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Sombor Index of c-Cyclic Chemical Graphs

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Abstract

The Sombor index, introduced by Ivan Gutman in 2020, has received intensive attention. The Sombor index of a graph G is defined as $SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2}$, where $E(G)$ denotes the edge set in G and d_u denotes the degree of vertex u in G. A graph with maximum degree at most 4 is called as a chemical graph.

Réti et al. [T. Réti, T. Došlić, A. Ali, On the Sombor index of graphs, Contrib. Math. 3 (2021) 11-18] proposed an open problem about determining the maximum Sombor index among all connected c-cyclic graph for $6 \leq c \leq n-2$. For $c = 1, 2, 3, 4$, the problem about finding the minimum (resp. maximum) Sombor index among all connected c-cyclic graph has already been solved. In this paper, we determine the minimum Sombor index among connected c-cyclic chemical graph for $c \geq 3, n \geq 5(c-1)$, which partially extends the results of Liu et al. [H. Liu, L. You, Y. Huang, Ordering chemical graphs by Sombor indices and its applications, MATCH Commun. Math. Comput. Chem. 87 (2022) 5-22] and Liu et al. [H. Liu, L. You, Y. Huang, Extremal Sombor indices of tetracyclic (chemical) graphs, MATCH Commun. Math. Comput. Chem. 88 (2022) 573-581].

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1 Introduction

1.1 Background

We use $|U|$ to denote the cardinality of set U. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let $N_G(u)$ be the neighbor set of vertex u in G, and $d_u(G) = |N_G(u)|$ is called as the degree of vertex u in G. $\Delta(G) = \max\{d_u(G) : u \in V(G)\}$ is called as the maximum degree of G. $\delta(G) = \min\{d_u(G) : u \in V(G)\}$ is called as the minimum degree of G. Let n_i be the number of vertices of G with degree i, and $m_{i,j}$ the number of edges of G joining a vertex of degree i and a vertex of degree j. An edge with end vertices of degree i and j can be called a (i,j)-edge for simply. A vertex with degree k is called as a k-vertex. A graph with $\Delta \leq 4$ is called a chemical graph. The minimum number of edges of a graph G whose removal makes G acyclic is known as the cyclomatic number, denoted by c. It also represent the number of linearly independent cycles of G and has the expression $c = m - n + 1$ for connected graphs [32]. A graph with cyclomatic number c is called a c-cyclic graph. The symbol "(G)" will be omitted if it is clear that G is the graph under consideration. In this paper, all notations and terminologies used but not defined can refer to Bondy and Murty [8].

Inspired by Euclidean metric, the Sombor index [18] of a graph G is defined as

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

A review paper about Sombor index can be found in [22]. The extremal Sombor index had been considered on (chemical) trees [9, 11, 13, 14, 16, 23, 31, 34], chemical graphs [9, 17, 21, 24, 35], c-cyclic graphs [12, 24, 25, 30], chemical applications [16, 21, 28, 29], spectral properties [26, 28] and so on.

Some topological indices of c-cyclic graphs had been considered for many years. Such as augmented Zagreb index [20], total irregularity [19], Sombor index [30], the first general Zagreb index and the first multiplicative Zagreb index [7], general Randić index [6], sigma index [1], second Zagreb index [4], symmetric division deg index [3], general sum-connectivity index [5, 32], vertex-degree-based topological indices [33] and so on.

Let $\mathcal{G}_{n,c}$ be the set of connected graphs with n vertices and cyclomatic number c. Let $\mathcal{CG}_{n,c}$ be the set of connected chemical graphs with n vertices and cyclomatic number c. The degree set of a graph G is the class of vertex degrees of G. A graph whose degree set has exactly two elements is called a bidegreed graph.

For a connected chemical graph with n vertices, we have

$$\sum_{i=1}^{4} n_i = n, \tag{1}$$

$$\sum_{i=1}^{4} in_i = 2(n+c-1), \tag{2}$$

$$\sum_{1\le j\le 4, j\ne i} m_{i,j} + 2m_{i,i} = in_i \ for \ i = 1,2,3,4. \tag{3}$$

1.2 Main results

Our main results are shown as follows.

Theorem 1.1. *Let $c \ge 3$, $n \ge 5(c-1)$, $G \in \mathcal{CG}_{n,c}$ with the minimum Sombor index. Then G is a bidegreed graph with degree set $\{2,3\}$, and $m_{2,3} = 2, m_{2,2} = n-2c+1, m_{3,3} = 3c-4$. Moreover, $SO(G) = (2n+5c-10)\sqrt{2} + 2\sqrt{13}$.*

Let $c = 3,4$. Then by Theorems 1.1, we have the following corollaries immediately, which are the results of [25].

Corollary 1.1. [25] *Let $n \ge 10$, $G \in \mathcal{CG}_{n,3}$ with the minimum Sombor index. Then G is a bidegreed graph with degree set $\{2,3\}$, and $m_{2,3} = 2, m_{2,2} = n-5, m_{3,3} = 5$. Moreover, $SO(G) = (2n+5)\sqrt{2} + 2\sqrt{13}$.*

Corollary 1.2. [25] *Let $n \ge 15$, $G \in \mathcal{CG}_{n,4}$ with the minimum Sombor index. Then G is a bidegreed graph with degree set $\{2,3\}$, and $m_{2,3} = 2, m_{2,2} = n-7, m_{3,3} = 8$. Moreover, $SO(G) = (2n+10)\sqrt{2} + 2\sqrt{13}$.*

Combining Theorem 1.1 with the conclusions of [25], we proposed the following conjecture.

Conjecture 1.1. *Let $c \geq 3$, $n \geq 5(c-1)$, $G \in \mathcal{G}_{n,c}$ with the minimum Sombor index. Then G is a bidegreed graph with degree set $\{2,3\}$, and $m_{2,3} = 2, m_{2,2} = n-2c+1, m_{3,3} = 3c-4$. Moreover, $SO(G) = (2n+5c-10)\sqrt{2} + 2\sqrt{13}$.*

2 Proof of Theorem 1.1

In the following, we first introduce some important lemmas.

Lemma 2.1. [27] *Let $x > a \geq 1, y > 0$, and $h(x,y) = \sqrt{x^2+y^2} - \sqrt{(x-a)^2+y^2}$. Then $h(x,y)$ is strictly increasing with x, strictly decreasing with y.*

Lemma 2.2. *Suppose that G is a connected graph, u,x,v,y are distinct vertices in G satisfied that $ux, vy \in E(G)$, $uv, uy, xv, xy \notin E(G)$, $d_u \geq d_v$, $d_y \geq d_x$. Let $G^* = G - \{ux, vy\} + \{uy, vx\}$. Then $SO(G^*) \leq SO(G)$, with equality if and only if $d_u = d_v$ or $d_y = d_x$.*

Proof. Let $f(x,y) = \sqrt{x^2+y^2}$. By the definition of Sombor index and Lemma 2.1, we have

$$SO(G) - SO(G^*) = (f(d_u,d_x) - f(d_v,d_x)) - (f(d_u,d_y) - f(d_v,d_y)) \geq 0,$$

with equality if and only if $d_u = d_v$ or $d_y = d_x$. ∎

For convenience, the edges ux, vy in G which satisfied the conditions of Lemma 2.2 are called two disjoint and non-adjacent edges in G. A connected (n,m) graph is a connected graph with n vertices and m edges.

Lemma 2.3. [2] *Let G be a connected (n,m) graph. If G has the minimum Sombor index, then $\Delta(G) - \delta(G) \leq 1$.*

Since $c = m-n+1$, then by Lemma 2.3, we have the following corollary.

Corollary 2.1. *Let $c \geq 1$, and $G \in \mathcal{G}_{n,c}$ with the minimum Sombor index. Then $\delta(G) \geq 2$.*

Lemma 2.4. [5] *Let $n \geq 5(c-1)$, $G \in \mathcal{G}_{n,c}$ and $\delta(G) \geq 2$, $\Delta(G) \geq 4$. Then $n_2 \geq 4$.*

Lemma 2.5. [10] *Let* $n \geq 5(c-1)$, $G \in \mathcal{G}_{n,c}$ *and* $\delta(G) \geq 2$, $\Delta(G) \geq 4$. *Then* $m_{2,2} \geq 1$.

Lemma 2.6. *Let* $c \geq 3$, $n \geq 5(c-1)$, *and* $G \in \mathcal{CG}_{n,c}$ *with the minimum Sombor index. Then* $\Delta(G) = 3$.

Proof. Let $f(x,y) = \sqrt{x^2+y^2}$. On the contrary, we suppose that $\Delta(G) \geq 4$. Since G is a chemical graph, then $\Delta(G) = 4$. By Corollary 2.1 and 2.5, $m_{2,2} \geq 1$.

Case 1. There is a 4-vertex that connecting to a 2-vertex of a $(2,2)$-edge in G.

Let $u_1u_2 \in E(G), u_2u_3 \in E(G)$ with $d_{u_1} = d_{u_2} = 2$, $d_{u_3} = 4$. Let $u_4 \neq u_1$ and $u_4 \in N_G(u_3) \setminus \{u_2\}$.

Subcase 1.1. $u_1 \notin N_G(u_3)$.

Let $G^* = G - u_3u_4 + u_2u_4$. Then $G^* \in \mathcal{CG}_{n,c}$. By Lemma 2.1, we have

$$\begin{aligned}
&SO(G) - SO(G^*)\\
=&f(2,4) - f(3,3) + f(2,2) - f(2,3) + (f(4,d_{u_4}) - f(3,d_{u_4}))\\
&+ \sum_{x \in N_G(u_3)\setminus\{u_2,u_4\}} (f(4,d_x) - f(3,d_x))\\
\geq&f(2,4) - f(3,3) + f(2,2) - f(2,3) + 3(f(4,4) - f(3,4))\\
=&11\sqrt{2} + 2\sqrt{5} - \sqrt{13} - 15 \approx 1.4229 > 0.
\end{aligned}$$

Subcase 1.2. $u_1 \in N_G(u_3)$.

Suppose that $N_G(u_3) = \{u_1, u_2, u_4, u_5\}$. Let $G^* = G - u_3u_4 + u_2u_4$. Then $G^* \in \mathcal{CG}_{n,c}$. Since $f(4,2) - f(3,2) > f(4,4) - f(3,4)$, then by Subcase 1.1, we have

$$\begin{aligned}
&SO(G) - SO(G^*)\\
=&f(2,4) - f(3,3) + f(2,2) - f(2,3) + (f(4,d_{u_4}) - f(3,d_{u_4}))\\
&+ (f(4,d_{u_5}) - f(3,d_{u_5})) + f(4,2) - f(3,2) > 0 \ .
\end{aligned}$$

Case 2. There is no any 4-vertex that connecting to a 2-vertex of a $(2,2)$-edge in G.

Let $w_1w_2 \in E(G), w_2w_3 \in E(G)$ with $d_{w_1} = d_{w_2} = 2$ and $d_{w_3} \neq 4$. Then $d_{w_3} = 2$ or 3. By Lemma 2.4, we have $n_2 \geq 4$.

Subcase 2.1. There is a 2-vertex that connecting to a 4-vertex in G.

Without loss of generality, we suppose $v_1v_2 \in E(G), v_2v_3 \in E(G)$ with $d_{v_2} = 2$, $d_{v_3} = 4$, then $d_{v_1} = 3$ or 4. Thus $v_2 \neq w_1$ and $v_2 \neq w_2$.

Subcase 2.1.1. $w_1w_3 \notin E(G)$.

If $v_1 \neq w_3$, we let $G^* = G - \{v_1v_2, w_1w_2, w_2w_3\} + \{w_2v_2, w_1w_3, w_2v_1\}$. Then $G^* \in \mathcal{CG}_{n,c}$ and $SO(G) = SO(G^*)$. In this case, there is a 4-vertex that connecting to a 2-vertex of a $(2, 2)$-edge in G^*. We return to the Case 1. By using the transformation of Case 1, we will obtain a contradiction.

If $v_1 = w_3$, then $d_{w_3} = 3$, otherwise there is a 4-vertex that connecting to a 2-vertex of a $(2, 2)$-edge in G, which is a contradiction. We let $G^* = G - \{w_1w_2, w_3v_2\} + \{w_1w_3, w_2v_2\}$. Then $G^* \in \mathcal{CG}_{n,c}$ and $SO(G) = SO(G^*)$. In this case, there is a 4-vertex that connecting to a 2-vertex of a $(2, 2)$-edge in G^*. We return to the Case 1. By using the transformation of Case 1, we will obtain a contradiction.

Subcase 2.1.2. $w_1w_3 \in E(G)$.

In this case, $w_1w_2 \in E(G), w_2w_3 \in E(G)$ with $d_{w_1} = d_{w_2} = 2$ and $d_{w_3} = 3$. $v_1v_2 \in E(G), v_2v_3 \in E(G)$ with $d_{v_2} = 2$, $d_{v_3} = 4$. Let $G^* = G - \{w_1w_3, v_2v_3\} + \{w_1v_2, w_3v_3\}$. Then $G^* \in \mathcal{CG}_{n,c}$ and by Lemma 2.1, $SO(G) - SO(G^*) = (f(2, 3) - f(2, 2)) - (f(3, 4) - f(2, 4)) > 0$, which is a contradiction.

Subcase 2.2. There is no any 2-vertex that connecting to a 4-vertex in G, i.e., $m_{2,4} = 0$.

By Lemma 2.2 and $G \in \mathcal{CG}_{n,c}$ with the minimum Sombor index, there are no two disjoint and non-adjacent $(3, 4)$-edges or $(2, 3)$-edges in G. Since $m_{2,4} = 0$ and G is a connected chemical graph, then $n_3 \geq 1$, thus $m_{3,4} \geq 1$. If $n_4 \geq 2$, then there are two disjoint and non-adjacent $(3, 4)$-edges in G, which is a contradiction. Thus $n_4 = 1$ and $m_{3,4} = 4$. By Lemma 2.5, $m_{2,2} \geq 1$. By Lemma 2.4, $n_4 \geq 4$. In this case, there are two disjoint and non-adjacent $(2, 3)$-edges in G, which is a contradiction.

Thus, the assumption $\Delta(G) \geq 4$ do not hold, and we get $\Delta(G) = 3$. ■

Lemma 2.7. *Let $c \geq 3$, $n \geq 5(c - 1)$, and $G \in \mathcal{CG}_{n,c}$ with the minimum Sombor index. Then $m_{2,3} = 2$.*

Proof. By Corollary 2.1 and Lemma 2.6, we know G is a bidegreed graph with degree set $\{2,3\}$. Since $c \geq 3$, then $m_{2,3} \geq 2$.

If $m_{2,3} \geq 3$, there are two disjoint and non-adjacent $(2,3)$-edges in G, by Lemma 2.2, we can obtained the graph G^* and $G^* \in \mathcal{CG}_{n,c}$. Then by Lemma 2.1, we have $SO(G) - SO(G^*) = 2f(2,3) - f(2,2) - f(3,3) = (f(2,3) - f(2,2)) - (f(3,3) - f(2,3)) > 0$, which is a contradiction with that $G \in \mathcal{CG}_{n,c}$ with the minimum Sombor index. Thus $m_{2,3} = 2$. This completes the proof. ■

Proof of Theorem 1.1. By Corollary 2.1 and Lemma 2.6, we know G is a bidegreed graph with degree set $\{2,3\}$. By Lemma 2.7, $m_{2,3} = 2$. By equations (1), (2) and Lemma 2.6, we have $n_2 + n_3 = n$ and $2n_2 + 3n_3 = 2m = 2(n + c - 1)$. Thus we have $n_3 = 2(c-1), n_2 = n - 2c + 2$. By equation (3) and Lemmas 2.6, 2.7, we have $2m_{2,2} + m_{2,3} = 2n_2$ and $m_{2,3} + 2m_{3,3} = 3n_3$. Since $m_{2,3} = 2$, then $m_{2,2} = n - 2c + 1, m_{3,3} = 3c - 4$, and $SO(G) = (2n + 5c - 10)\sqrt{2} + 2\sqrt{13}$. This completes the proof. ■

3 Conclusions

In this paper, we determine the minimum Sombor index among connected c-cyclic chemical graph for $c \geq 3, n \geq 5(c-1)$, which partially extends the results of [24] and [25] for $c = 3, 4$. The problem about finding the maximum Sombor index among all connected c-cyclic graph has already been solved for $c = 1, 2, 3, 4, 5$ in [30] and for $c = 6$ in [15]. However, the problem of determining the maximum Sombor index among connected c-cyclic (chemical) graph for $c \geq 7$ is still open. We intend to consider Conjecture 1.1 and the above challenging problems in the future.

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