



## Szeged Index of Bipartite Unicyclic Graphs

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**ABSTRACT.** The Szeged index of a connected graph  $G$  is defined as the sum of products  $n_1(e|G)n_2(e|G)$  over all edges  $e=uv$  of  $G$ , where  $n_1(e|G)$  and  $n_2(e|G)$  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  $u$ . In this paper, we determine the  $n$ -vertex bipartite unicyclic graphs with the first, the second, the third and the fourth smallest Szeged indices.

**Keywords:** Szeged index, unicyclic graphs, bipartite graphs, distance.

### 1. INTRODUCTION: ZAGREB INDICES

Topological indices are numerical graph invariants that quantitatively characterize molecular structure. The Wiener index is one of the oldest and the most thoroughly studied topological indices [1]. The Szeged index is another such topological index which coincides to the Wiener index on trees [2].

Let  $G$  be a simple connected graph with vertex set  $V(G)$  and edge set  $E(G)$ . For  $e = uv \in E(G)$ , let  $n_1(e|G)$  and  $n_2(e|G)$  be 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  $u$ . The Szeged index of the graph  $G$  is defined as [2]

$$Sz(G) = \sum_{e \in E(G)} n_1(e|G)n_2(e|G).$$

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Gutman [2] determined the  $n$ -vertex unicyclic graphs with the smallest and the largest Szeged indices for  $n \geq 3$ . Zhou et al. [3] determined (in Proposition 3 there) the  $n$ -vertex unicyclic graphs with the second, the third and the fourth smallest Szeged indices as well as (in Proposition 5 there) the  $n$ -vertex unicyclic graphs with the first a few largest Szeged indices for  $n \geq 6$ .

The number of vertices of a graph  $G$  is denoted by  $|G|$ . Let  $P_n$  and  $C_n$  be respectively the  $n$ -vertex path and cycle. Note that a unicyclic graph is bipartite if and only if its unique cycle length is even. Let  $C(n; T_1, T_2, \dots, T_r)$  be the unicyclic graph with cycle  $C_r = v_1 v_2 \dots v_r v_1$ , where the deletion of edges of the cycle results in vertex-disjoint trees  $T_1, T_2, \dots, T_r$  such that  $\sum_{i=1}^r |T_i| = n$  and  $v_i \in V(T_i)$  for  $i = 1, 2, \dots, r$ . The trees  $T_1, T_2, \dots, T_r$  are called the branches of  $C(n; T_1, T_2, \dots, T_r)$ .

For nonnegative integers  $a$  and  $b$ , let  $P(r, s, a, b)$  be the unicyclic graph obtained by attaching a path  $P_a$  at one terminal vertex to  $v_1$  and a path  $P_b$  at one terminal vertex to  $v_s$  of the cycle  $C_r$ , where  $s = 1, 2, \dots, \left\lfloor \frac{r}{2} \right\rfloor + 1$ . Let

$$P_{n,r} = P\left(r, \frac{r}{2} + 1, \left\lfloor \frac{n-r}{2} \right\rfloor, \left\lfloor \frac{n-r}{2} \right\rfloor\right) \text{ for even } r, \text{ and } P_{n,r} = P(r, 1, n-r, 0) \text{ for odd } r.$$

For odd  $n \geq 7$ , let  $H_n$  be the set of graphs  $C(n; T_1, T_2, \dots, T_{n-3})$  with  $|T_1| = |T_j| = |T_s| = 2$ ,  $|T_i| = 1$  for  $i \neq 1, j, s$ , and either  $1 < j \leq \left\lfloor \frac{n+1}{4} \right\rfloor < \frac{n-1}{2} \leq s \leq \frac{n-5}{2} + j$  or  $n-2-s \geq s-j \geq j-1 \geq \left\lfloor \frac{n+1}{4} \right\rfloor$ .

For even integer  $r \geq 4$ , let  $S(r, l, 2, 1)$  be the unicyclic graph obtained by attaching two pendent vertices to  $v_1$  and a pendent vertex to  $v_l$  of the cycle  $C_r$ , where  $l = 1, 2, \dots, \frac{r}{2} + 1$ .

By inspection the bipartite graphs in Proposition 5 of [3], we have immediately the following.

**Proposition 1.** Among  $n$ -vertex bipartite unicyclic graphs with  $n \geq 6$ ,

- (i) if  $n$  is even, then  $C_n$ ,  $P\left(n-2, \frac{n}{2}, 1, 1\right)$  and  $P(n-2, 1, 2, 0)$  are respectively the unique graphs with the first, the second and the third largest Szeged indices, which

are equal to  $\frac{n^3}{4}$ ,  $\frac{1}{4}(n^3 - 2n^2 + 8n - 8)$  and  $\frac{1}{4}(n^3 - 2n^2 + 8n - 12)$  respectively, and

$P\left(n-2, \frac{n}{2} - (s-3), 1, 1\right)$  for  $s = 4, \dots, \frac{n+4}{2}$  is the unique graph with the  $s$ -th largest Szeged index, which is equal to  $\frac{1}{4}(n^3 - 2n^2 + 8n - 8) - 2(s-3)$ ;

(ii) if  $n$  is odd, then  $P_{n,n-1}$ ,  $P\left(n-3, \frac{n-1}{2}, 2, 1\right)$  and  $P(n-3, 1, 3, 0)$  are respectively the unique graphs with the first, the second and the third largest Szeged indices, which are equal to  $\frac{1}{4}(n^3 - n^2 + 3n - 3)$ ,  $\frac{1}{4}(n^3 - 3n^2 + 15n - 21)$  and  $\frac{1}{4}(n^3 - 3n^2 + 15n - 29)$  respectively,

(a) for  $n = 7$ ,  $P\left(n-3, \frac{n-3}{2}, 2, 1\right)$ ,  $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$  and graphs in  $H_n$  are the unique graphs with the fourth largest Szeged index, which is equal to  $\frac{1}{4}(n^3 - 3n^2 + 11n - 9)$ , for

$n = 9$ ,  $P\left(n-3, \frac{n-3}{2}, 2, 1\right)$  is the unique graph with the fourth largest Szeged index, which is equal to  $\frac{1}{4}(n^3 - 3n^2 + 15n - 37)$ , while  $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$  and graphs in  $H_n$  are

the unique graphs with the fifth largest Szeged index, which is equal to  $\frac{1}{4}(n^3 - 3n^2 + 11n - 9)$ , and for  $n = 11$ ,  $P\left(n-3, \frac{n-3}{2}, 2, 1\right)$  is the unique graph with the fourth largest Szeged index, which is equal to  $\frac{1}{4}(n^3 - 3n^2 + 15n - 37)$ , while

$P\left(n-3, \frac{n-5}{2}, 2, 1\right)$ ,  $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$  and graphs in  $H_n$  are the unique graphs with the fifth largest Szeged index, which is equal to  $\frac{1}{4}(n^3 - 3n^2 + 11n - 9)$ ,

(b) for  $n \geq 13$ ,  $P\left(n-3, \frac{n-1}{2} - (s-4), 2, 1\right)$  for  $s = 5, \dots, \left\lceil \frac{n+9}{4} \right\rceil$  is the unique graph with the  $(s-1)$ -th largest Szeged index, which is equal to  $\frac{1}{4}(n^3 - 3n^2 + 15n - 21) - 4(s-4)$ , for  $s = \frac{n+13}{4}$  with  $n \equiv 3 \pmod{4}$ ,

$P\left(n-3, \frac{n-1}{2} - (s-4), 2, 1\right)$ ,  $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$  and graphs in  $H_n$  are the unique graphs with the  $(s-1)$ -th largest Szeged index, which is equal to  $\frac{1}{4}(n^3 - 3n^2 + 11n - 9)$ ,

and for  $s = \frac{n+15}{4}$  with  $n \equiv 1 \pmod{4}$ ,  $S\left(n-3, \frac{n-1}{2}, 2\right)$  and graphs in  $H_n$  are the unique graphs with the  $(s-1)$ -th largest Szeged index, which is equal to

$$\frac{1}{4}(n^3 - 3n^2 + 11n - 9).$$

However, by similar inspection of Proposition 3 of [3], we find all the  $n$ -vertex unicyclic graphs with the first, the second, the third and the fourth smallest Szeged indices are not bipartite for  $n \geq 6$ . Therefore it is interesting to determine the  $n$ -vertex bipartite unicyclic graphs with the first a few smallest Szeged indices for  $n \geq 6$ .

## 2. Preliminaries

For  $u, v \in V(G)$ , let  $d(u, v | G)$  be the distance between  $u$  and  $v$  in  $G$ , and let

$$D(u | G) = \sum_{v \in V(G)} d(u, v | G). \text{ Recall that Wiener index of the graph } G \text{ is defined as}$$

$$W(G) = \sum_{\{u, v\} \subseteq V(G)} d(u, v | G) = \frac{1}{2} \sum_{u \in V(G)} D(u | G) \text{ and that if } G \text{ is a tree then } W(G) = Sz(G).$$

Let  $S_n$  be the  $n$ -vertex star.

**Lemma 1.** [4] Let  $G = C(n; T_1, T_2, \dots, T_r)$ , where  $r$  is even. Then

$$Sz(G) = \sum_{i=1}^r W(T_i) + \sum_{i=1}^r (n - |T_i|) D(v_i | T_i) + \sum_{i=1}^r \sum_{j=1}^r |T_i| |T_j| d(v_i, v_j | C_r).$$

**Lemma 2.** [1] Let  $T$  be an  $n$ -vertex tree different from  $S_n$ . Then

$$W(T) > W(S_n) = (n-1)^2.$$

**Lemma 3.** [5] Let  $T$  be an  $n$ -vertex tree with  $u \in V(T)$ , where  $n \geq 3$ . Let  $x$  be the center of the star  $S_n$ . Then  $D(u | T) \geq D(x | S_n) = n-1$  with equality if and only if  $T = S_n$  and  $u = x$ .

Let  $P_4 = v_1 v_2 v_3 v_4$ . Let  $S_n'$  be the tree obtained from  $P_4$  by attaching  $n-4$  pendent vertices to  $v_2$  for  $n \geq 5$ , and  $S_n''$  the tree obtained from  $P_4$  by attaching  $n-5$  pendent vertices to  $v_2$  and a pendent vertex to  $v_3$  for  $n \geq 6$ .

**Lemma 4.** [5] Among the  $n$ -vertex trees with  $n \geq 6$ ,  $S_n'$  and  $S_n''$  are respectively the unique trees with the second and the third smallest Wiener indices, which are equal to  $n^2 - n - 2$  and  $n^2 - 7$ , respectively.

**Lemma 5.** [5] Let  $T$  be an  $n$ -vertex tree with  $n \geq 6$ ,  $T \neq S_n$ ,  $u \in V(T)$ , where  $u$  is not the vertex of maximal degree if  $T = S_n'$ . Let  $x$  and  $y$  be the vertex of maximal degree in  $S_n'$  and  $S_n''$ , respectively. Then  $D(u | T) \geq D(y | S_n'') > D(x | S_n') = n$ .

Let  $S_{n,r}$  be the unicyclic graph obtained by attaching  $n-r$  pendent vertices to a vertex of the cycle  $C_r$ , where  $3 \leq r \leq n$ .

**Lemma 6.** [3] Let  $G$  be an  $n$ -vertex unicyclic graph with cycle length  $r$ , where  $4 \leq r \leq n$  and  $r$  is even. Then  $S_z(G) \geq (n-1)(n-r) + \frac{r^2}{4}(2n-r)$  with equality if and only if  $G = S_{n,r}$ .

### 3. Results

Let  $\Lambda_n$  be the set of graphs  $C(n; T_1, T_2, T_3, T_4)$  with three trivial branches. Let  $\Gamma_n$  be the set of graphs  $C(n; T_1, T_2, T_3, T_4)$  in which there are exactly two trivial branches. Let  $\Psi_n$  be the set of graphs  $C(n; T_1, T_2, T_3, T_4)$  in which there is exactly one trivial branch. Let  $\Phi_n$  be the set of graphs  $C(n; T_1, T_2, T_3, T_4)$  with no trivial branch. Suppose without loss of generality that  $|T_1| \geq \max\{|T_2|, |T_3|, |T_4|\}$  in  $C(n; T_1, T_2, T_3, T_4)$ .

**Lemma 7.**  $S_{n,4}$  is the unique  $n$ -vertex bipartite unicyclic graph with the smallest Szeged index, which is equal to  $n^2 + 3n - 12$ .

**Proof.** Let  $G$  be an  $n$ -vertex bipartite unicyclic graph with cycle length  $r$ , where  $r$  is even and  $4 \leq r \leq n$ . From Lemma 6, we have

$$S_z(G) \geq S_z(S_{n,r}) = (n-1)(n-r) + \frac{r^2}{4}(2n-r).$$

Let  $f(x) = (n-1)(n-x) + \frac{x^2}{4}(2n-x)$ , where  $4 \leq x \leq n$ . It is easily seen that

$$f'(x) = -\frac{3}{4}x^2 + nx - (n-1) \geq \min\{f'(4), f'(n)\} = \min\left\{3n-11, \frac{1}{4}(n-2)^2\right\} > 0.$$

Thus for fixed  $n$ ,  $S_z(S_{n,r}) = f(r)$  is increasing for  $4 \leq r \leq n$ . The result follows easily.  $\square$

Let  $S_n(a, b, c, d)$  be the  $n$ -vertex unicyclic graph formed by attaching  $a-1$ ,  $b-1$ ,  $c-1$  and  $d-1$  pendent vertices to the four vertices of quadrangle consecutively, where  $a, b, c, d \geq 1$ , and  $a+b+c+d = n$ .

For  $n \geq 6$ , let  $B_n'$  be the  $n$ -vertex unicyclic graph formed by attaching  $n-6$  pendent vertices and a path  $P_2$  to one vertex of a quadrangle. For  $n \geq 7$ , let  $B_n''$  be the

$n$ -vertex unicyclic graph formed by attaching  $n-7$  pendent vertices and the star  $S_3$  at its center to one vertex of a quadrangle. Evidently,  $B'_n, B''_n \in \Lambda_n$ .

**Lemma 8.** Among the graphs in  $\Lambda_n$  with  $n \geq 7$ ,  $B'_n$  and  $B''_n$  are respectively the unique graphs with the second and the third smallest Szeged indices, which are equal to  $n^2 + 4n - 15$  and  $n^2 + 5n - 20$ , respectively.

**Proof.** Let  $G = C(n; T_1, T_2, T_3, T_4) \in \Lambda_n$ . Note that  $|T_1| = n-3$  and  $T_2, T_3, T_4$  are all trivial. By Lemma 1, we have

$$Sz(G) = W(T_1) + 3D(v_1|T_1) + 8(n-2)$$

which, together with Lemmas 4 and 5, implies that  $B'_n$  and  $B''_n$  are respectively the unique graphs in  $\Lambda_n$  with the second and the third smallest Szeged indices, where

$$Sz(B'_n) = W(S'_{n-3}) + 3(n-5+2) + 8(n-2) = n^2 + 4n - 15,$$

$$Sz(B''_n) = W(S''_{n-3}) + 3(n-6+4) + 8(n-2) = n^2 + 5n - 20.$$

This proves the result. □

**Lemma 9.** Among the graphs in  $\Gamma_n$  with  $n \geq 8$ ,  $S_n(n-4, 2, 1, 1)$  and  $S_n(n-5, 3, 1, 1)$  are respectively the unique graphs with the first and the second smallest Szeged indices, which are equal to  $n^2 + 5n - 22$  and  $n^2 + 7n - 36$ , respectively.

**Proof.** Let  $G = C(n; T_1, T_2, T_3, T_4) \in \Gamma_n$  with  $|T_1| = a, |T_2| = b, |T_3| = c$ , and  $|T_4| = d$ . It is easily seen that

$$Sz(S_n(a, b, c, d)) = n^2 - 5n + 4 + 2ab + 4ac + 2ad + 2bc + 4bd + 2cd.$$

Suppose that  $G \neq S_n(n-4, 2, 1, 1)$ . Note that  $a \geq b, c, d$ . There are two cases.

**Case 1.**  $c = d = 1$ . Then  $a + b = n - 2$  and  $(a, b) \neq (n - 4, 2)$ . By Lemmas 1-3,

$$Sz(G) \geq Sz(S_n(a, b, 1, 1)) = n^2 + n + 2ab - 6.$$

Obviously, for  $n \geq 8$ ,  $n^2 + n + 2ab - 6$  is minimal if and only if  $(a, b) = (n - 5, 3)$ . Thus  $Sz(G) \geq n^2 + 7n - 36$  with equality if and only if  $G = S_n(n - 5, 3, 1, 1)$ . Note that  $Sz(S_n(n - 4, 2, 1, 1)) = n^2 + 5n - 22$ . It follows that

$$\begin{aligned} Sz(G) &> Sz(S_n(n - 5, 3, 1, 1)) = n^2 + 7n - 36 \\ &> Sz(S_n(n - 4, 2, 1, 1)) = n^2 + 5n - 22 \end{aligned}$$

if  $G \neq S_n(n - 4, 2, 1, 1)$ ,  $S_n(n - 5, 3, 1, 1)$ .

**Case 2.**  $b = d = 1$ . Then  $a + c = n - 2$ . By Lemmas 1-3, we have

$$\begin{aligned} Sz(G) &\geq Sz(S_n(a, 1, c, 1)) = n^2 - n + 4ac \\ &\geq n^2 - n + 4(n - 4) \cdot 2 \end{aligned}$$

$$\begin{aligned}
 &= n^2 + 7n - 32 \\
 &> n^2 + 7n - 36 \\
 &= Sz(S_n(n-5, 3, 1, 1)) \\
 &> Sz(S_n(n-4, 2, 1, 1)).
 \end{aligned}$$

By combining Cases 1 and 2, the result follows. □

**Lemma 10.** Let  $G \in \Psi_n$ , where  $n \geq 8$ . Then

$$Sz(G) > Sz(S_n(n-5, 3, 1, 1)) = n^2 + 7n - 36.$$

**Proof.** Let  $G = C(n; T_1, T_2, T_3, T_4) \in \Psi_n$  with  $|T_1| = a$ ,  $|T_2| = b$ ,  $|T_3| = c$ , and  $|T_4| = d$ . Note that  $a \geq b, c, d$ . Suppose without loss of generality that  $b \geq d$ . Then there are three cases.

**Case 1.**  $d = 1$  and  $a \geq b \geq c$ . Then  $a + b + c = n - 1$ ,  $\frac{n-1-c}{2} \leq a \leq n-1-2c$ , and  $2 \leq c \leq \frac{n-1}{3}$ . Let  $f(a, b, c) = 2ab + 4ac + 2bc + 2a + 4b + 2c$ . It is easily seen that

$$Sz(S_n(a, b, c, 1)) = n^2 - 5n + 4 + f(a, b, c).$$

Note that

$$\begin{aligned}
 f(a, b, c) &= 2a(n-1-c-a) + 4ac + 2(n-1-c-a)c \\
 &\quad + 2a + 4(n-1-c-a) + 2c \\
 &= -2a^2 + 2(n-2)a - 2c^2 + 2(n-2)c + 4(n-1) \\
 &\geq \min \left\{ f\left(\frac{n-1-c}{2}, b, c\right), f(n-1-2c, b, c) \right\}.
 \end{aligned}$$

Thus  $Sz(S_n(a, b, c, 1)) \geq \min \left\{ Sz\left(S_n\left(\frac{n-1-c}{2}, b, c, 1\right)\right), Sz(S_n(n-1-2c, b, c, 1)) \right\}$ . It is not

difficult to check that

$$\begin{aligned}
 Sz\left(S_n\left(\frac{n-1-c}{2}, b, c, 1\right)\right) &= n^2 - 5n + 4 - 2\left(\frac{n-1-c}{2}\right)^2 \\
 &\quad + 2(n-2)\left(\frac{n-1-c}{2}\right) - 2c^2 + 2(n-2)c + 4(n-1) \\
 &= -\frac{5}{2}c^2 + (2n-3)c + \frac{3}{2}n^2 - 3n + \frac{3}{2} \\
 &= \frac{3}{2}n^2 + n - \frac{29}{2} \\
 &> n^2 + 7n - 36 = Sz(S_n(n-5, 3, 1, 1)),
 \end{aligned}$$

and

$$\begin{aligned}
 Sz(S_n(n-1-2c, b, c, 1)) &= n^2 - 5n + 4 - 2(n-1-2c)^2 \\
 &\quad + 2(n-2)(n-1-2c) - 2c^2 + 2(n-2)c + 4(n-1) \\
 &= -10c^2 + (6n-4)c + n^2 - 3n + 2 \\
 &\geq -10 \cdot 2^2 + (6n-4) \cdot 2 + n^2 - 3n + 2 \\
 &= n^2 + 9n - 46 \\
 &> n^2 + 7n - 36 = Sz(S_n(n-5, 3, 1, 1)).
 \end{aligned}$$

Thus by Lemmas 1-3, we have

$$Sz(G) \geq Sz(S_n(a, b, c, 1)) > Sz(S_n(n-5, 3, 1, 1)) = n^2 + 7n - 36 \text{ for } n \geq 8.$$

**Case 2.**  $d=1$  and  $a \geq c > b$ . Then  $a+b+c = n-1$ ,  $\frac{n-1-b}{2} \leq a < n-1-2b$ , and

$2 \leq b < \frac{n-1}{3}$ . Let

$$\begin{aligned}
 f(a, b, c) &= 2ab + 4a(n-1-a-b) + 2b(n-1-a-b) + 2a + 4b + 2(n-1-a-b) \\
 &= -4a^2 + 4(n-1-b)a - 2b^2 + 2nb + 2(n-1).
 \end{aligned}$$

Then

$$\begin{aligned}
 f(a, b, c) &> f(n-1-2b, b, c) \\
 &= -10b^2 + (6n-4)b + 2(n-1) \\
 &\geq -10 \cdot 2^2 + (6n-4) \cdot 2 + 2(n-1) \\
 &= 14n - 50.
 \end{aligned}$$

It follows that

$$\begin{aligned}
 Sz(S_n(a, b, c, 1)) &= n^2 - 5n + 4 + f(a, b, c) \\
 &> n^2 - 5n + 4 + 14n - 50 \\
 &= n^2 + 9n - 46 \\
 &> n^2 + 7n - 36 = Sz(S_n(n-5, 3, 1, 1)).
 \end{aligned}$$

By Lemmas 1-3, we have  $Sz(G) \geq Sz(S_n(a, b, c, 1)) > Sz(S_n(n-5, 3, 1, 1)) = n^2 + 7n - 36$ .

**Case 3.**  $c=1$  and  $a \geq b \geq d$ . Then  $a+b+d = n-1$ ,  $\frac{n-1-d}{2} \leq a \leq n-1-2d$ ,

$2 \leq d \leq \frac{n-1}{3}$ . Thus by similar arguments as in Case 2, we have

$$Sz(G) \geq Sz(S_n(a, b, 1, d)) > Sz(S_n(n-5, 3, 1, 1)) = n^2 + 7n - 36.$$

By combining Cases 1-3, the result follows. □

**Lemma 11.** Let  $G \in \Phi_n$ , where  $n \geq 8$ . Then



$$Sz(G) > Sz(S_n(n-5, 3, 1, 1)) = n^2 + 7n - 36.$$

**Proof.** Let  $G = C(n; T_1, T_2, T_3, T_4) \in \Phi_n$  with  $|T_1| = a$ ,  $|T_2| = b$ ,  $|T_3| = c$ , and  $|T_4| = d$ . Suppose without loss of generality that  $b \geq d$ . It is easily seen that

$$\begin{aligned} & Sz(S_n(a+1, b, c, d-1)) - Sz(S_n(a, b, c, d)) \\ &= 2(a+1)b + 4(a+1)c + 2(a+1)(d-1) + 4b(d-1) + 2c(d-1) \\ &\quad - (2ab + 4ac + 2ad + 4bd + 2cd) \\ &= 2(c + d - a - b - 1) < 0, \end{aligned}$$

and then  $Sz(S_n(a, b, c, d)) > Sz(S_n(a+1, b, c, d-1))$ . If  $G = S_n(a, b, c, d)$ , then by Lemma 10, we have

$$\begin{aligned} Sz(G) &= Sz(S_n(a, b, c, d)) > Sz(S_n(a+1, b, c, d-1)) \\ &> \dots > Sz(S_n(a+d-1, b, c, 1)) \\ &> Sz(S_n(n-5, 3, 1, 1)) = n^2 + 7n - 36 \end{aligned}$$

and if  $G \neq S_n(a, b, c, d)$ , then by Lemmas 1-3, we have

$$Sz(G) > Sz(S_n(a, b, c, d)) > Sz(S_n(n-5, 3, 1, 1)) = n^2 + 7n - 36.$$

The proof is now completed. □

**Proposition 2.** Among  $n$ -vertex bipartite unicyclic graphs with  $n \geq 6$ ,

(i) for  $n = 6$ ,  $S_6(2, 2, 1, 1)$  and  $B_6'$  are respectively the unique bipartite unicyclic graphs with the second and the third smallest Szeged indices, which are equal to 44 and 45, respectively;

(ii) for  $n = 7$ ,  $B_7'$  and  $S_7(3, 2, 1, 1)$  are the unique bipartite unicyclic graphs with the second smallest Szeged index, which is equal to 62, while  $B_7''$  is the unique bipartite unicyclic graphs with the third smallest Szeged index, which is equal to 64;

(iii) for  $n \geq 8$ ,  $B_n'$ ,  $S_n(n-4, 2, 1, 1)$  and  $B_n''$  are respectively the unique bipartite unicyclic graphs with the second, the third and the fourth smallest Szeged indices, which are  $n^2 + 4n - 15$ ,  $n^2 + 5n - 22$  and  $n^2 + 5n - 20$ , respectively.

**Proof.** The cases  $n = 6, 7$  may be checked easily. Suppose that  $n \geq 8$ .

By Lemma 8,  $B_n'$  and  $B_n''$  are respectively the unique graphs in  $\Lambda_n$  with the second and the third smallest Szeged indices, which are equal to  $n^2 + 4n - 15$  and  $n^2 + 5n - 20$ , respectively. By Lemma 9,  $S_n(n-4, 2, 1, 1)$  and  $S_n(n-5, 3, 1, 1)$  are respectively the unique graphs in  $\Gamma_n$  with the first and the second smallest Szeged indices, which are equal to  $n^2 + 5n - 22$  and  $n^2 + 7n - 36$ . By Lemmas 10 and 11, if  $G \in \Psi_n \cup \Phi_n$ , then  $Sz(G) > Sz(S_n(n-5, 3, 1, 1)) = n^2 + 7n - 36$ . It follows that, among  $n$ -vertex bipartite

unicyclic graphs with cycle length four, the graphs  $B_n'$ ,  $S_n(n-4, 2, 1, 1)$  and  $B_n''$  are respectively the unique graphs with the second, the third and the fourth smallest Szeged indices.

From the proof of Lemma 7, for any  $n$ -vertex bipartite unicyclic graph  $G$  with cycle length at least six, we have

$$Sz(G) \geq Sz(S_{n,6}) = n^2 + 11n - 48 > n^2 + 7n - 36 = Sz(S_n(n-5, 3, 1, 1)).$$

The result follows easily. □

Let  $G$  be a graph with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$  and edge set  $E(G) = \{e_1, e_2, \dots, e_m\}$ , thus possessing  $n$  vertices and  $m$  edges. The degree  $d(v)$  of the vertex  $v \in V(G)$  is the number of first neighbors of  $v$ . The edge of the graph  $G$ , connecting the vertices  $u$  and  $v$ , will be denoted by  $uv$ . Throughout this paper, the graphs considered are assumed to be connected.

In mathematical chemistry, two simple graph invariants

$$M_1 = M_1(G) := \sum_{v \in V(G)} d(v)^2 \quad \text{and} \quad M_2 = M_2(G) := \sum_{uv \in E(G)} d(u)d(v)$$

were first time encountered in connection with the study of the structure-dependency of total  $\pi$ -electron energy [1] and soon thereafter used for modeling of branching-based properties of alkanes [2]. Eventually, these two structure-descriptors were named *Zagreb group indices* [3]. Nowadays these are commonly referred to as the *first* ( $M_1$ ) and *second* ( $M_2$ ) *Zagreb indices*.

For information on the two Zagreb indices and a number of similar molecular structure descriptors, the readers should consult the books [4-6] and/or the reviews [7-11]. Of the countless published papers on Zagreb indices, we mention only the most recent ones [12-32], in which references to earlier works can be found.

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