

# Extremal Sombor Indices of Tetracyclic (Chemical) Graphs

Hechao Liu<sup>1</sup>, Lihua You<sup>1,\*</sup>, Yufei Huang<sup>2</sup>

<sup>1</sup>*School of Mathematical Sciences, South China Normal University,  
Guangzhou, 510631, P. R. China*

hechaoliu@m.scnu.edu.cn, ylhua@scnu.edu.cn

<sup>2</sup>*Department of Mathematics Teaching, Guangzhou Civil Aviation College,  
Guangzhou, 510403, P. R. China*

fayger@qq.com

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## Abstract

Based on elementary geometry, Gutman proposed the novel graph invariant called the Sombor index, which was defined as  $SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}$ , where  $d_u$  denotes the degree of vertex  $u$ . It has been proved that the Sombor index could predict some physicochemical properties. In this paper, we first give the classification of non-pendent tetracyclic (chemical) graphs with respect to the Sombor index, and we determine the minimum Sombor indices of tetracyclic (chemical) graphs.

## 1 Introduction

In this paper, all graphs are simple, with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$  and edge set  $E(G)$ . Let  $|V(G)| = n$  and  $|E(G)| = m$ . Let  $N_G(u)$  be the set of vertices which are neighbors of vertex  $u$ . Let  $d_u = |N_G(u)|$  be the degree of vertex  $u$ . If  $d_u = 1$ , then  $u$  is called a pendent vertex. Denote by  $\Delta(G)$  and  $\delta(G)$  the maximum degree and minimum degree of  $G$ . We denote  $n_i$  the number of vertices with degree  $i$ , and  $m_{i,j}$  the number of edges joining a vertex of degree  $i$  and a vertex of degree  $j$ .

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\*Corresponding author

Chemical graphs are the graphs with  $d_u \leq 4$  for all  $u \in V(G)$ . Tetracyclic graphs are the graphs with cyclomatic  $c = 4$  (i.e.,  $m = n + 3$ ). For all notations and terminology used, but not defined here, we refer to the textbook [4].

Inspired by Euclidean metric, Gutman proposed the Sombor index and the reduced Sombor index [13], which are defined as,

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

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

Recently, many research devote to the study of Sombor index. Redžepović [24] considered the chemical applicability of Sombor index. Deng et al. [11] determined the maximum Sombor indices of chemical trees. Cruz et al. [6] considered the extremal Sombor indices of some chemical graphs. Chen et al. [5] considered the extremal values of the Sombor indices of trees with some given parameters, including matching number, pendent vertices, diameter, segment number, branching number. Liu et al. [19] determined maximum and minimum (reduced) Sombor indices of chemical trees with given pendent vertices, and characterized their extremal graphs. Liu et al. [20] also ordered the minimal Sombor indices of chemical trees, chemical unicyclic graphs, chemical bicyclic graphs and chemical tricyclic graphs, respectively. Das et al. [9] determined the maximum Sombor indices of  $c$ -cycle graphs. One can refer to [1, 2, 7, 10, 12, 14, 16–18, 21–23, 25–28] for more details about Sombor indices.

Inspired by the results of [9] and [20], it is natural to consider the minimum Sombor indices of tetracyclic (chemical) graphs. In this paper, we first give the classification of tetracyclic (chemical) graphs with  $n_1(G) = 0$ . Then we determine the minimum Sombor indices of tetracyclic (chemical) graphs.

## 2 Main results

For convenience, the set of graphs with  $|V(G)| = n$  and  $|E(G)| = m$  are called  $(n, m)$  graphs. Denote by  $\mathcal{TG}_n$  (resp.  $\mathcal{CTG}_n$ ) the set of tetracyclic graphs (resp. tetracyclic chemical graphs) with  $n$  vertices.

**Lemma 2.1** [1] *Let  $G$  be a connected  $(n, m)$  graph. If  $G$  has the minimum Sombor index, then  $\Delta(G) - \delta(G) \leq 1$ .*

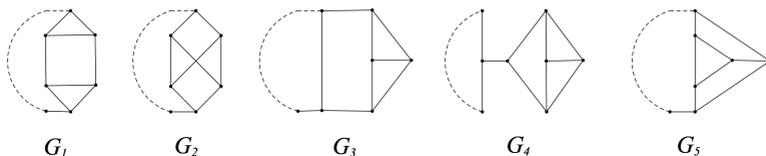
**Lemma 2.2** [15] *There exists a connected tetracyclic graph  $G$  of order  $n$  with  $n_1(G) = 0$  if and only if  $G$  belongs to one of the equivalence classes given in Table 1.*

**Table 1.** Vertex degree distributions (DD) of  $\mathcal{TG}_n$  with  $n_1 = 0$ .

DD	$n_8$	$n_7$	$n_6$	$n_5$	$n_4$	$n_3$	$n_2$	$n_1$	$n_i (i \geq 9)$
$H_1$	1	0	0	0	0	0	$n - 1$	0	0
$H_2$	0	1	0	0	0	1	$n - 2$	0	0
$H_3$	0	0	1	0	1	0	$n - 2$	0	0
$H_4$	0	0	1	0	0	2	$n - 3$	0	0
$H_5$	0	0	0	2	0	0	$n - 2$	0	0
$H_6$	0	0	0	1	1	1	$n - 3$	0	0
$H_7$	0	0	0	1	0	3	$n - 4$	0	0
$H_8$	0	0	0	0	3	0	$n - 3$	0	0
$H_9$	0	0	0	0	2	2	$n - 4$	0	0
$H_{10}$	0	0	0	0	1	4	$n - 5$	0	0
$H_{11}$	0	0	0	0	0	6	$n - 6$	0	0

We give the edge degree distributions of all connected tetracyclic graphs with  $n_1(G) = 0$  in  $H_k$ ,  $1 \leq k \leq 11$ , and their Sombor indices which are shown in Tables 2-6. Note that the relevant data of Tables 2-6 except the values of Sombor indices are from [3]. There are some writing errors in these tables of [3], we correct it.

Let  $\xi = \xi^* \cup \xi^{**}$ , where  $\xi^* = \{G|G \in \mathcal{TG}_n, n_1 = 0\}$ ,  $\xi^{**} = \{G|G \in \mathcal{TG}_n, n_1 \geq 1\}$ . Then  $\xi^* = \cup_{i=1}^{11} H_i = \cup_{i=1}^{95} \xi_i$  (see Tables 1-6). Note that  $\xi_7 = \{G|G \in \xi^*, m_{3,3} = 8, m_{3,2} = 2, m_{2,2} = n - 7\}$ . It is easy to verify that  $\xi_7 = \{G_1, G_2, G_3, G_4, G_5\}$ , see Figure 1. In the following, we will determine  $\xi_7$  is the set of graphs with the minimum (reduced) Sombor index among  $\mathcal{TG}_n$ .



**Figure 1.** The minimum graphs  $G_i (1 \leq i \leq 5)$ .

**Lemma 2.3** *Let  $G \in \xi_7$ . Then  $SO(G) = 2\sqrt{2}n + 2\sqrt{13} + 10\sqrt{2} \approx 2\sqrt{2}n + 21.35323$ .*

By Lemmas 2.1, 2.2 and 2.3, we have the following results.

**Theorem 2.4** Let  $G \in \mathcal{T}\mathcal{G}_n$  ( $n \geq 9$ ). Then

$$SO(G) \geq 2\sqrt{2}n + 2\sqrt{13} + 10\sqrt{2},$$

with equality if and only if  $G \in \xi_7$ , i.e.,  $G \cong G_i$ ,  $1 \leq i \leq 5$ , see Figure 1.

*Proof.* Suppose that  $G^* \in \mathcal{T}\mathcal{G}_n$  ( $n \geq 9$ ) and  $G^*$  has the minimum Sombor index. If  $n_1(G^*) \geq 1$ , then  $\Delta(G^*) - \delta(G^*) \geq 2$ , which is a contradiction with the conclusion of Lemma 2.1. Thus  $n_1(G^*) = 0$ . All connected tetracyclic graphs with  $n_1(G) = 0$  in  $H_k$ ,  $1 \leq k \leq 11$  and their Sombor indices are shown in Tables 2-6. By comparing these values of Sombor indices in Tables 2-6, we obtain the desired results. ■

We can easily verify the conclusion of Lemma 2.1 also holds for the reduced Sombor index. Similarly, we also have

**Theorem 2.5** Let  $G \in \mathcal{T}\mathcal{G}_n$  ( $n \geq 9$ ). Then

$$SO_{red}(G) \geq \sqrt{2}n + 2\sqrt{5} + 9\sqrt{2},$$

with equality if and only if  $G \in \xi_7$ , i.e.,  $G \cong G_i$ ,  $1 \leq i \leq 5$ , see Figure 1.

Since these minimum tetracyclic graphs (i.e.,  $G \cong G_i$ ,  $1 \leq i \leq 5$ ) are all chemical graphs, thus we have

**Corollary 2.6** Let  $G \in \mathcal{CT}\mathcal{G}_n$  ( $n \geq 9$ ). Then

$$SO(G) \geq 2\sqrt{2}n + 2\sqrt{13} + 10\sqrt{2},$$

$$SO_{red}(G) \geq \sqrt{2}n + 2\sqrt{5} + 9\sqrt{2}.$$

with equality if and only if  $G \in \xi_7$ , i.e.,  $G \cong G_i$ ,  $1 \leq i \leq 5$ , see Figure 1.

**Table 2.** Edge degree distributions (DD) of  $\mathcal{T}\mathcal{G}_n$  with  $n_1 = 0$  and  $\Delta = 3$ .

No.	DD	$m_{3,3}$	$m_{3,2}$	$m_{2,2}$	SO
$\xi_1$	$H_{11}$	2	14	$n - 13$	$2\sqrt{2}n + 22.19344$
$\xi_2$	$H_{11}$	3	12	$n - 12$	$2\sqrt{2}n + 22.05341$
$\xi_3$	$H_{11}$	4	10	$n - 11$	$2\sqrt{2}n + 21.91337$
$\xi_4$	$H_{11}$	5	8	$n - 10$	$2\sqrt{2}n + 21.77334$
$\xi_5$	$H_{11}$	6	6	$n - 9$	$2\sqrt{2}n + 21.63330$
$\xi_6$	$H_{11}$	7	4	$n - 8$	$2\sqrt{2}n + 21.49327$
$\xi_7$	$H_{11}$	8	2	$n - 7$	$2\sqrt{2}n + 21.35323$

**Table 3.** Edge degree distributions (*DD*) of  $\mathcal{T}\mathcal{G}_n$  with  $n_1 = 0$  and  $\Delta = 4$ .

<i>No.</i>	<i>DD</i>	$m_{4,4}$	$m_{4,3}$	$m_{4,2}$	$m_{3,3}$	$m_{3,2}$	$m_{2,2}$	<i>SO</i>
$\xi_8$	$H_8$	0	0	12	0	0	$n - 9$	$2\sqrt{2n} + 28.20978$
$\xi_9$	$H_8$	1	0	10	0	0	$n - 8$	$2\sqrt{2n} + 27.75079$
$\xi_{10}$	$H_8$	2	0	8	0	0	$n - 7$	$2\sqrt{2n} + 27.29180$
$\xi_{11}$	$H_8$	3	0	6	0	0	$n - 6$	$2\sqrt{2n} + 26.83281$
$\xi_{12}$	$H_9$	0	0	8	0	6	$n - 11$	$2\sqrt{2n} + 26.29769$
$\xi_{13}$	$H_9$	0	0	8	1	4	$n - 10$	$2\sqrt{2n} + 26.15766$
$\xi_{14}$	$H_9$	0	1	7	0	5	$n - 10$	$2\sqrt{2n} + 26.04843$
$\xi_{15}$	$H_9$	0	1	7	1	3	$n - 9$	$2\sqrt{2n} + 24.49418$
$\xi_{16}$	$H_9$	1	0	6	0	6	$n - 10$	$2\sqrt{2n} + 25.83870$
$\xi_{17}$	$H_9$	0	2	6	0	4	$n - 9$	$2\sqrt{2n} + 25.79917$
$\xi_{18}$	$H_9$	1	0	6	1	4	$n - 9$	$2\sqrt{2n} + 25.69867$
$\xi_{19}$	$H_9$	0	2	6	1	2	$n - 8$	$2\sqrt{2n} + 25.65914$
$\xi_{20}$	$H_9$	1	1	5	0	5	$n - 9$	$2\sqrt{2n} + 25.58944$
$\xi_{21}$	$H_9$	0	3	5	0	3	$n - 8$	$2\sqrt{2n} + 25.54991$
$\xi_{22}$	$H_9$	1	1	5	1	3	$n - 8$	$2\sqrt{2n} + 25.44941$
$\xi_{23}$	$H_9$	0	3	5	1	1	$n - 7$	$2\sqrt{2n} + 25.40988$
$\xi_{24}$	$H_9$	1	2	4	0	4	$n - 8$	$2\sqrt{2n} + 25.34018$
$\xi_{25}$	$H_9$	0	4	4	0	2	$n - 7$	$2\sqrt{2n} + 25.30065$
$\xi_{26}$	$H_9$	1	2	4	1	2	$n - 7$	$2\sqrt{2n} + 25.20015$
$\xi_{27}$	$H_9$	0	4	4	1	0	$n - 6$	$2\sqrt{2n} + 25.16062$
$\xi_{28}$	$H_9$	1	3	3	0	3	$n - 7$	$2\sqrt{2n} + 25.09092$
$\xi_{29}$	$H_9$	1	3	3	1	1	$n - 6$	$2\sqrt{2n} + 24.95089$
$\xi_{30}$	$H_9$	1	4	2	0	2	$n - 6$	$2\sqrt{2n} + 24.84166$
$\xi_{31}$	$H_9$	1	4	2	1	0	$n - 5$	$2\sqrt{2n} + 24.70163$
$\xi_{32}$	$H_{10}$	0	0	4	0	12	$n - 13$	$2\sqrt{2n} + 24.38560$
$\xi_{33}$	$H_{10}$	0	0	4	1	10	$n - 12$	$2\sqrt{2n} + 24.24557$
$\xi_{34}$	$H_{10}$	0	1	3	0	11	$n - 12$	$2\sqrt{2n} + 24.13634$
$\xi_{35}$	$H_{10}$	0	0	4	2	8	$n - 11$	$2\sqrt{2n} + 24.10553$
$\xi_{36}$	$H_{10}$	0	1	3	1	9	$n - 11$	$2\sqrt{2n} + 23.99631$
$\xi_{37}$	$H_{10}$	0	0	4	3	6	$n - 10$	$2\sqrt{2n} + 23.96550$
$\xi_{38}$	$H_{10}$	0	2	2	0	10	$n - 11$	$2\sqrt{2n} + 23.88708$
$\xi_{39}$	$H_{10}$	0	1	3	2	7	$n - 10$	$2\sqrt{2n} + 23.85627$
$\xi_{40}$	$H_{10}$	0	0	4	4	4	$n - 9$	$2\sqrt{2n} + 23.82546$
$\xi_{41}$	$H_{10}$	0	2	2	1	8	$n - 10$	$2\sqrt{2n} + 23.74705$
$\xi_{42}$	$H_{10}$	0	1	3	3	5	$n - 9$	$2\sqrt{2n} + 23.71624$
$\xi_{43}$	$H_{10}$	0	3	1	0	9	$n - 10$	$2\sqrt{2n} + 23.63782$
$\xi_{44}$	$H_{10}$	0	0	4	5	2	$n - 8$	$2\sqrt{2n} + 23.68543$
$\xi_{45}$	$H_{10}$	0	2	2	2	6	$n - 9$	$2\sqrt{2n} + 23.60701$

**Table 4.** Continued of Table 3.

<i>No.</i>	<i>DD</i>	$m_{4,4}$	$m_{4,3}$	$m_{4,2}$	$m_{3,3}$	$m_{3,2}$	$m_{2,2}$	<i>SO</i>
$\xi_{46}$	$H_{10}$	0	1	3	4	3	$n - 8$	$2\sqrt{2n} + 23.57620$
$\xi_{47}$	$H_{10}$	0	3	1	1	7	$n - 9$	$2\sqrt{2n} + 23.49779$
$\xi_{48}$	$H_{10}$	0	2	2	3	4	$n - 8$	$2\sqrt{2n} + 23.46698$
$\xi_{49}$	$H_{10}$	0	4	0	0	8	$n - 9$	$2\sqrt{2n} + 23.38856$
$\xi_{50}$	$H_{10}$	0	1	3	5	1	$n - 7$	$2\sqrt{2n} + 23.43617$
$\xi_{51}$	$H_{10}$	0	3	1	2	5	$n - 8$	$2\sqrt{2n} + 23.35775$
$\xi_{52}$	$H_{10}$	0	2	2	4	2	$n - 7$	$2\sqrt{2n} + 23.32694$
$\xi_{53}$	$H_{10}$	0	4	0	1	6	$n - 8$	$2\sqrt{2n} + 23.24853$
$\xi_{54}$	$H_{10}$	0	3	1	3	3	$n - 7$	$2\sqrt{2n} + 23.21772$
$\xi_{55}$	$H_{10}$	0	2	2	5	0	$n - 6$	$2\sqrt{2n} + 23.18691$
$\xi_{56}$	$H_{10}$	0	4	0	2	4	$n - 7$	$2\sqrt{2n} + 23.10849$
$\xi_{57}$	$H_{10}$	0	3	1	4	1	$n - 6$	$2\sqrt{2n} + 23.07768$
$\xi_{58}$	$H_{10}$	0	4	0	3	2	$n - 6$	$2\sqrt{2n} + 22.96846$

**Table 5.** Edge degree distributions (*DD*) of  $\mathcal{T}\mathcal{G}_n$  with  $n_1 = 0$  and  $\Delta = 5$ .

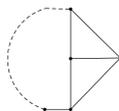
<i>No.</i>	<i>DD</i>	$m_{5,5}$	$m_{5,4}$	$m_{5,3}$	$m_{5,2}$	$m_{4,3}$	$m_{4,2}$	$m_{3,3}$	$m_{3,2}$	$m_{2,2}$	<i>SO</i>
$\xi_{59}$	$H_5$	0	0	0	10	0	0	0	0	$n - 7$	$2\sqrt{2n} + 34.05265$
$\xi_{60}$	$H_5$	1	0	0	8	0	0	0	0	$n - 6$	$2\sqrt{2n} + 33.18182$
$\xi_{61}$	$H_6$	0	0	0	5	0	4	0	3	$n - 9$	$2\sqrt{2n} + 30.17517$
$\xi_{62}$	$H_6$	0	0	0	5	1	3	0	2	$n - 8$	$2\sqrt{2n} + 29.92591$
$\xi_{63}$	$H_6$	0	0	1	4	0	4	0	2	$n - 8$	$2\sqrt{2n} + 29.84384$
$\xi_{64}$	$H_6$	0	1	0	4	0	3	0	3	$n - 8$	$2\sqrt{2n} + 29.54942$
$\xi_{65}$	$H_6$	0	0	1	4	1	3	0	1	$n - 7$	$2\sqrt{2n} + 29.59458$
$\xi_{66}$	$H_6$	0	1	0	4	1	2	0	2	$n - 7$	$2\sqrt{2n} + 29.30016$
$\xi_{67}$	$H_6$	0	1	1	3	0	3	0	2	$n - 7$	$2\sqrt{2n} + 29.21809$
$\xi_{68}$	$H_6$	0	1	1	3	1	2	0	1	$n - 6$	$2\sqrt{2n} + 28.96883$
$\xi_{69}$	$H_7$	0	0	0	5	0	0	0	9	$n - 11$	$2\sqrt{2n} + 28.26308$
$\xi_{70}$	$H_7$	0	0	0	5	0	0	1	7	$n - 10$	$2\sqrt{2n} + 28.12305$
$\xi_{71}$	$H_7$	0	0	0	5	0	0	2	5	$n - 9$	$2\sqrt{2n} + 27.98301$
$\xi_{72}$	$H_7$	0	0	1	4	0	0	0	8	$n - 10$	$2\sqrt{2n} + 27.93175$
$\xi_{73}$	$H_7$	0	0	0	5	0	0	3	3	$n - 8$	$2\sqrt{2n} + 27.84298$
$\xi_{74}$	$H_7$	0	0	1	4	0	0	1	6	$n - 9$	$2\sqrt{2n} + 27.79171$
$\xi_{75}$	$H_7$	0	0	1	4	0	0	2	4	$n - 8$	$2\sqrt{2n} + 27.65168$
$\xi_{76}$	$H_7$	0	0	2	3	0	0	0	7	$n - 9$	$2\sqrt{2n} + 27.60041$
$\xi_{77}$	$H_7$	0	0	1	4	0	0	3	2	$n - 7$	$2\sqrt{2n} + 27.51164$
$\xi_{78}$	$H_7$	0	0	2	3	0	0	1	5	$n - 8$	$2\sqrt{2n} + 27.46037$
$\xi_{79}$	$H_7$	0	0	2	3	0	0	2	3	$n - 7$	$2\sqrt{2n} + 27.32034$
$\xi_{80}$	$H_7$	0	0	3	2	0	0	0	6	$n - 8$	$2\sqrt{2n} + 27.26907$
$\xi_{81}$	$H_7$	0	0	2	3	0	0	3	1	$n - 6$	$2\sqrt{2n} + 27.18030$
$\xi_{82}$	$H_7$	0	0	3	2	0	0	1	4	$n - 7$	$2\sqrt{2n} + 27.12904$
$\xi_{83}$	$H_7$	0	0	3	2	0	0	2	2	$n - 6$	$2\sqrt{2n} + 26.98900$
$\xi_{84}$	$H_7$	0	0	3	2	0	0	3	0	$n - 5$	$2\sqrt{2n} + 26.84897$

**Table 6.** Edge degree distributions ( $DD$ ) of  $\mathcal{T}\mathcal{G}_n$  with  $n_1 = 0$  and  $\Delta = 6, 7, 8$ .

No.	$DD$	$m_{8,2}$	$m_{7,3}$	$m_{7,2}$	$m_{6,4}$	$m_{6,3}$	$m_{6,2}$	$m_{4,2}$	$m_{3,3}$	$m_{3,2}$	$m_{2,2}$	$SO$
$\xi_{85}$	$H_4$	0	0	0	0	0	6	0	0	6	$n-9$	$2\sqrt{2n} + 34.12479$
$\xi_{86}$	$H_4$	0	0	0	0	0	6	0	1	4	$n-8$	$2\sqrt{2n} + 33.98476$
$\xi_{87}$	$H_4$	0	0	0	0	1	5	0	0	5	$n-8$	$2\sqrt{2n} + 33.73131$
$\xi_{88}$	$H_4$	0	0	0	0	1	5	0	1	3	$n-7$	$2\sqrt{2n} + 33.59128$
$\xi_{89}$	$H_4$	0	0	0	0	2	4	0	0	4	$n-7$	$2\sqrt{2n} + 33.33784$
$\xi_{90}$	$H_4$	0	0	0	0	2	4	0	1	2	$n-6$	$2\sqrt{2n} + 33.19780$
$\xi_{91}$	$H_3$	0	0	0	0	0	6	4	0	0	$n-7$	$2\sqrt{2n} + 36.03688$
$\xi_{92}$	$H_3$	0	0	0	1	0	5	3	0	0	$n-6$	$2\sqrt{2n} + 35.27972$
$\xi_{93}$	$H_2$	0	0	7	0	0	0	0	0	3	$n-7$	$2\sqrt{2n} + 41.97843$
$\xi_{94}$	$H_2$	0	1	6	0	0	0	0	0	2	$n-6$	$2\sqrt{2n} + 41.53697$
$\xi_{95}$	$H_1$	8	0	0	0	0	0	0	0	0	$n-5$	$2\sqrt{2n} + 51.82755$

### 3 Concluding Remarks

The minimum Sombor indices had been studied on trees [13], unicyclic and bicyclic graphs [7], chemical tricyclic graphs [20]. In this paper, we give the classification of non-pendent tetracyclic (chemical) graphs with respect to the Sombor index, and we determine the minimum Sombor indices of tetracyclic (chemical) graphs. By calculating the (reduced) Sombor indices of connected tricyclic graphs in Table 2 of [8], we can easily determine the minimum tricyclic graphs is the tricyclic graph with  $m_{2,3} = 2$ ,  $m_{3,3} = 5$ ,  $m_{2,2} = n-5$ . The minimum tricyclic graphs with respect to (reduced) Sombor indices depicted in Figure 2.

**Figure 2.** The minimum tricyclic graph.

It is natural to consider the second (resp. third) minimum tricyclic and tetracyclic (chemical) graphs with respect to Sombor index. Thus we propose the following questions.

**Problem 3.1** Determine the second (resp. third) minimum tricyclic and tetracyclic (chemical) graphs.

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