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Research article

Extreme graphs on the Sombor indices

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Abstract: Gutman proposed the concept of Sombor index. It is defined via the term $\sqrt{d_F(v_i)^2 + d_F(v_j)^2}$, where $d_F(v_i)$ is the degree of the vertex v_i in graph F. Also, the reduced Sombor index and the Average Sombor index have been introduced recently, and these topological indices have good predictive potential in mathematical chemistry. In this paper, we determine the extreme molecular graphs with the maximum value of Sombor index and the extremal connected graphs with the maximum (reduced) Sombor index. Some inequalities relations among the chemistry indices are presented, these topology indices including the first Banhatti-Sombor index, the first Gourava index, the Second Gourava index, the Sum Connectivity Gourava index, Product Connectivity Gourava index, and Eccentric Connectivity index. In addition, we characterize the graph where equality occurs.

Keywords: Sombor index; reduced Sombor index; molecular graph
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1. Introduction

For a graph F with vertex set $V(F)$ and edge set $E(F)$, we let $e(F)$, $\delta(F)$, $\Delta(F)$ and $\overline{F}$ denote the number of edges, minimum degree, maximum degree, and complement of F, respectively.

Throught this paper, $F = (V(F), E(F))$ denotes a finite simple graph, it has no loops and parallel edges in graph F, for a nonempty subset S of F, the subgraph $F[S]$ of F induced by S, more generally, the graph $F - S$ is the induced subgraph $F[V - S]$ of F, the complement $\overline{F}$ of a graph F is that graph with vertex set $V(F)$ such that no vertices are adjacent in $\overline{F}$ if and only if these vertices are not adjacent in F. We refer the readers to the book [1] for undefined notations and terminologies.

Recently, a new index, introduced by Gutman [16], is defined as

$$\mathrm{SO} = \mathrm{SO}(F) = \sum_{v_iv_j \in E(F)} \sqrt{d_F(v_i)^2 + d_F(v_j)^2}, \tag{1.1}$$

where $\deg_F(v_i)$ is the degree of the vertex v_i in F. This new parameter is called Sombor index. Gutman [16] also proposed another concept

$$\mathrm{SO}_{\mathrm{red}} = \mathrm{SO}_{\mathrm{red}}(F) = \sum_{v_iv_j \in E(F)} \sqrt{(d_F(v_i) - 1)^2 + (d_F(v_j) - 1)^2} \tag{1.2}$$

and this new parameter is called reduced Sombor index.

Some bounds for $\mathrm{SO}(F)$ of trees and general graphs are presented in [16] and some properties are established. Deng et al. [13] gave an upper bound for all chemical trees with fixed order, and characterized extremal trees. Redžepović [21] examined the potentials of (reduced, average) Sombor index. Cruz et al. [2] characterized the extremal graphs on the Sombor index for chemical graphs, chemical trees, and hexagonal systems. In [6, 8, 12], Das et al. gave some bounds for Sombor index in terms of different graph parameters. In [7, 22], the authors characterized the maximal graph of Sombor index among all connected ν-cyclic graphs of order n, where $0 \leq \nu \leq n-2$.

For an integer $n \geq 2$, P_n is a path of order n with $n-1$ edges. A chemical tree (or molecular tree) is a tree with degree at most 4. A graph is called molecular graph if its maximum degree is at most four.

Deng et al. [13] proposed the following problems.

Problem 1. *[13] Which molecular trees with perfect matching reach the maximum value of* SO *and* $\mathrm{SO}_{\mathrm{red}}$*?*

Problem 2. *[13] Which molecular graphs reach the maximum value of* SO *and* $\mathrm{SO}_{\mathrm{red}}$*?*

Problem 3. *[13] Which connected graphs of order n and size m reach the extremal (minimum and maximum) of the (reduced) Sombor index?*

Cruz and Rada [3] partly solved Problem 2. But the others remain open. Gutman [16] derived the following bounds for Sombor index.

Theorem 1.1. *[16] Let F be a graph of order n. Then*

$$0 \leq \mathrm{SO}(F) \leq \frac{n(n-1)^2}{\sqrt{2}}$$

with equality if and only if $F \cong \overline{K_n}$ or $F \cong K_n$. Recall that $\mathrm{SO}(\overline{K_n}) = 0$ *and* $\mathrm{SO}(K_n) = \frac{n(n-1)^2}{\sqrt{2}}$.

Theorem 1.2. *[16] Let T be a tree of order n. Then*

$$2\sqrt{5} + 2(n-3)\sqrt{2} \leq \mathrm{SO}(T) \leq (n-1)\sqrt{n^2 - 2n + 2}$$

with equality if and only if $T \cong P_n$ or $T \cong S_n$, where S_n is a star with n vertices. Recall that $\mathrm{SO}(S_n) = (n-1)\sqrt{n^2 - 2n + 2}$ *and* $\mathrm{SO}(P_n) = 2\sqrt{5} + 2(n-3)\sqrt{2}$.

This paper is scheduled as follows. In Section 2, we determine the extreme graphs with the maximum value of Sombor index and the extremal connected graphs with the (reduced) Sombor index. In Section 3, some relations among the chemistry indexes are presented. In Section 4, we conclude this paper.

2. Extreme molecular graphs for SO and SO_{red}

Here are some properties of (reduced) Sombor index.

Theorem 2.1. *[13] Let F be a graph with n vertices. Then*

$$0 \leq SO_{red}(F) \leq \frac{\sqrt{2}}{2} n(n-1)(n-2)$$

with equality if and only if $F \cong tK_2 \cup (n-2)K_1$ *or* $F \cong K_n$. *Recall that* $SO_{red}(tK_2 \cup (n-2t)K_1) = 0$, $0 \leq t \leq \lfloor \frac{n}{2} \rfloor$ *and* $SO(K_n) = \frac{\sqrt{2}}{2} n(n-1)(n-2)$.

Let CG_n be the set of molecular graphs with n vertices.

Theorem 2.2. *[2] Let* $F \in CG_n$, $n \geq 5$. *Then*

$$2\sqrt{5} + 2(n-3)\sqrt{2} \leq SO(F) \leq 8n\sqrt{2}$$

with equality if and only if $F \cong P_n$ *or F is a* 4*-regular graph of order n.*

Lemma 2.1. *For any graph F, we have*

$$\sum_{v_i v_j \in E(F)} (d_F(v_i) + d_F(v_j)) = \sum_{v_i \in V(F)} d_F(v_i)^2. \tag{2.1}$$

Proof. Suppose that F is connected. Consider the edge weight sum by double counting method for every edge $v_i v_j \in E(F)$. The weight sum that the vertex v_i contributes to its adjacent edges is $d_F(v_i)^2$. On the other hand, let us calculate the edge weight sum by counting each edge, this implies that we have completed the proof of Eq (2.1).

Suppose that F is a disconnected graph. Let $F = H_1 \cup H_2 \cup \cdots \cup H_p$, where H_k $(k = 1, 2, \ldots, p)$ is the k-th connected component in F. From the above result, we conclude that

$$\sum_{v_i v_j \in E(F)} \left(d_F(v_i) + d_F(v_j)\right) = \sum_{k=1}^{p} \sum_{v_i v_j \in E(H_k)} \left(d_{H_k}(v_i) + d_{H_k}(v_j)\right) = \sum_{k=1}^{p} \sum_{v_i \in V(H_k)} d_{H_k}(v_i)^2 = \sum_{v_i \in V(F)} d_F(v_i)^2.$$

□

Liu et al. has solved Problem 2 in [24].

Theorem 2.3. *[24] Let* $F \in CG_n$. *Then*

$$SO_{red}(F) \leq 6n\sqrt{2}.$$

The equality holds if and only if H is a 4*-regular graph of order n.*

Let CG_n^k be the set of connected graphs with n vertices such that the degree of each vertex is at most k. we calculate the maximum value of Sombor index in CG_n^k. We now give an bound on CG_n^k about (reduced) Sombor index as below.

Theorem 2.4. *Let $F \in CG_n^k$. Then*

$$(n-3)\sqrt{2}+2 \leq \mathrm{SO}_{\mathrm{red}}(F) \leq \frac{\sqrt{2}}{2}nk(k-1).$$

The left (right, respectively) equality holds if and only if $F \cong P_n$ ($F \cong G_k$, respectively), where G_k stands for a k-regular graph of order n. Recall that $\mathrm{SO}_{red}(G_k) = \frac{\sqrt{2}}{2}nk(k-1)$ and $\mathrm{SO}_{red}(P_n) = (n-3)\sqrt{2}+2$.

Proof. For any graph F (with no isolated vertices), let $s_i = s_i(F)$ be the number of vertices of degree i in F, and let $e_{i,j} = e_{i,j}(F)$ be the number of edges in F connecting the vertices of degrees i and j.

It means that

$$\sum_{i=1}^{k} s_i = n. \tag{2.2}$$

It is well-known that the following relations hold: for two integers $i, j \in \{1, 2, \cdots, k\}$,

$$\sum_{j=1}^{k} \delta_{i,j} e_{i,j} = i s_i, \tag{2.3}$$

where

$$\delta_{i,j} = \begin{cases} 2, & i = j; \\ 1, & i \neq j. \end{cases} \tag{2.4}$$

Let $\Upsilon = \{(i, j)|(i, j) \in \mathbb{N} \times \mathbb{N}, 1 \leq i \leq j \leq k\}$ and $\Omega = \{(i, j)|(i, j) \in \Upsilon, (i, j) \neq (k, k)\}$. By (2.2) and (2.3), we have

$$\sum_{(i,j)\in\Upsilon} \left(\frac{1}{i} + \frac{1}{j}\right) e_{i,j} = n.$$

Note that the value of reduced Sombor index of molecular graphs with n vertex is equivalent to

$$\mathrm{SO}_{\mathrm{red}}(F) = \sum_{(i,j)\in\Upsilon} e_{i,j}\sqrt{(i-1)^2 + (j-1)^2}.$$

Thus,

$$\begin{aligned}
\mathrm{SO}_{red}(F) &= \sum_{(i,j)\in\Upsilon} e_{i,j}\sqrt{(i-1)^2 + (j-1)^2} \\
&= \sum_{(i,j)\in\Omega} e_{i,j}\sqrt{(i-1)^2 + (j-1)^2} + e_{k,k}\sqrt{(k-1)^2 + (k-1)^2} \\
&= \sum_{(i,j)\in\Omega} e_{i,j}\sqrt{(i-1)^2 + (j-1)^2} + (k-1)e_{k,k}\sqrt{2} \\
&= \sum_{(i,j)\in\Omega} e_{i,j}\sqrt{(i-1)^2 + (j-1)^2} + (k-1)\sqrt{2} \times \frac{k}{2} \times \left(n - \sum_{(i,j)\in\Omega}\left(\frac{1}{i} + \frac{1}{j}\right)e_{i,j}\right)
\end{aligned}$$

$$= \frac{k(k-1)n}{2}\sqrt{2} + \sum_{(i,j)\in\Omega} e_{i,j}\left\{\sqrt{(i-1)^2+(j-1)^2} - \frac{k(k-1)}{2}\sqrt{2}\left(\frac{1}{i}+\frac{1}{j}\right)\right\}.$$

Let $h(i,j) = \sqrt{(i-1)^2+(j-1)^2} - \frac{k(k-1)}{2}\sqrt{2}(\frac{1}{i}+\frac{1}{j})$. where $(i,j)\in\Omega$, it is easy to see that $h(k,k)=0$ and $h(i,j)<0$ for $(i,j)\in\Omega$, and then

$$\mathrm{SO_{red}}(F) = \frac{k(k-1)n}{2}\sqrt{2} + \sum_{(i,j)\in\Omega} e_{i,j}\left\{\sqrt{(j-1)^2+(i-1)^2} - \frac{k(k-1)}{2}\sqrt{2}\left(\frac{1}{i}+\frac{1}{j}\right)\right\},$$

we have

$$\mathrm{SO_{red}}(F) \le \frac{k(k-1)n}{2}\sqrt{2}.$$

It implies that $e(i,j)=0$ for all $(i,j)\in\Omega$, in the sake of reaching the maximum value of $\mathrm{SO_{red}}(F)$. Then F is a k-regular graph. Conversely, if F is a k-regular graph, then $\mathrm{SO_{red}}(F) = \frac{k(k-1)n}{2}\sqrt{2}$. Recall that F is an extremal graph which is a k-regular graph. For lower bound, it is similarly to the proof of Theorem 1.2, so, we give the result without proof. □

Similarly to the proof of Theorem 2.4, we have a result as below.

Corollary 2.1. *Let $F \in CG_n^k$. Then*

$$2\sqrt{5} + 2(n-3)\sqrt{2} \le \mathrm{SO}(F) \le \frac{\sqrt{2}}{2} nk^2,$$

with left (right, respectively) equality holds if and only if $F \cong P_n$ ($F \cong G_k$, respectively), where G_k stands for a k-regular graph of order n. Recall that $\mathrm{SO}(G_k) = \frac{\sqrt{2}}{2}nk^2$ and $\mathrm{SO}(P_n) = 2\sqrt{5}+2(n-3)\sqrt{2}$.

Let $CG_{n,m}$ be the class of graphs with n vertices and m edges. We now consider Problem 3. Let us calculate the minimum value of Sombor index for $F \in CG_{n,m}$.

Theorem 2.5. *Let $F \in CG_{n,m}$.*
(i)

$$\mathrm{SO}(F) \ge \frac{2\sqrt{2}m^2}{n}$$

with equality if and only if F is regular with order n.
(ii) *If F is triangle-free, then*

$$\mathrm{SO}(F) \le mn$$

with equality if and only if $F \cong \overline{K_n}$.

Proof. The following fact is immediate.

Fact 1. *For $\omega_1, \omega_2 \in \mathbb{R}^+$, we have*

$$\omega_1 + \omega_2 \ge \sqrt{\omega_1^2+\omega_2^2} \ge \frac{\sqrt{2}}{2}(\omega_1+\omega_2). \tag{2.5}$$

Moreover, the left (right) equality holds if $\omega_1\omega_2 = 0$ ($\omega_1 = \omega_2$).

(i) By Lemma 2.1 and Cauchy-Schwarz inequality, it follows that

$$\sum_{v_iv_j\in E(F)}\Big(d_F(v_i)+d_F(v_i)\Big)=\sum_{v_i\in V(F)}d_F(v_i)^2\geq\frac{\Big(\sum_{v_i\in V(F)}d_F(v_i)\Big)^2}{n}.$$

The right equality holds if $d_F(v_1)=d_F(v_2)=\cdots=d_F(v_n)$. Using the above result with Handshaking theorem, we have

$$\sum_{v_i\in V(F)}d_F(v_i)=2|E(F)|=2m,$$

it admits that

$$\sum_{v_iv_j\in E(F)}(d_F(v_i)+d_F(v_j))=\sum_{v_i\in V(F)}d_F(v_i)^2\geq\frac{4m^2}{n},\tag{2.6}$$

where equality holds if $d_F(v_1)=d_F(v_2)=\cdots=d_F(v_n)$. We take $\omega_1=d_F(v_i)$ and $\omega_2=d_F(v_j)$ in Fact 1, and the right inequality (2.5) will become

$$\sum_{v_iv_j\in E(F)}\sqrt{d_F(v_i)^2+d_F(v_j)^2}\geq\frac{\sqrt{2}}{2}\sum_{v_iv_j\in E(F)}\Big(d_F(v_i)+d_F(v_j)\Big)\geq\frac{2\sqrt{2}m^2}{n}$$

by (2.6). Moreover, the equality holds if F is a regular graph of order n.

(ii) For $v_iv_j\in E(F)$, since F is triangle-free, it follows that v_i and v_j cannot have a common neighbor, and hence $d_F(v_i)+d_F(v_j)\leq n$. Summing this inequality over all the edges, we have

$$\sum_{v_iv_j\in E(F)}\Big(d_F(v_i)+d_F(v_j)\Big)\leq mn.$$

By Lemma 2.1, we have

$$\sum_{v_i\in V(F)}d_F(v_i)^2=\sum_{v_iv_j\in E(F)}\Big(d_F(v_i)+d_F(v_j)\Big)\leq mn.\tag{2.7}$$

For $\omega_1=d_F(v_i)$ and $\omega_2=d_F(v_j)$, the left inequality (2.5) is transformed into

$$\sum_{v_iv_j\in E(F)}\sqrt{d_F(v_i)^2+d_F(v_j)^2}\leq\sum_{v_iv_j\in E(F)}\Big(d_F(v_i)+d_F(v_j)\Big)\leq mn$$

by (2.7). In addition, the equality holds if $d_F(v_i)\,d_F(v_j)=0$ for $v_iv_j\in E(F)$, *i.e.*, $F\cong\overline{K_n}$. □

Theorem 2.6. *Let $F\in CG_{n,m}$.*
(i)

$$\mathrm{SO}_{red}(F)\geq\frac{2\sqrt{2}m^2}{n}-m\sqrt{2}$$

with equality if F is regular with $|V(F)|=n$.
(ii) *If F is triangle-free, then*

$$\mathrm{SO}_{red}(F)\leq mn-2m$$

with equality if F is isomorphic to S_n.

Proof. The proof is very similar to Theorem 2.5.

Fact 2. *For $\tau_1 \geq 1$ and $\tau_2 \geq 1$, $\tau_1, \tau_2 \in \mathbb{R}^+$ the following inequality holds:*

$$\tau_1 + \tau_2 - 2 \geq \sqrt{(\tau_1 - 1)^2 + (\tau_2 - 1)^2} \geq \frac{\sqrt{2}}{2}(\tau_1 + \tau_2 - 2). \tag{2.8}$$

Moreover, the left (right) equality holds if $(\tau_1 - 1)(\tau_2 - 1) = 0$ ($\tau_1 = \tau_2$).

(i) For $\tau_1 = d_F(v_i)$ and $\tau_2 = d_F(v_j)$, according to the above result, it is easy to see that

$$\begin{aligned}\sum_{v_iv_j \in E(F)} \sqrt{(d_F(v_i) - 1)^2 + (d_F(v_j) - 1)^2} &\geq \frac{\sqrt{2}}{2} \sum_{v_iv_j \in E(F)} \Big(d_F(v_i) + d_F(v_j) - 2\Big) \\ &\geq \frac{2\sqrt{2}m^2}{n} - m\sqrt{2}\end{aligned}$$

by (2.6). Moreover, the equality holds if and only if F is a regular graph of order n.
(ii) Since F is triangle-free, one can easily see that $(d_F(v_i) - 1) + (d_F(v_j) - 1) \leq n - 2$ for $v_iv_j \in E(F)$. Summing this inequality over all the edges, we obtain

$$\sum_{v_iv_j \in E(F)} \Big[\Big(d_F(v_i) - 1\Big) + \Big(d_F(v_j) - 1\Big)\Big] \leq m(n-2) = mn - 2m.$$

For $\tau_1 = d(v_i)$ and $\tau_2 = d(v_j)$, it follows from (3.1) that

$$\sum_{v_iv_j \in E(F)} \sqrt{(d_F(v_i) - 1)^2 + (d_F(v_j) - 1)^2} \leq \sum_{v_iv_j \in E(F)} \Big(d_F(v_i) + d_F(v_j) - 2\Big) \leq mn - 2m.$$

Moreover, the equality holds if and only if $d_F(v_i) = 1$ or $d_F(v_j) = 1$ for $v_iv_j \in E(F)$, and $d_F(v_i) + d_F(v_j) = n$ for $v_iv_j \in E(F)$, that is, if and only if $F \cong S_n$. □

Theorem 2.7. *Let $F \in CG_{n,m}$. Then*

$$\mathrm{SO}(F) \leq \sqrt{2}m(n-1) \quad and \quad \mathrm{SO}_{red}(F) \leq \sqrt{2}m(n-2)$$

with equality if $F \cong K_n$.

Proof. Since $\Delta \leq n - 1$, it follows that

$$\sqrt{d_F(v_i)^2 + d_F(v_j)^2} \leq \sqrt{2}(n-1),$$

for $v_iv_j \in E(F)$. Similarly,

$$\sqrt{\Big(d_F(v_i) - 1\Big)^2 + \Big(d_F(v_j) - 1\Big)^2} \leq \sqrt{2}(n-2),$$

for $v_iv_j \in E(F)$. Then

$$\mathrm{SO}(F) = \sum_{v_iv_j \in E(F)} \sqrt{d_F(v_i)^2 + d_F(v_j)^2} \leq \sum_{v_iv_j \in E(F)} \sqrt{2}(n-1) = \sqrt{2}m(n-1),$$

where equality holds if and only if $d_F(v) = n-1$ for any $v \in V(F)$, $F \cong K_n$. Moreover,

$$\mathrm{SO}_{red}(F) = \sum_{v_iv_j \in E(F)} \sqrt{\left(d_F(v_i)-1\right)^2 + \left(d_F(v_j)-1\right)^2} \leq \sqrt{2}m(n-2)$$

with equality if and only if $F \cong K_n$. □

We now give an upper bound on $\mathrm{SO}(F)$ and $\mathrm{SO}_{red}(F)$ in terms of m only.

Proposition 2.1. *Let F be a graph with m edges. Then* $\mathrm{SO}(F) \leq m(m+1)$ *where equality holds if and only if* $F \cong \overline{K}_n$. *Moreover,* $\mathrm{SO}_{red}(F) \leq m^2 - m$ *where equality holds if and only if* $F \cong S_n$.

Proof. For $v_iv_j \in E(F)$, since $d_F(v_i) + d_F(v_j) \leq m+1$, it follows that

$$\mathrm{SO}(F) = \sum_{v_iv_j \in E(F)} \sqrt{d_F(v_i)^2 + d_F(v_j)^2} \leq \sum_{v_iv_j \in E(F)} \left(d_F(v_i) + d_F(v_j)\right) \leq m\,(m+1).$$

Moreover, the equality holds if $F \cong \overline{K}_n$. Therefore,

$$\mathrm{SO}_{red}(F) = \sum_{v_iv_j \in E(F)} \sqrt{\left(d_F(v_i)-1\right)^2 + \left(d_F(v_j)-1\right)^2} \leq \sum_{v_iv_j \in E(F)} \left(d_F(v_i) + d_F(v_j) - 2\right) \leq m\,(m-1).$$

The equality holds if and only if $F \cong S_n$. □

Let $CG^{\ell}\{n,m\}$ be the set of graphs with n vertices and m edges such that $d_F(v_i) + d_F(v_j) \leq \ell$.

Now consider the following question: to determine the maximum value of $\mathrm{SO}(F)$ among all connected graphs of order n with m edges such that $d_F(v_i) + d_F(v_j) \leq \ell$.

Using a proof similar to the Theorem 2.5, we obtain an upper bound.

Corollary 2.2. *Let* $F \in CG^{l}\{n,m\}$. *Then* $\mathrm{SO}(F) \leq m\,\ell$.

For $n, \rho_1, \rho_2, \rho_3 \in \mathbb{Z}^+$ and $\sum_{i=1}^{i=3} \rho_i = n-3$, $U(n, \rho_1, \rho_2, \rho_3)$ is a unicyclic graph obtained from a 3-cycle C_3 with $V(C_3) = \{u, v, w\}$ by adding ρ_1, ρ_2 and ρ_3 pendent vertices to the vertices u, v and w, respectively. $B_{2,0}(n, n-4, 0, 0)$ stands for two copies of K_3 by sharing an edge and connecting the remaining hanging edges to a vertex on the sharing edge.

Cruz and Rada [3] characterized the extremal graphs restricted in unicyclic graphs and bicyclic graphs, respectively.

Theorem 2.8. *[3] If F is the unicyclic graph of order n* ($n \geq 4$)*, then*

$$\mathrm{SO}(F) \leq \mathrm{SO}(U(n, n-3, 0, 0)).$$

Theorem 2.9. *[3] If F is a bicyclic graph of order n* ($n \geq 6$)*, then*

$$\mathrm{SO}(F) \leq \mathrm{SO}(B_{2,0}(n, n-4, 0, 0)).$$

For convenience, for a subgraph H_0 of K_n, denote by $K_n - H_0$ the graph obtained by deleting all edges of H_0 from K_n. From the structure of $K_n - H_0$, $\overline{K_n - H_0} = \overline{K_{n-|V(H_0)|}} \cup H_0$. In particular, let $H_1(n) = K_n - 2K_2$ and $H_2(n) = K_n - P_3$.

Proposition 2.2. *Let* $F \in CG_{n,m}$ *with* $m = \binom{n}{2} - 2$ $(n \geq 5)$. *Then*

$$\mathrm{SO}(F) \leq \mathrm{SO}(K_n - P_3),$$

where

$$\mathrm{SO}(K_n - P_3) = 2(n-3)\sqrt{(n-1)^2 + (n-2)^2} + (n-3)\sqrt{(n-1)^2 + (n-3)^2} + \binom{n-3}{2}(n-1)\sqrt{2} + (n-2)\sqrt{2}.$$

Proof. Since $F \in CG_{n,m}$ for $m = \binom{n}{2} - 2$, it must satisfy $F \cong H_1(n) = K_n - 2K_2$ or $F \cong H_2(n) = K_n - P_3$. For graph $K_n - 2K_2$, there are four vertices, say v_1, v_2, v_3 and v_4, of degree $n-2$. Suppose v_1v_2 and v_3v_4 denote $2K_2$, then $NE_{\ell_1,\ell_2} = \{uv | deg_F(u) = \ell_1, deg_F(v) = \ell_2\}$ by the definition of Sombor index. It follows that

$$\begin{aligned} SO(K_n - 2K_2) = & \sum_{v_iv_j \in NE_{n-2,n-1}} (d_F(v_i)^2 + d_F(v_j)^2) \\ & + \sum_{v_iv_j \in NE_{n-2,n-2}} (d_F(v_i)^2 + d_F(v_j)^2) \\ & + \sum_{v_iv_j \in NE_{n-1,n-1}} (d_F(v_i)^2 + d_F(v_j)^2) \\ = & 4(n-4)\sqrt{(n-2)^2 + (n-1)^2} + 4\sqrt{(n-2)^2 + (n-2)^2} + \binom{n-4}{2}(n-1)\sqrt{2}. \end{aligned}$$

Similarly, we have

$$\mathrm{SO}(K_n - P_3) = 2(n-3)\sqrt{(n-1)^2 + (n-2)^2} + (n-3)\sqrt{(n-3)^2 + (n-1)^2} + \binom{n-3}{2}(n-1)\sqrt{2} + (n-2)\sqrt{2}.$$

$$\begin{aligned} \mathrm{SO}(K_n - P_3) - \mathrm{SO}(K_n - 2K_2) = & \Big(2(n-3)\sqrt{(n-2)^2 + (n-1)^2} + (n-3)\sqrt{(n-3)^2 + (n-1)^2} \\ & + \binom{n-3}{2}(n-1)\sqrt{2} + (n-2)\sqrt{2}\Big) - \Big(4(n-4)\sqrt{(n-2)^2 + (n-1)^2} \\ & + 4\sqrt{(n-2)^2 + (n-2)^2} + \binom{n-4}{2}(n-1)\sqrt{2}\Big) \\ = & \sqrt{2}n^2 + \Big(\sqrt{2}\sqrt{n^2 - 4n + 5} - 2\sqrt{2n^2 - 6n + 5} - 8\sqrt{2}\Big)n \\ & - 3\sqrt{2}\sqrt{n^2 - 4n + 5} + 10\sqrt{2n^2 - 6n + 5} + 10\sqrt{2} \\ \geq & \Big(10\sqrt{2} + \sqrt{2}n^2 + 10\sqrt{2n^2 - 6n + 5} + \sqrt{2}n\sqrt{n^2 - 4n + 5}\Big) \\ & - \Big(3\sqrt{2}\sqrt{n^2 - 4n + 5} + 8n\sqrt{2} + 2n\sqrt{2n^2 - 6n + 5}\Big) \geq 0. \end{aligned}$$

Thus, $\mathrm{SO}(F - P_3) \geq \mathrm{SO}(F - 2K_2)$ for $n \geq 5$. □

Suppose that F is a connected graph with order n and size m. Clearly, $\binom{n}{2} = \frac{n(n-1)}{2} \geq m \geq n-1$. Let $F(m, n)$ be a graph giving the maximum value of the Sombor index. Then $\mathrm{SO}(F) \leq \mathrm{SO}(F(m, n)) = f(m, n)$. If $m = n-1$, then F is a tree. By Theorem 1.2, $\mathrm{SO}(F) \leq (n-1)\sqrt{n^2 - 2n + 2}$ where equality holds if and only if $F \cong S_n$, where S_n is the star of order n. Naturally, $f(n-1, n) = (n-1)\sqrt{n^2 - 2n + 2}$ and $F(n-1, n) = S_n$.

If $m = \binom{n}{2} = \frac{n(n-1)}{2}$, then F is a complete graph. By Theorem 1.1, $\mathrm{SO}(F) \leq \frac{n(n-1)^2}{\sqrt{2}}$, where the equality holds if and only if $F \cong K_n$. Then $f(\binom{n}{2}, n) = \frac{n(n-1)^2}{\sqrt{2}}$ and $F(\binom{n}{2}, n) = K_n$.

If $m = \binom{n}{2} - 1 = \frac{n^2-n-2}{2}$, then F is $K_n - K_2$, and hence

$$\mathrm{SO}(K_n - K_2) = 2(n-2)\sqrt{(n-1)^2 + (n-2)^2} + \binom{n-1}{2}(n-1)\sqrt{2}.$$

So,

$$f(\binom{n}{2} - 1, n) = 2(n-2)\sqrt{(n-1)^2 + (n-2)^2} + \binom{n-1}{2}(n-1)\sqrt{2}$$

and

$$G(\binom{n}{2}, n) = K_n - K_2.$$

By Theorem 2.2,

$$f(\binom{n}{2} - 2, n) = 2(n-3)\sqrt{(n-2)^2 + (n-1)^2} + (n-3)\sqrt{(n-3)^2 + (n-1)^2} + \binom{n-3}{2}(n-1)\sqrt{2} + (n-2)\sqrt{2}$$

and

$$F(\binom{n}{2} - 2, n) = K_n - P_3.$$

We now consider the general situation, for any integer n, m, $n - 1 \leq m \leq \binom{n}{2}$.

Algorithm A1, which gives a graph $F(m, n)$:

Algorithm A1 Extremal Graphs algorithm

```
procedure EXTREMAL GRAPH(m, n)                      ▷ m = |E(F)| and n = |V(F)|
    V(F) ← {v_1, v_2, ..., v_n}
    E_0 ← ∅                                          ▷ E(F)_0 := E_0
    f_1 ← n
    r ← 1
    t ← 2
    ℓ ← 0
    while r ≤ f_1 do                                 ▷ edge condition
        while t ≤ f_1 and ℓ ≤ m do
            E(F)_r ← E(F)_{r−1} ∪ {v_r v_t}          ▷ adding edge
            t ← t + 1
            ℓ ← ℓ + 1
        end while
        r ← r + 1
        t ← r + 1
        if ℓ ≥ m then break.
        end if
    end while
    return E(F)                                      ▷ F = (V(F), E(F))
end procedure
```

Let $1 \leq p \leq n-1$, $s_p = \sum_{i=1}^{p} (n-i)$, $k = \min\{p \mid s_p \leq m < s_{p+1}\}$, $t = m - s_k$. Then

$$\begin{aligned} f(m,n) &= \binom{k}{2}(n-1)\sqrt{2} + (n-k-t-1)k\sqrt{(n-1)^2+k^2} + kt\sqrt{(n-1)^2+(k+1)^2} \\ &+ t\sqrt{(k+1)^2+(k+t)^2} + k\sqrt{(n-1)^2+(k+t)^2}. \end{aligned}$$

Based on the theorem above, we propose the following problem.

Problem 4. *Let $F \in CG_{n,m}$ be a connected graph. Then*

$$\mathrm{SO}(F) \leq f(m,n)$$

with equality if and only if $F \cong F(m,n)$, where $F(m,n)$ is given by Algorithm A1, that is, $\mathrm{SO}(F(m,n)) = f(m,n)$.

3. Relation between SO and the others indices

The average Sombor index is defined as follows:

$$\mathrm{ASO}(F) = \sum_{uv \in E(F)} \sqrt{\left(d_u - \frac{2m}{n}\right)^2 + \left(d_v - \frac{2m}{n}\right)^2}.$$

The average Sombor index is introduced by Gutman [16] in 2021, it is a variant of Sombor index, which is a better measure of the chemical properties of molecular compounds.

Theorem 3.1. *Let K_{ℓ_1,ℓ_2} be a complete bipartite graph of order n. Then we have*

$$\mathrm{ASO}(F) \leq max\Big\{f(t_1), f(t_2)\Big\},$$

where

$$f(x) = x(n-x)\sqrt{\left(x - \frac{2x(n-x)}{n}\right)^2 + \left(n - x - \frac{2x(n-x)}{n}\right)^2},\ for\ x = t_1 or\ t_2,$$

$$t_1 = \left\lfloor \frac{1}{4}\left(2n - \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}n\right)\right\rfloor\ and\ t_2 = \left\lceil \frac{1}{4}\left(2n - \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}n\right)\right\rceil.$$

Proof. For K_{ℓ_1,ℓ_2} $(n = \ell_1 + \ell_2,\ \ell_1 \leq \ell_2)$, we have $m = \ell_1\,\ell_2 = \ell_1\,(n - \ell_1)$ and

$$\begin{aligned}\mathrm{ASO}(K_{\ell_1,\ell_2}) &= \ell_1\ell_2\sqrt{\left(\ell_1 - \frac{2m}{n}\right)^2 + \left(\ell_2 - \frac{2m}{n}\right)^2}\\ &= \ell_1(n-\ell_1)\sqrt{\left(\ell_1 - \frac{2\ell_1(n-\ell_1)}{n}\right)^2 + \left(n - \ell_1 - \frac{2\ell_1(n-\ell_1)}{n}\right)^2},\quad 1 \leq \ell_1 \leq \left\lfloor\frac{n}{2}\right\rfloor.\end{aligned}$$

Consider the following function

$$f(x) = x(n-x)\sqrt{\left(x - \frac{2x(n-x)}{n}\right)^2 + \left(n - x - \frac{2x(n-x)}{n}\right)^2}\ \text{for}\ 1 \leq x \leq \left\lfloor\frac{n}{2}\right\rfloor.$$

Then find the derivative of function $f(x)$,

$$f'(x) = \frac{2\Big[x(n-x)\big(\frac{x-2n}{x} + \frac{2x}{n}\big)\big(\frac{n^2+2x^2-3xn}{n}\big) + \big(\frac{x-n}{n} + \frac{2x}{n}\big)\big(\frac{2x^2-nx}{n}\big)\Big]}{\sqrt{\left(\frac{n^2+2x^2-3xn}{n}\right)^2 + \left(\frac{2x^2-nx}{n}\right)^2}}$$

$$+ (n-x)\sqrt{\left(\frac{n^2+2x^2-3xn}{n}\right)^2 + \left(\frac{2x^2-nx}{n}\right)^2} - x\sqrt{\left(\frac{n^2+2x^2-3xn}{n}\right)^2 + \left(\frac{2x^2-nx}{n}\right)^2}.$$

Set $f'(x) = 0$, the set of real roots of this equation is as showing below:

$$\left\{\frac{n}{4}\left(2 - \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}\right), \frac{n}{4}\left(2 + \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}\right)\right\}.$$

One can easily check that for $1 \leq x \leq \frac{n}{4}\left(2 - \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}\right)$, it follows that $f'(x) \geq 0$ and for $\frac{n}{4}\left(2 - \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}\right) \leq x \leq \lfloor\frac{n}{2}\rfloor$, it follows that $f'(x) \leq 0$. So, we know $f(x)$ is an increasing function on $1 \leq x \leq \frac{n}{4}\left(2 - \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}\right)$ and a decreasing function on $\frac{n}{4}\left(2 - \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}\right) \leq x \leq \lfloor\frac{n}{2}\rfloor$.

Hence,

$$\mathrm{ASO}(K_{\ell_1,\ell_2}) \quad = \quad f(\ell_1) \leq \max\{f(t_1), f(t_2)\},$$

where $t_1 = \left\lfloor \frac{n}{4}\left(2 - \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}\right)\right\rfloor$ and $t_2 = \left\lceil \frac{n}{4}\left(2 - \sqrt{\frac{1}{2}\left(\sqrt{17}-1\right)}\right)\right\rceil$. □

To illustrate the above Theorem 3.1, we give some extremal graphs for $1 \leq n \leq 1000$. For $n \in \{2,3,4,5,6,7\}$, the extremal graph is $K_{1,n-1} \cong S_{1,n-1}$ and $S_{1,k}$ is a star graph. For $n \geq 8$ and integers r, t with $0 \leq r \leq 15$, if $n - 8 = 16t + r$, then the extremal graph $K_{\ell,n-\ell}$ satisfies

$$\ell = \begin{cases} 3t+2, & \text{if } 0 \leq r \leq 5, \\ 3t+3, & \text{if } 6 \leq r \leq 10, \\ 3t+4, & \text{if } 11 \leq r \leq 15. \end{cases}$$

Kulli [18] proposed the first Banhatti-Sombor index of a connected graph F which is defined as

$$\mathrm{BSO}(F) = \sum_{uv\in E(F)} \sqrt{\frac{1}{d_F^2(u)} + \frac{1}{d_F^2(v)}},$$

which is also inspired by Sombor indices.

Theorem 3.2. *Let F be a connected graph. Then*

$$\frac{1}{\Delta^2} SO(F) \leq BSO(F) \leq \frac{1}{\delta^2} SO(F)$$

with equality if and only if F is a regular graph.

Proof. Since $\delta^2 \leq d_F(u)d_F(v) \leq \Delta^2$, we have

$$\begin{aligned} \sum_{uv\in E(F)} \sqrt{\frac{1}{d_F^2(u)} + \frac{1}{d_F^2(v)}} &\leq \max\left\{\frac{1}{d_F(u)d_F(v)} | uv \in E(F)\right\} \sum_{uv\in E(F)} \sqrt{d_F^2(u) + d_F^2(v)} \\ &\leq \frac{1}{\delta^2} \sum_{uv\in E(F)} \sqrt{d_F^2(u) + d_F^2(v)} \end{aligned}$$

and

$$\begin{aligned} \sum_{uv\in E(F)} \sqrt{\frac{1}{d_F^2(u)} + \frac{1}{d_F^2(v)}} &\geq \min\left\{\frac{1}{d_F(u)d_F(v)} | uv \in E(F)\right\} \sum_{uv\in E(F)} \sqrt{d_F^2(u) + d_F^2(v)} \\ &\geq \frac{1}{\Delta^2} \sum_{uv\in E(F)} \sqrt{d_F^2(u) + d_F^2(v)}. \end{aligned}$$

Then

$$\delta^2\, BSO(F) \leq SO(F) \leq \Delta^2\, BSO(F).$$

Moreover, both equalities hold if and only if F is a regular graph. □

Inspired by the definations of the Zagreb indices with applications, Kulli [20] introduced the first Gourava index defined as

$$GO_1(F) = \sum_{uv \in E(F)} [d_F(u) + d_F(v) + d_F(u)d_F(v)],$$

for the molecular graph F, and the Second Gourava index [19]

$$GO_2(F) = \sum_{uv \in E(F)} [d_F(u) + d_F(v)]\, d_F(u)d_F(v),$$

for the molecular graph F. The forgotten topological index is defined as [17]

$$F_1(F) = \sum_{uv \in E(F)} \Big(d_F(u)^2 + d_F(v)^2\Big) = \sum_{u \in V(F)} d_F(u)^3.$$

We now give an upper bound on $GO_1(F)$ and characterize the extremal graphs.

Theorem 3.3. *Let F be a connected graph. Then $GO_1(F) \le F_1(F)$ with equality if and only if $F \cong P_n$ or $F \cong C_n$.*

Proof. Let $uv \in E(F)$. Without loss of generality, we can assume that $d_F(u) \ge d_F(v)$. Also let

$$\begin{aligned} A &= d_F(u)^2 + d_F(v)^2 - \Big[d_F(u) + d_F(v) + d_F(u)d_F(v)\Big] \\ &= \Big(d_F(u) - d_F(v)\Big)^2 + \Big(d_F(u) - 1\Big)\Big(d_F(v) - 1\Big) - 1. \end{aligned} \tag{3.1}$$

If $\Big(d_F(u),\, d_F(v)\Big) \in \{(2,1),\,(2,2)\}$, then from (3.1), $A = 0$. Otherwise, $\Big(d_F(u),\, d_F(v)\Big) \notin \{(2,1),\,(2,2)\}$. Since F is connected, $d_F(u) \ge 3$. We consider the following two cases:

Case 1. $d_F(u) > d_F(v)$.

If $d_F(u) \ge d_F(v) + 2$, then we have

$$\Big(d_F(u) - d_F(v)\Big)^2 + \Big(d_F(u) - 1\Big)\Big(d_F(v) - 1\Big) \ge 4 \quad \text{and hence } A > 0.$$

Otherwise, $d_F(u) = d_F(v) + 1$. Therefore $d_F(u) \ge 3$ and $d_F(v) \ge 2$. Thus we obtain

$$\Big(d_F(u) - d_F(v)\Big)^2 + \Big(d_F(u) - 1\Big)\Big(d_F(v) - 1\Big) \ge 3 \quad \text{and hence } A > 0.$$

Case 2. $d_F(u) = d_F(v) \ge 3$.

Then $\Big(d_F(u) - 1\Big)\Big(d_F(v) - 1\Big) \ge 4$ and hence $A > 0$.

Thus we conclude that $A \ge 0$ with equality if and only if $\Big(d_F(u),\, d_F(v)\Big) \in \{(2,1),\,(2,2)\}$. Hence

$$GO_1(F) = \sum_{uv \in E(F)} [d_F(u) + d_F(v) + d_F(u)d_F(v)] \le \sum_{uv \in E(F)} \Big(d_F(u)^2 + d_F(v)^2\Big) = \sum_{u \in V(F)} d_F(u)^3 = F_1(F).$$

Moreover, the above equality holds if and only if $F \cong P_n$ or $F \cong C_n$. □

Theorem 3.4. *Let F be a connected graph. Then*

$$GO_2(F) \ge \frac{\delta}{m} SO(F)^2 \tag{3.2}$$

with equality if and only if F is a regular graph.

Proof. By Cauchy-Schwarz inequality, we obtain

$$\left(\sum_{uv\in E(F)} \sqrt{d_F^2(u)+d_F^2(v)}\right)^2 \leq m \sum_{uv\in E(F)} \left(d_F(u)^2+d_F(v)^2\right)$$

with equality if and only if $d_F^2(u)+d_F^2(v) = d_F^2(w)+d_F^2(z)$ for any edges $uv \in E(F)$ and $wz \in E(F)$. Using the above result, we obtain

$$\begin{aligned} GO_2(F) &= \sum_{uv\in E(F)} \left(d_F(u)+d_F(v)\right) d_F(u)d_F(v) \\ &\geq \delta \sum_{uv\in E(F)} \left(d_F(u)^2+d_F(v)^2\right) \\ &\geq \frac{\delta}{m}\left(\sum_{uv\in E(F)} \sqrt{d_F^2(u)+d_F^2(v)}\right)^2 \\ &= \frac{\delta}{m} SO(F)^2. \end{aligned} \tag{3.3}$$

Moreover, the equality holds in (3.2) if and only if $d_F(u) = \delta$ for all $u \in V(F)$. Hence the equality holds in (3.2) if and only if F is a regular graph. □

Theorem 3.5. *Let F be a connected graph. Then*

$$GO_2(F) \geq \frac{M_1(F)^2}{n} \tag{3.4}$$

with equality if and only if F is a bipartite semiregular graph or F is a regular graph.

Proof. Since

$$M_1(F) = \sum_{uv\in E(F)} \left(d_F(u)+d_F(v)\right)$$

and

$$\sum_{uv\in E(F)} \frac{d_F(u)+d_F(v)}{d_F(u)\,d_F(v)} = \sum_{uv\in E(F)} \left(\frac{1}{d_F(u)}+\frac{1}{d_F(v)}\right) = \sum_{u\in V(F)} d_F(u)\,\frac{1}{d_F(u)} = n$$

by weighted arithmetic-harmonic-mean inequality, we obtain

$$\frac{\sum\limits_{uv\in E(F)} \left(d_F(u)+d_F(v)\right) d_F(u)d_F(v)}{\sum\limits_{uv\in E(F)} \left(d_F(u)+d_F(v)\right)} \geq \frac{\sum\limits_{uv\in E(F)} \left(d_F(u)+d_F(v)\right)}{\sum\limits_{uv\in E(F)} \dfrac{d_F(u)+d_F(v)}{d_F(u)\,d_F(v)}},$$

that is,

$$GO_2(F) \geq \frac{M_1(F)^2}{n}.$$

Moreover, the equality holds if and only if $d_F(u)d_F(v) = d_F(w)d_F(x)$ for any edges $uv \in E(F)$ and $wx \in E(F)$, that is, if and only if the bipartite semiregular graph or the regular graph. □

Kulli [19] introduced the sum connectivity Gourava index and the product connectivity Gourava index for a molecular graph F, which is defined as

$$SGO_1(F) = \sum_{uv\in E(F)} \frac{1}{\sqrt{(d_F(u) + d_F(v)) + (d_F(u)d_F(v))}}$$

and

$$SGO_2(F) = \sum_{uv\in E(F)} \frac{1}{\sqrt{(d_F(u) + d_F(v))(d_F(u)d_F(v))}},$$

respectively.

Theorem 3.6. *Let F be a connected graph. Then*

$$SO(F) \geq \sqrt{\frac{2}{2n-2}\frac{m^2}{SGO_2(F)}}$$

with equality if and only if F is a complete graph.

Proof. By inequality between arithmetic and harmonic means for any number $\sqrt{d_F(u)d_F(v)}$ where $uv \in E(F)$, it follows that

$$\begin{aligned}
\sqrt{2n-2}SO(F) &= \sqrt{2n-2} \sum_{uv\in E(G)} \sqrt{d_F^2(u) + d_F^2(v)} \\
&\geq \sqrt{2(2n-2)} \sum_{uv\in E(F)} \sqrt{d_F(u)d_G(v)} \\
&\geq \frac{\sqrt{2(2n-2)}m^2}{\sum_{uv\in E(G)} \frac{1}{\sqrt{d_F(u)d_F(v)}}} \\
&\geq \frac{\sqrt{2}m^2}{\sum_{uv\in E(G)} \frac{1}{\sqrt{d_F(u)d_G(v)}} \frac{1}{\sqrt{(2n-2)}}} \\
&\geq \frac{\sqrt{2}m^2}{\sum_{uv\in E(G)} \frac{1}{\sqrt{d_F(u)d_F(v)}} \frac{1}{\sqrt{d_F(u)+d_F(v)}}} \\
&\geq \frac{\sqrt{2}m^2}{\sum_{uv\in E(F)} \frac{1}{\sqrt{d_F(u)d_F(v)d_F(u)+d_F(v)}}} \\
&\geq \frac{\sqrt{2}m^2}{SGO_2(F)}.
\end{aligned}$$

Then

$$SO(F) \geq \sqrt{\frac{2}{2n-2}\frac{m^2}{SGO_2(F)}}$$

with equality if and only if $d_F(u) = d_F(v)$ and $d_F(u) + d_F(v) = 2n - 2$. □

Using the proof strategy for Theorem 3.6, we have the following similar result.

Theorem 3.7. *Let F be a connected triangle-free graph. Then*

$$SO(F) \geq \sqrt{\frac{2}{n-1}} \frac{m^2}{SGO_2(F)}.$$

The eccentricity $\varepsilon_F(v)$ of a vertex $v \in V(F)$ is the distance between v and a vertex farthest from v in F. The eccentric connectivity index was introduced by Sharma, Goswami and Madan [23] as

$$\zeta^e(F) = \sum_{v \in V(F)} d_F(v)\, \varepsilon_F(v) = \sum_{uv \in E(F)} \Big(\varepsilon_F(u) + \varepsilon_F(v)\Big).$$

For its basic mathematical properties, including lower and upper bounds, see [5, 9–11, 14] and the references cited therein. The sum of eccentricities of all vertices of F is called the total eccentricity of F [4] and denoted by $\zeta(F)$, $\zeta(F) = \sum_{v \in V(F)} \varepsilon_F(v)$.

Lemma 3.1. *[15] Let F be a nontrivial connected graph of order n. For each vertex $v \in V(F)$, $d_F(v) \leq n - \varepsilon_F(v)$ with equality if and only if $F \cong P_4$ or $F \cong K_n - sK_2$ $(0 \leq s \leq \lfloor \frac{n}{2} \rfloor)$, where $K_n - sK_2$ denotes the graph obtained from the complete graph by removing s independent edges.*

Theorem 3.8. *Let F be a connected graph of order n with m edges and minimum degree δ. Then*

$$SO(F) \leq 2nm - \zeta^e(F) - (2 - \sqrt{2})\, m\, \delta \tag{3.5}$$

with equality if and only if $F \cong P_4$ or F is isomorphic to an $(n-2)$-regular graph (n is even) or $F \cong K_n$.

Proof. First, we have to prove that for any edge $uv \in E(F)$ $\Big(d_F(u) \geq d_F(v)\Big)$,

$$d_F(u) + (\sqrt{2} - 1)\, d_F(v) \geq \sqrt{d_F(u)^2 + d_F(v)^2}, \tag{3.6}$$

that is,

$$d_F(u)^2 + (3 - 2\sqrt{2})\, d_F(v)^2 + 2(\sqrt{2} - 1)\, d_F(u)\, d_F(v) \geq d_F(u)^2 + d_F(v)^2,$$

that is,

$$\Big(d_F(u) - d_F(v)\Big)\, d_F(v) \geq 0,$$

which is always true. Moreover, the equality holds in (3.6) if and only if $d_F(u) = d_F(v)$. Now,

$$\sum_{uv \in E(F)} d_F(v) \geq m\, \delta \tag{3.7}$$

with equality if and only if $d_F(v) = \delta$ for every edge $uv \in E(F)$. Using the above results with Lemma 3.1, we obtain

$$\begin{aligned} SO(F) = \sum_{uv \in E(F)} \sqrt{d_F^2(u) + d_F^2(v)} &\leq \sum_{uv \in E(F)} \Big(d_F(u) + (\sqrt{2} - 1)\, d_F(v)\Big) \\ &= \sum_{uv \in E(F)} \Big(d_F(u) + d_F(v)\Big) - (2 - \sqrt{2}) \sum_{uv \in E(F)} d_F(v) \end{aligned}$$

$$\leq \sum_{v\in V(F)} d_F^2(v) - (2-\sqrt{2})\, m\,\delta$$

$$\leq \sum_{v\in V(F)} d_F(v)\Big(n-\varepsilon_F(v)\Big) - (2-\sqrt{2})\, m\,\delta \tag{3.8}$$

$$= n \sum_{v\in V(F)} d_F(v) - \sum_{v\in v(F)} d_F(v)\,\varepsilon_F(v) - (2-\sqrt{2})\, m\,\delta$$

$$= 2nm - \zeta^e(F) - (2-\sqrt{2})\, m\,\delta.$$

Both (3.6) and (3.7) equalities hold if and only if $d_F(u) = d_F(v) = \delta$ for any edge $uv \in E(F)$. From the equality in (3.8), we have $F \cong P_4$ or $F \cong K_n - sK_2$ $(0 \leq s \leq \lfloor \frac{n}{2} \rfloor)$ by Lemma 3.1. Hence the equality holds in (3.5) if and only if $F \cong P_4$ or F is isomorphic to an $(n-2)$-regular graph (n is even) or $F \cong K_n$. □

Theorem 3.9. *Let F be a connected graph of order n with size m and maximum degree Δ. Then*

$$SO(F) \leq \sqrt{2m^2 n\Delta - m\Delta\zeta^e(F)}. \tag{3.9}$$

The above equality holds if and only if $F \cong P_4$ or F is isomorphic to an $(n-2)$-regular graph (n is even) or $F \cong K_n$.

Proof. By Cauchy-Schwarz inequality, we obtain

$$SO^2(F) = \left(\sum_{uv\in E(F)} \sqrt{d_F^2(u)+d_F^2(v)}\right)^2$$

$$\leq m \sum_{uv\in E(F)} \Big(d_F^2(u)+d_F^2(v)\Big) \tag{3.10}$$

$$= m \sum_{v\in v(F)} d_F^3(v) \leq m \sum_{v\in v(F)} d_F^2(v)\Big(n-\varepsilon_F(v)\Big) \tag{3.11}$$

$$= m \sum_{v\in v(F)} d_F(v)\Big(d_F(v)n - d_F(v)\,\varepsilon_F(v)\Big)$$

$$\leq m\Delta \sum_{v\in v(F)} \Big(d_F(v)n - d_F(v)\,\varepsilon_F(v)\Big) \tag{3.12}$$

$$= m\Delta\left(n \sum_{v\in v(F)} d_F(v) - \sum_{v\in v(F)} d_F(v)\,\varepsilon_F(v)\right)$$

$$= m\Delta\Big(2mn - \zeta^e(F)\Big).$$

The first part of the proof is done. □

Suppose equality holds in (3.9). Then all the inequalities in the above argument occur as equalities. From equality in (3.10), we obtain $d_F^2(u) + d_F^2(v) = d_F^2(w) + d_F^2(x)$ for any two edges $uv \in E(F)$ and

$wx \in E(F)$, that is, F is a semiregular graph as F is connected. From the equality in (3.11), we have $F \cong P_4$ or $F \cong K_n - sK_2$ ($0 \le s \le \lfloor \frac{n}{2} \rfloor$), by Lemma 3.1. From equality in (3.12), we obtain $d_F(v) = \Delta$ for all $v \in V(F)$ as $d_F(v)n > d_F(v)\,\varepsilon_F(v)$ with connected graph F. From these results, we obtain $F \cong P_4$ or F is isomorphic to an $(n-2)$-regular graph (n is even) or $F \cong K_n$.

Conversely, let $F \cong P_4$. Then $m = n = 4$, $\Delta = 2$, $\zeta^e(F) = 16$ and hence

$$SO(F) = 8\sqrt{2} = \sqrt{m\Delta\left(2mn - \zeta^e(F)\right)}.$$

Let F be a graph which is isomorphic to an $(n-2)$-regular graph (n is even). Then $2m = n(n-2)$, $\Delta = n-2$ and $\zeta^e(F) = 2n\,(n-2)$. Thus we have

$$SO(F) = \frac{n(n-2)^2}{\sqrt{2}} = \sqrt{m\Delta\left(2mn - \zeta^e(F)\right)}.$$

Let $F \cong K_n$. Then $2m = n(n-1)$, $\Delta = n-1$ and $\zeta^e(F) = n\,(n-1)$. Thus we have

$$SO(F) = \frac{n(n-1)^2}{\sqrt{2}} = \sqrt{m\Delta\left(2mn - \zeta^e(F)\right)}.$$

By the same way, we have the following result and we omit the details proof of it.

Theorem 3.10. *Let F be a connected graph of order n. Then*

$$SO(F) \le \Delta\left(n^2 - \zeta(F)\right) - (2 - \sqrt{2})\,m\,\delta$$

with equality if and only if $F \cong P_4$ or F is isomorphic to an $(n-2)$-regular graph (n is even) or $F \cong K_n$.

Proof. Since $d_F(v) \le \Delta$ for all $v \in V(F)$, from (3.8), we obtain the required result. Moreover, the equality holds if and only if $F \cong P_4$ or F is isomorphic to an $(n-2)$-regular graph (n is even) or $F \cong K_n$. □

4. Conclusions

In this paper, we studied some extremal values on the (reduced) Sombor index of molecular graphs. Furthermore, some relations among the chemistry indexes are presented, in particular, we obtained relationship between Sombor index and the other topological indices, and characterized the extreme graphs. Specifically, we obtained inequalities for Sombor index relating other indices, *i.e.*, the first Banhatti-Sombor index, the first Gourava index, the Second Gourava index, the Sum Connectivity Gourava index, Product Connectivity Gourava index, and Eccentric Connectivity index.

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Conflict of interest

The authors declare no conflict of interest.

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