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MAXIMUM VALUES OF SOMBOR INDEX OF BICYCLIC GRAPHS WITH A GIVEN MATCHING NUMBER

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Abstract. Sombor index is a popular vertex-degree-based topological index recently. In this paper, the maximum values of Sombor index for the class of all bicyclic graphs with a given matching number are wholly determined, then the extremal graphs with these maximum values are also characterized.

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1. Introduction

In chemical graph theory and mathematical chemistry, a topological index known as a connectivity index is a type of molecular descriptor calculated based on the molecular graph of a chemical compound. Since the first topological index (Wiener index) has been introduced in 1947, many definitions of topological indices are given as well. Recently, based on the idea of Euclidean norm, the famous Sombor index of a graph G is defined in 2021 by Gutman [8] as follows

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2},$$

where $G = (V(G), E(G))$ is a simply connected graph with vertex set $V(G)$ and edge set $E(G)$, d_u is vertex u's degree. Notwithstanding the definition of Sombor index was indtroduced in 2021, many papers have been published in [1, 3, 4, 7], and the chemical utilizations of this index were displayed in [10]. Results of trees, unicyclic graphs and bicyclic graphs for Sombor index, see [5, 6]. Most of results relative to Sombor index were summarized in [11].

Now we give the definitions and notations throughout this paper. We denote $\mathfrak{B}_n$ the set consists of bicyclic graphs of order n. Denoted by $\mathfrak{B}_{n,m}$ the family of bicyclic graphs with maximum matching number m of order n. Denoted by $\widehat{\mathfrak{B}}_n$ the family of all bicyclic graphs without pendant edges of order n. $N(x)$ denotes the neighborhood of x. Denoted by $P(G)$, $P(x)$ the set consists of pendant vertices in G and pendant neighbors of x respectively. Symbol $M = M(G)$ denotes the maximum matching of G. Write $|M| = m$, and $\mathfrak{B}_{2m,m}$ the set consists of all bicyclic graphs of order $2m$ with maximum matching number m. If we denote $\mathfrak{B}_n^1, \mathfrak{B}_n^2, \mathfrak{B}_n^3, \mathfrak{B}_n^4, \mathfrak{B}_n^5$ the family of bicyclic graphs constructed by attaching an edge between two disjoint cycles, the family of bicyclic

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graphs constructed by jointing a path (length ≥ 2) between two disjoint cycles, the family of bicyclic graphs constructed by combining two vertices from different cycles, the family of bicyclic graphs constructed by adding an edge between two non-adjacent vertices, the family of bicyclic graphs constructed by adding a path (length ≥ 2) between two non-adjacent vertices in those two cycles respectively, then $\widehat{\mathfrak{B}}_n = \mathfrak{B}_n^1 \cup \mathfrak{B}_n^2 \cup \mathfrak{B}_n^3 \cup \mathfrak{B}_n^4 \cup \mathfrak{B}_n^5$. Other definitions and notations refer to [2].

This paper will be written in the following way. In section 2, we will introduced several lemmas which are necessary to determine the maximum Sombor index, the proofs of these lemmas are given as well. In section 3, the main results are obtained that the bicyclic graphs with a given matching number of maximum Sombor index are completely characterized.

2. Lemmas

In this section, we show all the lemmas which will play important role to determine the maximum values for Sombor index. Denoted by $\mathfrak{U}_{2m,m}$ the set consist of all unicyclic graphs with maximum matching number m of order n. Zhou *et al.* [12] determined the following result (see Fig. 1).

Lemma 2.1. [12] *If $G \in \mathfrak{U}_{2m,m}$, then*

$$SO(G) \leq SO(U_{2m,m}) = m\sqrt{(m+1)^2+4} + \sqrt{(m+1)^2+1} + (m-2)\sqrt{5} + 2\sqrt{2}.$$

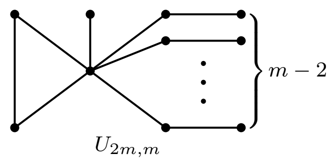

Figure 1. Unicyclic graphs $U_{2m,m}$

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Lemma 2.2. [13] *If $G \in \mathfrak{B}_{n,m}$ and $|P(G)| \geq 1$, then there exists a maximum matching M and a pendant vertex u such that u is not M-saturated.*

Lemma 2.3. [9] *Let G be a connected graph and uv be a non-pendent cut edge in G. Denote by G' the graph obtained by the contraction of uv onto the vertex u and adding a pendent vertex v to u. Then $SO(G) < SO(G')$.*

Lemma 2.4. *Function $\rho(t) = (t-3)\sqrt{t^2+1} - (t-4)\sqrt{(t-1)^2+1} + 2\sqrt{t^2+4} - 2\sqrt{(t-1)^2+4}$ is increasing when $t \in [3, +\infty)$.*

Proof. Let $\gamma(s) = \sqrt{s^2+1} + \dfrac{s(s-3)}{\sqrt{s^2+1}} + \dfrac{2s}{\sqrt{s^2+4}}$, $s \geq 3$. By derivation,

$$\begin{aligned}
\gamma'(s) &= \frac{s}{\sqrt{s^2+1}} + \frac{(2s-3)\sqrt{s^2+1} - s(s-3)\frac{s}{\sqrt{s^2+1}}}{s^2+1} + 2\frac{\sqrt{s^2+4} - \frac{s^2}{\sqrt{s^2+4}}}{s^2+4} \\
&= \frac{s}{\sqrt{s^2+1}} + \frac{s^3+2s-3}{(s^2+1)\sqrt{s^2+1}} + \frac{8}{(s^2+4)\sqrt{s^2+4}} > 0.
\end{aligned}$$

It means $\gamma(t) > \gamma(t-1)$. Hence,

$$\rho'(t) = \sqrt{t^2+1} - \sqrt{(t-1)^2+1} + \frac{(t-3)t}{\sqrt{t^2+1}} - \frac{(t-4)(t-1)}{\sqrt{(t-1)^2+1}} + 2\frac{t}{\sqrt{t^2+4}} - 2\frac{t-1}{\sqrt{(t-1)^2+4}}$$

$$= \gamma(t) - \gamma(t-1) > 0.$$

It follows function $\rho(t)$ is increasing when $t \geq 3$. $\square$

Lemma 2.5. *Function*

$$\begin{aligned}\sigma(t) = & t\sqrt{(t+1)^2+4} + \sqrt{(t+1)^2+1} + \sqrt{5}(t-2) \\ & - \left[(t-3)\sqrt{5} + (t+1)\sqrt{(t+2)^2+4} + \sqrt{(t+2)^2+1}\right]\end{aligned}$$

is decreasing when $t \geq 3$.

Proof. By derivation,

$$\begin{aligned}\sigma'(t) = & \left[\sqrt{(t+1)^2+4} + \frac{t(t+1)}{\sqrt{(t+1)^2+4}} + \frac{t+1}{\sqrt{(t+1)^2+1}}\right] \\ & - \left[\sqrt{(t+2)^2+4} + \frac{(t+1)(t+2)}{\sqrt{(t+2)^2+4}} + \frac{t+2}{\sqrt{(t+2)^2+1}}\right].\end{aligned}$$

And the derivation of function

$$\alpha(s) = \sqrt{(s+1)^2+4} + \frac{s(s+1)}{\sqrt{(s+1)^2+4}} + \frac{s+1}{\sqrt{(s+1)^2+1}},\ s \geq 3$$

satisfy

$$\begin{aligned}\alpha'(s) &= \frac{s+1}{\sqrt{(s+1)^2+4}} + \frac{(2s+1)\sqrt{(s+1)^2+4} - \frac{s(s+1)^2}{\sqrt{(s+1)^2+4}}}{(s+1)^2+4} + \frac{\sqrt{(s+1)^2+1} - \frac{(s+1)^2}{\sqrt{(s+1)^2+1}}}{(s+1)^2+1} \\ &= \frac{s+1}{\sqrt{(s+1)^2+4}} + \frac{(s+1)^3+4(2s+1)}{[(s+1)^2+4]\sqrt{(s+1)^2+4}} + \frac{1}{[(s+1)^2+1]\sqrt{(s+1)^2+1}} > 0,\end{aligned}$$

which means $\alpha(t+1) > \alpha(t)$. It is deduced that $\sigma'(t) = \alpha(t) - \alpha(t+1) < 0$. Hence, function $\sigma(t)$ is decreasing when $t \geq 3$. $\square$

Lemma 2.6. *Assume G is connected, $d_x = 2$, $N(x) = \{y, z\}$ such that $d_y \geq 2$ and $yz \notin E(G)$. Write $G' = G - xz + yz$, then $SO(G') > SO(G)$.*

Proof. Let $d_y = a \geq 2$ and $N(y) = \{y = x, y_1, \cdots, y_{a-1}\}$. Then

$$\begin{aligned}& SO(G') - SO(G) \\ = & \left(\sum_{i=1}^{a-1}\sqrt{(a+1)^2+d_{y_i}^2} + \sqrt{(a+1)^2+1} + \sqrt{(a+1)^2+d_z^2}\right) \\ & - \left(\sum_{i=1}^{a-1}\sqrt{a^2+d_{y_i}^2} + \sqrt{a^2+2^2} + \sqrt{2^2+d_z^2}\right) \\ > & \sqrt{(a+1)^2+1} - \sqrt{a^2+2^2} > 0.\end{aligned}$$

Hence, $SO(G') > SO(G)$. $\square$

Now based on the partition of $\widehat{\mathfrak{B}}_n$ in section 1 and Lemma 2.6 above, we get the following lemma which is necessary to get maximum Sombor index for the bicyclic graphs with a given matching number.

Lemma 2.7. *Assume $G \in \mathfrak{B}_{2m,m} \setminus \{BC_1\}$, bicyclic graphs BC_1 and $BC_{6,3}$ are defigured in Figure 2. If $m > 2$ and there is no pendant edge such that its one end has degree two, then*

$$SO(G) \leq (m-3)\sqrt{5} + (m+1)\sqrt{(m+2)^2+4} + \sqrt{(m+2)^2+1} + 4\sqrt{2}.$$

Specially, when $m = 3$ and $G \cong BC_{6,3}$,

$$\begin{aligned} SO(G) = SO(BC_{6,3}) &= \left[(m-3)\sqrt{5} + (m+1)\sqrt{(m+2)^2+4} + \sqrt{(m+2)^2+1} + 4\sqrt{2}\right]\Big|_{m=3} \\ &= \sqrt{26} + 4\sqrt{29} + 4\sqrt{2}. \end{aligned}$$

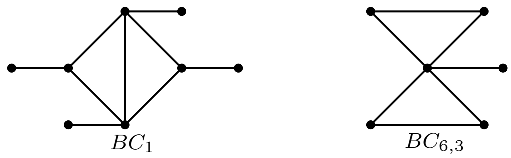

FIGURE 2. Bicyclic graphs $BC_1, BC_{6,3}$.

Proof. Assume the order of maximum matching $M(G)$ is m and for every $x \in V(G)$, $|N(x) \cap P(x)| \leq 1$. Hence, G is a graph constructed by adding pendant edges onto some $\widehat{G} \in \mathfrak{B}_l$, $m \leq l \leq 2m$.

Case 1 If G contains no 2-degree vertex, then $l = m$ or $l = m+1$. At this time, $\widehat{G} \in \cup_{i=1}^{5} \mathfrak{B}_m^i$ or $\widehat{G} \in \mathfrak{B}_{m+1}^1 \cup \mathfrak{B}_{m+1}^4$.

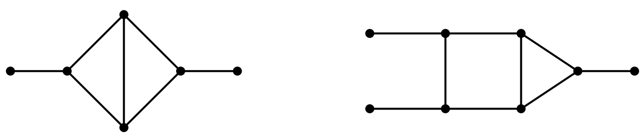

FIGURE 3. Bicyclic graphs Y_1 and Y_2.

Assume $m = 3$, then $G \cong Y_1$ (see Fig. 3). Obviously,

$$\begin{aligned} SO(Y_1) &= 2\sqrt{10} + 15\sqrt{2} < \sqrt{26} + 4\sqrt{29} + 4\sqrt{2} \\ &= \left[(m-3)\sqrt{5} + (m+1)\sqrt{(m+2)^2+4} + \sqrt{(m+2)^2+1} + 4\sqrt{2}\right]\Big|_{m=3}. \end{aligned}$$

Assume $m = 4$, in view of $G \ncong BC_1$, $G \cong Y_2$ (see Fig. 3). Obviously,

$$\begin{aligned} SO(Y_2) &= 3\sqrt{10} + 18\sqrt{2} < \sqrt{5} + 10\sqrt{10} + \sqrt{37} + 4\sqrt{2} \\ &= \left[(m-3)\sqrt{5} + (m+1)\sqrt{(m+2)^2+4} + 4\sqrt{2} + \sqrt{(m+2)^2+1}\right]\Big|_{m=4}. \end{aligned}$$

Assume $m \geq 5$. If $\widehat{G} \in \mathfrak{B}_m^1 \cup \mathfrak{B}_m^4$, then $SO(G) = 2\sqrt{17} + 4\sqrt{2} + 20 + (m-2)\sqrt{10} + (3m-12)\sqrt{2}$. If $\widehat{G} \in \mathfrak{B}_m^2 \cup \mathfrak{B}_m^5$, then $SO(G) = 2\sqrt{17} + 30 + (m-2)\sqrt{10} + 3(m-5)\sqrt{2}$. If $\widehat{G} \in \mathfrak{B}_m^3$, then $SO(G) = \sqrt{26} + 4\sqrt{34} +$

$(m-1)\sqrt{10}+3(m-3)\sqrt{2}$. If $\widehat{G} \in \mathfrak{B}^1_{m+1} \cup \mathfrak{B}^4_{m+1}$, then $SO(G) = (m-1)\sqrt{10}+3(m+2)\sqrt{2}$. Consider function

$$\begin{aligned}\beta(t) &= \left[\sqrt{26}+4\sqrt{34}+(t-1)\sqrt{10}+3(t-3)\sqrt{2}\right] - \left[(t-3)\sqrt{5}+(t+1)\sqrt{(t+2)^2+4}\right.\\ &\quad \left.+\sqrt{(t+2)^2+1}+4\sqrt{2}\right]\\ &= \sqrt{26}+4\sqrt{34}+(t-1)\sqrt{10}+(3t-5)\sqrt{2}-(t-3)\sqrt{5}-(t+1)\sqrt{(t+2)^2+4}\\ &\quad -\sqrt{(t+2)^2+1},\ t \geq 5.\end{aligned}$$

By derivation,

$$\beta'(t) = \sqrt{10}+3\sqrt{2}-\sqrt{5}-\sqrt{(t+2)^2+4}-\frac{(t+1)(t+2)}{\sqrt{(t+2)^2+4}}-\frac{t+2}{\sqrt{(t+2)^2+1}} < 0.$$

It gives $\beta(t)$ is decreasing when $t \geq 5$. Hence, $\beta(t) \leq \beta(5) < 0$. Therefore,

$$SO(G) \leq (m-3)\sqrt{5}+(m+1)\sqrt{(m+2)^2+4}+\sqrt{(m+2)^2+1}+4\sqrt{2}.$$

Case 2. G contains a 2-degree vertex x. Let $N(x) = \{y, z\}$. Obviously, $d_y \geq 2$ and $d_z \geq 2$. Now suppose $xy \in M$.

Subcase 2.1. Assume there is no 2-degree vertex in cycles of G. Base on the condition that there is no pendant edge, its one end has degree two, we get $\widehat{G} \in \mathfrak{B}^2_k$ and x is not in cycles in G. Hence, yz is not an edge in $E(G)$. Write $G' = G - xz + yz$. Then $G' \in \mathfrak{B}_{2m,m}$ and $SO(G') > SO(G)$ by Lemma 2.6. By repeating applying the same argument as above until no vertex is of degree 2. Then by Case 1, we obtain the result in lemma.

Subcase 2.2. Now assume x is in a cycle of G. Then $G_1 = G - xz \in \mathfrak{U}_{2m,m}$. By combining the facts $2 \leq d_y, d_z = b \leq 5$, function $\sqrt{t^2+4}-\sqrt{t^2+1}$ is decreasing for $t \geq 2$, $|N(z) \cap P(z)| \leq 1$ and function $\sqrt{d_z^2+s^2}-\sqrt{(d_z-1)^2+s^2}$ is decreasing for $s \geq 1$, we get

$$\begin{aligned}SO(G) &= SO(G_1)+\sqrt{d_z^2+4}+\left(\sqrt{d_y^2+4}-\sqrt{d_y^2+1}\right)\\ &\quad +\sum_{w \in N(z)\setminus\{x\}}\left(\sqrt{d_z^2+d_w^2}-\sqrt{(d_z-1)^2+d_w^2}\right)\\ &\leq SO(G_1)+\sqrt{d_z^2+4}+\left(\sqrt{8}-\sqrt{5}\right)+\left(\sqrt{d_z^2+1}-\sqrt{(d_z-1)^2+1}\right)\\ &\quad +(b-2)\left(\sqrt{d_z^2+4}-\sqrt{(d_z-1)^2+4}\right)\\ &\leq SO(G_1)+\sqrt{5^2+4}+\left(\sqrt{8}-\sqrt{5}\right)+\left(\sqrt{26}-\sqrt{17}\right)+(b-2)\left(\sqrt{5^2+4}-\sqrt{4^2+4}\right)\\ &\leq SO(G_1)+4\sqrt{29}+2\sqrt{2}-7\sqrt{5}+\sqrt{26}-\sqrt{17},\end{aligned} \tag{2.1}$$

equality admits iff $d_y = 2, d_z = b = 5$.

If $G_1 \cong C_3(1,1,1)$, then $G \cong Y_3$ or $G \cong Y_4$ (see Fig. 4). By calculating, $SO(Y_3) = \sqrt{10}+11\sqrt{2}+2\sqrt{13}$, $SO(Y_4) = \sqrt{10}+\sqrt{17}+\sqrt{13}+2\sqrt{5}+3\sqrt{2}+10$, it follows $SO(Y_3) < SO(Y_4) < SO(BC_{6,3}) = 4\sqrt{2}+4\sqrt{29}+\sqrt{26}$. Hence, the consequence in lemma holds.

If $G_1 \cong F_1$ (see Fig. 5), then from (2.1),

$$\begin{aligned}SO(G) &\leq SO(F_1)+4\sqrt{29}+2\sqrt{2}-7\sqrt{5}+\sqrt{26}-\sqrt{17}\\ &= \left[3\sqrt{5}+\sqrt{17}+10+2\sqrt{10}+3\sqrt{2}\right]+\left[4\sqrt{29}+2\sqrt{2}-7\sqrt{5}+\sqrt{26}-\sqrt{17}\right]\end{aligned}$$

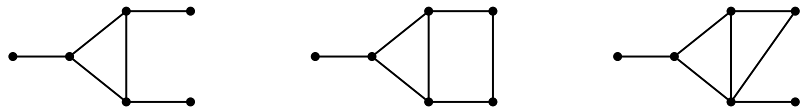

FIGURE 4. Unicyclic graph $C_3(1,1,1)$ and Bicyclic graphs Y_3, Y_4.

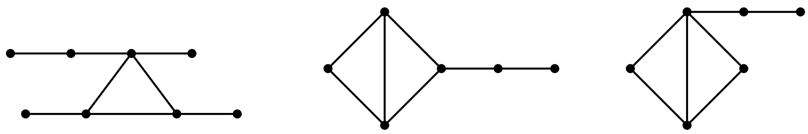

FIGURE 5. Bicyclic graphs F_1, F_2, F_3.

$$\leq \left[(m-3)\sqrt{5}+(m+1)\sqrt{(m+2)^2+4}+4\sqrt{2}+\sqrt{(m+2)^2+1}\right]\Big|_{m=4}.$$

Now if $G \ncong C_3(1,1,1)$ and $G \ncong F_1$, then by Lemma 2.1, (2.1) can be rewritten as

$$\begin{aligned}
&SO(G)\\
&\leq SO(G_1)+4\sqrt{29}+2\sqrt{2}-11\sqrt{5}+\sqrt{26}-\sqrt{17}\\
&\leq \left[m\sqrt{(m+1)^2+4}+\sqrt{(m+1)^2+1}+\sqrt{5}(m-2)+2\sqrt{2}\right]+4\sqrt{29}+2\sqrt{2}-7\sqrt{5}+\sqrt{26}-\sqrt{17},\\
&\leq (m-3)\sqrt{5}+(m+1)\sqrt{(m+2)^2+4}+\sqrt{(m+2)^2+1}+4\sqrt{2}.
\end{aligned}$$

equality admits iff $d_y = 2, b = 5$, that is, $G_1 \cong U_{6,3}$ and $G \cong BC_{6,3}$. □

3. MAIN RESULTS

In this section, by using the lemmas above, we will wholly determine the maximum values of Sombor index for graphs with a given matching number. At begin with, we first get $BC_{2m,m}$ (see Fig. 8) has the maximum value of Sombor index in graph $G \in \mathfrak{B}_{2m,m} \setminus \{BC_1\}$ in the following theorem.

Theorem 3.1. *Assume $G \in \mathfrak{B}_{2m,m} \setminus \{BC_1\}$. If $m > 2$, then*

$$SO(G) \leq SO(BC_{2m,m}) = (m-3)\sqrt{5}+(m+1)\sqrt{(m+2)^2+4}+\sqrt{(m+2)^2+1}+4\sqrt{2}.$$

Proof. We apply inductive method. Assume $m = 3$. By Lemma 2.2, if $d_x = 1$ and $xy \in E(G)$, then $d_y = 2$. Hence, $G \cong F_2$ or $G \cong F_3$ (see Fig. 5). By calculating,

$$SO(F_2) = \sqrt{5}+9\sqrt{2}+3\sqrt{13},\ SO(F_3) = 7\sqrt{5}+2\sqrt{13}+5.$$

Obviously, $SO(G) \leq SO(BC_{6,3})$.

Now assume the consequence when $G \in \mathfrak{B}_{2m-2,m-1}$ for $m > 3$ admits.

If there is no pendant edge such that its another end has degree two, then by Lemma 2.7, the consequence in theorem admits.

If there is a pendant edge xy, such that $d_y = 1, d_x = 2$, then $G' = G - \{x,y\} \in \mathfrak{B}_{2m-2,m-1}$ and $xy \in M$. Write $z \neq y$, $xz \in E(G)$. At this moment, $2 \leq d_z \leq m+2$.

Now if $G' \cong BC_1$, then $d_z \leq 5$. Hence,

$$\begin{aligned}
SO(G) &= SO(BC_1) + \sum_{z_i \in N(z)\setminus\{x\}} \left(\sqrt{d_z^2+d_w^2} - \sqrt{(d_z-1)^2+d_w^2}\right) + \sqrt{d_z^2+2^2} + \sqrt{5} \\
&\leq SO(BC_1) + \sum_{w \in N(z)\setminus\{x\}} \left(\sqrt{5^2+d_w^2} - \sqrt{4^2+d_w^2}\right) + \sqrt{5^2+4} + \sqrt{5} \\
&\leq \left(2\sqrt{10}+2\sqrt{17}+20+4\sqrt{2}\right) + \left(\sqrt{5^2+1}-\sqrt{4^2+1}\right) + \left(\sqrt{5^2+2^2}-\sqrt{4^2+2^2}\right) \\
&\quad + 2\left(\sqrt{5^2+3^2}-\sqrt{4^2+3^2}\right) + \left(\sqrt{5^2+4^2}-\sqrt{4^2+4^2}\right) + \sqrt{5^2+4} + \sqrt{5} \\
&\leq \left[(m-3)\sqrt{5} + (m+1)\sqrt{(m+2)^2+4} + \sqrt{(m+2)^2+1} + 4\sqrt{2}\right]\Big|_{m=5} \\
&= SO(BC_{10,5}).
\end{aligned}$$

If $G' \ncong BC_1$, note that $d_z = a \leq m+2$ and $G' \in \mathfrak{B}_{2m-2,m-1}$, then

$$\begin{aligned}
SO(G) &\leq SO(G') + \sum_{w \in N(z)\setminus\{x\}} \left[\sqrt{d_z^2+d_w^2} - \sqrt{(d_z-1)^2+d_w^2}\right] + \sqrt{2^2+1} + \sqrt{d_z^2+2^2} \\
&\leq \left[(m-4)\sqrt{5} + m\sqrt{(m+1)^2+4} + \sqrt{(m+1)^2+1} + 4\sqrt{2}\right] + \sqrt{5} + \sqrt{a^2+4} \\
&\quad + \left[\sqrt{a^2+1} - \sqrt{(a-1)^2+1}\right] + (a-2)\left[\sqrt{a^2+4} - \sqrt{(a-1)^2+4}\right] \\
&\leq \left[(m-4)\sqrt{5} + m\sqrt{(m+1)^2+4} + \sqrt{(m+1)^2+1} + 4\sqrt{2}\right] + \sqrt{5} + \sqrt{(m+2)^2+4} \\
&\quad + \left[\sqrt{(m+2)^2+1} - \sqrt{(m+1)^2+1}\right] + m\left[\sqrt{(m+2)^2+4} - \sqrt{(m+1)^2+4}\right] \\
&= (m-3)\sqrt{5} + (m+1)\sqrt{(m+2)^2+4} + \sqrt{(m+2)^2+1} + 4\sqrt{2},
\end{aligned}$$

specially, equality admits when $G \cong BC_{2m,m}$. □

By using Lemma 2.4 and Lemma 2.6, the maximum Sombor index of $G \in \mathfrak{B}_{n,2}$ is completely determined in the following theorem.

Theorem 3.2. *If $G \in \mathfrak{B}_{n,2}$, then*

$$SO(G) \leq SO(BC_{n,n-1,3}) = (n-4)\sqrt{(n-1)^2+1} + 2\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+9} + 2\sqrt{13}.$$

Proof. We consider the following cases.

Case 1. If $n = 4$, then $G \cong Z_1$ (see Fig. 6) and

$$\begin{aligned}
SO(G) = SO(Z_1) &= 4\sqrt{13} + 3\sqrt{2} \\
&= \left[(n-4)\sqrt{(n-1)^2+1} + 2\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+9} + 2\sqrt{13}\right]\Big|_{n=4}.
\end{aligned}$$

The consequence holds in Theorem 3.2.

Case 2. If $n = 5$, then $G \in \{Z_i : 2 \leq i \leq 6\}$. By calculating, $SO(Z_2) = 6\sqrt{13}$, $SO(Z_3) = 4\sqrt{13} + 5\sqrt{2}$, $SO(Z_4) = 8\sqrt{5} + 4\sqrt{2}$, $SO(Z_5) = \sqrt{10} + 9\sqrt{2} + 2\sqrt{13}$, $SO(Z_6) = \sqrt{17} + 5 + 4\sqrt{5} + 2\sqrt{13}$. Hence, assertion holds in Theorem 3.2.

Case 3. If $n \geq 6$, then we consider three subcases.

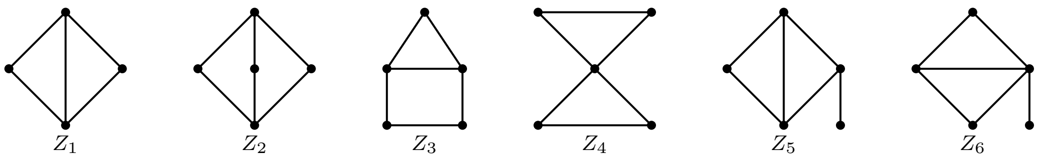

FIGURE 6. Bicyclic graphs $Z_1, Z_2, Z_3, Z_4, Z_5, Z_6$.

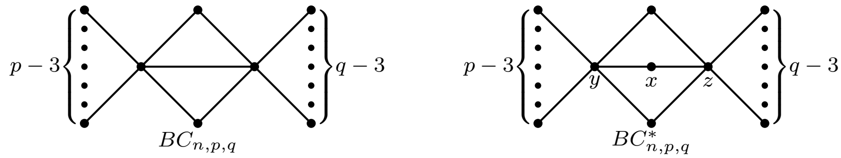

FIGURE 7. Bicyclic graphs $BC_{n,p,q}$ and $BC^*_{n,p,q}$.

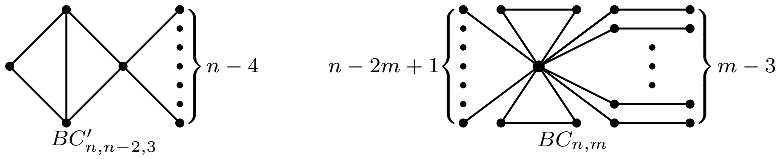

FIGURE 8. Bicyclic graphs $BC'_{n,n-2,3}$ and $BC_{n,m}$.

Subcase 3.1. $G \cong BC_{n,p,q}$ (see Fig. 7), $p \geq q$. Then

$$
\begin{aligned}
& SO(BC_{n,p+1,q-1}) - SO(BC_{n,p,q}) \\
= & \Big((p-2)\sqrt{(p+1)^2+1} + (q-4)\sqrt{(q-1)^2+1} + \sqrt{(p+1)^2+(q-1)^2} \\
& + 2\sqrt{(p+1)^2+4} + 2\sqrt{(q-1)^2+4}\Big) - \Big(2\sqrt{p^2+4} + 2\sqrt{q^2+4} + (p-3)\sqrt{p^2+1} \\
& +(q-3)\sqrt{q^2+1} + \sqrt{p^2+q^2}\Big) \\
> & \Big((p-2)\sqrt{(p+1)^2+1} - (p-3)\sqrt{p^2+1} + 2\sqrt{(p+1)^2+4} - 2\sqrt{p^2+4}\Big) \\
& - \Big((q-3)\sqrt{q^2+1} - (q-4)\sqrt{(q-1)^2+1} + 2\sqrt{q^2+4} - 2\sqrt{(q-1)^2+4}\Big) \\
= & \rho(p+1) - \rho(q) > 0
\end{aligned}
$$

since Lemma 2.4. It conclude $SO(BC_{n,p,q}) < SO(BC_{n,p+1,q-1}) < SO(BC_{n,p+2,q-2}) < \cdots < SO(BC_{n,n-1,3}) = (n-4)\sqrt{n^2+1} + 2\sqrt{n^2+4} + \sqrt{n^2+9} + 2\sqrt{13}$.

Subcase 3.2. $G \cong BC'_{n,n-2,3}$ (see Fig. 8). Then

$$
\begin{aligned}
& SO(BC_{n,n-1,3}) - SO(BC'_{n,n-2,3}) \\
& = (n-4)\sqrt{(n-1)^2+1} + 2\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+9} + 2\sqrt{13} \\
& \quad - \Big[(n-4)\sqrt{(n-2)^2+1} + 2\sqrt{(n-2)^2+9} + 3\sqrt{2} + 2\sqrt{13}\Big] \\
& > 2\sqrt{(n-1)^2+4} - 2\sqrt{(n-2)^2+9} + \sqrt{(n-1)^2+9} - 3\sqrt{2} > 0
\end{aligned}
$$

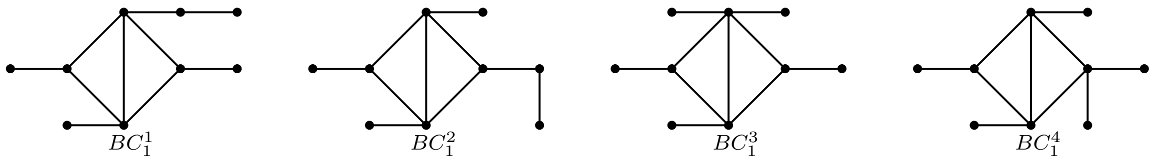

FIGURE 9. Bicyclic graphs $BC_1^1, BC_1^2, BC_1^3, BC_1^4$.

since $n \geq 4$.

Subcase 3.3. $G \cong BC^*_{n,p,q}$ (see Fig. 7), $p \geq q$.

Assume $d_x = 2$, $N(x) = \{x_1, x_2\}$. Now if write $G' = G - xx_2 + x_1x_2$, then $G' \cong BC_{n,p+1,q}$ and $SO(G') > SO(BC_{n,p+1,q})$ since Lemma 2.6. Consequently, by Case 1, $SO(G) \leq SO(BC_{n,n-1,3})$. We finish the proof. □

Now we show the maximum Sombor index of $G \in \mathfrak{B}_{n,m}$ in the following theorem.

Theorem 3.3. *Assume $G \in \mathfrak{B}_{n,m}$. If $G \ncong BC_1$ and $3 \leq m \leq \lfloor \frac{n}{2} \rfloor$, then*

$$\begin{aligned} SO(G) \leq SO(BC_{n,m}) = (m-3)\sqrt{5} + (m+1)\sqrt{(n-m+2)^2+4} + 4\sqrt{2} \\ +(n-2m+1)\sqrt{(n-m+2)^2+1}. \end{aligned}$$

Proof. We apply inductive method on n.

Assume that $n = 2m$, by Theorem 3.1, the consequence in theorem admits.

Assume that $n \geq 2m+1$ (see Fig. 7), the consequence in theorem admits.

Now we consider two cases.

Case 1. If $|P(G)| = 0$, then $G \in \widehat{\mathfrak{B}}_{2m+1}$. By calculating, if $G \in \mathfrak{B}^1_{2m+1} \cup \mathfrak{B}^4_{2m+1}$, then $SO(G) = 3\sqrt{2} + 4\sqrt{13} + 2(2m-3)\sqrt{2}$. If $G \in \mathfrak{B}^2_{2m+1} \cup \mathfrak{B}^5_{2m+1}$, then $SO(G) = 6\sqrt{13} + 2(2m-4)\sqrt{2}$. If $G \in \mathfrak{B}^3_{2m+1}$, then $SO(G) = 8\sqrt{5} + 4(m-1)\sqrt{2}$. Hence,

$$\begin{aligned} & SO(G) - SO(BC_{2m+1,m}) \\ \leq & \left[8\sqrt{5} + 4(m-1)\sqrt{2}\right] - \left[(m-3)\sqrt{5} + (m+1)\sqrt{(m+3)^2+4} + 4\sqrt{2} + 2\sqrt{(m+2)^2+1}\right] \\ < & \ 0 \end{aligned}$$

since $m \geq 3$. It follows $SO(G) < SO(BC_{2m+1,m})$.

Case 2. If $|P(G)| \geq 1$, then by Lemma 2.2, there exists $xy \notin M$, where M is maximum matching of G, $d_x = 1, d_y \geq 2$. Obviously, $G' = G - x \in \mathfrak{B}_{n-1,m}$. Now by the construction of G', we get $2 \leq d_y = a \leq n - m + 2$ and $|P(y)| = b \leq n - 2m + 1$.

Subcase 2.1. If $G' \cong BC_1$, then $a \leq 5$. Hence, $G \cong BC_1^1$ or $G \cong BC_1^2$ or $G \cong BC_1^3$ or $G \cong BC_1^4$ (see Fig. 9). By calculating,

$$\begin{aligned} SO(BC_1^1) &= \sqrt{5} + 2\sqrt{10} + \sqrt{17} + 2\sqrt{5} + 20 + 4\sqrt{2}, \\ SO(BC_1^2) &= \sqrt{5} + \sqrt{10} + 2\sqrt{17} + \sqrt{13} + 20 + 4\sqrt{2}, \\ SO(BC_1^3) &= 2\sqrt{10} + \sqrt{17} + 2\sqrt{26} + 10 + 2\sqrt{34} + \sqrt{41}, \\ SO(BC_1^4) &= \sqrt{10} + 4\sqrt{17} + 10 + 12\sqrt{2}. \end{aligned}$$

Therefore, $SO(BC_1^i) \leq SO(BC_{9,4})$, $i = 1, 2, 3, 4$.

Subcase 2.2. Assume $G' \ncong BC_1$. Now by the fact that $xy \notin M$ and there are at least $n-2m$ vertices admitting non-M-saturated, then $|P(y)|-1 \leq n-2m$, that is, $|P(y)| \leq n-2m+1$. Hence,

$$\begin{aligned}
SO(G) &= SO(G') + \sum_{w \in N(y)\backslash\{x\}} \left[\sqrt{d_y^2+d_w^2} - \sqrt{(d_y-1)^2+d_w^2}\right] + \sqrt{d_y^2+1} \\
&\leq SO(G') + (n-2m)\left[\sqrt{d_y^2+1} - \sqrt{(d_y-1)^2+1}\right] + \sqrt{d_y^2+1} \\
&\quad + ((n+2-m)-(n-2m+1))\left[\sqrt{d_y^2+2^2} - \sqrt{(d_y-1)^2+2^2}\right] \\
&\leq (m-3)\sqrt{5} + (m+1)\sqrt{(n-m+1)^2+4} + 4\sqrt{2} + (n-2m)\sqrt{(n-m+1)^2+1} \\
&\quad + (n-2m)\left[\sqrt{(n+2-m)^2+1} - \sqrt{(n+1-m)^2+1}\right] + \sqrt{(n+2-m)^2+1} \\
&\quad + (m+1)\left[\sqrt{(n+2-m)^2+2^2} - \sqrt{(n+1-m)^2+2^2}\right] \\
&= (m-3)\sqrt{5} + (m+1)\sqrt{(n-m+2)^2+4} + 4\sqrt{2} + (n-2m+1)\sqrt{(n-m+2)^2+1},
\end{aligned}$$

where the equality admits iff $G' \cong BC_{n-1,m}$, that is, $G \cong BC_{n,m}$. □

According to the result of Theorem 3.3, one can obtain the following corollary which is a consequence in [4].

Corollary 3.4. *[4] Assume $G \in \mathfrak{B}_n$. If $n \geq 4$, then*

$$SO(G) \leq SO(BC_{n,n-1,3}) = (n-4)\sqrt{(n-1)^2+1} + 2\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+9} + 2\sqrt{13}.$$

Proof. Write M the maximum matching of G.

If $|M| = 2$, then by Theorem 3.2, $SO(G) \leq SO(BC_{n,n-1,3}) = (n-4)\sqrt{(n-1)^2+1} + 2\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+9} + 2\sqrt{13}$.

If $|M| = 3$, then by Theorem 3.3,

$$SO(G) \leq SO(BC_{n,3}) = 4\sqrt{(n-1)^2+4} + 4\sqrt{2} + (n-5)\sqrt{(n-1)^2+1}.$$

Now by calculating,

$$\begin{aligned}
&SO(BC_{n,n-1,3}) - SO(BC_{n,3}) \\
&= \left[(n-4)\sqrt{(n-1)^2+1} + 2\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+9} + 2\sqrt{13}\right] \\
&\quad - \left[4\sqrt{(n-1)^2+4} + 4\sqrt{2} + (n-5)\sqrt{(n-1)^2+1}\right] \\
&> 0,
\end{aligned}$$

which means the consequence of corollary holds.

Assume that $|M| \geq 4$. If $G \cong BC_1$, then $SO(G) = 2\sqrt{10} + 2\sqrt{17} + 20 + 4\sqrt{2} \leq 20\sqrt{2} + \sqrt{58} + 2\sqrt{53} + 2\sqrt{13} = SO(BC_{8,7,3})$. If $G \ncong BC_1$, then by Lemma 2.6 and Theorem 3.3, we get $SO(G) < SO(BC_{n,m}) < SO(BC_{n,m-1}) < \cdots < SO(BC_{n,3}) < SO(BC_{n,n-1,3})$. □

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