

Ordering Chemical Graphs by Sombor Indices and Its Applications

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Abstract

Topological indices are a class of numerical invariants that predict certain physical and chemical properties of molecules. Recently, two novel topological indices, named as Sombor index and reduced Sombor index, were introduced by Gutman, defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G^2(u) + d_G^2(v)},$$

$$SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_G(u) - 1)^2 + (d_G(v) - 1)^2},$$

where $d_G(u)$ denotes the degree of vertex u in G .

In this paper, our aim is to order the chemical trees, chemical unicyclic graphs, chemical bicyclic graphs and chemical tricyclic graphs with respect to Sombor index and reduced Sombor index. We determine the first fourteen minimum chemical trees, the first four minimum chemical unicyclic graphs, the first three minimum chemical bicyclic graphs, the first seven minimum chemical tricyclic graphs. At last, we consider the applications of reduced Sombor index to octane isomers.

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1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Denote by $N_G(u)$ the set of vertices adjacent to u in G for every $u \in V(G)$. The degree $d_G(u)$ of u in G is the cardinality of $N_G(u)$. Let $\Delta(G)$ (or simply Δ) be the maximum degree of G . Let $n_i(G)$ (or simply n_i) be the number of vertices with degree i in G . Denote by $m_{i,j}(G)$ the numbers of edges connected a vertex with degree i and a vertex with degree j in G . In this paper, all notations and terminologies used but not defined can refer to the textbook [4].

The Sombor index ($SO(G)$ for short) and reduced Sombor index ($SO_{red}(G)$ for short) of a graph G are defined as [10]

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G^2(u) + d_G^2(v)},$$

$$SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_G(u) - 1)^2 + (d_G(v) - 1)^2}.$$

Shortly after, Deng et al. [9] determined the maximum Sombor indices of chemical trees. Cruz et al. [5] determined the extremal values of some chemical graphs. Also, Redžepović [24] studied chemical applicability of Sombor indices. Milovanović et al. [23] considered the bounds of Sombor indices and the relations between Sombor indices and other indices. Furthermore, Liu et al. [22] obtained some bounds for reduced Sombor index of graphs with given several parameters and some special graphs, they also obtained the expected values of reduced Sombor index in random polyphenyl chains, the bounds of reduced Sombor spectrum radius and energy. For more details of Sombor indices, we refer to [2, 8, 10, 11, 18, 25, 26].

The chemical graph is a graph with $d_G(u) \leq 4$ for all $u \in V(G)$. Ordering chemical graphs by some topological indices is an interesting problem. Ghalavand and Ashrafi had done a lot of work on ordering chemical graphs by some topological indices such as Wiener polarity index [3], sum exdeg index [12], total irregularity [13], forgotten coindex [14], Randić index and sum-connectivity index [15] and hyper-Zagreb index [16]. For more related papers can be find in [1, 17, 19] and references cited therein.

Motivated by [15, 17], our aim is to consider the similar issues regarding (reduced) Sombor index. In this paper, we determine the first fourteen minimum chemical trees, the first four minimum chemical unicyclic graphs, the first three minimum chemical bi-

cyclic graphs, the first seven minimum chemical tricyclic graphs. At last, we consider the applications of reduced Sombor index to octane isomers.

2 Preliminaries

Here are some important transformations that will be used in the proof of main results.

Lemma 2.1 *Let G_0 be a connected graph with vertices u_1, u_2, u_3, u_4 ($d_{G_0}(u_1) = 1$, $d_{G_0}(u_2) = 2$, $d_{G_0}(u_3) = 3$ or 4 , $d_{G_0}(u_4) = 1$, $\{u_1u_2, u_3u_4\} \subseteq E(G_0)$). Suppose that $P = v_1v_2 \cdots v_l$ is a path. Denote by G_1 the graph gotten from G_0 , P by attaching vertices u_1v_1 . Let $G_2 = G_1 - u_1v_1 + u_4v_1$. Then $SO(G_1) > SO(G_2)$ and $SO_{red}(G_1) > SO_{red}(G_2)$.*

Proof. By the definition of Sombor index, we have

$$\begin{aligned} SO(G_2) - SO(G_1) &= \sqrt{1^2 + 2^2} + \sqrt{d_{G_0}^2(u_3) + 2^2} - [\sqrt{2^2 + 2^2} + \sqrt{d_{G_0}^2(u_3) + 1^2}] \\ &= \sqrt{5} + \sqrt{d_{G_0}^2(u_3) + 4} - 2\sqrt{2} - \sqrt{d_{G_0}^2(u_3) + 1^2}. \end{aligned}$$

If $d_{G_0}^2(u_3) = 3$, then $SO(G_2) - SO(G_1) = \sqrt{5} + \sqrt{13} - 2\sqrt{2} - \sqrt{10} < 0$.

If $d_{G_0}^2(u_3) = 4$, then $SO(G_2) - SO(G_1) = \sqrt{5} + \sqrt{20} - 2\sqrt{2} - \sqrt{17} < 0$.

Therefore $SO(G_1) > SO(G_2)$. In a similar way, we also have $SO_{red}(G_1) > SO_{red}(G_2)$.

This completes the proof. ■

Lemma 2.2 *Let G_0 , G be two connected graphs with vertices $x \in V(G_0)$, $y \in V(G)$ ($d_{G_0}(x) = 1$ or 2 and $d_{G_0}(y) = 2$ or 3). Suppose that $P_1 = u_1u_2 \cdots u_k$ and $P_2 = v_1v_2 \cdots v_l$ are two paths. Denote by G_1 the graph gotten from G_0 , G , P_1 and P_2 by attaching vertices v_1x , u_1x and u_ky . Let $G_2 = G_1 - \{u_1x, u_ky\} + \{xy, u_1v_l\}$. Then $SO(G_1) > SO(G_2)$ and $SO_{red}(G_1) > SO_{red}(G_2)$.*

Proof. We consider the following two cases.

Case 1. $l = 1$.

$$\begin{aligned} SO(G_2) - SO(G_1) &= \sqrt{1^2 + 2^2} + \sqrt{(d_{G_0}(x) + 2)^2 + (d_{G_0}(y) + 1)^2} \\ &\quad - [\sqrt{(d_{G_0}(x) + 2)^2 + 1^2} + \sqrt{(d_{G_0}(y) + 1)^2 + 2^2}]. \end{aligned}$$

Since $d_{G_0}(x) = 1$ or 2 and $d_{G_0}(y) = 2$ or 3 .

If $d_{G_0}(x) = 1$ and $d_{G_0}(y) = 2$, then $SO(G_2) - SO(G_1) = \sqrt{5} + 3\sqrt{2} - \sqrt{10} - \sqrt{13} < 0$.

If $d_{G_0}(x) = 1$ and $d_{G_0}(y) = 3$, then $SO(G_2) - SO(G_1) = \sqrt{5} + 5 - \sqrt{10} - \sqrt{20} < 0$.

If $d_{G_0}(x) = 2$ and $d_{G_0}(y) = 2$, then $SO(G_2) - SO(G_1) = \sqrt{5} + 5 - \sqrt{17} - \sqrt{13} < 0$.

If $d_{G_0}(x) = 2$ and $d_{G_0}(y) = 3$, then $SO(G_2) - SO(G_1) = \sqrt{5} + 4\sqrt{2} - \sqrt{17} - \sqrt{20} < 0$.

Case 2. $l \geq 2$.

$$SO(G_2) - SO(G_1) = \sqrt{2^2 + 2^2} + \sqrt{(d_{G_0}(x) + 2)^2 + (d_{G_0}(y) + 1)^2} \\ - [\sqrt{(d_{G_0}(x) + 2)^2 + 2^2} + \sqrt{(d_{G_0}(y) + 1)^2 + 2^2}].$$

Since $d_{G_0}(x) = 1$ or 2 and $d_{G_0}(y) = 2$ or 3 .

If $d_{G_0}(x) = 1$ and $d_{G_0}(y) = 2$, then $SO(G_2) - SO(G_1) = 2\sqrt{2} + 3\sqrt{2} - \sqrt{13} - \sqrt{13} < 0$.

If $d_{G_0}(x) = 1$ and $d_{G_0}(y) = 3$, then $SO(G_2) - SO(G_1) = 2\sqrt{2} + 5 - \sqrt{13} - \sqrt{20} < 0$.

If $d_{G_0}(x) = 2$ and $d_{G_0}(y) = 2$, then $SO(G_2) - SO(G_1) = 2\sqrt{2} + 5 - \sqrt{20} - \sqrt{13} < 0$.

If $d_{G_0}(x) = 2$ and $d_{G_0}(y) = 3$, then $SO(G_2) - SO(G_1) = 2\sqrt{2} + 4\sqrt{2} - \sqrt{20} - \sqrt{20} < 0$.

Therefore $SO(G_1) > SO(G_2)$. In a similar way, we also have $SO_{red}(G_1) > SO_{red}(G_2)$.

This completes the proof. ■

Lemma 2.3 *Let G_0 be a connected graph with the vertex x ($d_{G_0}(x) = 1$ or 2). Suppose that $P_1 = u_1u_2 \cdots u_k$ and $P_2 = v_1v_2 \cdots v_l$ are two paths. Denote by G_1 the graph gotten from G_0 , P_1 and P_2 by attaching vertices u_1x and v_1x . Let $G_2 = G_1 - u_1x + u_1v_l$. Then $SO(G_1) > SO(G_2)$ and $SO_{red}(G_1) > SO_{red}(G_2)$.*

Proof. Let $d_{G_0}(x) = t = 1$ or 2 , $N_{G_0}(x) = \{z_1, z_2, \dots, z_t\}$, $d_{G_0}(z_i) = d_i$, $1 \leq i \leq t$.

Case 1. $k = l = 1$.

$$SO(G_2) - SO(G_1) = \sqrt{1^2 + 2^2} + \sqrt{(t+1)^2 + 2^2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+1)^2} \\ - [\sqrt{(t+2)^2 + 1^2} + \sqrt{(t+2)^2 + 1^2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+2)^2}] \\ < \sqrt{5} + \sqrt{(t+1)^2 + 2^2} - 2\sqrt{(t+2)^2 + 1^2}.$$

If $t = 1$, then $SO(G_2) - SO(G_1) < \sqrt{5} + 2\sqrt{2} - 2\sqrt{10} < 0$.

If $t = 2$, then $SO(G_2) - SO(G_1) < \sqrt{5} + \sqrt{13} - 2\sqrt{17} < 0$.

Case 2. $k = 1, l \geq 2$.

$$SO(G_2) - SO(G_1) < 2\sqrt{2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+1)^2} - [\sqrt{(t+2)^2 + 1^2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+2)^2}] \\ < 2\sqrt{2} - \sqrt{(t+2)^2 + 1^2}.$$

If $t = 1$, then $SO(G_2) - SO(G_1) < 2\sqrt{2} - \sqrt{10} < 0$.

If $t = 2$, then $SO(G_2) - SO(G_1) < 2\sqrt{2} - \sqrt{17} < 0$.

Case 3. $k \geq 2, l = 1$.

The conclusion holds from Case 2 and symmetry.

Case 4. $k \geq 2, l \geq 2$.

$$\begin{aligned} SO(G_2) - SO(G_1) &= 2\sqrt{2^2 + 2^2} + \sqrt{(t+1)^2 + 2^2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+1)^2} \\ &\quad - [\sqrt{1^2 + 2^2} + 2\sqrt{(t+2)^2 + 2^2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+2)^2}] \\ &< 4\sqrt{2} + \sqrt{(t+1)^2 + 2^2} - \sqrt{5} - 2\sqrt{(t+2)^2 + 2^2}. \end{aligned}$$

If $t = 1$, then $SO(G_2) - SO(G_1) < 6\sqrt{2} - 2\sqrt{13} - \sqrt{5} < 0$.

If $t = 2$, then $SO(G_2) - SO(G_1) < \sqrt{13} + 4\sqrt{2} - 5\sqrt{5} < 0$.

Therefore $SO(G_1) > SO(G_2)$. In a similar way, we also have $SO_{red}(G_1) > SO_{red}(G_2)$.

This completes the proof. ■

Lemma 2.4 *Let G_0 be a connected graph with vertices x and y ($d_{G_0}(x) = 2$ or 3 , $d_{G_0}(y) = 2$ or 3). Suppose that $P_1 = u_1u_2 \cdots u_k$ and $P_2 = v_1v_2 \cdots v_l$ are two paths. Denote by G_1 the graph gotten from G_0 , P_1 and P_2 by attaching vertices u_1x and v_1y . Let $G_2 = G_1 - u_1x + u_1v_l$. Then $SO(G_1) > SO(G_2)$ and $SO_{red}(G_1) > SO_{red}(G_2)$.*

Proof. Let $d_{G_0}(x) = t = 2$ or 3 , $N_{G_0}(x) = \{z_1, z_2, \dots, z_t\}$, $d_{G_0}(z_i) = d_i$, $1 \leq i \leq t$.

Case 1. $k = l = 1$.

$$\begin{aligned} SO(G_2) - SO(G_1) &= \sqrt{1^2 + 2^2} + \sqrt{(d_{G_0}(y) + 1)^2 + 2^2} + \sum_{i=1}^t \sqrt{d_i^2 + t^2} \\ &\quad - \left[\sqrt{(d_{G_0}(y) + 1)^2 + 1^2} + \sqrt{(t+1)^2 + 1^2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+1)^2} \right] \\ &< \sqrt{5} + \sqrt{(d_{G_0}(y) + 1)^2 + 4} - \left[\sqrt{(d_{G_0}(y) + 1)^2 + 1^2} + \sqrt{(t+1)^2 + 1^2} \right]. \end{aligned}$$

Since $d_{G_0}(y) = 2$ or 3 and $t = 2$ or 3 .

If $d_{G_0}(y) = 2$ and $t = 2$, then $SO(G_2) - SO(G_1) < \sqrt{5} + \sqrt{13} - \sqrt{10} - \sqrt{10} < 0$.

If $d_{G_0}(y) = 2$ and $t = 3$, then $SO(G_2) - SO(G_1) < \sqrt{5} + \sqrt{13} - \sqrt{10} - \sqrt{17} < 0$.

If $d_{G_0}(y) = 3$ and $t = 2$, then $SO(G_2) - SO(G_1) < \sqrt{5} + \sqrt{20} - \sqrt{10} - \sqrt{17} < 0$.

If $d_{G_0}(y) = 3$ and $t = 3$, then $SO(G_2) - SO(G_1) < \sqrt{5} + \sqrt{20} - \sqrt{17} - \sqrt{17} < 0$.

Case 2. $k = 1, l \geq 2$.

$$\begin{aligned} SO(G_2) - SO(G_1) &= \sqrt{2^2 + 2^2} + \sum_{i=1}^t \sqrt{d_i^2 + t^2} - [\sqrt{(t+1)^2 + 1^2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+1)^2}] \\ &< 2\sqrt{2} - \sqrt{(t+1)^2 + 1^2}. \end{aligned}$$

Since $t = 2$ or 3 .

$$\text{If } t = 2, \text{ then } SO(G_2) - SO(G_1) < 2\sqrt{2} - \sqrt{10} < 0.$$

$$\text{If } t = 3, \text{ then } SO(G_2) - SO(G_1) < 2\sqrt{2} - \sqrt{17} < 0.$$

Case 3. $k \geq 2, l = 1$.

$$\begin{aligned} SO(G_2) - SO(G_1) &= \sqrt{2^2 + 2^2} + \sqrt{(d_{G_0}(y) + 1)^2 + 2^2} + \sum_{i=1}^t \sqrt{d_i^2 + t^2} \\ &\quad - \left[\sqrt{(d_{G_0}(y) + 1)^2 + 1^2} + \sqrt{(t+1)^2 + 2^2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+1)^2} \right] \\ &< 2\sqrt{2} + \sqrt{(d_{G_0}(y) + 1)^2 + 4} - \left[\sqrt{(d_{G_0}(y) + 1)^2 + 1^2} + \sqrt{(t+1)^2 + 4} \right]. \end{aligned}$$

Since $d_{G_0}(y) = 2$ or 3 and $t = 2$ or 3 .

$$\text{If } d_{G_0}(y) = 2 \text{ and } t = 2, \text{ then } SO(G_2) - SO(G_1) < 2\sqrt{2} + \sqrt{13} - \sqrt{10} - \sqrt{13} < 0.$$

$$\text{If } d_{G_0}(y) = 2 \text{ and } t = 3, \text{ then } SO(G_2) - SO(G_1) < 2\sqrt{2} + \sqrt{13} - \sqrt{10} - \sqrt{20} < 0.$$

$$\text{If } d_{G_0}(y) = 3 \text{ and } t = 2, \text{ then } SO(G_2) - SO(G_1) < 2\sqrt{2} + \sqrt{20} - \sqrt{17} - \sqrt{13} < 0.$$

$$\text{If } d_{G_0}(y) = 3 \text{ and } t = 3, \text{ then } SO(G_2) - SO(G_1) < 2\sqrt{2} + \sqrt{20} - \sqrt{17} - \sqrt{20} < 0.$$

Case 4. $k \geq 2, l \geq 2$.

$$\begin{aligned} SO(G_2) - SO(G_1) &= 2\sqrt{2^2 + 2^2} + \sum_{i=1}^t \sqrt{d_i^2 + t^2} \\ &\quad - [\sqrt{1^2 + 2^2} + \sqrt{(t+1)^2 + 2^2} + \sum_{i=1}^t \sqrt{d_i^2 + (t+1)^2}] \\ &< 4\sqrt{2} - \sqrt{5} - \sqrt{(t+1)^2 + 4}. \end{aligned}$$

Since $t = 2$ or 3 .

$$\text{If } t = 2, \text{ then } SO(G_2) - SO(G_1) < 4\sqrt{2} - \sqrt{5} - \sqrt{13} < 0.$$

$$\text{If } t = 3, \text{ then } SO(G_2) - SO(G_1) < 4\sqrt{2} - \sqrt{5} - \sqrt{20} < 0.$$

Therefore $SO(G_1) > SO(G_2)$. In a similar way, we also have $SO_{red}(G_1) > SO_{red}(G_2)$.

This completes the proof. ■

3 Main results

Denote by CT_n , CU_n , CB_n , CTG_n the set of chemical trees, chemical unicyclic graphs, chemical bicyclic graphs, chemical tricyclic graphs with n vertices, respectively. If G has t_i vertices of degree d_i for $1 \leq i \leq s$, then we denote the degree sequence of G as $D(G) \triangleq (d_1^{t_1}, d_2^{t_2}, \dots, d_s^{t_s})$, where $\sum_{i=1}^s t_i = n$.

3.1 Chemical trees

Let $\Phi(n) = \{T \in (4^1, 2^{n-5}, 1^4) | m_{1,2}(T) = m_{2,4}(T) = 4, m_{1,4}(T) = 0, m_{2,2}(T) = n - 9\}$, $n \geq 9$, and $\Omega(n) = \{T \in (3^3, 2^{n-8}, 1^5) | m_{1,2}(T) = m_{2,3}(T) = 5, m_{1,3}(T) = 0, m_{3,3}(T) = 2, m_{2,2}(T) = n - 13\}$, $n \geq 13$.

If $T \in \Phi(n)$, then

$$SO(T) = 2\sqrt{2}n + 12\sqrt{5} - 18\sqrt{2} \approx 2\sqrt{2}n + 1.376971607, \quad (1)$$

$$SO_{red}(T) = \sqrt{2}n + 4 + 4\sqrt{10} - 9\sqrt{2} \approx \sqrt{2}n + 3.921188579. \quad (2)$$

If $T \in \Omega(n)$, then

$$SO(T) = 2\sqrt{2}n + 5\sqrt{5} + 5\sqrt{13} - 20\sqrt{2} \approx 2\sqrt{2}n + 0.923825017, \quad (3)$$

$$SO_{red}(T) = \sqrt{2}n + 5 + 5\sqrt{5} - 9\sqrt{2} \approx \sqrt{2}n + 3.452417826. \quad (4)$$

Recall that n_i is the numbers of vertices with degree i in G . If $G \in CT_n$, since $\sum_{i=1}^4 n_i = n$ and $n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n - 1)$, then $n_1 = n_3 + 2n_4 + 2$ and $n_2 = n - 2n_3 - 3n_4 - 2$.

Theorem 3.1 *Let $T^* \in CT_n$ ($n \geq 9$), $\Delta(T^*) = 4$. If $T^* \notin \Phi(n)$, then there exists $T \in \Phi(n)$, such that $SO(T) < SO(T^*)$ and $SO_{red}(T) < SO_{red}(T^*)$.*

Proof. We consider the following two cases.

Case 1. If $T^* \in (4^1, 2^{n-5}, 1^4)$, then T^* meets at least one of the following conditions $m_{1,2}(T^*) \neq 4$, $m_{2,4}(T^*) \neq 4$, $m_{1,4}(T^*) \neq 0$, $m_{2,2}(T^*) \neq n - 9$, i.e., $m_{1,2}(T^*) < 4$, $m_{2,4}(T^*) < 4$, $m_{1,4}(T^*) > 0$, $m_{2,2}(T^*) > n - 9$. By the transformation of Lemma 2.1, we can obtain a chemical tree $T \in \Phi(n)$, so we have $SO(T) < SO(T^*)$.

Case 2. If $T^* \notin (4^1, 2^{n-5}, 1^4)$. By the transformation of Lemma 2.3, we can obtain a chemical tree $T \in (4^1, 2^{n-5}, 1^4)$. If $T \in \Phi(n)$, by Lemma 2.3, we have $SO(T) < SO(T^*)$. If $T \notin \Phi(n)$, we are back to Case 1 and the conclusion holds.

Therefore $SO(T) < SO(T^*)$. In a similar way, we also have $SO_{red}(T) < SO_{red}(T^*)$. This completes the proof. ■

Theorem 3.2 Let $T^* \in CT_n$ ($n \geq 13$), $\Delta(T^*) = 3$, $n_3(T^*) \geq 3$. If $T^* \notin \Omega(n)$, then there exists $T \in \Omega(n)$, such that $SO(T) < SO(T^*)$ and $SO_{red}(T) < SO_{red}(T^*)$.

Proof. We consider the following two cases.

Case 1. If $T^* \in (3^3, 2^{n-8}, 1^5)$, then T^* meets at least one of the following conditions $m_{1,2}(T^*) \neq 5$, $m_{2,3}(T^*) \neq 5$, $m_{1,3}(T^*) \neq 0$, $m_{3,3}(T^*) \neq 2$, $m_{2,2}(T^*) \neq n - 13$, i.e., $m_{1,2}(T^*) < 5$, $m_{2,3}(T^*) > 5$, $m_{1,3}(T^*) > 0$, $m_{3,3}(T^*) < 2$, $m_{2,2}(T^*) > n - 13$. By the transformation of Lemma 2.1 and Lemma 2.2, we can obtain a chemical tree $T \in \Omega(n)$, so we have $SO(T) < SO(T^*)$.

Case 2. If $T^* \notin (3^3, 2^{n-8}, 1^5)$, since $n_1(T^*) = n_3(T^*) + 2$ and $n_3(T^*) \geq 3$, then $n_3(T^*) \geq 4$. By the transformation of Lemma 2.3, we can obtain a chemical tree $T \in (3^3, 2^{n-8}, 1^5)$. If $T \in \Omega(n)$, by Lemma 2.3, we have $SO(T) < SO(T^*)$. If $T \notin \Omega(n)$, we are back to Case 1 and the conclusion holds.

Therefore $SO(T) < SO(T^*)$. In a similar way, we also have $SO_{red}(T) < SO_{red}(T^*)$. This completes the proof. ■

In what follows, we determine the extremal chemical trees with respect to (reduced) Sombor index. It is worth noting that the relevant data of Table 1 \sim 8 except the values of (reduced) Sombor indices are from [15, 17].

Table 1. CT_n with $\Delta \leq 3$, $n_3 \leq 2$ and their (reduced)Sombor index.

	$m_{3,3}$	$m_{2,3}$	$m_{1,2}$	$m_{1,3}$	$m_{2,2}$	$SO(G)$	$SO_{red}(G)$
A_1	0	0	2	0	$n - 3$	$(2\sqrt{2}n - 4.013145419)$	$(\sqrt{2}n - 2.242640687)$
A_2	0	1	1	2	$n - 5$	$(2\sqrt{2}n - 1.975961050)$	$(\sqrt{2}n + 0.165000165)$
A_3	0	2	2	1	$n - 6$	$(2\sqrt{2}n - 2.125046582)$	$(\sqrt{2}n - 0.013145419)$
A_4	0	3	3	0	$n - 7$	$(2\sqrt{2}n - 2.274132114)$	$(\sqrt{2}n - 0.191291004)$
A_5	0	2	0	4	$n - 7$	$(2\sqrt{2}n + 0.061223318)$	$(\sqrt{2}n + 2.572641018)$
A_6	0	3	1	3	$n - 8$	$(2\sqrt{2}n - 0.087862213)$	$(\sqrt{2}n + 2.394495433)$
A_7	0	4	2	2	$n - 9$	$(2\sqrt{2}n - 0.236947745)$	$(\sqrt{2}n + 2.216349848)$
A_8	1	1	1	3	$n - 7$	$(2\sqrt{2}n - 0.227896952)$	$(\sqrt{2}n + 2.165000165)$
A_9	0	5	3	1	$n - 10$	$(2\sqrt{2}n - 0.386033277)$	$(\sqrt{2}n + 2.038204263)$
A_{10}	1	2	2	2	$n - 8$	$(2\sqrt{2}n - 0.376982484)$	$(\sqrt{2}n + 1.986854580)$
A_{11}	0	6	4	0	$n - 11$	$(2\sqrt{2}n - 0.535118809)$	$(\sqrt{2}n + 1.860058678)$
A_{12}	1	3	3	1	$n - 9$	$(2\sqrt{2}n - 0.526068016)$	$(\sqrt{2}n + 1.808708995)$
A_{13}	1	4	4	0	$n - 10$	$(2\sqrt{2}n - 0.675153548)$	$(\sqrt{2}n + 1.630563411)$

Theorem 3.3 If $n \geq 13$, $T_1 \in A_1$, $T_2 \in A_4$, $T_3 \in A_3$, $T_4 \in A_2$, $T_5 \in A_{13}$, $T_6 \in A_{11}$, $T_7 \in A_{12}$, $T_8 \in A_9$, $T_9 \in A_{10}$, $T_{10} \in A_7$, $T_{11} \in A_8$, $T_{12} \in A_6$, $T_{13} \in A_5$, $T_{14} \in \Omega_n$, and

$T \in CT_n \setminus \{T_1, T_2, \dots, T_{14}\}$, then $SO(T_1) < SO(T_2) < SO(T_3) < SO(T_4) < SO(T_5) < SO(T_6) < SO(T_7) < SO(T_8) < SO(T_9) < SO(T_{10}) < SO(T_{11}) < SO(T_{12}) < SO(T_{13}) < SO(T_{14}) < SO(T)$.

Proof. By Table 1 and the Sombor index of chemical trees among $\Omega(n)$, we have $SO(T_1) < SO(T_2) < SO(T_3) < SO(T_4) < SO(T_5) < SO(T_6) < SO(T_7) < SO(T_8) < SO(T_9) < SO(T_{10}) < SO(T_{11}) < SO(T_{12}) < SO(T_{13}) < SO(T_{14})$.

If $\Delta(T) \leq 3$ and $n_3(T) \leq 2$, the conclusion holds. If $\Delta(T) = 3$ and $n_3(T) \geq 3$, then by Theorem 3.2, the conclusion holds. If $\Delta(T) = 4$, then by Equation (1),(3) and Theorem 3.1, the conclusion holds. ■

Similar to the proof of Theorem 3.3, we have

Theorem 3.4 *If $n \geq 13$, $T_1 \in A_1$, $T_2 \in A_4$, $T_3 \in A_3$, $T_4 \in A_2$, $T_5 \in A_{13}$, $T_6 \in A_{12}$, $T_7 \in A_{11}$, $T_8 \in A_{10}$, $T_9 \in A_9$, $T_{10} \in A_8$, $T_{11} \in A_7$, $T_{12} \in A_6$, $T_{13} \in A_5$, $T_{14} \in \Omega_n$, and $T \in CT_n \setminus \{T_1, T_2, \dots, T_{14}\}$, then $SO_{red}(T_1) < SO_{red}(T_2) < SO_{red}(T_3) < SO_{red}(T_4) < SO_{red}(T_5) < SO_{red}(T_6) < SO_{red}(T_7) < SO_{red}(T_8) < SO_{red}(T_9) < SO_{red}(T_{10}) < SO_{red}(T_{11}) < SO_{red}(T_{12}) < SO_{red}(T_{13}) < SO_{red}(T_{14}) < SO_{red}(T)$.*

3.2 Chemical unicyclic graphs

In this subsection, we consider the extremal chemical unicyclic graphs with respect to (reduced) Sombor index.

Table 2. Degree distributions (DD) of CU_n with $n_1 \leq 2$.

	n_4	n_3	n_2	n_1
H_1	0	0	n	0
H_2	0	1	$n-2$	1
H_3	1	0	$n-3$	2
H_4	0	2	$n-4$	2

Lemma 3.5 *[15, 17] $G \in CU_n$ and $n_1(G) \leq 2$ if and only if G belongs to one of equivalence classes given in Table 2.*

Theorem 3.6 *If $n \geq 7$, $G_1 \in \alpha_1$, $G_2 \in \alpha_3$, $G_3 \in \alpha_2$, $G_4 \in \alpha_9$ in Table 3. $G \in CU_n \setminus \{G_1, G_2, G_3, G_4\}$, then $SO(G_1) < SO(G_2) < SO(G_3) < SO(G_4) < SO(G)$.*

Proof. By Table 3, we have $SO(G_1) < SO(G_2) < SO(G_3) < SO(G_4)$.

Table 3. CU_n with $n_1 \leq 2$ and their (reduced)Sombor index.

	DD	$m_{1,2}$	$m_{1,3}$	$m_{1,4}$	$m_{2,3}$	$m_{2,4}$	$m_{3,3}$	$m_{2,2}$	$SO(G)$	$SO_{red}(G)$
α_1	H_1	0	0	0	0	0	0	n	$(2\sqrt{2}n)$	$(\sqrt{2}n)$
α_2	H_2	0	1	0	2	0	0	$n-3$	$(2\sqrt{2}n+1.888)$	$(\sqrt{2}n+2.229)$
α_3	H_2	1	0	0	3	0	0	$n-4$	$(2\sqrt{2}n+1.739)$	$(\sqrt{2}n+2.051)$
α_4	H_3	0	0	2	0	2	0	$n-4$	$(2\sqrt{2}n+5.876)$	$(\sqrt{2}n+6.667)$
α_5	H_3	1	0	1	0	3	0	$n-5$	$(2\sqrt{2}n+5.633)$	$(\sqrt{2}n+6.415)$
α_6	H_3	2	0	0	0	4	0	$n-6$	$(2\sqrt{2}n+5.390)$	$(\sqrt{2}n+6.163)$
α_7	H_4	0	2	0	2	0	1	$n-5$	$(2\sqrt{2}n+3.636)$	$(\sqrt{2}n+4.229)$
α_8	H_4	1	1	0	3	0	1	$n-6$	$(2\sqrt{2}n+3.487)$	$(\sqrt{2}n+4.051)$
α_9	H_4	2	0	0	4	0	1	$n-7$	$(2\sqrt{2}n+3.337)$	$(\sqrt{2}n+3.873)$
α_{10}	H_4	0	2	0	4	0	0	$n-6$	$(2\sqrt{2}n+3.776)$	$(\sqrt{2}n+4.458)$
α_{11}	H_4	1	1	0	5	0	0	$n-7$	$(2\sqrt{2}n+3.627)$	$(\sqrt{2}n+4.280)$
α_{12}	H_4	2	0	0	6	0	0	$n-8$	$(2\sqrt{2}n+3.478)$	$(\sqrt{2}n+4.102)$

If $n_1(G) \leq 2$, by Table 3, the conclusion holds. If $n_1(G) \geq 3$, by the transformations of Lemma 2.3 and Lemma 2.4, we can obtain a chemical unicyclic graphs G^* with $n_1(G^*) = 2$, so we have $SO(G) > SO(G^*)$. By Table 3, $SO(G_4) \leq SO(G^*)$. Thus, the conclusion holds. ■

Similar to the proof of Theorem 3.6, we have

Theorem 3.7 *If $n \geq 7$, $G_1 \in \alpha_1$, $G_2 \in \alpha_3$, $G_3 \in \alpha_2$, $G_4 \in \alpha_9$ in Table 3. $G \in CU_n \setminus \{G_1, G_2, G_3, G_4\}$, then $SO_{red}(G_1) < SO_{red}(G_2) < SO_{red}(G_3) < SO_{red}(G_4) < SO_{red}(G)$.*

3.3 Chemical bicyclic graphs

In this subsection, we consider the extremal chemical bicyclic graphs with respect to (reduced) Sombor index.

Table 4. Degree distributions (DD) of CB_n with $n_1 \leq 1$.

	n_4	n_3	n_2	n_1
B_1	1	0	$n-1$	0
B_2	0	2	$n-2$	0
B_3	1	1	$n-3$	1
B_4	0	3	$n-4$	1

Lemma 3.8 *[15, 17] $G \in CB_n$ and $n_1(G) \leq 1$ if and only if G belongs to one of equivalence classes given in Table 4.*

Theorem 3.9 *If $n \geq 6$, $G_1 \in \beta_2$, $G_2 \in \beta_3$, $G_3 \in \beta_9$ in Table 5. $G \in CB_n \setminus \{G_1, G_2, G_3\}$, then $SO(G_1) < SO(G_2) < SO(G_3) < SO(G)$.*

Table 5. CB_n with $n_1 \leq 1$ and their (reduced)Sombor index.

	DD	$m_{1,2}$	$m_{1,3}$	$m_{1,4}$	$m_{2,3}$	$m_{2,4}$	$m_{3,3}$	$m_{3,4}$	$m_{2,2}$	$SO(G)$	$SO_{red}(G)$
β_1	B_1	0	0	0	0	4	0	0	$n-3$	$(2\sqrt{2n}+9.403)$	$(\sqrt{2n}+8.406)$
β_2	B_2	0	0	0	4	0	1	0	$n-4$	$(2\sqrt{2n}+7.351)$	$(\sqrt{2n}+6.115)$
β_3	B_2	0	0	0	6	0	0	0	$n-5$	$(2\sqrt{2n}+7.491)$	$(\sqrt{2n}+6.345)$
β_4	B_3	0	0	1	2	2	0	1	$n-5$	$(2\sqrt{2n}+11.136)$	$(\sqrt{2n}+10.331)$
β_5	B_3	1	0	0	2	3	0	1	$n-6$	$(2\sqrt{2n}+10.893)$	$(\sqrt{2n}+10.079)$
β_6	B_3	0	0	1	3	3	0	0	$n-6$	$(2\sqrt{2n}+11.385)$	$(\sqrt{2n}+10.709)$
β_7	B_3	1	0	0	3	4	0	0	$n-7$	$(2\sqrt{2n}+11.142)$	$(\sqrt{2n}+10.457)$
β_8	B_4	0	1	0	2	0	3	0	$n-5$	$(2\sqrt{2n}+8.959)$	$(\sqrt{2n}+7.886)$
β_9	B_4	1	0	0	3	0	3	0	$n-6$	$(2\sqrt{2n}+8.810)$	$(\sqrt{2n}+7.708)$
β_{10}	B_4	0	1	0	4	0	2	0	$n-6$	$(2\sqrt{2n}+9.099)$	$(\sqrt{2n}+8.115)$
β_{11}	B_4	1	0	0	5	0	2	0	$n-7$	$(2\sqrt{2n}+8.950)$	$(\sqrt{2n}+7.937)$
β_{12}	B_4	0	1	0	6	0	1	0	$n-7$	$(2\sqrt{2n}+9.239)$	$(\sqrt{2n}+8.345)$
β_{13}	B_4	1	0	0	7	0	1	0	$n-8$	$(2\sqrt{2n}+9.090)$	$(\sqrt{2n}+8.167)$
β_{14}	B_4	0	1	0	8	0	0	0	$n-8$	$(2\sqrt{2n}+9.379)$	$(\sqrt{2n}+8.574)$
β_{15}	B_4	1	0	0	9	0	0	0	$n-9$	$(2\sqrt{2n}+9.230)$	$(\sqrt{2n}+8.396)$

Proof. By Table 5, we have $SO(G_1) < SO(G_2) < SO(G_3)$.

If $n_1(G) \leq 1$, by Table 5, the conclusion holds. If $n_1(G) \geq 2$, by the transformations of Lemma 2.3 and Lemma 2.4, we can obtain a chemical bicyclic graphs G^* with $n_1(G^*) = 1$, so we have $SO(G') > SO(G^*)$. By Table 5, $SO(G_3) \leq SO(G^*)$. Thus, the conclusion holds. \blacksquare

Similar to the proof of Theorem 3.9, we have

Theorem 3.10 *If $n \geq 6$, $G_1 \in \beta_2$, $G_2 \in \beta_3$, $G_3 \in \beta_9$ in Table 5. $G \in CB_n \setminus \{G_1, G_2, G_3\}$, then $SO_{red}(G_1) < SO_{red}(G_2) < SO_{red}(G_3) < SO_{red}(G)$.*

3.4 Chemical tricyclic graphs

In this subsection, we consider the extremal chemical tricyclic graphs with respect to (reduced) Sombor index.

Table 6. Degree distributions (DD) of CTG_n with $n_1 \leq 1$.

	n_4	n_3	n_2	n_1
E_1	2	0	$n-2$	0
E_2	1	2	$n-3$	0
E_3	0	4	$n-4$	0
E_4	2	1	$n-4$	1
E_5	1	3	$n-5$	1
E_6	0	5	$n-6$	1

Table 7. CTG_n with $n_1 \leq 1$ and their (reduced)Sombor index.

	DD	$m_{1,2}$	$m_{1,3}$	$m_{1,4}$	$m_{2,3}$	$m_{2,4}$	$m_{3,3}$	$m_{3,4}$	$m_{4,4}$	$m_{2,2}$	$SO(G)$	$SO_{red}(G)$
γ_1	E_1	0	0	0	0	8	0	0	0	$n-6$	$(2\sqrt{2n}+18.806)$	$(\sqrt{2n}+16.812)$
γ_2	E_1	0	0	0	0	6	0	0	1	$n-5$	$(2\sqrt{2n}+18.347)$	$(\sqrt{2n}+16.145)$
γ_3	E_2	0	0	0	2	2	1	2	0	$n-5$	$(2\sqrt{2n}+16.255)$	$(\sqrt{2n}+13.765)$
γ_4	E_2	0	0	0	3	3	1	1	0	$n-6$	$(2\sqrt{2n}+16.505)$	$(\sqrt{2n}+14.143)$
γ_5	E_2	0	0	0	4	4	1	0	0	$n-7$	$(2\sqrt{2n}+16.754)$	$(\sqrt{2n}+14.522)$
γ_6	E_2	0	0	0	4	2	0	2	0	$n-6$	$(2\sqrt{2n}+16.395)$	$(\sqrt{2n}+13.994)$
γ_7	E_2	0	0	0	5	3	0	1	0	$n-7$	$(2\sqrt{2n}+16.645)$	$(\sqrt{2n}+14.373)$
γ_8	E_2	0	0	0	6	4	0	0	0	$n-8$	$(2\sqrt{2n}+16.894)$	$(\sqrt{2n}+14.751)$
γ_9	E_3	0	0	0	2	0	5	0	0	$n-5$	$(2\sqrt{2n}+14.282)$	$(\sqrt{2n}+11.543)$
γ_{10}	E_3	0	0	0	4	0	4	0	0	$n-6$	$(2\sqrt{2n}+14.422)$	$(\sqrt{2n}+11.772)$
γ_{11}	E_3	0	0	0	6	0	3	0	0	$n-7$	$(2\sqrt{2n}+14.562)$	$(\sqrt{2n}+12.002)$
γ_{12}	E_3	0	0	0	8	0	2	0	0	$n-8$	$(2\sqrt{2n}+14.702)$	$(\sqrt{2n}+12.231)$
γ_{13}	E_3	0	0	0	10	0	1	0	0	$n-9$	$(2\sqrt{2n}+14.842)$	$(\sqrt{2n}+12.461)$
γ_{14}	E_3	0	0	0	12	0	0	0	0	$n-10$	$(2\sqrt{2n}+14.982)$	$(\sqrt{2n}+12.690)$
γ_{15}	E_4	0	0	1	1	3	0	2	1	$n-6$	$(2\sqrt{2n}+19.831)$	$(\sqrt{2n}+17.691)$
γ_{16}	E_4	1	0	0	1	4	0	2	1	$n-7$	$(2\sqrt{2n}+19.588)$	$(\sqrt{2n}+17.439)$
γ_{17}	E_4	0	0	1	2	4	0	1	1	$n-7$	$(2\sqrt{2n}+20.080)$	$(\sqrt{2n}+18.069)$
γ_{18}	E_4	1	0	0	2	5	0	1	1	$n-8$	$(2\sqrt{2n}+19.837)$	$(\sqrt{2n}+17.818)$
γ_{19}	E_4	0	0	1	3	5	0	0	1	$n-8$	$(2\sqrt{2n}+20.329)$	$(\sqrt{2n}+18.448)$
γ_{20}	E_4	1	0	0	3	6	0	0	1	$n-9$	$(2\sqrt{2n}+20.086)$	$(\sqrt{2n}+18.196)$
γ_{21}	E_4	0	0	1	1	5	0	2	0	$n-7$	$(2\sqrt{2n}+20.290)$	$(\sqrt{2n}+18.359)$
γ_{22}	E_4	1	0	0	1	6	0	2	0	$n-8$	$(2\sqrt{2n}+20.047)$	$(\sqrt{2n}+18.107)$
γ_{23}	E_4	0	0	1	2	6	0	1	0	$n-8$	$(2\sqrt{2n}+20.539)$	$(\sqrt{2n}+18.737)$
γ_{24}	E_4	1	0	0	2	7	0	1	0	$n-9$	$(2\sqrt{2n}+20.296)$	$(\sqrt{2n}+18.485)$
γ_{25}	E_4	0	0	1	3	7	0	0	0	$n-9$	$(2\sqrt{2n}+20.788)$	$(\sqrt{2n}+16.116)$
γ_{26}	E_4	1	0	0	3	8	0	0	0	$n-10$	$(2\sqrt{2n}+20.545)$	$(\sqrt{2n}+18.864)$
γ_{27}	E_5	0	0	1	2	0	2	3	0	$n-6$	$(2\sqrt{2n}+17.848)$	$(\sqrt{2n}+15.460)$
γ_{28}	E_5	0	0	1	4	0	1	3	0	$n-7$	$(2\sqrt{2n}+17.988)$	$(\sqrt{2n}+15.689)$
γ_{29}	E_5	0	0	1	6	0	0	3	0	$n-8$	$(2\sqrt{2n}+18.128)$	$(\sqrt{2n}+15.919)$
γ_{30}	E_5	0	0	1	1	1	3	2	0	$n-6$	$(2\sqrt{2n}+17.958)$	$(\sqrt{2n}+15.609)$
γ_{31}	E_5	0	0	1	3	1	2	2	0	$n-7$	$(2\sqrt{2n}+18.098)$	$(\sqrt{2n}+15.838)$
γ_{32}	E_5	0	0	1	5	1	1	2	0	$n-8$	$(2\sqrt{2n}+18.238)$	$(\sqrt{2n}+16.068)$
γ_{33}	E_5	0	0	1	7	1	0	2	0	$n-9$	$(2\sqrt{2n}+18.378)$	$(\sqrt{2n}+16.297)$
γ_{34}	E_5	0	0	1	2	2	3	1	0	$n-7$	$(2\sqrt{2n}+18.207)$	$(\sqrt{2n}+15.988)$
γ_{35}	E_5	0	0	1	4	2	2	1	0	$n-8$	$(2\sqrt{2n}+18.347)$	$(\sqrt{2n}+16.217)$
γ_{36}	E_5	0	0	1	6	2	1	1	0	$n-9$	$(2\sqrt{2n}+18.487)$	$(\sqrt{2n}+16.447)$
γ_{37}	E_5	0	0	1	8	2	0	1	0	$n-10$	$(2\sqrt{2n}+18.627)$	$(\sqrt{2n}+16.676)$
γ_{38}	E_5	0	0	1	3	3	3	0	0	$n-8$	$(2\sqrt{2n}+18.456)$	$(\sqrt{2n}+16.366)$
γ_{39}	E_5	0	0	1	5	3	2	0	0	$n-9$	$(2\sqrt{2n}+18.596)$	$(\sqrt{2n}+16.596)$
γ_{40}	E_5	0	0	1	7	3	1	0	0	$n-10$	$(2\sqrt{2n}+18.736)$	$(\sqrt{2n}+16.825)$

Table 8. CTG_n with $n_1 \leq 1$ and their (reduced)Sombor index.

	DD	$m_{1,2}$	$m_{1,3}$	$m_{1,4}$	$m_{2,3}$	$m_{2,4}$	$m_{3,3}$	$m_{3,4}$	$m_{4,4}$	$m_{2,2}$	$SO(G)$	$SO_{red}(G)$
γ_{41}	E_5	0	0	1	9	3	0	0	0	$n - 11$	$(2\sqrt{2n} + 18.876)$	$(\sqrt{2n} + 17.055)$
γ_{42}	E_5	1	0	0	0	1	3	3	0	$n - 6$	$(2\sqrt{2n} + 17.465)$	$(\sqrt{2n} + 14.978)$
γ_{43}	E_5	1	0	0	2	1	2	3	0	$n - 7$	$(2\sqrt{2n} + 17.605)$	$(\sqrt{2n} + 15.208)$
γ_{44}	E_5	1	0	0	4	1	1	3	0	$n - 8$	$(2\sqrt{2n} + 17.745)$	$(\sqrt{2n} + 15.437)$
γ_{45}	E_5	1	0	0	6	1	0	3	0	$n - 9$	$(2\sqrt{2n} + 17.885)$	$(\sqrt{2n} + 15.667)$
γ_{46}	E_5	1	0	0	1	2	3	2	0	$n - 7$	$(2\sqrt{2n} + 17.714)$	$(\sqrt{2n} + 15.357)$
γ_{47}	E_5	1	0	0	3	2	2	2	0	$n - 8$	$(2\sqrt{2n} + 17.854)$	$(\sqrt{2n} + 15.587)$
γ_{48}	E_5	1	0	0	5	2	1	2	0	$n - 9$	$(2\sqrt{2n} + 17.994)$	$(\sqrt{2n} + 15.816)$
γ_{49}	E_5	1	0	0	7	2	0	2	0	$n - 10$	$(2\sqrt{2n} + 18.134)$	$(\sqrt{2n} + 16.045)$
γ_{50}	E_5	1	0	0	2	3	3	1	0	$n - 8$	$(2\sqrt{2n} + 17.964)$	$(\sqrt{2n} + 15.736)$
γ_{51}	E_5	1	0	0	4	3	2	1	1	$n - 9$	$(2\sqrt{2n} + 18.104)$	$(\sqrt{2n} + 15.965)$
γ_{52}	E_5	1	0	0	6	3	1	1	0	$n - 10$	$(2\sqrt{2n} + 18.244)$	$(\sqrt{2n} + 16.195)$
γ_{53}	E_5	1	0	0	8	3	0	1	0	$n - 11$	$(2\sqrt{2n} + 18.384)$	$(\sqrt{2n} + 16.424)$
γ_{54}	E_5	1	0	0	3	4	3	0	0	$n - 9$	$(2\sqrt{2n} + 18.213)$	$(\sqrt{2n} + 16.114)$
γ_{55}	E_5	1	0	0	5	4	2	0	0	$n - 10$	$(2\sqrt{2n} + 18.353)$	$(\sqrt{2n} + 16.344)$
γ_{56}	E_5	1	0	0	7	4	1	0	0	$n - 11$	$(2\sqrt{2n} + 18.493)$	$(\sqrt{2n} + 16.573)$
γ_{57}	E_5	1	0	0	9	4	0	0	0	$n - 12$	$(2\sqrt{2n} + 18.633)$	$(\sqrt{2n} + 16.803)$
γ_{58}	E_6	0	1	0	2	0	6	0	0	$n - 7$	$(2\sqrt{2n} + 16.030)$	$(\sqrt{2n} + 13.543)$
γ_{59}	E_6	0	1	0	4	0	5	0	0	$n - 8$	$(2\sqrt{2n} + 16.170)$	$(\sqrt{2n} + 13.772)$
γ_{60}	E_6	0	1	0	6	0	4	0	0	$n - 9$	$(2\sqrt{2n} + 16.310)$	$(\sqrt{2n} + 14.002)$
γ_{61}	E_6	0	1	0	8	0	3	0	0	$n - 10$	$(2\sqrt{2n} + 16.450)$	$(\sqrt{2n} + 14.231)$
γ_{62}	E_6	0	1	0	10	0	2	0	0	$n - 11$	$(2\sqrt{2n} + 16.590)$	$(\sqrt{2n} + 14.461)$
γ_{63}	E_6	0	1	0	12	0	1	0	0	$n - 12$	$(2\sqrt{2n} + 16.730)$	$(\sqrt{2n} + 14.690)$
γ_{64}	E_6	0	1	0	14	0	0	0	0	$n - 13$	$(2\sqrt{2n} + 16.870)$	$(\sqrt{2n} + 14.920)$
γ_{65}	E_6	1	0	0	1	0	7	0	0	$n - 7$	$(2\sqrt{2n} + 15.741)$	$(\sqrt{2n} + 13.135)$
γ_{66}	E_6	1	0	0	3	0	6	0	0	$n - 8$	$(2\sqrt{2n} + 15.881)$	$(\sqrt{2n} + 13.365)$
γ_{67}	E_6	1	0	0	5	0	5	0	0	$n - 9$	$(2\sqrt{2n} + 16.021)$	$(\sqrt{2n} + 13.594)$
γ_{68}	E_6	1	0	0	7	0	4	0	0	$n - 10$	$(2\sqrt{2n} + 16.161)$	$(\sqrt{2n} + 13.824)$
γ_{69}	E_6	1	0	0	9	0	3	0	0	$n - 11$	$(2\sqrt{2n} + 16.301)$	$(\sqrt{2n} + 14.053)$
γ_{70}	E_6	1	0	0	11	0	2	0	0	$n - 12$	$(2\sqrt{2n} + 16.441)$	$(\sqrt{2n} + 14.283)$
γ_{71}	E_6	1	0	0	13	0	1	0	0	$n - 13$	$(2\sqrt{2n} + 16.581)$	$(\sqrt{2n} + 14.512)$
γ_{72}	E_6	1	0	0	15	0	0	0	0	$n - 14$	$(2\sqrt{2n} + 16.721)$	$(\sqrt{2n} + 14.742)$

Lemma 3.11 [15, 17] $G \in CTG_n$ and $n_1(G) \leq 1$ if and only if G belongs to one of equivalence classes given in Table 6.

Theorem 3.12 If $n \geq 6$, $G_1 \in \gamma_9$, $G_2 \in \gamma_{10}$, $G_3 \in \gamma_{11}$, $G_4 \in \gamma_{12}$, $G_5 \in \gamma_{13}$, $G_6 \in \gamma_{14}$, $G_7 \in \gamma_{65}$ in Table 7 and Table 8. $G \in CTG_n \setminus \{G_1, G_2, G_3, G_4, G_5, G_6, G_7\}$, then $SO(G_1) < SO(G_2) < SO(G_3) < SO(G_4) < SO(G_5) < SO(G_6) < SO(G_7) < SO(G)$.

Proof. By Table 7 and Table 8, we have $SO(G_1) < SO(G_2) < SO(G_3) < SO(G_4) <$

$$SO(G_5) < SO(G_6) < SO(G_7).$$

If $n_1(G) \leq 1$, by Table 7 and Table 8, the conclusion holds. If $n_1(G) \geq 2$, by the transformations of Lemma 2.3 and Lemma 2.4, we can obtain a chemical tricyclic graphs G^* with $n_1(G^*) = 1$, so we have $SO(G) > SO(G^*)$. By Table 7 and Table 8, $SO(G_7) \leq SO(G^*)$. Thus, the conclusion holds. ■

Similar to the proof of Theorem 3.12, we have

Theorem 3.13 *If $n \geq 6$, $G_1 \in \gamma_9$, $G_2 \in \gamma_{10}$, $G_3 \in \gamma_{11}$, $G_4 \in \gamma_{12}$, $G_5 \in \gamma_{13}$, $G_6 \in \gamma_{14}$, $G_7 \in \gamma_{65}$ in Table 7 and Table 8. $G \in CTG_n \setminus \{G_1, G_2, G_3, G_4, G_5, G_6, G_7\}$, then $SO_{red}(G_1) < SO_{red}(G_2) < SO_{red}(G_3) < SO_{red}(G_4) < SO_{red}(G_5) < SO_{red}(G_6) < SO_{red}(G_7) < SO_{red}(G)$.*

4 Applications of reduced Sombor index to octane isomers

Deng et al. [9], considered the correlation between some physico-chemical properties of octane isomers with Sombor index. In this section, we study the correlation between these physico-chemical properties of octane isomers with reduced Sombor index. We also compare the reduced Sombor index with some other topological indices.

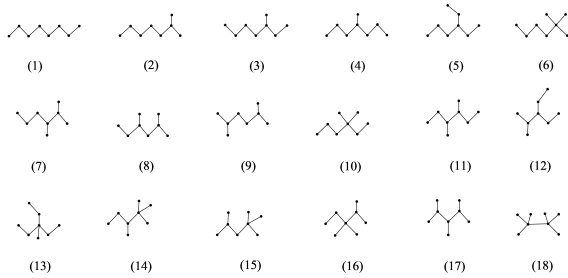


Figure 1. Chemical graphs of octane isomers.

The chemical graphs of 18 octane isomers can see in Figure 1. We can calculate the values of reduced Sombor index for the 18 octane isomers in Figure 1 as [9.0710, 11.4787, 11.3005, 11.3005, 11.1224, 15.9907, 13.4787, 13.7082, 13.8663, 15.7387, 13.3005, 13.3005, 15.4868, 17.8416, 18.3983, 17.7678, 15.6568, 22.2426]. Based on the values of Acentric Factors (Entropy, SNar, HNar) of the 18 octane isomers (see [7, 9]) in Figure 1, we can also obtain

the regression models of the reduces Sombor index (similar to the results of [9]).

$$AcenFac = 0.4881 - 0.0105 \times SO_{red}, R^2 = 0.9213. \quad (5)$$

$$Entropy = 124.5 - 1.317 \times SO_{red}, R^2 = 0.8922. \quad (6)$$

$$SNar = 5.003 - 0.1015 \times SO_{red}, R^2 = 0.9736. \quad (7)$$

$$HNar = 1.793 - 0.02654 \times SO_{red}, R^2 = 0.9341. \quad (8)$$

Table 9. R^2 values between indices and Acentric Factors, Entropy, SNar, HNar.

Physico-chemical property	SO_{red}	M_1	M_2	F	R	SCI	SDD	M_N
Acentric Factors	0.9213	0.9468	0.973	0.9313	0.8176	0.8647	0.8118	0.98915
Entropy	0.8922	0.9107	0.8868	0.9077	0.8205	0.8518	0.8276	0.90746
SNar	0.9736	0.9974	0.8940	0.9453	0.9487	0.9710	0.9252	0.9477
HNar	0.9341	0.9774	0.8941	0.9453	0.9487	0.9710	0.9252	0.9115

The correlation (R) between Acentric Factors(resp. Entropy, SNar, HNar) and reduced Sombor indices of the octane isomers is about -0.959(resp. -0.944, -0.986, -0.966). It shows a good linear relation. Therefore, the reduced Sombor index can help to predict these physico-chemical properties. We compare the reduced Sombor index with some existing topological indices, we found that sometimes the reduced Sombor index shows better predictive power than the existing indices. It is worth noting that [24] (before our paper) also consider the correlation between Sombor index and Entropy of octane isomers, however, for the sake of the integrity of the article, we have not removed the results about our results of Entropy. We also considered other physico-chemical properties, such as Acentric Factors, SNar and HNar, which do not appear in the [24].

5 Concluding Remarks

In this paper, we determine the first fourteen minimum chemical trees, the first four minimum chemical unicyclic graphs, the first three minimum chemical bicyclic graphs, the first seven minimum chemical tricyclic graphs. At last, we consider applications of reduced Sombor index to octane isomers. However, obtaining a more detailed ordering is still an open problem.

Problem 5.1 *Further ordering chemical graphs by their Sombor indices.*

We intend to elaborate this matter in the near future.

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