AIMS Mathematics

http://www.aimspress.com/journal/Math

AIMS Mathematics, 8(3): 5369–5390.
DOI: 10.3934/math.2023270
Received: 27 September 2022
Accepted: 24 October 2022
Published: 15 December 2022

Research article

On optimal molecular trees with respect to Sombor indices

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Abstract: The Sombor index and reduced Sombor index, introduced by mathematical chemist Ivan Gutman [MATCH Commun. Math. Comput. Chem. 86 (2021) 11–16], are the recently proposed degree-based graph invariants that attained a lot of attention from researchers in a very short time. In this paper, the best possible upper bounds on the both aforementioned indices for molecular trees are obtained in terms of order and number of branching vertices or vertices of degree 2. The optimal molecular trees achieving the obtained bounds are also completely characterized.

Keywords: topological index; Sombor indices; molecular trees; optimization
Mathematics Subject Classification: 05C09, 05C90, 05C92

1. Introduction

The graphs considered throughout this paper are finite and connected. The graph-theoretical terminology and notation that are used in this study without explaining here can be found in the books [1,2].

A graph invariant is a function f defined on the set of all graphs with the condition that $f(G_1) = f(G_2)$ whenever G_1 and G_2 are isomorphic. The real-valued graph invariants are commonly known as topological indices in mathematical chemistry, particularly in chemical graph theory [20].

The Sombor index and the reduced Sombor index abbreviated as SO and SO_{red}, respectively, are the topological indices introduced recently by mathematical chemist Ivan Gutman in his seminal paper [9]. The Sombor index SO has attained attention from many scientific groups all over the world in a very short time, which resulted in many publications; for example, see the review papers [8,15] and associated papers listed therein. The chemical applicability of the indices SO and SO_{red} is also well documented. Redžepović [17] examined the discriminating and predictive ability of the indices SO and

SO_{red} on a large class of isomers and found that both of these indices have good discriminating and predictive potential. Deng et al. [7] compared the predictive ability of SO on octane isomers with that of similar kind of existing topological indices and showed that SO has a higher accuracy in predicting physico-chemical properties of the the aforementioned chemical compounds; Liu et al. [13] conducted a similar comparative study for SO_{red} and concluded that SO_{red} outperforms in several cases. Also, it was demonstrated in [14] that boiling points of benzenoid hydrocarbons are highly correlated with SO and SO_{red}. By considering these chemical applications of SO and SO_{red}, it make sense to study further these indices, particularly for molecular graphs (these are graphs of maximum degree at most 4).

In chemical graph theory, molecular trees play an important role because a certain class of chemical compounds can be viewed by using the concept of molecular trees. Thereby, in the present paper, we study the topological indices SO and SO_{red} for molecular trees under certain constraints. Deng et al. [7] determined the trees possessing the maximum and minimum values of SO and SO_{red} among all molecular trees of a given order; see also [5, 18] where the same problem regarding SO was solved independently. Let us consider the following problem.

Problem 1. *Characterize the trees possessing the maximum and minimum values of SO and SO_{red} among all molecular trees of a given order and with a fixed number of (i) branching vertices (ii) vertices of degree* 2.

The minimal part of Problem 1 concerning SO has already been solved in [3] where several other interesting extremal problems were also resolved. The main objective of this study is to give a solution to the maximal part of Problem 1. Detail about the mathematical study of the Sombor index for general trees can be found in [5, 6, 10, 12, 19, 21, 22].

2. Preliminaries

Let $V(G)$ and $E(G)$ denote the set of vertices and edges, respectively, in the graph G. For the vertex $v \in V(G)$, the degree of v is denoted by $d_G(v)$ (or simply by d_v if only one graph is under consideration). A vertex $u \in V(G)$ is said to be a pendent vertex or a branching vertex if $d_u = 1$ or $d_u \geq 3$, respectively. The set $N_G(u)$ consists of the vertices of the graph G that are adjacent to the vertex u. Let $n_i(G)$ denotes the count of vertices having degree i in the graph G. Denote by $x_{i,j}(G)$ the cardinality of the set consisting of the edges connecting the vertex of degree i with the vertex of degree j in the graph G. A graph of order n is also known as an n-vertex graph.

For a graph G, the Sombor index and reduced Sombor index abbreviated as SO and SO_{red}, respectively, are defined [9] as

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

3. Auxiliary results

We start this section with the following elementary result, noted in [16].

Lemma 1. *The function f defined as*

$$f(x, y) = \sqrt{x^2 + y^2} - \sqrt{(x - c)^2 + y^2},$$

with $1 \leq c < x$ and $y > 0$, is strictly decreasing in y and strictly increasing in x.

For $r \geq 3$, each of the vertices $u_2, u_3, \cdots, u_{r-1}$ of the path $P : u_1u_2 \cdots u_r$ in a graph is called internal vertex of P. Denote by $P_{i,j}(C)$ (or simply $P_{i,j}$) the path from a branching vertex of degree i to a branching vertex of degree j in a molecular tree C such that all the internal vertices (if exist) of $P_{i,j}$ have degree 2.

Lemma 2. *If the molecular tree C contains a path $P_{4,4} : v_1v_2 \cdots v_s$ and an edge uw such that $d_u = 1$ and $d_w = 3$ with the condition that v_1 lies on the $w - v_s$ path, then for the molecular tree C' obtained from C by deleting the edges v_1v_2, uw and adding new edges v_2w, v_1u, the inequalities $SO(C) < SO(C')$ and $SO_{red}(C) < SO_{red}(C')$ hold, where C and C' have the same degree sequence.*

Proof. Clearly, the trees C and C' have the same degree sequence. Also, we note that

$$SO(C) = SO(C') + \sqrt{10} - \sqrt{17} + \sqrt{4 + d_{v_2}^2} - \sqrt{9 + d_{v_2}^2} < SO(C')$$

and

$$SO_{red}(C) = SO_{red}(C') + 2 - 3 + \sqrt{9 + (d_{v_2} - 1)^2} - \sqrt{4 + (d_{v_2} - 1)^2} < SO(C').$$

■

Lemma 3. *For a molecular tree C, if $x_{1,3}(C) > 0$ such that C contains the paths $P_{3,4} : u_1u_2 \cdots u_t$ and $P'_{4,3} : u_tu_{t+1} \cdots u_{s-1}u_s$, where $t \geq 2$, $s \geq 3$, and $t < s$, then a molecular tree C' can be obtained with $x_{1,3}(C') < x_{1,3}(C)$ such that $SO(C) < SO(C')$ and $SO_{red}(C) < SO_{red}(C')$, where C and C' have the same degree sequence.*

Proof. Suppose that $uv \in E(C)$ such that $d_u = 1$ and $d_v = 3$. We prove the result by considering two possible cases.
Case I. $s \leq 4$.

Note that one of the paths $P_{4,3}$ and $P'_{4,3}$ contains exactly one internal vertex and the other contains no internal vertex. Thus, without loss of generality it can be assumed that $t = 2$. If $s = 3$, then we take $C' = C - \{uv, u_1u_2, u_2u_3\} + \{u_1u_3, uu_2, u_2v\}$, and for $s = 4$, we take $C' = C - \{u_1u_2, u_3u_4, uv\} + \{u_1u_4, uu_2, u_3v\}$. In either case, we note that both C and C' have the same degree sequence, $x_{1,3}(C') < x_{1,3}(C)$, and

$$SO(C) = SO(C') + 5 + \sqrt{10} - 3\sqrt{2} - \sqrt{17} < SO(C')$$

$$SO_{red}(C) = SO_{red}(C') + \sqrt{13} - 1 - 2\sqrt{2} < SO_{red}(C'),$$

as required.
Case II. $s > 4$.

If $t = 2$ or $t = s - 1$, the result is proved in a fully analogous way as in Case I. In what follows, suppose that $2 < t < s - 2$. When $s = 5$ then ($t = 3$ and) we take $C' = C - \{u_2u_3, u_4u_5, uv\} + \{u_2u_5, u_3u, u_4v\}$, and otherwise (that is, if $s \geq 6$ then) we take $C' = C - \{u_2u_3, u_{t-1}u_t, u_{s-1}u_s, uv\} + \{u_2u_s, uu_t, u_{s-1}u_3, u_{t-1}v\}$. In either case, we observe that both C and C' have the same degree sequence, $x_{1,3}(C') < x_{1,3}(C)$, and

$$SO(C) = SO(C') + \sqrt{10} + 2\sqrt{5} - \sqrt{13} - \sqrt{17} < SO(C'),$$

$$SO_{red}(C) = SO_{red}(C') + \sqrt{10} - 1 - \sqrt{5} < SO_{red}(C'),$$

as desired. ■

Lemma 4. *Let C be a molecular tree with $xy, uv, wz \in E(C)$, where the vertices x, y, u, v, w, z are chosen in such a way that $d_u = 1$, $d_x = 3 = d_y$, $d_v = d_w = d_z = 4$, and w lies on one of the three paths $v - z$, $x - z$, $y - z$ paths, and that $x_{1,3}(C) = 0$. If $N_C(z) = \{w, z_1, z_2, z_3\}$ and $C' = C - \{xy, z_1z, z_2z, z_3z, uv\} + \{xu, uy, z_1u, z_2u, z_3v\}$ then $SO(C) < SO(C')$ and $SO_{red}(C) < SO_{red}(C')$, where C and C' have the same degree sequence.*

Proof. It can be easily observed that C and C' have the same degree sequence. Also, after elementary calculations, we arrive at $SO(C) = SO(C') + 7\sqrt{2} - 10 < SO(C')$ and $SO_{red}(C) = SO_{red}(C') + 5\sqrt{2} - 2\sqrt{13} < 0$. ■

Lemma 5. *Let C be a molecular tree with $uv, z'w, wz \in E(C)$, where the vertices $u, v, w, z, z' \in V(C)$ are chosen in such a way that $d_w = 2$ and $\min\{d_u, d_v, d_z, d_{z'}\} \geq 3$ provided that $d_u + d_v > d_z + d_{z'}$. If $C' = C - \{uv, z'w, wz\} + \{z'z, uw, wv\}$, then $SO(C) < SO(C')$ and $SO_{red}(C) < SO_{red}(C')$, where C and C' have the same degree sequence.*

Proof. We observe that both the trees C and C' have the same degree sequence and

$$\begin{aligned} SO(C) &= SO(C') + \sqrt{d_u^2 + d_v^2} + \sqrt{4 + d_{z'}^2} + \sqrt{4 + d_z^2} - \sqrt{4 + d_v^2} \\ &\quad - \sqrt{4 + d_u^2} - \sqrt{d_z^2 + d_{z'}^2} \\ &= SO(C') + I_1 \end{aligned}$$

and

$$\begin{aligned} SO_{red}(C) &= SO_{red}(C') + \sqrt{(d_u - 1)^2 + (d_v - 1)^2} + \sqrt{1 + (d_{z'} - 1)^2} + \sqrt{1 + (d_z - 1)^2} \\ &\quad - \sqrt{1 + (d_u - 1)^2} - \sqrt{1 + (d_v - 1)^2} - \sqrt{(d_z - 1)^2 + (d_{z'} - 1)^2} \\ &= SO_{red}(C') + I_2, \end{aligned}$$

where

$$I_1 = \sqrt{d_u^2 + d_v^2} + \sqrt{4 + d_{z'}^2} + \sqrt{4 + d_z^2} - \sqrt{4 + d_v^2} - \sqrt{4 + d_u^2} - \sqrt{d_z^2 + d_{z'}^2}$$

and

$$\begin{aligned} I_2 = &\sqrt{(d_u - 1)^2 + (d_v - 1)^2} + \sqrt{1 + (d_{z'} - 1)^2} + \sqrt{1 + (d_z - 1)^2} - \sqrt{1 + (d_u - 1)^2} \\ &- \sqrt{1 + (d_v - 1)^2} - \sqrt{(d_z - 1)^2 + (d_{z'} - 1)^2}. \end{aligned}$$

To complete the proof, it is enough to show that $I_1 < 0$ and $I_2 < 0$. Recall that $d_u + d_v \in \{7, 8\}$ and hence we consider two cases accordingly.

i) If $d_u + d_v = 8$ then $d_u = 4 = d_v$ and hence $d_z + d_{z'} \in \{6, 7\}$, and therefore we get $I_1 < 0$ and $I_2 < 0$

ii) If $d_u + d_v = 7$ then $d_u = 3$ and $d_v = 4$ (or $d_u = 4$ and $d_v = 3$) and hence $d_z = 3 = d_{z'}$ and thence we have $I_1 < 0$ and $I_2 < 0$.

■

Lemma 6. *Let C be a molecular tree with $uv, vw, xy \in E(C)$, where the vertices u, v, w, x, y are chosen in such a way that $d_u = 2 = d_v$, $d_w \geq 2$, and $\min\{d_x, d_y\} \geq 3$. If $C' = C - \{uv, vw, xy\} + \{uw, xv, vy\}$ then $SO(C) < SO(C')$ and $SO_{red}(C) < SO_{red}(C')$, where C and C' have the same degree sequence.*

Proof. Clearly, the degree sequences of C and C' is the same. Since $d_x, d_y \in \{3, 4\}$, we have

$$SO(C) = SO(C') + 2\sqrt{2} + \sqrt{d_x^2 + d_y^2} - \sqrt{4 + d_x^2} - \sqrt{4 + d_y^2} < SO(C')$$

and

$$\begin{aligned} SO_{red}(C) = SO_{red}(C') + \sqrt{2} + \sqrt{(d_x - 1)^2 + (d_y - 1)^2} \\ - \sqrt{1 + (d_x - 1)^2} - \sqrt{1 + (d_y - 1)^2} \\ < SO_{red}(C'). \end{aligned}$$

■

4. Main results

For $n \geq 4$, denote by C_{n,n_b} the collection of all n-vertex molecular trees with n_b branching vertices, where $n_b \leq \frac{1}{2}(n-2)$. As the path P_n is the unique graph in $C_{n,0}$, where $SO(P_n) = 2\sqrt{2}(n-3) + 2\sqrt{5}$ and $SO_{red}(P_n) = \sqrt{2}(n-3) + 2$, and C_1 (depicted in Figure 1) is the unique graph in $C_{4,1}$ (whose (reduced) Sombor index value is given in Table 1), in rest of the investigation we assume that $n > 4$ and $n_b \geq 1$. We also define the sub-classes C_p and C_q^* of C_{n,n_b} as follows:

$$C_p = \{C \in C_{n,n_b} : n_2(C) = 0,\ n_3(C) \geq 0\}, \tag{4.1}$$

$$C_q^* = \{C \in C_{n,n_b} : n_3(C) = 0,\ n_2(C) \geq 0\}. \tag{4.2}$$

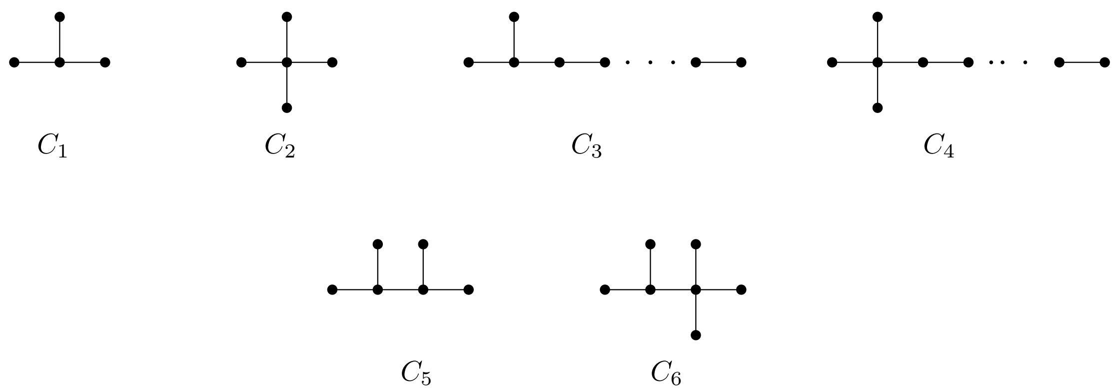

Figure 1. The molecular trees $C_1, C_2, \cdots, C_6$.

Lemma 7. *If C_b is a molecular tree with the maximum Sombor index (respectively, reduced Sombor index) over the class C_{n,n_b}, then either $C_b \in C_p$ or $C_b \in C_q^*$.*

Proof. Contrarily, assume that $C_b \in C_{n,n_b} \setminus (C_p \cup C_q^*)$. There must be vertices u and v in C_b with $d_u = 3$ and $d_v = 2$. Let $N_u(C_b) = \{u_1, u_2, u_3\}$ and $N_v(C_b) = \{v_1, v_2\}$, where v_2 and u_3 lie on the $u - v$ path. If $uv \in E(C)$ then we take $v_2 = u$ and $u_3 = v$, and also it possible that $u_3 = v_2$. If C' is the tree deduced

Table 1. The (reduced) Sombor indices of the trees $C_1, C_2, \cdots, C_6$.

	$SO(C_i)$	$SO_{red}(C_i)$
C_1	$3\sqrt{10}$	6
C_2	$4\sqrt{17}$	12
C_3	$2\sqrt{2}(n-5)+2\sqrt{10}+\sqrt{13}+\sqrt{5}$	$\sqrt{2}(n-5)+5+\sqrt{5}$
C_4	$2\sqrt{2}(n-6)+3(\sqrt{17}+\sqrt{5})$	$\sqrt{2}(n-6)+10+\sqrt{10}$
C_5	$4\sqrt{10}+3\sqrt{2}$	$2\sqrt{2}+8$
C_6	$2\sqrt{10}+3\sqrt{17}+5$	$\sqrt{13}+13$

from C by dropping the edges uu_1, uu_2 and adding two new edges vu_1, vu_2 in C, then $C' \in \mathcal{C}_{n,n_b}$ and (by keeping in mind Lemma 1, we have)

$$\begin{aligned}
SO(C_b) &= SO(C') + \sum_{i=1}^{3}\sqrt{9+d_{u_i}^2} + \sum_{j=1}^{2}\sqrt{4+d_{v_j}^2} - \sqrt{1+d_{u_3}^2} \\
&\quad - \sum_{i=1}^{2}\sqrt{16+d_{u_i}^2} - \sum_{j=1}^{2}\sqrt{16+d_{v_j}^2} \\
&< SO(C') + \sqrt{9+d_{u_3}^2} - \sqrt{1+d_{u_3}^2} \\
&\quad + \sum_{j=1}^{2}\left(\sqrt{4+d_{v_j}^2} - \sqrt{16+d_{v_j}^2}\right) \\
&\le SO(C') + \sum_{j=1}^{2}\left(\sqrt{4+d_{v_j}^2} - \sqrt{16+d_{v_j}^2}\right) + \sqrt{13} - \sqrt{5} \\
&\le SO(C') + 3\sqrt{5} + \sqrt{13} - 8\sqrt{2} < SO(C'),
\end{aligned}$$

which is contradicting our assumption concerning the choice of C_b.
Similarly, we have

$$\begin{aligned}
SO_{red}(C_b) &= SO_{red}(C') + \sum_{i=1}^{3}\sqrt{4+(d_{u_i}-1)^2} + \sum_{j=1}^{2}\sqrt{1+(d_{v_j}-1)^2} \\
&\quad - \sqrt{(d_{u_3}-1)^2} - \sum_{i=1}^{2}\sqrt{9+(d_{u_i}-1)^2} - \sum_{j=1}^{2}\sqrt{9+(d_{v_j}-1)^2} \\
&< SO_{red}(C') + \sqrt{4+(d_{u_3}-1)^2} - \sqrt{(d_{u_3}-1)^2} \\
&\quad + \sum_{j=1}^{2}\sqrt{1+(d_{v_j}-1)^2} - \sum_{j=1}^{2}\sqrt{9+(d_{v_j}-1)^2} \\
&\le SO_{red}(C') + \sum_{j=1}^{2}\sqrt{1+(d_{v_j}-1)^2} - \sum_{j=1}^{2}\sqrt{9+(d_{v_j}-1)^2} + \sqrt{5} - 1 \\
&\le SO_{red}(C') + \sqrt{5} + 2\sqrt{10} - 6\sqrt{2} - 1 < SO_{red}(C'),
\end{aligned}$$

a contradiction. ■

Lemma 8. *For $n_b > 1$, if C_b is the tree with the maximum Sombor index (respectively reduced Sombor index) in the class $\mathcal{C}_{n,n_b}$, then $x_{1,2}(C_b) = 0$.*

Proof. Contrariwise, assume that there is a path $P : v_1v_2 \cdots v_t$ in C_b, where $t \geq 3$ such that $d_{v_1} = 1$, $d_{v_t} > 2$ and $d_{v_j} = 2$ for all $2 \leq j \leq t-1$. Since $n_2(C_b) \geq 1$, by Lemma 7 we must have $d_{v_t} = 4$. Also, at least one of the neighbors of v_t different from v_{t-1} is non-pendent because $n_b > 1$. Take $w \in N_{C_b}(v_t) \setminus \{v_{t-1}\}$ such that $d_w \geq 2$. As $n_3(C_b) = 0$ by Lemma 7, we have $d_w \in \{2, 4\}$. If $C' = C_b - \{v_1v_2, v_{t-1}v_1, uw\} + \{v_1v_t, uv_2, v_{t-1}w\}$, then we have $C' \in \mathcal{C}_{n,n_b}$ and

$$SO(C_b) = SO(C') + \sqrt{5} - \sqrt{17} + \sqrt{16 + d_w^2} - \sqrt{4 + d_w^2} < SO(C'),$$

and

$$SO_{red}(C_b) = SO_{red}(C') + 1 - 3 + \sqrt{9 + (d_w - 1)^2} - \sqrt{1 + (d_w - 1)^2} < SO_{red}(C').$$

a contradiction.

■

For a non-trivial molecular tree C of order n, the following identities hold:

$$n = n_1(C) + n_2(C) + n_3(C) + n_4(C), \tag{4.3}$$

$$n_1(C) + 2n_2(C) + 3n_3(C) + 4n_4(C) = 2(n-1), \tag{4.4}$$

$$n_b = n_3(C) + n_4(C). \tag{4.5}$$

The results in the following lemma directly follows from Eqs (4.3)–(4.5).

Lemma 9. *For a molecular tree $C \in \mathcal{C}_{n,n_b}$, the following statements hold:*
(i) If $C \in \mathcal{C}_p$, then $n_1(C) = n - n_b$, $n_3(C) = 3n_b - n + 2$ and $n_4(C) = n - 2n_b - 2$.
(ii) If $C \in \mathcal{C}_q^*$, then $n_1(C) = 2n_b + 2$, $n_2(C) = n - 3n_b - 2$ and $n_4(C) = n_b$.
(iii) $C \in \mathcal{C}_p \cap \mathcal{C}_q^*$ if and only if $n_b = \frac{n-2}{3}$.

Lemma 10. *For a molecular tree C with the maximum Sombor index (respectively reduced Sombor index) over the class $\mathcal{C}_{n,n_b}$, $n_2(C) \geq 1$ if and only if $0 \leq n_b < \frac{n-2}{3}$ or $n \geq 3n_b + 3$.*

Proof. If $n_2(C) \geq 1$, then $n_3(C) = 0$ by Lemma 7 and hence $C \in \mathcal{C}_q^*$; now, by using the result $n_2(C) = n - 3n_b - 2$ of Lemma 9 it is deduced that $n_b < \frac{n-2}{3}$ or $n \geq 3n_b + 3$.
Conversely, suppose that $0 \leq n_b < \frac{n-2}{3}$ or $n \geq 3n_b + 3$ with $n_b \geq 0$. Contrarily, assume that $n_2(C) = 0$. From Eqs (4.3)–(4.5), it follows that $2n_b + n_4(C) = n - 2$, which together with the assumption $n \geq 3n_b + 3$ implies that $n_4(C) \geq n_b + 1$, which is a contradiction. ■

Note that C_2 and C_3 with $n = 5$ (see Figure 1) are the only molecular trees in $\mathcal{C}_{5,1}$, and it can be easily observed that $SO(C_2) > SO(C_3)$ (respectively $SO_{red}(C_2) > SO_{red}(C_3)$); see Table 1. For $n \geq 5$, we define the the following sub-classes of $\mathcal{C}_{n,n_b}$:
$B_0 = \{C \in \mathcal{C}_q^* : n_b = 1 \text{ and } x_{1,2}(C) = 1\}$,
$B_1 = \{C \in \mathcal{C}_q^* : 1 < n_b < \frac{n-1}{4} \text{ and } x_{1,2}(C) = 0 = x_{4,4}(C)\}$,
$B_2 = \{C \in \mathcal{C}_q^* : \frac{n-1}{4} \leq n_b < \frac{n-2}{3} \text{ and } x_{1,2}(C) = 0 = x_{2,2}(C)\}$,

$B_3 = \{C \in \mathcal{C}_p : \frac{n-2}{3} < n_b \leq \frac{3n-7}{8}$ and $x_{1,3}(C) = 0 = x_{3,3}(C)\}$,
$B_4 = \{C \in \mathcal{C}_p : \frac{3n-7}{8} < n_b \leq \frac{2n-6}{5}$ and $x_{1,3}(C) = 0 = x_{4,4}(C)$ and $x_{3,3} \neq 0\}$,
$B_5 = \{C \in \mathcal{C}_p : \frac{2n-6}{5} < n_b \leq \frac{n-2}{2}$ and $x_{4,4} = 0$ and $x_{3,3} = n_3(C) - 1\}$,
where $\mathcal{C}_p$ and $\mathcal{C}_q^*$ are defined in (4.1) and (4.2). For a molecular tree C, we have

$$\sum_{1 \leq j \leq 4;\ j \neq i} x_{i,j}(C) + 2x_{i,i}(C) = i \cdot n_i \quad \textit{where } i = 1, 2, 3, 4. \tag{4.6}$$

Theorem 1. *If $n \geq 6$ and $C \in \mathcal{C}_{n,1}$, then*
i) $SO(C) \leq 2\sqrt{2}(n-6) + 3\sqrt{5} + 3\sqrt{17}$,
ii) $SO_{red}(C) \leq \sqrt{2}(n-6) + 10 + \sqrt{10}$.
The equalities occur if and only if $C \cong B_0$.

Proof. Let $n > 5$ and $C_1 \in \mathcal{C}_{n,1}$ be a molecular tree with the maximum Sombor index (respectively reduced Sombor index). Let v be the unique branching vertex of C_1.
Claim 1. $d_v = 4$.

Contrariwise, suppose that $d_v = 3$. The constraint $n > 5$ ensures that there is a vertex u of degree 2 in C_1 which is adjacent to a pendent vertex, say w. Let C' be the new tree obtained from C_1 by deleting the edge uw and adding the new edge vw. Certainly, we have $C' \in \mathcal{C}_{n,1}$.
Note that

$$SO(C_1) = SO(C') + \sum_{z \in N_{C_1}(v)} \sqrt{9 + d_z^2} + \xi - \sum_{z \in N_{C_1}(v)} \sqrt{16 + d_z^2} - \sqrt{17} < SO(C'),$$

and

$$\begin{aligned} SO_{red}(C_1) &= SO_{red}(C') + \sum_{z \in N_{C_1}(v)} \sqrt{4 + (d_z - 1)^2} + \eta - \sum_{z \in N_{C_1}(v)} \sqrt{9 + (d_z - 1)^2} - 3. \\ &< SO_{red}(C'), \end{aligned}$$

which leads to the contradiction to our assumption concerning C_1, where

$$\xi = \begin{cases} \sqrt{5} & \text{if } uv \in V(C_1), \\ \sqrt{8} & \text{if } uv \notin V(C_1), \end{cases} \quad \text{and} \quad \eta = \begin{cases} 1 & \text{if } uv \in V(C_1), \\ \sqrt{2} & \text{if } uv \notin V(C_1). \end{cases}$$

Claim 2. The vertex v has exactly one non pendent neighbor.

Since $n \geq 6$, the vertex v has at least one non pendent neighbor. Contrarily assume that $P_1 : v_1v_2 \cdots v_rv$ and $P_2 : w_1w_2 \cdots w_sv$ are two paths in C_1 with $d_{v_1} = 1 = d_{w_1}$ and $d_{v_i} = 2 = d_{w_j}$ for $2 \leq i \leq r$ and $2 \leq j \leq s$. If $C' = C_1 - \{v_2v_1, v_rv\} + \{v_1v, v_rw_1\}$, then we have $C' \in \mathcal{C}_{n,1}$ and

$$SO(C_1) = SO(C') + \sqrt{4 + d_v^2} - \sqrt{1 + d_v^2} + \sqrt{5} - \sqrt{8} < SO(C'),$$

and

$$SO_{red}(C_1) = SO_{red}(C') + \sqrt{1 + (d_v - 1)^2} - \sqrt{(d_v - 1)^2} + 1 - \sqrt{2} < SO_{red}(C'),$$

a contradiction (where $d_v = 4$ by Claim 1).
Now, the desired result follows from Claims 1 and 2. ∎

Theorem 2. *If $C \in \mathcal{C}_{n,n_b}$ and $1 < n_b < \frac{n-1}{4}$, then*
(i) $SO(C) \leq 2\sqrt{2}(n-1) + 2\sqrt{17}(n_b+1) + 4\sqrt{5}(n_b-1) - 8\sqrt{2}n_b$,
(ii) $SO_{red}(C) \leq \sqrt{2}(n-4n_b-1) + 2\sqrt{10}(n_b-1) + 6(n_b+1)$,
and the equalities occur if and only if $C \cong B_1$.

Proof. Denote by C_b the molecular tree with the maximum Sombor index (respectively reduced Sombor index) in the class $\mathcal{C}_{n,n_b}$, for $1 < n_b < \frac{n-1}{4}$. Since $n_b < \frac{n-1}{4} < \frac{n-2}{3}$, Lemma 10 ensures that $n_2(C_b) > 0$, which together with Lemma 7 implies that $C_b \in \mathcal{C}_q^*$, and hence by Lemma 9(b) one has $n_1(C_b) = 2n_b + 2$, $n_2(C_b) = n - 3n_b - 2$ and $n_4(C_b) = n_b$. Because of the constraint $n_b > 1$, Lemma 8 guaranties that

$$x_{1,2}(C_b) = 0, \tag{4.7}$$

plugging it into (4.6) for $i = 1$, we get

$$x_{1,4}(C_b) = n_1(C_b) = 2n_b + 2. \tag{4.8}$$

Since $n_b < \frac{n-1}{4}$ or $4n_b < n-1$ which gives $n_4(C_b) - 1 = n_b - 1 < n - 3n_b - 2 = n_2(C_b)$ and therefore

$$n_4(C_b) \leq n_2(C_b). \tag{4.9}$$

We claim that $x_{2,2}(C_b) \neq 0$. Contrarily, assume that $x_{2,2}(C_b) = 0$. Then, (4.6) with $i = 2$ gives

$$x_{2,4}(C_b) = 2n_2(C_b). \tag{4.10}$$

Equations (4.3) and (4.4) implies that

$$n_1(C_b) - 2n_4(C_b) = 2 \tag{4.11}$$

Also, (4.6) with $i = 4$ yields

$$2x_{4,4}(C_b) = 4n_4(C_b) - x_{1,4}(C_b) - x_{2,4}(C_b) \tag{4.12}$$

Using (4.8)–(4.11) in (4.12), we have

$$2x_{4,4}(C_b) = 4n_4(C_b) - n_1(C_b) - 2n_2(C_b) \leq 4n_4(C_b) - n_1(C_b) - 2n_4(C_b) = -2,$$

a contradiction. Hence, the claim $x_{2,2}(C_b) \neq 0$ is true.

We also claim that

$$x_{4,4}(C_b) = 0. \tag{4.13}$$

Suppose to the contrary that $x_{4,4}(C_b) \neq 0$. Take $xy \in E(C_b)$ such that $d_x = d_y = 4$. Since $x_{2,2}(C_b) \neq 0$, take $uv, vw \in E(C_b)$ such that $d_u = d_v = 2$ and $d_w \geq 2$. If C' is the tree obtained by applying the transformation mentioned in the statement of Lemma 6, then Lemma 6 guaranties that $SO(C_b) < SO(C')$ and $SO_{red}(C_b) < SO_{red}(C')$, which is a contradiction to the definition of C_b. Therefore, $x_{4,4}(C_b) = 0$.

Now, by using Eqs (4.6)–(4.8) and (4.13), we get $x_{2,4}(C_b) = 2n_b - 2$ and $x_{2,2}(C_b) = n - 4n_b - 1$. Hence, $SO(C_b) = 2\sqrt{2}(n-1) + 2\sqrt{17}(n_b+1) + 4\sqrt{5}(n_b-1) - 8\sqrt{2}n_b$ and $SO_{red}(C_b) = \sqrt{2}(n - 4n_b - 1) + 2\sqrt{10}(n_b-1) + 6(n_b+1)$, which completes the proof. ■

Theorem 3. *If $C \in \mathcal{C}_{n,n_b}$ such that $\frac{n-1}{4} \leq n_b < \frac{n-2}{3}$, then*
i) $SO(C) \leq 4\sqrt{5}(n-3n_b-2) - 4\sqrt{2}(n-4n_b-1) + 2\sqrt{17}(n_b+1)$,
ii) $SO_{red}(C) \leq 2\sqrt{10}(n-3n_b-2) - 3\sqrt{2}(n-4n_b-1) + 6(n_b+1)$,
and the equalities occur if and only if $C \cong B_2$.

Proof. Denote by C_b the molecular tree with the maximum Sombor index (respectively reduced Sombor index) from the class $\mathcal{C}_{n,n_b}$ for $\frac{n-1}{4} \leq n_b < \frac{n-2}{3}$. By Lemma 10, the inequality $n_2(C_b) > 0$ holds for $n_b < \frac{n-2}{3}$ and ultimately we have $C_b \in \mathcal{C}_q^*$ or $n_3(C_b) = 0$ because of Lemma 7. The equations $n_1(C_b) = 2n_b + 2$, $n_2(C_b) = n - 3n_b - 2$ and $n_4(C_b) = n_b$ follow from (b) part of Lemma 9, and (4.7) and (4.8) hold by Lemma 8. Also, the inequality $n_2(C_b) \leq n_4(C_b) - 1$ is obtained from $\frac{n-1}{4} \leq n_b$. By using the method used in the proof of Theorem 2, we get $x_{2,2}(C_b) = 0$, $x_{2,4}(C_b) = 2n_2(C_b) = 2n - 6n_b - 4$ and $x_{4,4}(C_b) = n_b - 1 - n_2(C_b) = 4n_b - n + 1$. Hence, $C_b \cong B_2$ or $SO(C_b) = 4\sqrt{5}(n-3n_b-2) - 4\sqrt{2}(n-4n_b-1) + 2\sqrt{17}(n_b+1)$ and $SO_{red}(C_b) = 2\sqrt{10}(n-3n_b-2) - 3\sqrt{2}(n-4n_b-1) + 6(n_b+1)$, which completes the proof. ■

Theorem 4. *Let $C \in \mathcal{C}_{n,n_b}$ be the molecular tree such that $n_b = \frac{n-2}{3}$, then*
i) $SO(C) = \frac{2\sqrt{17}}{3}(n+1) + \frac{4\sqrt{2}}{3}(n-5)$,
ii) $SO_{red}(C) = 2(n+1) + \sqrt{2}(n-5)$.

Proof. The part (c) of Lemma 9 ensures that $C \in \mathcal{C}_p \cap \mathcal{C}_q^*$, which implies that $n_3(C) = 0 = n_2(C)$. Thus, $x_{1,4}(C) = n - n_b = \frac{2}{3}(n+1)$ and $x_{4,4}(C) = n_b - 1 = \frac{1}{3}(n-5)$. ■

Theorem 5. *If $C \in \mathcal{C}_{n,n_b}$ such that $\frac{n-2}{3} < n_b \leq \frac{3n-7}{8}$, then*
i) $SO(C) \leq \sqrt{17}(n-n_b) + 5(9n_b-3n+6) + 4\sqrt{2}(3n-8n_b-7)$,
ii) $SO_{red}(C) \leq 3(n-n_b) + \sqrt{13}(9n_b-3n+6) + 3\sqrt{2}(3n-8n_b-7)$,
and the equalities occur if and only if $C \cong B_3$.

Proof. Denote by C_b the molecular tree with the maximum Sombor index (respectively reduced Sombor index) in the class $\mathcal{C}_{n,n_b}$, for $\frac{n-2}{3} < n_b \leq \frac{3n-7}{8}$. By Lemma 10, we have $n_2(C_b) = 0$ (as $\frac{n-2}{3} < n_b$), which implies that $C_b \in \mathcal{C}_p$. Also, Lemma 9(a) guaranties that $n_1(C_b) = n - n_b$, $n_3(C_b) = 3n_b - n + 2$ and $n_4(C_b) = n - 2n_b - 2$. Now, the inequality $n_b \leq \frac{3n-7}{8}$ can be written as $6n_b - 2n + 5 < n - 2n_b - 2$, which leads us to the fact that $2n_3(C_b) + 1 \leq n_4(C_b)$. Using Lemmas 2–4 and keeping in mind the fact $n_4(C_b) \geq 2n_3(C_b) + 1$, we have

$$x_{1,3}(C_b) = 0 \tag{4.14}$$

and

$$x_{1,4}(C_b) = n - n_b. \tag{4.15}$$

Now, using Lemmas 2–4 and Eqs (4.6), (4.14) and (4.15), we have $x_{3,3}(C_b) = 0$, $x_{3,4}(C_b) = 3n_3(C_b) = 9n_b - 3n + 6$, $x_{4,4}(C_b) = n_4(C_b) - 2n_3(C_b) - 1 = 3n - 8n_b - 7$. Hence, $SO(C_b) = \sqrt{17}(n-n_b) + 5(9n_b - 3n + 6) + 4\sqrt{2}(3n - 8n_b - 7)$, and $SO_{red}(C_b) = 3(n-n_b) + \sqrt{13}(9n_b - 3n + 6) + 3\sqrt{2}(3n - 8n_b - 7)$. This completes the proof. ■

Theorem 6. *If $C \in \mathcal{C}_{n,n_b}$ such that $\frac{3n-7}{8} < n_b \leq \frac{2n-6}{5}$, then*
i) $SO(C) \leq \sqrt{17}(n-n_b) + 3\sqrt{2}(8n_b-3n+7) + 5(3n-7n_b-8)$,
ii) $SO_{red}(C) \leq 3(n-n_b) + 2\sqrt{2}(8n_b-3n+7) + \sqrt{13}(3n-7n_b-8)$,
and the equalities occur if and only if $C \cong B_4$.

Proof. Denote by C_b the molecular tree with the maximum Sombor index (respectively reduced Sombor index) from the class C_{n,n_b} for $\frac{3n-7}{8} < n_b \leq \frac{2n-6}{5}$. By using Lemma 10 it is easy to check that $n_2(C_b) = 0$ as $\frac{n-2}{3} < \frac{3n-7}{8} < n_b$, which implies that $C_b \in C_p$ and further (a) part of Lemma 9 concludes that $n_1(C_b) = n - n_b$, $n_3(C_b) = 3n_b - n + 2$ and $n_4(C_b) = n - 2n_b - 2$. Note that $n_b \leq \frac{2n-6}{5}$ can be easily written as $3n_b - n + 4 \leq n - 2n_b - 2$, which leads us to the fact $n_3(C_b) + 2 \leq n_4(C_b)$.

From Lemmas 2–4 it is clear that we have to place the vertices as described in the proof of Theorem 5. Keeping in mind the fact $2n_3(C_b)+1 > n_4(C_b) \geq n_3(C_b)+2$ and Eqs (4.6), (4.14) and (4.15), we have $x_{3,3}(C_b) = 2n_3(C_b)+1-n_4(C_b) = 8n_b-3n+7$, $x_{3,4}(C_b) = n_3(C_b)+2+2(n_4(C_b)-(n_3(C_b)+2)) = 3n - 7n_b - 8$ and $x_{4,4}(C_b) = 0$. Hence, $SO(C_b) = \sqrt{17}(n - n_b) + 3\sqrt{2}(8n_b - 3n + 7) + 5(3n - 7n_b - 8)$ and $SO_{red}(C_b) = 3(n - n_b) + 2\sqrt{2}(8n_b - 3n + 7) + \sqrt{13}(3n - 7n_b - 8)$, which completes the proof. ■

Theorem 7. *If $C \in C_{n,n_b}$ such that $\frac{2n-6}{5} < n_b \leq \frac{n-2}{2}$, then*
i) $SO(C) \leq (5 + 3\sqrt{17})(n - 2n_b - 2) - \sqrt{10}(2n - 5n_b - 6) - 3\sqrt{2}(n - 3n_b - 1)$,
ii) $SO_{red}(C) \leq (5n - 8n_b - 6) + \sqrt{13}(n - 2n_b - 2) - 2\sqrt{2}(n - 3n_b - 1)$,
and the equalities occur if and only if $C_b \cong B_5$.

Proof. Denote by C_b the molecular tree with the maximum Sombor index (respectively reduced Sombor index) from the class C_{n,n_b} for $\frac{2n-6}{5} < n_b \leq \frac{n-2}{2}$. By using Lemma 10 it is easy to check that $n_2(C_b) = 0$ as $\frac{n-2}{3} < \frac{2n-6}{5} < n_b$, which implies that $C_b \in C_p$ and further (a) part of Lemma 9 concludes that $n_1(C_b) = n - n_b$, $n_3(C) = 3n_b - n + 2$ and $n_4(C_b) = n - 2n_b - 2$. Note that $n_b > \frac{2n-6}{5}$ can be easily written as $3n_b - n + 4 > n - 2n_b - 2$, which leads us to the fact $n_3(C_b) + 2 > n_4(C_b)$. From Lemmas 2–4 it is clear that we have to place the vertices of degree 4 between the pendent vertices and the vertices of degree 3. The fact $n_3(C_b) + 2 > n_4(C_b)$ gives the result

$$x_{1,4}(C_b) = 3n_4(C_b) = 3n - 6n_b - 6, \tag{4.16}$$

and

$$x_{1,3}(C_b) = 5n_b - 2n + 6. \tag{4.17}$$

Now, using (4.6), (4.16) and (4.17), we have $x_{3,3}(C_b) = n_3(C_b) - 1 = 3n_b - n + 1$, $x_{3,4}(C_b) = n_4(C_b) = n-2n_b-2$ and $x_{4,4}(C_b) = 0$. Hence, $SO(C_b) = (5+3\sqrt{17})(n-2n_b-2)-\sqrt{10}(2n-5n_b-6)-3\sqrt{2}(n-3n_b-1)$ and $SO_{red}(C_b) = (5n - 8n_b - 6) + \sqrt{13}(n - 2n_b - 2) - 2\sqrt{2}(n - 3n_b - 1)$, which completes the proof. ■

Denote by $C^*_{n,q}$ the class of all n-vertex molecular trees, where q is the number of vertices of degree 2. Next, we are going to obtain the upper bounds for the molecular trees with respect to Sombor index and reduced Sombor index from the collection of molecular trees $C^*_{n,q}$ for $0 \leq q \leq n - 2$. It is obvious that the path graph P_n is the unique graph for $q = n - 2$, and there does not exist any graph corresponding to the value $q = n - 3$ in the collection $C^*_{n,q}$. Hence, we proceed with the assumption that $0 \leq q \leq n - 4$.

Lemma 11. *If the molecular tree $C \in C^*_{n,q}$ is the tree with the maximum Sombor index (respectively reduced Somber index) , then $n_3(C) \leq 2$.*

Proof. Suppose contrarily that $n_3(C) > 2$, and there are vertices u, w and z of degree 3 such that w is located on the unique $u - z$ path. Consider $N_z(C) = \{z_1, z_2, z_3\}$ with the assumption that the vertex z_3 lies on the $u - z$ path in C (z_3 may coincide with w). Now, a tree C' can be obtained from the collection $C^*_{n,q}$ such as $C' = C - \{zz_1, zz_2\} + \{uz_1, wz_2\}$, which gives the following result:

$$SO(C) \;=\; SO(C') + \sum_{x \in N_C(u)} \sqrt{d_x^2 + 9} + \sum_{y \in N_C(w)} \sqrt{d_y^2 + 9}$$

$$
\begin{aligned}
& + \sum_{i=1}^{3} \sqrt{d_{z_i}^2 + 9} - \sum_{x \in N_C(u)} \sqrt{d_x^2 + 16} - \sum_{y \in N_C(w)} \sqrt{d_y^2 + 16} \\
& - \sum_{i=1}^{2} \sqrt{d_{z_i}^2 + 16} - \sqrt{d_{z_3}^2 + 1} \\
< \; & SO(C') + \sum_{x \in N_C(u)} \sqrt{d_x^2 + 9} + \sum_{i=1}^{3} \sqrt{d_{z_i}^2 + 9} \\
& - \sum_{x \in N_C(u)} \sqrt{d_x^2 + 16} - \sum_{i=1}^{2} \sqrt{d_{z_i}^2 + 16} - \sqrt{d_{z_3}^2 + 1} \\
\leq \; & SO(C') + 5(5) - 20\sqrt{2} + \sqrt{10} - \sqrt{2} < SO(C'),
\end{aligned}
$$

a contradiction for the chosen C.
Similarly

$$
\begin{aligned}
SO_{red}(C) \; = \; & SO_{red}(C') + \sum_{x \in N_C(u)} \sqrt{(d_x - 1)^2 + 4} + \sum_{y \in N_C(w)} \sqrt{(d_y - 1)^2 + 4} \\
& + \sum_{i=1}^{3} \sqrt{(d_{z_i} - 1)^2 + 4} - \sum_{x \in N_C(u)} \sqrt{(d_x - 1)^2 + 9} \\
& - \sum_{y \in N_C(w)} \sqrt{(d_y - 1)^2 + 9} - \sum_{i=1}^{2} \sqrt{(d_{z_i} - 1)^2 + 9} - \sqrt{(d_{z_3} - 1)^2} \\
< \; & SO_{red}(C') + 5\sqrt{13} - 15\sqrt{2} + 2 < SO_{red}(C'),
\end{aligned}
$$

which also leads to a contradiction. ■

Lemma 12. *If $C \in C^*_{n,q}$, then*
i) $n_3(C) = 0$ if and only if $n - q - 2 \equiv 0$ (mod 3), $n_4(C) = \frac{n-q-2}{3}$ and
$n_1(C) = \frac{2}{3}(n - q + 1)$,
ii) $n_3(C) = 1$ if and only if $n - q - 1 \equiv 0$ (mod 3), $n_4(C) = \frac{n-q-4}{3}$ and
$n_1(C) = \frac{2}{3}(n - q - 1) + 1$,
iii) $n_3(C) = 2$ if and only if $n - q \equiv 0$ (mod 3), $n_4(C) = \frac{n-q-6}{3}$ and
$n_1(C) = \frac{2}{3}(n - q)$.

Proof. The following equation can be drawn by using Eqs (4.3) and (4.4):

$$n_1(C) = n_3(C) + 2n_4(C) + 2. \tag{4.18}$$

Now, using Eqs (4.3) and (4.18), we get

$$n - q - 2 - 2n_3(C) = 3n_4(C) \tag{4.19}$$

or

$$n - q - 2 - 2n_3(C) \equiv 0(mod3). \tag{4.20}$$

By solving the Eqs (4.4) and (4.18) for the values of $n_1(C)$ and $n_4(C)$, we get

$$n_1(C) = \frac{2n - 2q + 2 - n_3(C)}{3}, \tag{4.21}$$

and

$$n_4(C) = \frac{n - q - 2 - 2n_3(C)}{3}. \tag{4.22}$$

The required results are directly followed by Eqs (4.20)–(4.22). ■

Lemma 13. *If $C \in C^*_{n,q}$ is the tree with the maximum Sombor index (respectively reduced Somber index) with $n-4 \leq q \leq n-5$, then $x_{1,2}(C) \leq 1$.*

Proof. Note that there is a unique branching vertex (say) u in C with the fact that $d_u = 3$ if $q = n-4$, and $d_u = 4$ if $q = n-5$. Let us assume that, for $l, m \geq 3$, there are paths $u_1u_2\cdots u_lu$ and $u'_1u'_2\cdots u'_mu$ in C such that $d_{u_i} = 2 = d_{u'_j}$ for all $2 \leq i \leq l$ and $2 \leq j \leq m$, and $d_{u_1} = 1 = d_{u'_1}$. If a tree C' in the class $C^*_{n,q}$ is chosen as $C' = C - \{u_{l-1}u_l\} + \{u_{l-1}u'_1\}$, then

$$SO(C) = SO(C') + \sqrt{4 + d_u^2} - \sqrt{1 + d_u^2} + \sqrt{5} - 2\sqrt{2},$$

and

$$SO_{red}(C) = SO_{red}(C') + \sqrt{1 + (d_u - 1)^2} - \sqrt{(d_u - 1)^2 + 1} - \sqrt{2},$$

by using the fact $d_u = 3$ or $d_u = 4$ in the above mentioned results it can easily be checked that $SO(C) < SO(C')$ and $SO_{red}(C) < SO_{red}(C')$, which is a contradiction. ■

Lemma 14. *If $C \in C^*_{n,q}$ is the tree with the maximum Sombor index (respectively reduced Somber index) such that $q \leq n-6$, then $x_{1,2}(C) = 0$.*

Proof. The results can be proved by using the same process as done in Lemma 8. ■

Note that $C^*_{4,0}$ and $C^*_{5,0}$ contain unique trees C_1 and C_2, respectively, with the Sombor and reduced Sombor index values given in Table 1. Further more, by using Lemma 13 it can be observed that C_5 and C_6 are the molecular trees with maximum (reduced) Somber index values (given in Table 1) among the graphs in $C^*_{6,0}$ and $C^*_{7,0}$, respectively. Among all the molecular trees $C^*_{n,q}$, where $q \geq 1$, If we consider $C_3 = \{C \in C^*_{n,q} : x_{1,3}(C) = 2, x_{1,2}(C) = 1, x_{2,3}(C) = 1, x_{2,2}(C) = n-5\}$ and $C_4 = \{C \in C^*_{n,q} : x_{1,4}(C) = 3, x_{1,2}(C) = 1, x_{2,4}(C) = 1, x_{2,2}(C) = n-6\}$ (given in Figure 1), the following result is observed:

Theorem 8. *For the molecular tree $C \in C^*_{n,q}$, where $n \geq 5$, the following results hold:*
a) If $C \in C^*_{n,n-4} \setminus C_3$, then $SO(C) < SO(C_3)$.
b) If $C \in C^*_{n,n-5} \setminus C_4$, then $SO(C) < SO(C_4)$.

Proof. Using Lemma 13, it can be concluded that C_3 among the class $C^*_{n,n-4}$ and C_4 among $C^*_{n,n-5}$, respectively, contain the maximum (reduced) Sombor index value (given in Table 1), which completes the proof. ■

Consider the following subsets of $C^*_{n,q}$:
$Q_0 = \{C \in C^*_{n,q}$: $q < n-5$ and $n_3(C) = 0$ such that $x_{1,4}(C) = \frac{2}{3}(n-q+1)$ and $x_{2,2}(C) = 0$ whenever $x_{4,4}(C) \neq 0\}$,
$Q_1 = \{C \in C^*_{n,q}$: $q < n-5$ and $n_3(C) = 1$ such that $x_{1,2}(C) = 0$ and $x_{1,3}(C) \neq 0$ implies that there does not exist $P_{4,4}$ in C moreover if $x_{2,j}(C) \neq 0$ for $2 \leq j \leq 3$, then $x_{4,4}(C) = 0\}$,
$Q_2 = \{C \in C^*_{n,q}$: $n_3(C) = 2$ such that $x_{1,2}(C) = 0$, $x_{1,3}(C) \neq 0 \Rightarrow P_{4,4} = 0$ and $P_{3,3} \neq 0$, and whenever $x_{1,3}(C) = 0$ along with $P_{3,3} \neq 0$, then $P_{4,4} = 0$, furthermore $x_{2,i}(C) \neq 0 \Rightarrow x_{j,k} = 0$, where $2 \leq i \leq 3$ and $3 \leq j,k \leq 4\}$.

Theorem 9. *Let $C \in C^*_{n,q}$ for $q < n-5$ such that $n_3(C) = 0$. Then*

$$SO(C) \leq \begin{cases} \frac{2\sqrt{17}}{3}(n-q+1) + \frac{4\sqrt{2}}{3}(n-4q-5) + 4\sqrt{5}q & \text{if } q < \frac{n-5}{4}, \\ \frac{2\sqrt{17}}{3}(n-q+1) + \frac{4\sqrt{5}}{3}(n-q-5) - \frac{2\sqrt{2}}{3}(n-4q-5) & \text{if } q \geq \frac{n-5}{4}. \end{cases}$$

And

$$SO_{red}(C) \leq \begin{cases} \sqrt{2}(n-4q-5) + 2(n-q+1) + 2\sqrt{10}q & \text{if } q < \frac{n-5}{4}, \\ 2(n-q+1) + \frac{2\sqrt{10}}{3}(n-q-5) - \frac{\sqrt{2}}{3}(n-4q-5) & \text{if } q \geq \frac{n-5}{4}. \end{cases}$$

Equalities hold if and only if $C \in Q_0$.

Proof. Denote by C_{q_0} the molecular tree having maximum Sombor index (or reduced Sombor index) among the collection $C^*_{n,q}$ such that $n_3(C_{q_0}) = 0$. By using Lemma 12 it follows that $n-q-2 \equiv 0 \pmod 3$, $n_4(C_{q_0}) = \frac{n-q-2}{3}$ and $n_1(C_{q_0}) = \frac{2}{3}(n-q+1)$. The vertices of degree 2 are to be placed according to the conditions proved in Lemmas 6 and 14, that is all the pendent vertices are to be attached to the vertices of degree 4 i.e., Lemma 14 concludes that

$$x_{1,2}(C_{q_0}) = 0, \tag{4.23}$$

which implies that

$$x_{1,4}(C_{q_0}) = \frac{2}{3}(n-q+1). \tag{4.24}$$

Further more, the vertices of degree 2 are to be placed between the vertices of degree 4 in such a way that if there is an edge connecting the vertices of degree 4, then no two vertices of degree 2 are adjacent. The above discussion leads us to the fact that $C_{q_0} \in Q_0$. Now the following two cases arise here:
Case I. $n_2(C_{q_0}) < n_4(C_{q_0}) - 1$ or $q < \frac{n-5}{4}$.

In this case, Lemma 6 implies that

$$x_{2,2}(C_{q_0}) = 0. \tag{4.25}$$

By using (4.6), (4.23)–(4.25), we have $x_{2,4}(C_{q_0}) = 2q$ and $x_{4,4}(C_{q_0}) = \frac{n-4q-5}{3}$. Hence, $SO(C_{q_0}) = \frac{2\sqrt{17}}{3}(n-q+1) + \frac{4\sqrt{2}}{3}(n-4q-5) + 4\sqrt{5}q$ and $SO_{red}(C_{q_0}) = \sqrt{2}(n-4q-5) + 2(n-q+1) + 2\sqrt{10}q$.
Case II. $n_2(C_{q_0}) \geq n_4(C_{q_0}) - 1$ or $q \geq \frac{n-5}{4}$.

In this case, by Lemma 6, we have

$$x_{4,4}(C_{q_0}) = 0. \tag{4.26}$$

Using (4.6), (4.23)–(4.26), we get $x_{2,2}(C_{q_0}) = \frac{4q-n+5}{3}$ and $x_{2,4}(C_{q_0}) = 2(n_4(C_{q_0}) - 1) = \frac{2}{3}(n-q-5)$. Hence, $SO(C_{q_0}) = \frac{2\sqrt{17}}{3}(n-q+1) + \frac{4\sqrt{5}}{3}(n-q-5) - \frac{2\sqrt{2}}{3}(n-4q-5)$ and $SO_{red}(C_{q_0}) = 2(n-q+1) + \frac{2\sqrt{10}}{3}(n-q-5) - \frac{\sqrt{2}}{3}(n-4q-5)$, which completes the proof. ■

Theorem 10. *Let $C \in C^*_{n,q}$ such that $n_3(C) = 1$. Then*

$$SO(C) \leq \begin{cases} 2\sqrt{10} + 3\sqrt{17} + 5 & \text{if } q = 0 \text{ and } n = 7, \\ 2\sqrt{2}(q-1) + 2\sqrt{5} + 2\sqrt{10} + 3\sqrt{17} + \sqrt{13} & \text{if } q = n - 7 \geq 1, \\ 6\sqrt{17} + \sqrt{10}(\sqrt{10} + 1) & \text{if } q = 0 \text{ and } n = 10, \\ 6\sqrt{17} + 5 + 2\sqrt{5} + \sqrt{13} + \sqrt{10} & \text{if } q = 1 \text{ and } n = 11, \\ 2\sqrt{2}(q-2) + 6\sqrt{17} + 4\sqrt{5} + 2\sqrt{13} + \sqrt{10} & \text{if } q \geq 2 \text{ and } n - q = 10, \\ (2\sqrt{5} - 5)q + 9\sqrt{17} + 15 & \text{if } q \leq 2 \text{ and } n - q = 13, \\ (2\sqrt{2})(q-3) + 9\sqrt{17} + 3(2\sqrt{5} + \sqrt{13}) & \text{if } q > 2 \text{ and } n - q = 13, \\ \frac{\sqrt{17}}{3}(2n - 2q + 1) + 4\sqrt{5}q & \\ +\frac{4\sqrt{2}}{3}(n - 4q - 13) + 15 & \text{if } q < \frac{n-13}{4}, \\ \frac{\sqrt{17}}{3}(2n - 2q + 1) + \frac{2\sqrt{5}}{3}(n + 2q - 13) & \\ +\frac{\sqrt{13}}{3}(4q - n + 13) + \frac{5}{3}(n - 4q - 4) & \text{if } \frac{n-13}{4} \leq q < \frac{n-4}{3}, \\ \frac{\sqrt{17}}{3}(2n - 2q + 1) + \frac{2\sqrt{2}}{3}(4q - n + 4) & \\ +\frac{2\sqrt{5}}{3}(2n - 2q - 15) + 3\sqrt{13} & \text{if } q \geq \frac{n-4}{3}. \end{cases}$$

And

$$SO_{red}(C) \leq \begin{cases} \sqrt{13}(\sqrt{13} + 1) & \text{if } q = 0 \text{ and } n = 7, \\ \sqrt{2}(q-1) + \sqrt{10} + \sqrt{5} + 13 & \text{if } q = n - 7 \geq 1, \\ 20 + 2\sqrt{13} & \text{if } q = 0 \text{ and } n = 10, \\ 20 + \sqrt{13} + \sqrt{10} + \sqrt{5} & \text{if } q = 1 \text{ and } n = 11, \\ \sqrt{2}(q-2) + 20 + 2\sqrt{10} + 2\sqrt{5} & \text{if } q \geq 2 \text{ and } n - q = 10, \\ \sqrt{13}(3 - q) + 27 + \sqrt{10}q & \text{if } q \leq 2 \text{ and } n - q = 13, \\ \sqrt{2}(q-3) + 27 + 3(\sqrt{5} + \sqrt{10}) & \text{if } q > 2 \text{ and } n - q = 13, \\ (2n - 2q + 1) + 2\sqrt{10}q & \\ +\sqrt{2}(n - 4q - 13) + 3\sqrt{13} & \text{if } q < \frac{n-13}{4}, \\ (2n - 2q + 1) + \frac{\sqrt{10}}{3}(n + 2q - 13) & \\ +\frac{\sqrt{5}}{3}(4q - n + 13) + \frac{\sqrt{13}}{3}(n - 4q - 4) & \text{if } \frac{n-13}{4} \leq q < \frac{n-4}{3}, \\ (2n - 2q + 1) + \frac{\sqrt{2}}{3}(4q - n + 4) & \\ +\frac{\sqrt{10}}{3}(2n - 2q - 15) + 3\sqrt{13} & \text{if } q \geq \frac{n-4}{3}. \end{cases}$$

Equalities hold if and only if $C \in Q_1$.

Proof. If C_{q_1} denotes the molecular tree having maximum Sombor index (or reduced Sombor index) among the collection $C^*_{n,q}$, where $n_3(C_{q_1}) = 1$, then by using Lemma 12 we have $n - q - 1 \equiv 0 \pmod 3$, $n_1(C_{q_1}) = \frac{2n-2q+1}{3}$, $n_4(C_{q_1}) = \frac{n-q-4}{3}$. Note that Lemmas 2, 14 and 5 show that $C_{q_1} \in Q_1$. This implies that

$$x_{1,2}(C_{q_1}) = 0, \tag{4.27}$$

and the vertices of degree 4 are to be placed in the three neighbors of the vertex of degree 3 in such a way that if a pendent vertex is present in C_{q_1} which is adjacent to the vertex of degree 3, then there must not exists a $P_{4,4}$ path in C_{q_1}. The following cases are possible:

Case 1. $n_4(C_{q_1}) = 1$

Subcase 1.1. $q = 0$.

In this case $n = 7$, $x_{2,j}(C_{q_1}) = 0$ for all $1 \leq j \leq 4$, $x_{3,4}(C_{q_1}) = 1$, $x_{1,3}(C_{q_1}) = 2$ and $x_{1,4}(C_{q_1}) = 3$. The graph here is C_6 given in Figure 1 with (reduced) Sombor index value given in Table 1.

Subcase 1.2. $q > 0$.

This holds for $n \geq 8$, by keeping in mind the Lemmas 5 and 6, and using the results in Eqs (4.6) and (4.27), we have $x_{3,4}(C_{q_1}) = 0$, $x_{2,3}(C_{q_1}) = 1 = x_{2,4}(C_{q_1})$, $x_{1,3}(C_{q_1}) = 2$, $x_{1,4}(C_{q_1}) = 3$ and $x_{2,2}(C_{q_1}) = q-1$. Hence, $SO(C_{q_1}) = 2\sqrt{2}(q-1) + 2\sqrt{5} + 2\sqrt{10} + 3\sqrt{17} + \sqrt{13}$ and $SO_{red} = \sqrt{2}(q-1) + \sqrt{10} + \sqrt{5} + 13$.

Case 2. $n_4(C_{q_1}) = 2$.

Subcase 2.1. $q = 0$

In this case we have $n = 10$, where Lemma 2 shows that

$$x_{3,4}(C_{q_1}) = 2. \tag{4.28}$$

By using Eqs (4.6), (4.27) and (4.28), we have $x_{1,3}(C_{q_1}) = 1$ and $x_{1,4}(C_{q_1}) = 6$, which gives $SO(C_{q_1}) = 6\sqrt{17} + \sqrt{10}(\sqrt{10} + 1)$ and $SO_{red}(C_{q_1}) = 20 + 2\sqrt{13}$.

Subcase 2.2. $q = 1$

Here $n = 11$, By using Eqs (4.6), (4.27), we have $x_{1,3}(C_{q_1}) = 1$, $x_{1,4}(C_{q_1}) = 6$ and $x_{3,4}(C_{q_1}) = 1 = x_{2,3}(C_{q_1}) = x_{2,4}(C_{q_1})$, which gives $SO(C_{q_1}) = 6\sqrt{17} + 5 + 2\sqrt{5} + \sqrt{13} + \sqrt{10}$ and $SO_{red}(C_{q_1}) = 20 + \sqrt{13} + \sqrt{10} + \sqrt{5}$.

Subcase 2.3. $q \geq 2$

This holds for $n \geq 12$, and by keeping in mind the Lemmas 5, 6 and the results in Eqs (4.6) and (4.27), we have $x_{1,3}(C_{q_1}) = 1$, $x_{1,4}(C_{q_1}) = 6$, $x_{2,4}(C_{q_1}) = 2 = x_{2,3}(C_{q_1})$ and $x_{2,2}(C_{q_1}) = q - 2$. Hence, $SO(C_{q_1}) = 2\sqrt{2}(q-2) + 6\sqrt{17} + 4\sqrt{5} + 2\sqrt{13} + \sqrt{10}$ and $SO_{red}(C_{q_1}) = \sqrt{2}(q-2) + 20 + 2\sqrt{10} + 2\sqrt{5}$.

Case 3. $n_4(C_{q_1}) = 3$

Lemma 2 gives

$$x_{1,3}(C_{q_1}) = 0. \tag{4.29}$$

Subcase 3.1. $q \leq 2$

Again Lemmas 5, 6 and the Eqs (4.6), (4.27) and (4.29) imply that, $x_{1,4}(C_{q_1}) = 9$, $x_{2,3}(C_{q_1}) = x_{2,4}(C_{q_1}) = q$, $x_{2,2}(C_{q_1}) = 0 = x_{4,4}(C_{q_1})$ and $x_{3,4}(C_{q_1}) = 3-q$. Hence, $SO(C_{q_1}) = (2\sqrt{5}-5)q + 9\sqrt{17} + 15$ and $SO_{red}(C_{q_1}) = \sqrt{13}(3-q) + 27 + \sqrt{10}q$.

Subcase 3.2. $q > 2$

Here $x_{1,4}(C_{q_1}) = 9$, $x_{2,3}(C_{q_1}) = x_{2,4}(C_{q_1}) = 3$, $x_{2,2}(C_{q_1}) = q - 3$ and $x_{3,4}(C_{q_1}) = 0$ are obtained by using Lemmas 5, 6 and the Eqs (4.6), (4.27) and (4.29). Hence, $SO(C_{q_1}) = (2\sqrt{2})(q-3) + 9\sqrt{17} + 3(2\sqrt{5} + \sqrt{13})$ and $SO_{red}(C_{q_1}) = \sqrt{2}(q-3) + 27 + 3(\sqrt{5} + \sqrt{10})$.

Case 4. $n_4(C_{q_1}) > 3$
Subcase 4.1. $q < \frac{n-13}{4}$

It is easy to check that $q < \frac{n-13}{4}$ implies that $q < n_4(C_{q_1}) - 3$ or $q < x_{4,4}(C_{q_1})$. Lemmas 5, 6 and the Eqs (4.6), (4.27) and (4.29) follow the results $x_{2,2}(C_{q_1}) = 0 = x_{2,3}(C_{q_1})$, $x_{2,4}(C_{q_1}) = q$, $x_{3,4}(C_{q_1}) = 3$, $x_{1,4}(C_{q_1}) = \frac{2n-2q+1}{3}$ and $x_{4,4}(C_{q_1}) = \frac{n-4q-13}{3}$. Hence, $SO(C_{q_1}) = \frac{\sqrt{17}}{3}(2n-2q+1) + 4\sqrt{5}q + \frac{4\sqrt{2}}{3}(n-4q-13) + 15$ and $SO_{red}(C_{q_1}) = (2n-2q+1) + 2\sqrt{10}q + \sqrt{2}(n-4q-13) + 3\sqrt{13}$.

Subcase 4.2. $\frac{n-13}{4} \leq q < \frac{n-4}{3}$

It gives $n_4(C_{q_1}) - 3 \leq q < n_4$, which implies that

$$x_{4,4}(C_{q_1}) = 0, \tag{4.30}$$

by keeping in mind the Lemmas 5, 6 and using the Eqs (4.27), (4.29) and (4.30) in (4.6), we have $x_{2,2}(C_{q_1}) = 0$, $x_{2,3}(C_{q_1}) = \frac{4q-n+13}{3}$, $x_{2,4}(C_{q_1}) = \frac{n+2q-13}{3}$, $x_{1,4}(C_{q_1}) = \frac{2n-2q+1}{3}$ and $x_{3,4}(C_{q_1}) = \frac{n-4q-4}{3}$. Hence, $SO(C_{q_1}) = \frac{\sqrt{17}}{3}(2n-2q+1) + \frac{2\sqrt{5}}{3}(n+2q-13) + \frac{\sqrt{13}}{3}(4q-n+13) + \frac{5}{3}(n-4q-4)$ and $SO_{red}(C_{q_1}) = (2n-2q+1) + \frac{\sqrt{10}}{3}(n+2q-13) + \frac{\sqrt{5}}{3}(4q-n+13) + \frac{\sqrt{13}}{3}(n-4q-4)$.

Subcase 4.3. $q \geq \frac{n-4}{3}$

This imply that $q \geq n_4(C)$, and Lemmas 5 and 6 conclude that

$$x_{3,4}(C_{q_1}) = 0, \tag{4.31}$$

and using the Eqs (4.27), (4.29)–(4.31) in (4.6), we have $x_{1,4}(C_{q_1}) = \frac{2n-2q+1}{3}$, $x_{2,2}(C_{q_1}) = \frac{4q-n+4}{3}$, $x_{2,3}(C_{q_1}) = 3$ and $x_{2,4}(C_{q_1}) = \frac{2n-2q-15}{3}$. Hence, $SO(C_{q_1}) = \frac{\sqrt{17}}{3}(2n-2q+1) + \frac{2\sqrt{2}}{3}(4q-n+4) + \frac{2\sqrt{5}}{3}(2n-2q-15) + 3\sqrt{13}$ and $SO_{red}(C_{q_1}) = (2n-2q+1) + \frac{\sqrt{2}}{3}(4q-n+4) + \frac{\sqrt{10}}{3}(2n-2q-15) + 3\sqrt{13}$.
■

Theorem 11. *Let $C \in C^*_{n,q}$, where $n_3(C) = 2$. Then*

$$
SO(C) \leq \begin{cases}
4\sqrt{10} + 3\sqrt{2} & \text{if } n-q = 6 \text{ and } q = 0,\\
2\sqrt{2}(q-1) + 4\sqrt{10} + 2\sqrt{13} & \text{if } n-q = 6 \text{ and } q > 0,\\
\frac{\sqrt{10}(18-n+q)}{3} + \frac{(3\sqrt{17}+5)(n-q-6)}{3} + 3\sqrt{2} & \text{if } 9 \leq n-q \leq 15 \text{ and } q = 0,\\
\frac{\sqrt{10}}{3}(18-n+q) + \sqrt{17}(n-q-6) & \\
+(\sqrt{13} + 2\sqrt{5} - 5)q + 3\sqrt{2} + 15 & \text{if } 9 \leq n-q \leq 15 \text{ and } 1 \leq q \leq \frac{n-6}{4},\\
\frac{\sqrt{10}}{3}(18-n+q) + \frac{(3\sqrt{17}+2\sqrt{5})}{3}(n-q-6) & \\
+\frac{\sqrt{13}}{3}(n-q) + \frac{2\sqrt{2}}{3}(4q-n+3) & \text{if } 9 \leq n-q \leq 15 \text{ and } q > \frac{n-6}{4},\\
\frac{2\sqrt{17}}{3}(n-q) + (\sqrt{13} + 2\sqrt{5})q + 5(4-q) + 3\sqrt{2} & \text{if } n-q = 18 \text{ and } 1 \leq q \leq 4,\\
\frac{2\sqrt{17}}{3}(n-q) + 6\sqrt{13} + 8\sqrt{5} + 2\sqrt{2}(q-5) & \text{if } n-q = 18 \text{ and } q > 4,\\
\frac{2\sqrt{17}}{3}(n-q) + (\sqrt{13} + 2\sqrt{5})q + 5(6-q) & \text{if } n-q = 21 \text{ and } 0 \leq q \leq 6,\\
\frac{2\sqrt{17}}{3}(n-q) + 6(\sqrt{13} + 2\sqrt{5}) + 2\sqrt{2}(q-6) & \text{if } n-q = 21 \text{ and } q > 6,\\
\frac{2\sqrt{17}}{3}(n-q) + 4\sqrt{5}q & \\
+\frac{4\sqrt{2}(n-4q-21)}{3} + 30 & \text{if } n-q > 21 \text{ and } q \leq \frac{n-21}{4},\\
\frac{2\sqrt{17}}{3}(n-q) + \frac{\sqrt{13}(4q-n+21)}{3} & \\
+\frac{2\sqrt{5}(n+2q-21)}{3} + \frac{5(n-4q-3)}{3} & \text{if } n-q > 21 \text{ and } \frac{n-21}{4} < q \leq \frac{n-3}{4},\\
\frac{2\sqrt{17}}{3}(n-q) + \frac{2\sqrt{2}(4q-n+3)}{3} + \frac{4\sqrt{5}(n-q-12)}{3} + 6\sqrt{13} & \text{if } n-q > 21 \text{ and } q > \frac{n-3}{4}.
\end{cases}
$$

And

$$
SO_{red}(C) \leq \begin{cases}
8 + 2\sqrt{2} & \text{if } n-q = 6 \text{ and } q = 0, \\
\sqrt{2}(q-1) + 8 + 2\sqrt{5} & \text{if } n-q = 6 \text{ and } q > 0, \\
\frac{2(18-n+q)}{3} + \frac{(9+\sqrt{13})(n-q-6)}{3} + 2\sqrt{2} & \text{if } 9 \leq n-q \leq 15 \text{ and } q = 0, \\
\frac{2(18-n+q)}{3} + 3(n-q-6)3 + (\sqrt{5} + \sqrt{10} & \\
-\sqrt{13})q + 2\sqrt{2} + 3\sqrt{13} & \text{if } 9 \leq n-q \leq 15 \text{ and } 1 \leq q \leq \frac{n-6}{4}, \\
\frac{2(18-n+q)}{3} + (9 + \sqrt{10})(n-q-6)3 & \\
+\frac{\sqrt{5}}{3}(n-q) + \frac{\sqrt{2}}{3}(4q-n+3) & \text{if } 9 \leq n-q \leq 15 \text{ and } q > \frac{n-6}{4}, \\
2(n-q) + (\sqrt{5} + \sqrt{10})q + \sqrt{13}(4-q) + 2\sqrt{2} & \text{if } n-q = 18 \text{ and } 1 \leq q \leq 4, \\
2(n-q) + 6\sqrt{5} + 4\sqrt{10} + \sqrt{2}(q-5) & \text{if } n-q = 18 \text{ and } q > 4, \\
2(n-q) + (\sqrt{5} + \sqrt{10})q + \sqrt{13}(6-q) & \text{if } n-q = 21 \text{ and } 0 \leq q \leq 6, \\
2(n-q) + 6(\sqrt{5} + \sqrt{10}) + \sqrt{2}(q-6) & \text{if } n-q = 21 \text{ and } q > 6, \\
2(n-q) + 2\sqrt{10}q + \sqrt{2}(n-4q-21) + 6\sqrt{13} & \text{if } n-q > 21 \text{ and } q \leq \frac{n-21}{4}, \\
2(n-q) + 2\sqrt{10}q + \frac{\sqrt{5}(4q-n+21)}{3} & \\
+\frac{\sqrt{10}(n+2q-21)}{3} + \frac{\sqrt{13}(n-4q-3)}{3} & \text{if } n-q > 21 \text{ and } \frac{n-21}{4} < q \leq \frac{n-3}{4}, \\
2(n-q) + 6\sqrt{5} + \frac{\sqrt{2}(4q-n+3)}{3} + \frac{2\sqrt{10}(n-q-12)}{3} & \text{if } n-q > 21 \text{ and } q > \frac{n-3}{4}.
\end{cases}
$$

Equalities hold if and only if $C \in Q_2$.

Proof. Let C_{q_2} denotes the molecular tree with maximum (reduced) Sombor index value among the class $C^*_{n,q}$, where $n_3(C_{q_2}) = 2$. By Lemma 12, $n - q \equiv 0 \pmod 3$, $n_1(C_{q_2}) = \frac{2n-2q}{3}$ and $n_4(C_{q_2}) = \frac{n-q-6}{3}$. By Lemma 14 it holds that

$$x_{1,2}(C_{q_2}) = 0, \tag{4.32}$$

and Lemmas 2–6 provide the consequence $C_{q_2} \in Q_2$. We consider the following cases:
Case 1. $n_4(C_{q_2}) = 0$ or $n - q = 6$
Subcase 1.1. $q = 0$

Here, using Eq (4.6), we have $x_{1,3}(C_{q_2}) = 4$ and $x_{3,3}(C_{q_2}) = 1$, which give $SO(C_{q_2}) = 4\sqrt{10} + 3\sqrt{2}$ and $SO_{red}(C_{q_2}) = 8 + 2\sqrt{2}$.
Subcase 1.2. $q > 0$

By using (4.32) in (4.6), it is easy to get $x_{1,3}(C_{q_2}) = 4$, $x_{2,2}(C_{q_2}) = q - 1$, $x_{2,3}(C_{q_2}) = 2$ and $x_{3,3}(C_{q_2}) = 0$, which give $SO(C_{q_2}) = 2\sqrt{2}(q-1) + 4\sqrt{10} + 2\sqrt{13}$ and $SO_{red}(C_{q_2}) = \sqrt{2}(q-1) + 8 + 2\sqrt{5}$.
Case 2. $1 \leq n_4(C_{q_2}) \leq 3$ or $9 \leq n - q \leq 15$

By using Lemmas 2–4 and Eq (4.32), we have

$$x_{1,3}(C_{q_2}) = 4 - n_4(C_{q_2}) = \frac{18 - n + q}{3}, \tag{4.33}$$

$$x_{1,4}(C_{q_2}) = n_1(C_{q_2}) - x_{1,3}(C_{q_2}) = n - q - 6. \tag{4.34}$$

and

$$x_{4,4}(C_{q_2}) = 0. \tag{4.35}$$

Subcase 2.1. $q = 0$

Using Eqs (4.32)–(4.35) in (4.6), we have $x_{3,3}(C_{q_2}) = 1$ and $x_{3,4}(C_{q_2}) = \frac{n-q-6}{3}$, which give $SO(C_{q_2}) = \frac{\sqrt{10}}{3}(18 - n + q) + (\sqrt{17} + \frac{5}{3})(n - q - 6) + 3\sqrt{2}$ and $SO_{red}(C_{q_2}) = \frac{2(18-n+q)}{3} + \frac{(9+\sqrt{13})(n-q-6)}{3} + 2\sqrt{2}$.

Subcase 2.2. $1 \le q \le \frac{n-6}{4}$

This case holds for $q \le n_4(C_{q_2})$, so by using Lemmas 5, 6 and the Eqs (4.32)–(4.35) in (4.6), we have $x_{3,3}(C_{q_2}) = 1$, $x_{3,4}(C_{q_2}) = 3 - q$, $x_{2,3}(C_{q_2}) = q = x_{2,4}(C_{q_2})$ and $x_{2,2}(C_{q_2}) = 0$, which give $SO(C_{q_2}) = \frac{\sqrt{10}}{3}(18 - n + q) + \sqrt{17}(n - q - 6) + (\sqrt{13} + 2\sqrt{5} - 5)q + 3\sqrt{2} + 15$ and $SO_{red}(C_{q_2}) = \frac{2(18-n+q)}{3} + 3(n - q - 6)3 + (\sqrt{5} + \sqrt{10} - \sqrt{13})q + 2\sqrt{2} + 3\sqrt{13}$.

Subcase 2.3. $q > \frac{n-6}{4}$

This holds for $q > n_4(C_{q_2})$, and again by keeping in mind the results used in Subcase 2.2, we may easily get $x_{3,3}(C_{q_2}) = 0 = x_{3,4}(C_{q_2})$, $x_{2,3}(C_{q_2}) = \frac{n-q}{3}$, $x_{2,4}(C_{q_2}) = \frac{n-q-6}{3}$ and $x_{2,2}(C_{q_2}) = \frac{4q-n+3}{3}$. Hence, $SO(C_{q_2}) = \frac{\sqrt{10}}{3}(18 - n + q) + \frac{(3\sqrt{17}+2\sqrt{5})}{3}(n - q - 6) + \frac{\sqrt{13}}{3}(n - q) + \frac{2\sqrt{2}}{3}(4q - n + 3)$ and $SO_{red}(C_{q_2}) = \frac{2(18-n+q)}{3} + (9 + \sqrt{10})(n - q - 6)3 + \frac{\sqrt{5}}{3}(n - q) + \frac{\sqrt{2}}{3}(4q - n + 3)$.

Case 3. $n - q = 18$ or $n_4(C_{q_2}) = 4$

In this case, Lemmas 2–4 and Eq. (4.32) show that (4.35) holds and

$$x_{1,3}(C_{q_2}) = 0, \tag{4.36}$$

also

$$x_{1,4}(C_{q_2}) = \frac{2n - 2q}{3}. \tag{4.37}$$

Consider the following possibilities:

Subcase 3.1. $0 \le q \le 4$

Keeping in mind Lemmas 5 and 6, also using the Eqs (4.6), (4.32) and (4.35)–(4.37), we have $x_{2,2}(C_{q_2}) = 0$, $x_{2,3}(C_{q_2}) = q = x_{2,4}(C_{q_2})$, $x_{3,3}(C_{q_2}) = 1$ and $x_{3,4}(C_{q_2}) = 4 - q$. Hence, $SO(C_{q_2}) = \frac{2\sqrt{17}}{3}(n-q)+(\sqrt{13}+2\sqrt{5})q+5(4-q)+3\sqrt{2}$ and $SO_{red}(C_{q_2}) = 2(n-q)+(\sqrt{5}+\sqrt{10})q+\sqrt{13}(4-q)+2\sqrt{2}$.

Subcase 3.2. $q > 4$

Taking into account the facts used in Subcase 3.1, we may check that $x_{2,2}(C_{q_2}) = q - 5$, $x_{2,3}(C_{q_2}) = 6$, $x_{2,4}(C_{q_2}) = 4$ and $x_{3,3}(C_{q_2}) = 0 = x_{3,4}(C_{q_2})$. Hence, $SO(C_{q_2}) = \frac{2\sqrt{17}}{3}(n-q)+6\sqrt{13}+8\sqrt{5}+2\sqrt{2}(q-5)$ and $SO_{red}(C_{q_2}) = 2(n - q) + 6\sqrt{5} + 4\sqrt{10} + \sqrt{2}(q - 5)$.

Case 4. $n - q > 18$ or $n_4(C_{q_2}) > 4$

Lemmas 2–4 imply that (4.36) and (4.37) hold and

$$x_{3,3}(C_{q_2}) = 0. \tag{4.38}$$

Subcase 4.1. $n - q = 21$ and $0 \le q \le 6$

Note that (4.35) holds in this case, further more Lemmas 5, 6 and the Eqs (4.6), (4.32), (4.35) and (4.36)–(4.38), we have $x_{2,2}(C_{q_2}) = 0$, $x_{2,3}(C_{q_2}) = q = x_{2,4}(C_{q_2})$ and $x_{3,4}(C_{q_2}) = 6 - q$. Hence, $SO(C_{q_2}) = \frac{2\sqrt{17}}{3}(n-q)+(\sqrt{13}+2\sqrt{5})q+5(6-q)$ and $SO_{red}(C_{q_2}) = 2(n-q)+(\sqrt{5}+\sqrt{10})q+\sqrt{13}(6-q)$.

Subcase 4.2. $n - q = 21$ and $q > 6$

Taking into account the facts used in Subcase 3.1, we have $x_{2,2}(C_{q_2}) = q-6$, $x_{2,3}(C_{q_2}) = 6 = x_{2,4}(C_{q_2})$ and $x_{3,4}(C_{q_2}) = 0$. Hence, $SO(C_{q_2}) = \frac{2\sqrt{17}}{3}(n-q) + 6(\sqrt{13} + 2\sqrt{5}) + 2\sqrt{2}(q-6)$ and $SO_{red}(C_{q_2}) = 2(n-q) + 6(\sqrt{5} + \sqrt{10}) + \sqrt{2}(q-6)$.

Subcase 4.3. $n - q > 21$ and $q \le \frac{n-21}{4}$

This case implies that $q \le n_4(C_{q_2}) - 5$ for which $x_{2,3}(C_{q_2}) = 0$ by Lemma 5. Now using Lemma 6 and Eqs (4.6), (4.32) and (4.36)–(4.38), we have $x_{2,2}(C_{q_2}) = 0$, $x_{2,4}(C_{q_2}) = 2q$, $x_{4,4}(C_{q_2}) = \frac{n-4q-21}{3}$ and $x_{3,4}(C_{q_2}) = 6$. Hence, $SO(C_{q_2}) = \frac{2\sqrt{17}}{3}(n-q) + 4\sqrt{5}q + \frac{4\sqrt{2}(n-4q-21)}{3} + 30$ and $SO_{red}(C_{q_2}) = 2(n-q) + 2\sqrt{10}q + \sqrt{2}(n-4q-21) + 6\sqrt{13}$.

Subcase 4.4. $n - q > 21$ and $\frac{n-21}{4} < q \le \frac{n-3}{4}$

(4.35) holds in this case and also using (4.6), (4.32) and (4.36)–(4.38), we have $x_{2,2}(C_{q_2}) = 0$, $x_{2,3}(C_{q_2}) = \frac{4q-n+21}{3}$, $x_{2,4}(C_{q_2}) = \frac{n+2q-21}{3}$ and $x_{3,4}(C_{q_2}) = \frac{n-4q-3}{3}$. Hence, $SO(C_{q_2}) = \frac{2\sqrt{17}}{3}(n-q) + \frac{\sqrt{13}(4q-n+21)}{3} + \frac{2\sqrt{5}(n+2q-21)}{3} + \frac{5(n-4q-3)}{3}$ and $SO_{red}(C_{q_2}) = 2(n-q) + 2\sqrt{10}q + \frac{\sqrt{5}(4q-n+21)}{3} + \frac{\sqrt{10}(n+2q-21)}{3} + \frac{\sqrt{13}(n-4q-3)}{3}$.

Subcase 4.5. $n - q > 21$ and $q > \frac{n-3}{4}$

Again using Lemmas 5, 6 and the Eqs (4.6), (4.32), (4.35) and (4.36)–(4.38), we have $x_{2,2}(C_{q_2}) = \frac{4q-n+3}{3}$, $x_{2,3}(C_{q_2}) = 6$, $x_{2,4}(C_{q_2}) = \frac{2(n-q-12)}{3}$ and $x_{3,4}(C_{q_2}) = 0$. Hence, $SO(C_{q_2}) = \frac{2\sqrt{17}}{3}(n-q) + \frac{2\sqrt{2}(4q-n+3)}{3} + \frac{4\sqrt{5}(n-q-12)}{3} + 6\sqrt{13}$ and $SO_{red}(C_{q_2}) = 2(n-q) + 6\sqrt{5} + \frac{\sqrt{2}(4q-n+3)}{3} + \frac{2\sqrt{10}(n-q-12)}{3}$. ■

5. Conclusions

In this paper, an extremal chemical-graph-theoretical problem concerning the Sombor index and the reduced Sombor index is addressed. Particularly, the problem of characterizing trees possessing the maximum values of the aforementioned two indices from the class of all molecular trees of a given order and with a fixed number of (i) branching vertices (ii) vertices of degree 2, is solved in this paper. A solution to the minimal version of this problem regarding the Sombor index was reported in [3]. It is believed that the minimal version of the problem under consideration regarding the reduced Sombor index is not difficult and can be solved by using the technique used in [3]; nevertheless, it still seems to be interesting to find such a solution. Solving Problem 1 for the multiplicative and exponential versions of the Sombor and reduced Sombor indices (for example, see [11]) is another possible direction for a future work concerning the present study.

Conflict of interest

The authors have no conflict of interest.

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