_1) > Sz^*(G_2) = Sz^*(C_1) = n^2 + 13n - 50$. ■

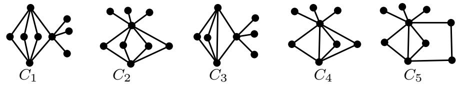

Figure 6. Using for the proof of Lemmas 3.5, 3.6, 3.7 and Theorem 3.12.

Lemma 3.6 *If G contains $\alpha_4(1,2,2,3)$ as its brace. Then $Sz^*(G) \geq Sz^*(C_5)$ with equality if and only if $G \cong C_5$.*

Proof. Mark the six vertices of $\alpha_4(1,2,2,3)$ as $x_1, x_2, \ldots, x_6$, see Fig. 4. Let ℓ_i be the number of pendants connected to x_i. Let G_1 be the graph formed from G by deleting the ℓ_4 pendants of x_4 and adding to x_3. We have

$$\begin{aligned}
t_{1,0} &= (\ell_1+\ell_5-\ell_3-\ell_4+2)^2 + (\ell_2+\ell_6-\ell_3-\ell_4+2)^2 \\
&\quad + (\ell_1+\ell_3+\ell_4+\ell_5+2)^2 + (\ell_2+\ell_3+\ell_4+\ell_6+2)^2 \\
&\quad + 2(\ell_1+\ell_5-\ell_2-\ell_6)^2 + 2(\ell_1+\ell_2+\ell_3+\ell_4-\ell_5-\ell_6+2)^2 \\
&\quad - (\ell_1+\ell_4+\ell_5-\ell_3+2)^2 - (\ell_2+\ell_4+\ell_6-\ell_3+2)^2 \\
&\quad - (\ell_1+\ell_3+\ell_5-\ell_4+2)^2 - (\ell_2+\ell_3+\ell_6-\ell_4+2)^2 \\
&\quad - 2(\ell_1+\ell_5-\ell_2-\ell_6)^2 - 2(\ell_1+\ell_2+\ell_3+\ell_4-\ell_5-\ell_6+2)^2 \\
&= 16\ell_3\ell_4 > 0.
\end{aligned}$$

If $\ell_2+\ell_6 \geq \ell_1+\ell_5 \geq 1$. G_2 denote the graph obtained from G_1 by deleting the all pendants of x_1 and x_5 and adding to x_2 and x_6, respectively. We get

$$\begin{aligned}
t_{2,1} &= 2(\ell_1+\ell_2+\ell_5+\ell_6)^2 + 2(\ell_1+\ell_2+\ell_3-\ell_5-\ell_6+2)^2 \\
&\quad + (\ell_3+2)^2 + (\ell_1+\ell_2+\ell_3+\ell_5+\ell_6+2)^2 + (2-\ell_3)^2 \\
&\quad + (\ell_1+\ell_2+\ell_5+\ell_6-\ell_3+2)^2 - (\ell_1+\ell_3+\ell_5+2)^2 \\
&\quad - (\ell_2+\ell_3+\ell_6+2)^2 - (\ell_1+\ell_5-\ell_3+2)^2 - (\ell_2+\ell_6-\ell_3+2)^2 \\
&\quad - 2(\ell_1+\ell_5-\ell_2-\ell_6)^2 - 2(\ell_1+\ell_2+\ell_3-\ell_5-\ell_6+2)^2 \\
&= 12(\ell_1\ell_2+\ell_1\ell_6+\ell_2\ell_5+\ell_5\ell_6) \geq 12(\ell_1+\ell_5)^2 > 0.
\end{aligned}$$

Let G_3 be the graph formed from G_2 by deleting the all pendants of x_3 and x_6 and adding to x_1. Observe that $G_3 \cong C_5$. We arrive at

$$\begin{aligned}
t_{3,2} &= 2(3-1)^2 + 4(\ell_2+\ell_3+\ell_6+2)^2 + 2(\ell_2+\ell_3+\ell_6)^2 \\
&\quad - (2-\ell_3)^2 - (\ell_2+\ell_6-\ell_3+2)^2 - (\ell_2+\ell_3+\ell_6+2)^2 \\
&\quad - (\ell_3+2)^2 - 2(\ell_2+\ell_6)^2 - 2(\ell_2+\ell_3-\ell_6+2)^2 \\
&= 8\ell_2\ell_3 + 8\ell_2\ell_6 + 16\ell_3\ell_6 + 8\ell_3 + 16\ell_6 \\
&\geq 8(\ell_2+1)(\ell_3+\ell_6) > 0.
\end{aligned}$$

Combining with Eq.(1), we have $Sz^*(G) > Sz^*(G_1) > Sz^*(G_2) > Sz^*(C_5)$, and

$$Sz^*(C_5) = \frac{3}{2}n^2 + 7n - 28 > n^2 + 13n - 50. \tag{4}$$

Therefore, the assertion is gotten, as required. ■

Lemma 3.7 *If G contains $\alpha_4(1,2,2,2)$ as its brace with $n \geq 8$. Then $Sz^*(G) \geq Sz^*(C_4)$ for $n \geq 8$. Especially, $Sz^*(C_4) \geq Sz^*(C_1)$ for $n \geq 20$, otherwise, $Sz^*(C_1) \geq Sz^*(C_4)$.*

Proof. Label the five vertices of $\alpha_4(1,2,2,2)$ as $x_1, x_2, \ldots, x_5$ with $d(x_1) = d(x_2) = 4$ and $d(x_i) = 2$ for $i \geq 3$. Let $\ell_i (\geq 0)$ be the number of pendants connecting to x_i.

The graph G_1 is formed from G by deleting the ℓ_i pendants of $x_i (i \geq 4)$ and adding to x_3. The graph G_2 is obtained from G_1 by deleting the ℓ_2 pendants of x_2 and adding to x_1. For $\ell_1, \ell_3 \geq 1$, let G_3 be the graph formed from G_2 by shifting ℓ_1 pendants form x_1 to x_3. Obviously, $G_3 \cong C_4$. We have that

$$\begin{aligned}
t_{2,1} &= (\ell_1 + \ell_2 - \ell_3 + 2)^2 + 2(\ell_1 + \ell_2 + \ell_3 + 2)^2 + (\ell_1 - \ell_2)^2 \\
&\quad + (\ell_3 - 2)^2 + 2(\ell_3 + 2)^2 - (\ell_1 - \ell_2)^2 - (\ell_1 - \ell_3 + 2)^2 \\
&\quad - (\ell_2 - \ell_3 + 2)^2 - 2(\ell_1 + \ell_3 + 2)^2 - 2(\ell_2 + \ell_3 + 2)^2 \\
&= 10\ell_1\ell_2 > 0,
\end{aligned}$$

$$\begin{aligned}
t_{3,2} &= 2(\ell_1 + \ell_3 - 2)^2 + 4(\ell_1 + \ell_3 + 2)^2 - (\ell_1 - \ell_3 + 2)^2 \\
&\quad - (\ell_3 - 2)^2 - (\ell_1)^2 - 2(\ell_1 + \ell_3 + 2)^2 - 2(\ell_3 + 2)^2 \\
&= 2\ell_1^2 + 10\ell_1\ell_3 - 4\ell_1 > 0,
\end{aligned}$$

$$\begin{aligned}
t_{1,0} &= (\ell_1 - \ell_3 - \ell_4 - \ell_5 + 2)^2 + (\ell_2 - \ell_3 - \ell_4 - \ell_5 + 2)^2 + (\ell_1 - \ell_2)^2 \\
&\quad + 2(\ell_1 + \ell_3 + \ell_4 + \ell_5 + 2)^2 + 2(\ell_2 + \ell_3 + \ell_4 + \ell_5 + 2)^2 - (\ell_1 - \ell_2)^2 \\
&\quad - (\ell_1 + \ell_4 + \ell_5 - \ell_3 + 2)^2 - (\ell_2 + \ell_4 + \ell_5 - \ell_3 + 2)^2 \\
&\quad - (\ell_1 + \ell_3 + \ell_5 - \ell_4 + 2)^2 - (\ell_2 + \ell_3 + \ell_5 - \ell_4 + 2)^2 \\
&\quad - (\ell_1 + \ell_3 + \ell_4 - \ell_5 + 2)^2 - (\ell_2 + \ell_3 + \ell_4 - \ell_5 + 2)^2 \\
&= 16(\ell_3\ell_4 + \ell_3\ell_5 + \ell_4\ell_5) > 0.
\end{aligned}$$

Combining with Eq. (2) and the above three relation, $Sz^*(G) \geq Sz^*(G_1) \geq Sz^*(G_2) > Sz^*(C_4)$ is gotten. Especially, $G_2 \cong C_3$ for $\ell_3 = 0$. Furthermore, we deduce that

$$\begin{aligned}
Sz^*(C_3) &= \frac{1}{4}(7n^2 + 4n - 44) > n^2 + 13n - 50 \text{ for } n \geq 12, \\
Sz^*(C_4) &= \frac{1}{4}(5n^2 + 28n - 114) > n^2 + 13n - 50 \text{ for } n \geq 20, \\
Sz^*(C_3) - Sz^*(C_4) &= \frac{1}{2}(n - 5)(n - 7).
\end{aligned} \tag{5}$$

We thus confirm the conclusion. ■

Theorem 3.8 *Let $G \in \mathscr{A}$ with n vertices. Then $Sz^*(G) \geq Sz^*(B_{11})$ for $n \geq 17$, $Sz^*(G) \geq Sz^*(B_{12})$ for $15 \geq n \geq 13$, $Sz^*(G) \geq Sz^*(B_{22})$ for $12 \geq n \geq 9$, $Sz^*(G) \geq Sz^*(B_{23})$ for $n \leq 7$. Especially, $Sz^*(G) \geq Sz^*(B_{1i})$ for $n = 16$ and $i = 1, 2$, $Sz^*(G) \geq Sz^*(B_{2i})$ for $n = 8$ and $i = 2, 3$.*

Proof. Since G belongs to $\mathscr{A}$. it contains one of $\alpha_i (i = 5, 6, \cdots, 15)$ as its brace. It is easy to find a vertex $x \in V(G)$ such that $G = H_1 \cdot H_2$ with $V(H_1) \cap V(H_2) = \{x\}$ and $|H_1| + |H_2| = n + 1$, where, H_1 is the bicyclic subgraph of G and H_2 is an unicyclic subgraph of G. By means of Lemma 2.3, we have that

$Sz^*(G) \geq Sz^*(H_1 \cdot S_{|H_2|,4})$ for $n \geq 13$, and, $Sz^*(G) \geq Sz^*(H_1 \cdot S_{|H_2|,3})$ for $n \leq 12$.

When $n \geq 13$, from Lemma 2.4, we deduce that

$$Sz^*(H_1 \cdot S_{|H_2|,4}) \geq Sz^*(A_1 \cdot S_{|H_2|,4}) = Sz^*(B_{11}) \quad \text{for}\, n \geq 17,$$

$$Sz^*(H_1 \cdot S_{|H_2|,4}) \geq Sz^*(A_2 \cdot S_{|H_2|,4}) = Sz^*(B_{12}) \quad \text{for}\, 15 \geq n \geq 13,$$

$$Sz^*(H_1 \cdot S_{|H_2|,4}) \geq Sz^*(A_i \cdot S_{|H_2|,4}) = Sz^*(B_{1i}) \quad \text{for}\, n = 16\, \text{and}\, i = 1, 2.$$

When $n \leq 12$, similarly, Lemma 2.5 results in

$$Sz^*(H_1 \cdot S_{|H_2|,3}) \geq Sz^*(A_2 \cdot S_{|H_2|,3}) = Sz^*(B_{22}) \quad \text{for}\, 12 \geq n \geq 9,$$

$$Sz^*(H_1 \cdot S_{|H_2|,3}) \geq Sz^*(A_3 \cdot S_{|H_2|,3}) = Sz^*(B_{23}) \quad \text{for}\, n \leq 7,$$

$$Sz^*(H_1 \cdot S_{|H_2|,3}) \geq Sz^*(A_i \cdot S_{|H_2|,3}) = Sz^*(B_{2i}) \quad \text{for}\, n = 8\, \text{and}\, i = 2, 3.$$

Thus, the proof is finished. ■

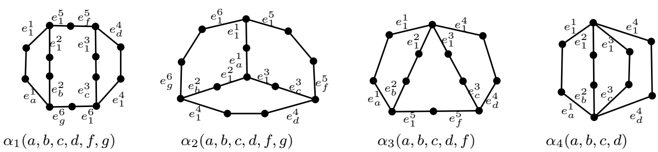

Figure 7. Labeling the edges of the four braces $\alpha_i (i = 1, 2, 3, 4)$.

Theorem 3.9 *Let $G \in \mathscr{G}_n^1$ with n vertices. Then $Sz^*(G) > n^2 + 13n - 50$ for $n \geq 11$, otherwise, $Sz^*(G) > \frac{7}{4}n^2 + n - 8$.*

Proof. Since G belongs to $\mathscr{G}_n^1$, G has a α_1 as its brace. We now choose 8 edges $e_1^1, e_a^1, e_1^2, e_c^3, e_1^4, e_d^4, e_1^5$ and e_1^6, see Fig.7, and consider $\delta(e)$ of these edges, e.g., $\delta(e_1^5) \leq n - 6$. It is easy to show that $\sum_{e \in E} \delta(e)^2 \leq 4(n-6)^2 + 4(n-4)^2 + (n-6)(n-2)^2 < n^3 - 2n^2 - 52n + 200$. Combining with Eq. (2), $Sz^*(G) > n^2 + 13n - 50$, as required. ■

Theorem 3.10 *Let $G \in \mathscr{G}_n^2$ with n vertices. Then $Sz^*(G) > n^2 + 13n - 50$.*

Proof. If $G \in \mathscr{G}_n^2$, Then G has the subgraph $\alpha_2(a, b, c, d, f, g)$ as its brace.

Case 1. There are at least three paths are more than 2.

Subcase 1.1 The three paths enclose a cycle.

Suppose the three paths are $P(g), P(a), P(b)$ by the symmetry of α_2. We now choose the 9 edges $e_1^1, e_a^1, e_1^2, e_b^2, e_c^3, e_d^4, e_f^5, e_1^6$ and e_g^6 (see Fig.7) and count the $\delta(e)$ of the nine edges, for instance, $\delta(e_1^1) \le n-6$. Consequently, it will result in $\sum_{e\in E}\delta(e)^2 \le 6(n-6)^2 + 3(n-4)^2 + (n-7)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Subcase 1.2 The three paths share a common vertex.

Assume that the three paths are $P(a), P(b), P(c)$ by the symmetry of α_2. We now choose the 9 edges $e_1^1, e_a^1, e_1^2, e_b^2, e_1^3, e_c^3, e_1^4, e_f^5$ and e_1^6 (see Fig.7) and count $\delta(e)$ of these edges, such as, $\delta(e_1^1) \le n-5$. It brings about $\sum_{e\in E}\delta(e)^2 \le 9(n-5)^2 + (n-7)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Subcase 1.3 The three paths consist of a new path.

By symmetry, let the three paths be $P(a), P(b), P(d)$. choosing the 9 edges e_1^1, e_a^1, e_1^2, $e_b^2, e_c^3, e_1^4, e_d^4, e_f^5$ and e_1^6 (see Fig.7), by the same way, we deduce that $\sum_{e\in E}\delta(e)^2 \le 8(n-5)^2 + (n-4)^2 + (n-7)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Case 2. there are just two paths are no less than 2 in α_2.

Subcase 2.1 The two paths belong to the same cycle in α_2.

By the symmetry, let the two paths be $P(a)$ and $P(b)$. Select the eight edges e_1^1, e_a^1, e_1^2, $e_b^2, e_1^3, e_1^4, e_1^5$ and e_1^6 (see Fig.7), and count the $\delta(e)$ of these edges, such as, $\delta(e_1^1) \le n-6$, it is easy to find that $\sum_{e\in E}\delta(e)^2 \le 2(n-6)^2 + 4(n-5)^2 + 2(n-4)^2 + (n-6)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Subcase 2.2 The two paths belong to two distinct cycles in α_2.

Using the similar way of Subcase 2.1, we get $\sum_{e\in E}\delta(e)^2 \le 4(n-6)^2 + 4(n-4)^2 + (n-6)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Case 3. There is only one path no less than 2 in α_2.

By the symmetry, assume that the path is $P(d)$ with $d \ge 2$. We claim that $d = 2$.(If not, $d \ge 3$, we obtain $\sum_{e\in E}\delta(e)^2 \le 3(n-6)^2 + 2(n-5)^2 + 3(n-4)^2 + (n-6)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.) It follows from Lemma 3.1 that $Sz^*(G) \ge Sz^*(C_{21})(\text{or}\, C_{22}) > n^2 + 13n - 50$.

Case 4. The six paths are isomorphic to $P(1)$.

Notice that $\alpha_2 \cong K_4$, let x_1, x_2, x_3, x_4 be its four vertices and ℓ_i be the pendants of x_i. Let G_1 be the graph which is obtained from G by shifting all pendants of other three vertices to x_1. If only one of $\ell_1, \ell_2, \ell_3, \ell_4$ is more than zero. Then $G \cong G_1$. Hence, assume that at least two of the four numbers are no less than one, e.g., $\ell_2, \ell_3 \geq 1$. We deduce that

$$t_{1,0} = 3(\ell_1 + \ell_2 + \ell_3 + \ell_4)^2 - (\ell_1 - \ell_2)^2 - (\ell_1 - \ell_3)^2$$

$$-(\ell_1 - \ell_4)^2 - (\ell_2 - \ell_3)^2 - (\ell_2 - \ell_4)^2 - (\ell_3 - \ell_4)^2$$

$$= 8(\ell_1\ell_2 + \ell_1\ell_3 + \ell_1\ell_4 + \ell_2\ell_3 + \ell_2\ell_4 + \ell_3\ell_4) > 0,$$

combining with Eq. (2), it follows that $Sz^*(G) > Sz^*(G_1) = Sz^*(C_{23}) = \frac{7}{4}n^2 + n - 8 > n^2 + 13n - 50$ for $n \geq 11$. Therefore, the proof is finished. ■

Theorem 3.11 *Let $G \in \mathscr{G}_n^3$ with n vertices. Then $Sz^*(G) \geq Sz^*(C_{14})$ for $n \geq 18$. Especially, $Sz^*(G) \geq Sz^*(C_{12})$ for $17 \geq n \geq 12$, $Sz^*(G) \geq Sz^*(C_{11})$ for $n \leq 10$ and $Sz^*(G) = Sz^*(C_{11})(or\, C_{12})$ for $n = 11$.*

Proof. Let G belongs to $\mathscr{G}_n^3$, then G includes a brace α_3. For the symmetry, suppose that $a, d \geq 2$. We will take part in the following cases to verify the conclusion.

Case 1. $a, d \geq 3$.

Subcase 1.1. $b = c = f = 1$.

select the 9 edges $e_1^1, e_2^1, e_a^1, e_1^2, e_1^3, e_1^4, e_2^4, e_d^4$ and e_1^5 (see Fig.7), and reckon $\delta(e)$ of these edges, e.g., $\delta(e_1^5)$. it will cause $\sum_{e\in E} \delta(e)^2 \leq (n-7)^2 + 4(n-6)^2 + 4(n-4)^2 + (n-7)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Subcase 1.2. At least one of the three numbers b, c, f more than 1.

Take the 9 edges $e_1^1, e_2^1, e_a^1, e_1^2, e_1^3, e_1^4, e_2^4, e_d^4$, e_1^5(see Fig.7), and count $\delta(e)$, by the same way, it will lead to $\sum_{e\in E} \delta(e)^2 \leq (n-7)^2 + 3(n-6)^2 + 4(n-5)^2 + (n-4)^2 + (n-7)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Since a and d with respect to α_3 have symmetry, showing the case $d \geq 3$ and $a = 2$ is same as the $a \geq 3$ and $d = 2$. So we now just discuss the following case.

Case 2. $a \geq 3$ and $d = 2$.

Subcase 2.1. $a \geq 4$ and $d = 2$.

We pick the 9 edges $e_1^1, e_2^1, e_3^1, e_a^1, e_1^2, e_1^3, e_1^4, e_2^4$,$e_1^5$(see Fig.7), and count $\delta(e)$ of these edges, such as, $\delta_2^4 \leq n - 4$, it will bring about $\sum_{e\in E} \delta(e)^2 \leq 2(n-6)^2 + 5(n-5)^2 + (n-4)^2 + (n-3)^2 + (n-7)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Subcase 2.2. $a = 3$, $d = 2$ and $b = c = f = 1$.

The Subcase is confirmed by Lemma 3.2.

Subcase 2.3. $a = 3$, $d = 2$ and at least one of ℓ, r, t is more than 1.

The proof of Subcase 2.3 is similar with Subcase 2.1, Hence, the proceeding is omitted here.

Case 3. $a = d = 2$.

Subcase 3.1. $b, c, f \geq 2$.

If $b, c, f \geq 2$. One can obtain that $\sum_{e\in E} \delta(e)^2 \leq 4(n-8)^2 + 4(n-6)^2 + (n-6)(n-2)^2 < n^3 - 2n^2 - 52n + 200$ by picking the 8 edges $e_1^1, e_2^1, e_1^2, e_b^2, e_1^3, e_r^3, e_1^4, e_2^4$(see Fig.7) and calculating $\delta(e)$ of these edges.

Subcase 3.2. Two of the three numbers b, c, f more than 1.

If $b, f \geq 2$(or $c, f \geq 2$). We select 8 edges $e_1^1, e_2^1, e_1^2, e_b^2, e_1^3, e_1^4, e_2^4, e_1^5$(see Fig.7), by the same way, and get that $\sum_{e\in E} \delta(e)^2 \leq 2(n-7)^2 + 2(n-6)^2 + 3(n-5)^2 + (n-4)^2 + (n-6)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

If $b, c \geq 2$. Taking edges $e_1^1, e_2^1, e_1^2, e_b^2, e_1^3, e_c^3, e_1^4, e_2^4$(see Fig.7) and computing $\delta(e)$ of the 8 edges we have $\sum_{e\in E} \delta(e)^2 \leq 4(n-6)^2 + 4(n-5)^2 + (n-6)(n-2)^2$.

Subcase 3.3. One of the three numbers b, c, f is more than 1.

If $b \geq 2$(or $c \geq 2$). Then, we deduce $\sum_{e\in E} \delta(e)^2 \leq 3(n-6)^2 + 3(n-5)^2 + 2(n-4)^2 + (n-6)(n-2)^2$ through choosing $e_1^1, e_2^1, e_1^2, e_b^2, e_1^3, e_1^4, e_2^4, e_1^5$(see Fig.7) and counting $\delta(e)$ of the 8 eight edges.

If $f \geq 3$. Picking 8 edges as $e_1^1, e_2^1, e_1^2, e_1^3, e_1^4, e_2^4, e_1^5, e_f^5$(see Fig.7) and figuring out $\delta(e)$ of these edges, one can check that $\sum_{e\in E} \delta(e)^2 \leq 2(n-6)^2 + 4(n-5)^2 + 2(n-4)^2 + (n-6)(n-2)^2$. If $f = 2$. Lemma 3.3 brings to $Sz^*(G) \geq Sz^*(C_{13}) > n^2 + 13n - 50$.

Subcase 3.4. $b = c = f = 1$.

Applying Lemma 3.4, we have that $Sz^*(G) \geq Sz^*(C_{12})$ for $n \geq 12$ and $Sz^*(G) \geq Sz^*(C_{11})$ for $n \geq 10$.

Note that $Sz^*(C_{12}) - Sz^*(C_{14}) = \frac{1}{4}(n-10)^2 - 10$ for $n \geq 18$ and $Sz^*(C_{15}) - Sz^*(C_{12}) = n - \frac{9}{4}$ for $n \geq 3$. Hence, together with Eqs. (2) and (3), the assertion is obtained, as required. ■

Theorem 3.12 *Let $G \in \mathscr{G}_n^4$ with $n(\geq 8)$ vertices. Then $Sz^*(G) \geq n^2 + 13n - 50$ for $n \geq 20$ and $Sz^*(G) \geq 5n^2 + 28n - 114$ for $n \leq 19$, the two equalities holds if and only if $G \cong C_1$ and $G \cong C_4$, respectively.*

Proof. Since $G \in \mathscr{G}_n^4$. Then there is some $\alpha_4(a,b,c,d)$ as its brace. Without loss of generality, suppose $1 \le a \le b \le c \le d$. We now divide three cases to show the result.

Case 1. $3 \le a \le b \le c \le d$.

Choose the eight edges $e_1^1, e_a^1, e_1^2, e_b^2, e_1^3, e_c^3, e_1^4, e_d^4$ as shown in Fig. 7. We deduce that $\sum_{e\in E(G)} \delta(e)^2 \le 8(n-6)^2 + (n-6)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Case 2. $a = 2$.

Subcase 2.1. At least one of b, c, d is more than 3.

Here, we just show the special case only one of b, c, d is more than 3. Other cases are verified by the same way of the special case. With loss of generality, assume that $d \ge 3$. Picking the eight edges $e_1^1, e_a^1, e_1^2, e_b^2, e_1^3, e_c^3, e_1^4, e_d^4$ in α_4 as shown in Fig.7 and computing their $\delta(e)$, it will bring about $Di(G) \le 8(n-5)^2 + (n-6)(n-2)^2 < n^3 - 2n^2 - 52n + 200$.

Subcase 2.2. $b = c = d = 2$.

The subcase can be verified by Lemma 3.5.

Case 3. $a = 1$.

Subcase 3.1. $3 \le b \le c \le d$.

We deduce that $Di(G) \le 3(n-8)^2 + 6(n-4)^2 + (n-7)(n-2)^2 < n^3 - 2n^2 - 52n + 200$ through selecting the nine edges $e_1^1, e_1^2, e_2^2, e_b^2, e_1^3, e_2^3, e_c^3, e_1^4, e_2^4, e_d^4$ in α_4 (see Fig. 7) and figuring out their $\delta(e)$.

Subcase 3.2. $b = 2$, $3 \le c \le d$.

The proof of Subcase 3.2 is similar with that of Subcase 3.1, so the process is omitted here.

Subcase 3.3. $b = c = 2$, $3 \le d$.

We claim that $d = 3$. If not, $d \ge 4$, we pick the 9 edges $e_1^1, e_1^2, e_2^2, e_1^3, e_2^3, e_1^4, e_2^4, e_3^4, e_d^4$ in α_4, as shown in Fig. 7 and count $\delta(e)$ of these edges. It is not difficult to deduce $\sum_{e\in E(G)} \delta(e)^2 \le (n-7)^2 + 4(n-5)^2 + 4(n-4)^2 + (n-7)(n-2)^2 < n^3 - 2n^2 - 52n + 200$. So $\alpha_4 \cong \alpha_4(1,2,2,3)$. Applying Lemma 3.6, we obtain that $Sz^*(G) \ge Sz^*(C_5) > Sz^*(C_1)$.

Subcase 3.4. $b = c = d = 2$.

The Subcase is verified through Lemma 3.7.

Therefore, the proof is complete. ■

In order to approve Theorem 1.3, applying Theorem3.8, Theorem 3.9, Theorem 3.10, Theorem 3.11 and Theorem 3.12, it just to compare the value of revised Szeged index of the extremal graphs are deduced in these Theorems.

Note that $Sz^*(B_{11}) = n^2 + 13n - 42 > Sz^*(C_1)$, $Sz^*(B_{12}) = \frac{5}{4}n^2 + 8n - 26 > Sz^*(C_1)$ for $n \geq 13$, $Sz^*(B_{22}) = \frac{3}{2}n^2 + 4n - \frac{31}{2} > Sz^*(C_1)$ for $n \geq 13$ and $Sz^*(B_{23}) = \frac{7}{4}n^2 + 3n - \frac{29}{2} > Sz^*(C_1)$. In addition, $Sz^*(C_{11}) = Sz^*(C_{23}) = \frac{7}{4}n^2 + n - 8 > Sz^*(C_4)$, $Sz^*(B_{12}) > Sz^*(C_4)$, $Sz^*(B_{22}) > Sz^*(C_4)$ and $Sz^*(B_{14}) > Sz^*(C_4)$. Bearing in mind the above relation, together with Eqs. (1), (2), (3) and (5), Theorem 1.3 is totally verified.

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References

[1] M. Aouchiche, P. Hansen, On a conjecture about the Szeged index, *Eur. J. Comb.* **31** (2010) 1662–1666.

[2] A. T. Balaban, *From Chemical Topology to Three–Dimensional Geometry*, Plenum Press, New York, 1997.

[3] M. Bonamy, M. Knor, B. Lužar, A. Pinlou, R. Škrekovski, On the difference between the Szeged and Wiener index, arxiv.org/pdf/1602.05184.

[4] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, Berlin, 2008.

[5] S. Cao, M. Dehmer, Y. Shi, Extremality of degree–based graph entropies, *Inf. Sci.* **278** (2014) 22–33.

[6] L. Chen, X. Li, M. Liu, The (revised) Szeged index and the Wiener index of a nonbipartite graph, *Eur. J. Comb.* **36** (2014) 237–246.

[7] L. Chen, X. Li, M. Liu, Tricyclic graphs with maximal revised Szeged index, *Discr. Appl. Math.* **177** (2014) 71–79.

[8] L. Chen, X. Li, M. Liu, I. Gutman, On a relation between the Szeged index and the Wiener index for bipartite graphs, *Trans. Comb.* **1** (2012) 43–49.

[9] J. Devillers, A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon & Breach, Amsterdam, 1999.

[10] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[11] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes New York* **27** (1994) 9–15.

[12] I. Gutman, S. Klavžar, B. Mohar (Eds.), Fifty Years of the Wiener Index, in: *MATCH Commun. Math. Comput. Chem.* **35** (1997) 1–259.

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

[14] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, III. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[15] I. Gutman, Y. N. Yeh, S.L. Lee, Y.L. Luo, Some recent results in the theory of the Wiener number, *Indian J. Chem.* **32A** (1993) 651–661.

[16] P. Hansen, *Computers and conjectures in chemical graph theory: some AutoGraphiX open conjectures*, in: Plenary talk at the International Conference on Mathematical Chemistry, Xiamen, China, August 4–7, 2010.

[17] S. Ji, X. Li, B. Huo, On reformulated Zagreb indices with respect to acyclic, unicyclic and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 723–732.

[18] S. Ji, X. Li, Y, Shi, The extremal matching energy of bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 697–706.

[19] S. Ji, M. Liu, J, Wu, The lower bound of revised Szeged index with respect to bicyclic graphs, *submitted*.

[20] S. Li, H. Zhang, Proofs of three conjectures on the quotients of the (revised) Szeged index and the Wiener index and beyond, *Discr. Math.* **340** (2017) 311–324.

[21] P. Khadikar, P. Kale, N. Deshpande, S. Karmarkar, V. Agrawal, Szeged indices of hexagonal chains, *MATCH Commun. Math. Comput. Chem.* **43** (2000) 7–15.

[22] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, J. Singh, A. Shrivastava, I. Lukovits, M. V. Diudea, Szeged index – Applications for drug modeling, *Lett. Drug Design Disc.* **2** (2005) 606–624.

[23] R. Lang, T. Li, D. Mo, Y. Shi, A novel method for analyzing inverse problem of topological indices of graphs using competitive agglomeration, *Appl. Math. Comput.* **291** (2016) 115–121.

[24] X. Li, M. Liu, Bicyclic graphs with maximal revised Szeged index, *Discr. Appl. Math.* **161** (2013) 2527–2531.

[25] X. Li, Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.

[26] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.

[27] M. J. Nadjafi–Arani, H. Khodashenas, A. R. Ashrafi, On the differences between Szeged and Wiener indices of graphs, *Discr. Math.* **311** (2011) 2233–2237.

[28] M. J. Nadjafi–Arani, H. Khodashenas, A. R. Ashrafi, Graphs whose Szeged and Wiener numbers differ by 4 and 5, *Math. Comput. Modell.* **55** (2012) 1644–1648.

[29] T. Pisanski, M. Randić, Use of the Szeged index and the revised Szeged index for measuring network bipartivity, *Discr. Appl. Math.* **158** (2010) 1936–1944.

[30] T. Pisanski, J. Žerovnik, Edge–contributions of some topological indices and arboreality of molecular graphs, *Ars Math. Contemp.* **2** (2009) 49–58.

[31] M. Randić, On generalization of Wiener index for cyclic structures, *Acta Chim. Slov.* **49** (2002) 483–496.

[32] S. Simić, I. Gutman, V. Baltić, Some graphs with extremal Szeged index, *Math. Slov.* **50** (2000) 1–15.

[33] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[34] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[35] J. Žerovnik, Szeged index of symmetric graphs, *J. Chem. Inf. Comput. Sci.* **39** (1999) 77–80.

[36] R. Xing, B. Zhou, On the revised Szeged index, *Discr. Appl. Math.* **159** (2011) 69–78.