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On the Reduced Sombor Index and Its Applications

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Abstract

Based on elementary geometry, a novel vertex-degree-based molecular structure descriptor was recently introduced by Gutman in the chemical graph theory, defined as $SO_{red}(G) = \sum_{uv\in E(G)} \sqrt{(d_u-1)^2+(d_v-1)^2}$, where d_u denotes the degree of vertex u in G, and named as reduced Sombor index. It was demonstrated that the reduced Sombor index can help to exert modest discriminative potential and predict physico-chemical properties of molecules, and it performs with slightly better predictive potential than the Sombor index [10, 27]. Based on the results of testing predictive potential of reduced Sombor indices, it may be successfully applied on modeling thermodynamic properties of compounds [27].

In this paper, we obtain some bounds for reduced Sombor index of graphs with given several parameters (such as maximum degree Δ, minimum degree δ, matching number β, chromatic number χ, independence number α, clique number ω), some special graphs (such as unicyclic grahs, bipartite graphs, graphs with no triangles, graphs with no K_{r+1} $(2 \le r \le n-1)$) and the Nordhaus-Gaddum-type results. We also characterize some extremal molecular graphs. Then we obtain the expected values of reduced Sombor index in random polyphenyl chains. At last, we apply the reduced Sombor index to graph spectrum and energy problems.

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1 Introduction

In this paper, notations and terminologies used but not defined here can refer to Bondy and Murty [3]. Inspired by Euclidean metric, a novel vertex-degree-based molecular structure descriptor was recently introduced by Gutman in the chemical graph theory, the reduced Sombor index [17], defined as

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

(reduced) Sombor index was developed as the geometric representation of vertex-degree-based molecular structure descriptor, and any vertex-degree-based descriptor can be viewed as a special case of a Sombor-type index [18].

Since the first paper [17] on the Sombor indices was published, a flood of papers were created to report the properties of Sombor indices. Recently, the Sombor index was studied on trees, unicyclic graphs and bicyclic graphs [6,29], molecular graphs [5,10]. Moreover, the mathematical properties of Sombor index were studied in [9,18,25,33]. Also, in [10,27] chemical applicability of Sombor indices was considered. One can refer [22,23] for more and some other details on the Sombor indices.

The rest of the paper is organized as follows. In Section 2 we obtain some bounds for reduced Sombor index of graphs with a given several parameters (such as maximum degree Δ, minimum degree δ, matching number β, chromatic number χ, independence number α, clique number ω), some special graphs (such as unicyclic grahs, bipartite graphs, graphs with no triangles, graphs with no K_{r+1} $(2 \le r \le n-1)$) and the Nordhaus-Gaddum-type results. In Section 3 We characterize the extremal graphs among molecular graphs. In Section 4 we obtain the expected values of reduced Sombor index in random polyphenyl chains. In Section 5 we apply the reduced Sombor index to graph spectrum and energy problems. In Section 6 we conclude this paper.

2 On the reduced Sombor index of graphs

2.1 Simple graphs

Here are three simple properties of reduced Sombor index.

Lemma 2.1 *[10] Let G be a simple graph with n vertices. Then*

$$0 \le SO_{red}(G) \le SO_{red}(K_n) = \frac{\sqrt{2}}{2} n(n-1)(n-2),$$

with left equality iff $G \cong tK_2 \cup (n-2t)K_1$ *where* $0 \le t \le \lfloor \frac{n}{2} \rfloor$*, right equality iff* $G \cong K_n$*.*

Lemma 2.2 *[10] Let G be a simple connected graph with n vertices. Then*

$$SO_{red}(P_n) \le SO_{red}(G) \le SO_{red}(K_n),$$

with left equality iff $G \cong P_n$*, right equality iff* $G \cong K_n$*.*

Lemma 2.3 *[10] Let T be a tree with n vertices. Then*

$$SO_{red}(P_n) \le SO_{red}(T) \le SO_{red}(S_n),$$

with left equality iff $T \cong P_n$*, right equality iff* $T \cong S_n$*.*

In 2014, Gutman et al. [20] proposed the reduced reciprocal Randić (RRR) index, which is defined as $RRR(G) = \sum\limits_{uv \in E(G)} \sqrt{(d_u-1)(d_v-1)}$. By the definition of reduced Sombor index, we have

Theorem 2.4 *Let G be a simple connected graph. Then*

$$SO_{red}(G) \ge \sqrt{2} RRR(G),$$

with equality iff G is a regular graph.

Let G be a simple connected graph with no pendent vertices. Denote $\psi(G) = \sum\limits_{uv \in E(G)} \frac{1}{\sqrt{(d_u-1)(d_v-1)}}$, then $\psi(G) \cdot RRR(G) \ge m^2$. By Theorem 2.4, we have

Theorem 2.5 *Let G be a simple connected graph with m edges and no pendent vertices. Then*

$$SO_{red}(G) \ge \frac{\sqrt{2} m^2}{\psi(G)},$$

with equality iff G is a regular graph.

In the following we consider the bounds of simple graphs with given some parameters. Denote Δ, δ the maximum and minimum degree of G, then we have the following results.

Theorem 2.6 *Let G be a simple connected graph with n vertices. Then*

$$\frac{\sqrt{2}}{2} n\delta(\delta - 1) \le SO_{red}(G) \le \frac{\sqrt{2}}{2} n\Delta(\Delta - 1),$$

with equality iff G is a regular graph.

Proof. It is obvious that $n\delta \leq \sum\limits_{v \in V(G)} d_v = 2m \leq n\Delta$, with equality iff $d_v = \Delta$ or δ for all $v \in V(G)$. Then we have

(1) $SO_{red}(G) = \sum\limits_{uv \in E(G)} \sqrt{(d_u-1)^2+(d_v-1)^2} \geq \sqrt{2}m(\delta-1) \geq \frac{\sqrt{2}}{2}n\delta(\delta-1)$, with equality iff $d_v = \delta$ for all $v \in V(G)$.

(2) $SO_{red}(G) = \sum\limits_{uv \in E(G)} \sqrt{(d_u-1)^2+(d_v-1)^2} \leq \sqrt{2}m(\Delta-1) \leq \frac{\sqrt{2}}{2}n\Delta(\Delta-1)$, with equality iff $d_v = \Delta$ for all $v \in V(G)$. ■

Lemma 2.7 *[18, 25] Let G be a simple connected graph with n vertices, m edges. $Z_g(G)$ is the first Zagreb index of the graph G. Then*

$$\frac{\sqrt{2}}{2}(Z_g(G)-2m) \leq SO_{red}(G) \leq Z_g(G)-2m,$$

with left equality iff $d_u = d_v$ for any $uv \in E(G)$, right equality iff $G \cong \frac{n}{2}K_2$ for even n.

Since $Z_g(G) \geq \frac{4m^2}{n}$ with equality iff G is a regular graph (see [14]). By Lemma 2.7, we have

Theorem 2.8 *Let G be a simple connected graph with n vertices, m edges. Then*

$$SO_{red}(G) \geq \frac{\sqrt{2}m}{n}(2m-n),$$

with equality iff G is a regular graph.

Since $Z_g(G) \leq n(2m-n+1)$ with equality iff $G \cong K_n, K_{1,n-1}$ or $\frac{n}{2}K_2$ (see [35]). By Lemma 2.7, we have

Theorem 2.9 *Let G be a simple graph with n vertices, m edges. Then*

$$SO_{red}(G) \leq (2m-n)(n-1),$$

with equality iff $G \cong \frac{n}{2}K_2$ for some even n.

In order to obtain the minimum value of the reduced Sombor index of unicyclic graphs, we need the following lemmas.

Theorem 2.10 *Let G be a simple connected graph with n vertices, m edges. Then*

(1) $SO_{red}(G) \geq \sqrt{2}m(\delta-1)$,

(2) $SO_{red}(G) \geq \frac{\sqrt{2}}{2}(2m(\frac{2m}{n}-1)+\frac{1}{2}(\Delta-\delta)^2) \geq \sqrt{2}m(\frac{2m}{n}-1)$.

with equality iff G is a regular graph.

Proof. (1) By Lemma 2.7 and $Z_g(G) \geq 2m\delta$, with equality iff G is a regular graph. Thus $SO_{red}(G) \geq \sqrt{2}m(\delta - 1)$, with equality iff G is a regular graph.

(2) By Lemma 2.7 and $Z_g(G) \geq \frac{4m^2}{n} + \frac{1}{2}(\Delta - \delta)^2$, with equality iff $d_2 = \cdots = d_{n-1} = \frac{d_1+d_n}{2}$ (see [1]). Thus $SO_{red}(G) \geq \frac{\sqrt{2}}{2}(2m(\frac{2m}{n} - 1) + \frac{1}{2}(\Delta - \delta)^2) \geq \sqrt{2}m(\frac{2m}{n} - 1)$, with equality iff G is a regular graph. ■

In the following, we obtain the minimum unicyclic graphs with respect to reduced Sombor index.

Theorem 2.11 *Let G be a unicyclic graph with n vertices. Then*

(1) $SO_{red}(G) \geq \sqrt{2}n(\delta - 1)$,

(2) $SO_{red}(G) \geq \sqrt{2}n + \frac{\sqrt{2}}{4}(\Delta - \delta)^2 \geq \sqrt{2}n$,

with equality iff $G \cong C_n$.

Proof. For unicyclic graph G, $n = |V(G)| = |E(G)| = m$. Combine with Theorem 2.10, we obtain the conclusions. ■

Since $\sum_{i=1}^{n} d_i^2 \geq d_1^2 + d_n^2 + \frac{(2m-d_1-d_n)^2}{n-2}$ with equality iff $d_2 = \cdots = d_{n-1} = \frac{d_1+d_n}{2}$, where $d_1 \geq d_2 \geq \cdots \geq d_n$ (see [8]). By Lemma 2.7, we have

Theorem 2.12 *Let G be a simple connected graph with n vertices, m edges. Then*

$$SO_{red}(G) \geq \frac{\sqrt{2}}{2}\left(\Delta^2 + \delta^2 + \frac{(2m - \Delta - \delta)^2}{n-2} - 2m\right),$$

with equality iff G is a regular graph.

Let Γ be the class of graphs with $d_2 = d_3 = \cdots = d_n$, and Δ_2 the second maximum degree of G. Since $Z_g(G) \geq \Delta^2 + \frac{(2m-\Delta)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}(\Delta_2 - \delta)^2$ with equality iff G is a regular graph or $G \in \Gamma$ (see [13]). By Lemma 2.7, we have that

Theorem 2.13 *Let G be a simple graph with n vertices, m edges. Then*

$$SO_{red}(G) \geq \frac{\sqrt{2}}{2}\left(\Delta^2 + \frac{(2m - \Delta)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}(\Delta_2 - \delta)^2 - 2m\right),$$

with equality iff G is a regular graph.

2.2 Simple graphs with no triangles

In the following we consider the bounds of simple graphs with no triangles or K_{r+1} $(2 \leq r \leq n-1)$.

Theorem 2.14 *Let G be a simple connected graph with n vertices and no triangles. Then*

$$SO_{red}(G) \leq \begin{cases} m\sqrt{(\delta-1)^2+(n-\delta-1)^2}, & if\ \Delta+\delta \leq n; \\ m\sqrt{(\Delta-1)^2+(n-\Delta-1)^2}, & if\ \Delta+\delta \geq n. \end{cases}$$

Proof. Since G be a simple connected graph with n vertices and no triangles, then $d_u + d_v \leq n$ for every $uv \in E(G)$. Let $f(x) = x^2 + (n-2-x)^2$ where $\delta - 1 \leq x \leq \Delta - 1$. It is obvious that $f'(x) < 0$ for $x \in [\delta - 1, \frac{n}{2} - 1]$, $f'(x) > 0$ for $x \in [\frac{n}{2} - 1, \Delta - 1]$. Thus (1) if $\Delta + \delta \leq n$, then $\sqrt{(d_u-1)^2+(n-1-d_v)^2} \leq \sqrt{(\delta-1)^2+(n-1-\delta)^2}$, (2) if $\Delta+\delta \geq n$, then $\sqrt{(d_u-1)^2+(n-1-d_v)^2} \leq \sqrt{(\Delta-1)^2+(n-1-\Delta)^2}$. From the definition of reduced Sombor index, we have

(1) If $\Delta + \delta \leq n$, then

$SO_{red}(G) \leq \sum\limits_{uv\in E(G)} \sqrt{(d_u-1)^2+(n-1-d_v)^2} \leq m\sqrt{(\delta-1)^2+(n-\delta-1)^2}$;

(2) If $\Delta + \delta \geq n$, then

$SO_{red}(G) \leq \sum\limits_{uv\in E(G)} \sqrt{(d_u-1)^2+(n-1-d_v)^2} \leq m\sqrt{(\Delta-1)^2+(n-\Delta-1)^2}$. ■

With the help of the following properties, we can obtain other bounds of simple graphs with no triangles or K_{r+1} $(2 \leq r \leq n-1)$.

Theorem 2.15 *Let G be a simple connected graph with minimum degree δ and $|E(G)| = m$. Then*

$$SO_{red}(G) \leq Z_g(G) - \sqrt{2}((\sqrt{2}-1)\delta + 1)m,$$

with equality iff G is a regular graph.

Proof. Without loss of generality, we suppose $d_u \geq d_v$ for every $uv \in E(G)$. It is obvious that $\sqrt{(d_u-1)^2+(d_v-1)^2} \leq d_u - 1 + (\sqrt{2}-1)(d_v-1) = d_u - \sqrt{2} + (\sqrt{2}-1)d_v$.

From the definition of reduced Sombor index, we have

$SO_{red}(G) = \sum\limits_{uv\in E(G)} \sqrt{(d_u-1)^2+(d_v-1)^2} \leq \sum\limits_{uv\in E(G), d_u\geq d_v} (d_u + (\sqrt{2}-1)d_v - \sqrt{2}) = \sum\limits_{uv\in E(G)} (d_u+d_v) - \sum\limits_{uv\in E(G), d_u\geq d_v} [(2-\sqrt{2})d_v + \sqrt{2}] \leq Z_g(G) - \sqrt{2}((\sqrt{2}-1)\delta+1)m$, with equality iff G is a regular graph. ■

Theorem 2.16 *Let G be a simple connected graph with n vertices, minimum degree δ and no triangles. Then*

$$SO_{red}(G) \leq m(n - \sqrt{2} - (2 - \sqrt{2})\delta),$$

with equality iff $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Proof. Since G be a simple connected graph with n vertices, minimum degree δ and no triangles. Then $Z_g(G) \leq mn$ with equality iff G is a complete bipartite graph (see [35]). Combine with Lemma 2.15, the conclusion holds. ■

Theorem 2.17 *Let G be a simple connected graph with n vertices, minimum degree δ and no K_{r+1} $(2 \leq r \leq n-1)$. Then*

$$SO_{red}(G) \leq \frac{2r-2}{r}mn - \sqrt{2}((\sqrt{2}-1)\delta + 1)m,$$

with equality iff G is a regular complete r-partite graph.

Proof. Since G is a simple connected graph with n vertices, minimum degree δ and no K_{r+1} $(2 \leq r \leq n-1)$. Then $Z_g(G) \leq \frac{2r-2}{r}mn$ with equality iff G is a complete 2-partite graph for $r = 2$ and a regular complete r-partite graph for $r \geq 3$ (see [37]). Combine with Lemma 2.15, the conclusion holds. ■

Except the above results, we also have the following results.

Theorem 2.18 *Let G be a simple connected graph with n vertices, m edges, and minimum degree δ. Then*

$$SO_{red}(G) \leq m\left(\frac{2m}{n-1} + n - (2+\sqrt{2}) - (2-\sqrt{2})\delta\right),$$

with equality iff $G \cong K_n$.

Proof. Since G is a simple connected graph with n vertices, m edges, and minimum degree δ. Then $Z_g(G) \leq m(\frac{2m}{n-1} + n - 2)$ with equality iff $G \cong K_n, K_{1,n-1}$, or $K_1 \cup K_{n-1}$ (see [35]). Combine with Lemma 2.15, the conclusion holds. ■

Theorem 2.19 *Let G be a simple connected graph with n vertices, m edges, and minimum degree δ. Then*

$$SO_{red}(G) \leq n(2m - n\delta) + \frac{n}{2}\left(\delta^2 + 1 + (\delta - 1)\sqrt{(\delta+1)^2 + 4(2m - n\delta)}\right) - \sqrt{2}((\sqrt{2}-1)\delta + 1)m,$$

with equality iff G is a regular graph.

Proof. Since G is a simple connected graph with n vertices, m edges, and minimum degree δ. Then $Z_g(G) \leq n(2m-n\delta)+\frac{n}{2}(\delta^2+1+(\delta-1)\sqrt{(\delta+1)^2+4(2m-n\delta)})$ with equality iff G is a regular graph or $G \cong K_{1,n-1}$ (see [35]). Combine with Lemma 2.15, the conclusion holds. ■

2.3 Bipartite graphs (with given matching number)

In the following we consider the bounds of bipartite graphs (with given matching number). The monotonicity of reduced Sombor index is obvious.

Lemma 2.20 *Let G be a graph and $u, v \in V(G)$, then*

(1) *if $e = uv \notin G$, then $SO_{red}(G) < SO_{red}(G+e)$;*

(2) *if $e = uv \in G$, then $SO_{red}(G) > SO_{red}(G-e)$.*

Theorem 2.21 *Let G be a bipartite graph with n vertices. Then*

$$SO_{red}(G) \leq \left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor \sqrt{\left(\left\lceil \frac{n}{2} \right\rceil - 1\right)^2 + \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right)^2},$$

with equality iff $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

Proof. Since G is a bipartite graph with n vertices, we suppose $p \geq q$. Then by Lemma 2.20, $SO_{red}(G) \leq SO_{red}(K_{p,q})$. Thus $SO_{red}(G) \leq SO_{red}(K_{p,q}) = pq\sqrt{(p-1)^2+(q-1)^2} = p(n-p)\sqrt{(p-1)^2+(n-p-1)^2}$.

Let $f(x) = x(n-x)\sqrt{(x-1)^2+(n-x-1)^2}$, where $\lceil \frac{n}{2} \rceil \leq x \leq n-1$. It is obvious that $f'(x) = \frac{x(n-x)(2x-n)+(n-2x)[(x-1)^2+(n-x-1)^2]}{(x-1)^2+(n-x-1)^2} \leq 0$ for $\lceil \frac{n}{2} \rceil \leq x \leq n-1$. Thus $SO_{red}(G) \leq p(n-p)\sqrt{(p-1)^2+(n-p-1)^2} \leq \lceil \frac{n}{2} \rceil \lfloor \frac{n}{2} \rfloor \sqrt{(\lceil \frac{n}{2} \rceil - 1)^2 + (\lfloor \frac{n}{2} \rfloor - 1)^2}$, with equality iff $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$. ■

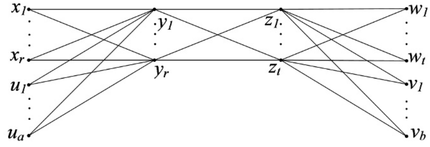


Figure 1: Bipartite graph $B(r,t,a,b)$.

Let $B(r,t,a,b)$ be the bipartite graph obtained from $G_1 = K_{r,r+a}$ and $G_2 = K_{t,t+b}$ by joining each vertex of r-part in G_1 to each vertex of t-part in G_2, where r,t,a,b are non-negative integers, see Figure 1.

Lemma 2.22 *[7] Let G be a bipartite graph of order n with bipartition (X, Y) and matching number β. Then there exists a bipartite graph $G' = B(r, t, a, b)$ such that*

(1) $I(G') \leq I(G)$ for the topological index I which decreases with addition of edges;

(2) $I(G') \geq I(G)$ for the topological index I which increases with addition of edges, with equality if and only if $G \cong B(r, t, a, b)$ for some non-negative integers r, t, a, b, where $r + t = \beta$, $r + t + a = |X|$ and $r + t + b = |Y|$.

Lemma 2.23 *If bipartite graph $B(r, t, a, b) \ncong K_{r+t,r+t+a+b}$. Then $SO_{red}(B(r, t, a, b)) < SO_{red}(K_{r+t,r+t+a+b})$.*

Proof. From the definition of reduced Sombor index, we have

$$\begin{aligned}
&SO_{red}(K_{r+t,r+t+a+b}) - SO_{red}(B(r, t, a, b))\\
&= (r + t)(r + t + a + b)\sqrt{(r + t + a + b - 1)^2 + (r + t - 1)^2}\\
&\quad - r(r + a)\sqrt{(r + t + a - 1)^2 + (r - 1)^2} - rt\sqrt{(r + t + a - 1)^2 + (r + t + b - 1)^2}\\
&\quad - t(t + b)\sqrt{(r + t + b - 1)^2 + (t - 1)^2}\\
&\geq (r(t + b) + t(r + a))\sqrt{(r + t + a + b - 1)^2 + (r + t - 1)^2}\\
&\quad - rt\sqrt{(r + t + a - 1)^2 + (r + t + b - 1)^2}\\
&\geq rt\left[\sqrt{4(r + t + a + b - 1)^2 + 4(r + t - 1)^2} - \sqrt{(r + t + a - 1)^2 + (r + t + b - 1)^2}\right]\\
&= rt\left[\frac{4(r + t + a + b - 1)^2 + 4(r + t - 1)^2 - (r + t + a - 1)^2 - (r + t + b - 1)^2}{\sqrt{4(r + t + a + b - 1)^2 + 4(r + t - 1)^2} + \sqrt{(r + t + a - 1)^2 + (r + t + b - 1)^2}}\right]\\
&> 0.
\end{aligned}$$

■

In the following, we obtain maximum bipartite graphs with given matching number.

Theorem 2.24 *Let G be a bipartite graph with n vertices and matching number β. Then*

$$SO_{red}(G) \leq SO_{red}(K_{\beta,n-\beta}) = \beta(n - \beta)\sqrt{(\beta - 1)^2 + (n - \beta - 1)^2},$$

with equality iff $G \cong K_{\beta,n-\beta}$.

Proof. Suppose that G is a bipartite graph with n vertices, bipartition (X, Y), and matching number β, such that its reduced Sombor index is as large as possible.

By Lemma 2.20, 2.22, there exists a bipartite graph $B(r, t, a, b)$ such that $SO_{red}(G) \leq SO_{red}(B(r, t, a, b))$ with equality iff $G \cong B(r, t, a, b)$, where $r + t = \beta$, $r + t + a = |X|$ and $r + t + b = |Y|$.

By Lemma 2.23, $SO_{red}(B(r, t, a, b)) \leq SO_{red}(K_{r+t,r+t+a+b})$ with equality iff $G \cong K_{r+t,r+t+a+b}$, i.e. $G \cong K_{\beta,n-\beta}$. This completes the proof. ■

2.4 Simple graphs with given chromatic number

Denote by $\mathcal{X}(n,\chi)$ the set of connected graphs with n vertices and chromatic number χ. By the monotonicity of reduced Sombor index and the definition of $\mathcal{X}(n,\chi)$, we have

Theorem 2.25 *Let $G \in \mathcal{X}(n,\chi)$. Then*

$$SO_{red}(G) \leq SO_{red}(K_{n_1,n_2,\ldots,n_\chi}),$$

with equality iff $G \cong K_{n_1,n_2,\ldots,n_\chi}$, where $\sum\limits_{i=1}^{\chi} n_i = n$.

The Turán graph $T_{n,k}$ is a special complete multipartite graph $K_{n_1,n_2,\ldots,n_k}$ with $|n_i - n_j| \leq 1$ for $1 \leq i,j \leq k$. Further describing the maximum reduced Sombor index in $K_{n_1,n_2,\ldots,n_\chi}$ is still an open problem. Therefore we propose the following conjecture.

Conjecture 2.1 *Let $G \in K_{n_1,n_2,\ldots,n_\chi}$. Then*

$$SO_{red}(G) \leq SO_{red}(T_{n,\chi}),$$

with equality iff $G \cong T_{n,\chi}$.

2.5 Simple graphs with given independence number

Let $CS(n,\alpha)$ be the complete split graph with n vertices and independence number α. In the following, we obtain maximum simple connected graphs with given independence number.

Theorem 2.26 *Let G be a simple connected graph with n vertices and independence number α. Then*

$$SO_{red}(G) \leq \sqrt{2}\binom{n-\alpha}{2}(n-2) + \alpha(n-\alpha)\sqrt{(n-\alpha-1)^2 + (n-2)^2},$$

with equality iff $G \cong CS(n,\alpha)$.

Proof. Since G is a simple connected graph with n vertices and independence number α. By Lemma 2.20, we have

$$SO_{red}(G) \leq SO_{red}(CS(n,\alpha)) = \sqrt{2}\binom{n-\alpha}{2}(n-2) + \alpha(n-\alpha)\sqrt{(n-\alpha-1)^2 + (n-2)^2},$$

with equality iff $G \cong CS(n,\alpha)$. ■

2.6 Simple graphs with given clique number

Theorem 2.27 *Let G be a simple graph with n vertices and clique number ω. Then*

$$SO_{red}(G) \geq \frac{\sqrt{2}}{2}\left(\frac{n^3}{\omega^2} + 2m(2n-1) - n^3\right),$$

with equality iff G is a k-regular graph and $\omega = \frac{n}{n-k}$.

Proof. Since G is a simple graph with n vertices and clique number ω. Then $Z_g(G) \geq 4mn + \frac{n^3}{\omega^2} - n^3$ with equality iff G is a regular graph of degree k and $\omega = \frac{n}{n-k}$ (see [15]). Combine with Lemma 2.7, the conclusion holds. ■

2.7 Nordhaus–Gaddum-type results

Theorem 2.28 *Let G be a simple graph with n vertices. Then*

$$\frac{\sqrt{2}}{4}n\{2\lfloor\frac{n}{2}\rfloor^2 - 2(n-1)\lfloor\frac{n}{2}\rfloor + (n-2)(n-1)\} \leq SO_{red}(G) + SO_{red}(\overline{G}) \leq \frac{\sqrt{2}}{2}n(n-1)(n-2),$$

with left equality iff G is a $\lfloor\frac{n}{2}\rfloor$-regular graph, right equality iff $G \cong K_n$ or $G \cong \overline{K_n}$.

Proof. Since $|E(G)| + |E(\overline{G})| = \binom{n}{2}$ and $\sqrt{(d_i-1)^2 + (d_j-1)^2} \leq \sqrt{2}(n-2)$ for $i \sim j$ in G or $\overline{G}$. Thus $SO_{red}(G) + SO_{red}(\overline{G}) \leq \binom{n}{2}\sqrt{2}(n-2) = \frac{\sqrt{2}}{2}n(n-1)(n-2)$, with equality iff $G \cong K_n$ or $G \cong \overline{K_n}$.

On the other hand, we have $SO_{red}(G) = \sum\limits_{i \sim j}\sqrt{(d_i-1)^2 + (d_j-1)^2} \geq \frac{\sqrt{2}}{2}\sum\limits_{i\sim j}[(d_i-1) + (d_j-1)] = \frac{\sqrt{2}}{2}\sum\limits_{i=1}^{n}(d_i-1)(d_i-1)$. And $SO_{red}(\overline{G}) = \sum\limits_{i\sim j}\sqrt{(n-2-d_i)^2 + (n-2-d_j)^2} \geq \frac{\sqrt{2}}{2}\sum\limits_{i\sim j}[(n-2-d_i) + (n-2-d_j)] = \frac{\sqrt{2}}{2}\sum\limits_{i=1}^{n}(n-2-d_i)(n-1-d_i)$. So $SO_{red}(G) + SO_{red}(\overline{G}) \geq \frac{\sqrt{2}}{2}\sum\limits_{i=1}^{n}[(d_i-1)(d_i-1) + (n-2-d_i)(n-1-d_i)] = \frac{\sqrt{2}}{2}\sum\limits_{i=1}^{n}[2d_i^2 - 2(n-1)d_i + (n-2)(n-1)] \geq \frac{\sqrt{2}}{2}n\{2\lfloor\frac{n}{2}\rfloor^2 - 2(n-1)\lfloor\frac{n}{2}\rfloor + (n-2)(n-1)\}$, with equality iff G is a $\lfloor\frac{n}{2}\rfloor$-regular graph. ■

3 On the reduced Sombor index of molecular graphs

A molecular graph is a graph with maximum degree at most 4. Cruza et al. [5], considered the Sombor index of molecular graphs. In the following, we obtain the extremal molecular graphs with respect to reduced Sombor index. Let G be a molecular graph. Denote by n_x the number of vertices of G with degree x, $m_{x,y}$ the number of edges connecting a vertex with degree x and a vertex with degree y. Thus, $n = \sum_{i=1}^{4} n_i$. Let $P = \{(x, y) \in N \times N : 1 \leq x \leq y \leq 4\}$, then $n = \sum_{(x,y)\in P} \frac{x+y}{xy} m_{x,y}$. Reduced Sombor index can be writed as $SO_{red}(G) = \sum_{(x,y)\in P} \sqrt{(x-1)^2 + (y-1)^2}\, m_{x,y}$.

Theorem 3.1 *Let G be a molecular graph with n vertices. Then*

$$SO_{red}(G) \leq 6\sqrt{2}n,$$

with equality iff G is a 4-regular molecular graph.

Proof. For convenience, we denote $Q = \{(x, y) \in P : (x, y) \neq (4, 4)\}$. Since $n = \sum_{(x,y)\in P} \frac{x+y}{xy} m_{x,y}$, then $m_{4,4} = 2(n - \sum_{(x,y)\in Q} \frac{x+y}{xy} m_{x,y})$. From the definition of reduced Sombor index, we have

$$\begin{aligned}
SO_{red}(G) =& 3\sqrt{2}m_{4,4} + \sum_{(x,y)\in Q} \sqrt{(x-1)^2 + (y-1)^2} m_{x,y} \\
=& 6\sqrt{2}\left(n - \sum_{(x,y)\in Q} \frac{x+y}{xy} m_{x,y}\right) + \sum_{(x,y)\in Q} \sqrt{(x-1)^2 + (y-1)^2} m_{x,y} \\
=& 6\sqrt{2}n + \sum_{(x,y)\in Q} \left(\sqrt{(x-1)^2 + (y-1)^2} - 6\sqrt{2}\frac{x+y}{xy}\right) m_{x,y} \\
=& 6\sqrt{2}n + \sum_{(x,y)\in P} \left(\sqrt{(x-1)^2 + (y-1)^2} - 6\sqrt{2}\frac{x+y}{xy}\right) m_{x,y} \leq 6\sqrt{2}n\ .
\end{aligned}$$

with equality iff $\sqrt{(x-1)^2 + (y-1)^2} = 6\sqrt{2}\frac{x+y}{xy}$ for $(x, y) \in P$, then $(x, y) = (4, 4)$, i.e., G is a 4-regular molecular graph. ∎

The minimum reduced Sombor index of molecular graph is obvious.

Theorem 3.2 *Let G be a molecular graph with n vertices. Then*

$$SO_{red}(G) \geq \begin{cases} 0, & if\ n \equiv 0(mod\ 2); \\ 2, & if\ n \equiv 1(mod\ 2). \end{cases}$$

And $SO_{red}(G) = 0$ with equality iff $G \cong \frac{n}{2}P_2$, $SO_{red}(G) = 2$ with equality iff $G \cong \frac{n-3}{2}P_2 \cup P_3$.

By Lemma 2.2 and 3.1, we have the following result.

Theorem 3.3 *Let G be a connected molecular graph with n vertices. Then*

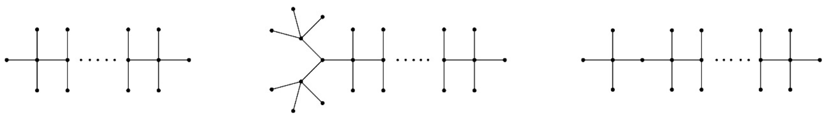
$$\sqrt{2}(n-3)+2 \leq SO_{red}(G) \leq 6\sqrt{2}n,$$

with left equality iff $G \cong P_n$, right equality iff G is a connected 4-regular molecular graph.

Deng et al. [10] obtain the maximum value of the reduced Sombor index and the corresponding extremal graphs for all molecular trees. Let $\mathcal{CT}_n$ be the set of molecular trees with n vertices.

Lemma 3.4 *[10] Let $T \in \mathcal{CT}_n$, $n \geq 5$. Then*

$$SO_{red}(T) \leq \begin{cases} (2+\sqrt{2})n+2-5\sqrt{2}, & n \equiv 2(mod\ 3); \\ (2+\sqrt{2})n+1+3\sqrt{13}-13\sqrt{2}, & n \equiv 1(mod\ 3); \\ (2+\sqrt{2})n+2\sqrt{10}-9\sqrt{2}, & n \equiv 0(mod\ 3). \end{cases}$$



(1) (2) (3)

Figure 2: Three types of maximum molecular trees.

The corresponding maximum molecular trees are depicted in Figure 2.

If $n \equiv 2(mod\ 3)$ $(n \geq 5)$, the maximum molecular trees are (1) of Figure 2.

If $n \equiv 1(mod\ 3)$ $(n \geq 13)$, the maximum molecular trees are (2) of Figure 2.

If $n \equiv 0(mod\ 3)$ $(n \geq 9)$, the maximum molecular trees are (3) of Figure 2.

Exponential reduced Sombor index is defined as

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

We conjecture that the maximum molecular trees of exponential reduced Sombor index and reduced Sombor index are the same.

Conjecture 3.1 *Let $T \in \mathcal{CT}_n$, $n \geq 5$. Then*

$$e^{SO_{red}}(T) \leq \begin{cases} \frac{2}{3}(n+1)e^3+\frac{1}{3}(n-5)e^{3\sqrt{2}}, & n \equiv 2(mod\ 3); \\ \frac{1}{3}(2n+1)e^3+\frac{1}{3}(n-13)e^{3\sqrt{2}}+3e^{\sqrt{13}}, & n \equiv 1(mod\ 3); \\ \frac{2}{3}ne^3+\frac{1}{3}(n-9)e^{3\sqrt{2}}+2e^{\sqrt{10}}, & n \equiv 0(mod\ 3). \end{cases}$$

The corresponding maximum molecular trees, also see Figure 2.

4 The expected values of reduced Sombor index in random polyphenyl chains

Random network theory is an important part of network science. In recent years, there are many results about the extreme values of topological indices of random molecular graphs, such as [24, 28, 32, 34, 39] and references cited therein. The polyphenyl chains are special molecular graphs. A polyphenyl chain PPC_h with h hexagons can be regarded as a polyphenyl chain PPC_{h-1} with $h-1$ hexagons to which a new terminal hexagon H_h has been adjoined by a cut edge. For $h \geq 3$, the terminal hexagon H_h can be attached in three ways, which results in the local arrangements, we describe as PPC_h^1, PPC_h^2, and PPC_h^3, respectively, see Figure 3.

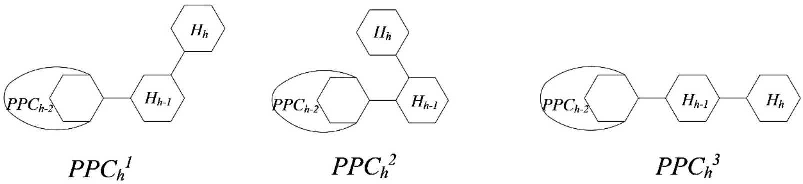


Figure 3: The three types of local arrangements in polyphenyl chains.

Suppose that the change from PPC_{h-1} to PPC_h is a random process. The probability from PPC_{h-1} to PPC_h is p_1, p_2 and $1-p_1-p_2$, respectively, see Figure 3. p_1, p_2 are constants, irrelative to h. Thus, the process is a zeroth-order Markov process. With associating probabilities, such a polyphenyl chain is called a random polyphenyl chain. We denote it by $PPC(h; p_1, p_2)$.

Denote by $\mathcal{M}_h = PPC(h; 1, 0)$ the polyphenyl meta-chain, $\mathcal{O}_h = PPC(h; 0, 1)$ the polyphenyl orth-chain, $\mathcal{P}_h = PPC(h; 0, 0)$ the polyphenyl para-chain, respectively.

Recall that $m_{x,y}(G)$ is the number of edges connecting a vertex with degree x and a vertex with degree y in G. Thus

$$SO_{red}(PPC_h) = \sqrt{2}m_{2,2}(PPC_h) + \sqrt{5}m_{2,3}(PPC_h) + 2\sqrt{2}m_{3,3}(PPC_h).$$

Denote by $E_h = E[SO_{red}(PPC(h; p_1, p_2))]$ the expected values of reduced Sombor index of random polyphenyl chain $PPC(h; p_1, p_2)$. In the following, we determine E_h.

Theorem 4.1 *Let $PPC(h; p_1, p_2)$ $(h \geq 2)$ be a random polyphenyl chain. Then*

$$E_h = [(3\sqrt{2} - 2\sqrt{5})p_2 + 4(\sqrt{2} + \sqrt{5})]h + 2(2\sqrt{5} - 3\sqrt{2})p_2 + 2(\sqrt{2} - 2\sqrt{5}).$$

Proof. When $h = 2$, then $E_2 = E[SO_{red}(PPC(2; p_1, p_2))] = 10\sqrt{2} + 4\sqrt{5}$.

When $h \geq 3$, $m_{2,2}(PPC_h)$, $m_{2,3}(PPC_h)$, $m_{3,3}(PPC_h)$ depend on the three possible constructions(see Figure 3).

Case 1. $PPC_{h-1} \to PPC_h^1$, with probability p_1.

$$m_{2,2}(PPC_h^1) = m_{2,2}(PPC_{h-1}) + 2;$$

$$m_{2,3}(PPC_h^1) = m_{2,3}(PPC_{h-1}) + 4;$$

$$m_{3,3}(PPC_h^1) = m_{3,3}(PPC_{h-1}) + 1.$$

Thus, $SO_{red}(PPC_h^1) = SO_{red}(PPC_{h-1}) + 4(\sqrt{2} + \sqrt{5})$.

Case 2. $PPC_{h-1} \to PPC_h^2$, with probability p_2.

$$m_{2,2}(PPC_h^2) = m_{2,2}(PPC_{h-1}) + 3;$$

$$m_{2,3}(PPC_h^2) = m_{2,3}(PPC_{h-1}) + 2;$$

$$m_{3,3}(PPC_h^2) = m_{3,3}(PPC_{h-1}) + 2.$$

Thus, $SO_{red}(PPC_h^2) = SO_{red}(PPC_{h-1}) + 7\sqrt{2} + 2\sqrt{5}$.

Case 3. $PPC_{h-1} \to PPC_h^3$, with probability $1 - p_1 - p_2$.

$$m_{2,2}(PPC_h^3) = m_{2,2}(PPC_{h-1}) + 2;$$

$$m_{2,3}(PPC_h^3) = m_{2,3}(PPC_{h-1}) + 4;$$

$$m_{3,3}(PPC_h^3) = m_{3,3}(PPC_{h-1}) + 1.$$

Thus, $SO_{red}(PPC_h^3) = SO_{red}(PPC_{h-1}) + 4(\sqrt{2} + \sqrt{5})$.

Thus, $E_h = E[SO_{red}(PPC(h; p_1, p_2))] = p_1 SO_{red}(PPC_h^1) + p_2 SO_{red}(PPC_h^2) + (1 - p_1 - p_2) SO_{red}(PPC_h^3) = SO_{red}(PPC_{h-1}) + (3\sqrt{2} - 2\sqrt{5})p_2 + 4(\sqrt{2} + \sqrt{5})$. Since $E[E_h] = E_h$, then

$$E_h = E_{h-1} + (3\sqrt{2} - 2\sqrt{5})p_2 + 4(\sqrt{2} + \sqrt{5}).$$

Since above equation is a first order constant coefficient linear difference equation, we can easily get $E_h = [(3\sqrt{2} - 2\sqrt{5})p_2 + 4(\sqrt{2} + \sqrt{5})]h + 2(2\sqrt{5} - 3\sqrt{2})p_2 + 2(\sqrt{2} - 2\sqrt{5})$. ■

Recall that $\mathcal{M}_h = PPC(h; 1, 0)$ is the polyphenyl meta-chain, $\mathcal{O}_h = PPC(h; 0, 1)$ is the polyphenyl orth-chain, $\mathcal{P}_h = PPC(h; 0, 0)$ is the polyphenyl para-chain. By Theorem 4.1, we have

Corollary 4.2 *The reduced Sombor index of* $\mathcal{M}_h$, $\mathcal{O}_h$ *and* $\mathcal{P}_h$ *are*

$SO_{red}(\mathcal{O}_h) = (7\sqrt{2} + 2\sqrt{5})h - 4\sqrt{2}$;

$SO_{red}(\mathcal{M}_h) = SO_{red}(\mathcal{P}_h) = 4(\sqrt{2} + \sqrt{5})h - 2(\sqrt{2} - 2\sqrt{5})$.

Corollary 4.3 *Among all polyphenyl chains* PPC_h, *we have*

$$(7\sqrt{2} + 2\sqrt{5})h + 4\sqrt{5} - 6\sqrt{2} \leq SO_{red}(PPC_h) \leq 4(\sqrt{2} + \sqrt{5})h - 2(\sqrt{2} - 2\sqrt{5}),$$

with left equality iff $G \cong \mathcal{O}_h$, *right equality iff* $G \cong \mathcal{P}_h$ *or* $G \cong \mathcal{M}_h$.

Denote by $\mathcal{PC}_h$ the set of all polyphenyl chains with h hexagons. The average value of reduced Sombor indices among $\mathcal{PC}_h$ can be characterized as

$$SO_{avr}(\mathcal{PC}_h) = \frac{1}{|\mathcal{PC}_h|} \sum_{G \in \mathcal{PC}_h} SO_{red}(G).$$

Since each element in $\mathcal{PC}_h$ has the same probability of occurrence, we have $p_1 = p_2 = 1 - p_1 - p_2 = \frac{1}{3}$. Then we have

Theorem 4.4 *The average values of reduced Sombor index among* $\mathcal{PC}_h$ *is*

$SO_{avr}(\mathcal{PC}_h) = \frac{5}{3}(3\sqrt{2} + 2\sqrt{5})h - \frac{8}{3}\sqrt{5}$.

We find that the average values of reduced Sombor index with respect to $\{\mathcal{M}_h, \mathcal{O}_h, \mathcal{P}_h\}$ are $\frac{SO_{red}(\mathcal{M}_h)+SO_{red}(\mathcal{O}_h)+SO_{red}(\mathcal{P}_h)}{3} = \frac{5}{3}(3\sqrt{2} + 2\sqrt{5})h - \frac{8}{3}\sqrt{5} = SO_{avr}(\mathcal{PC}_h)$.

The expected values of (reduced) Sombor index for random hexagonal chains, random phenylene chains can be obtained by a similar method.

5 Applying reduced Sombor index to graph spectrum and energy problems

5.1 Reduced Sombor spectral radius and energy of simple graph

Let G be a simple graph, the adjacent matrix $A(G)$ is defined as

$$(A(G))_{ij} = \begin{cases} 1, & u_i u_j \in E(G); \\ 0, & others. \end{cases}$$

Let the eigenvalues of $A(G)$ be $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$, and $\lambda_1(G)$ is the spectral radius of G. The energy of G is defined as $E_A(G) = \sum_{i=1}^{n} |\lambda_i|$ (see [19]). The energy levels of the electrons in the molecule represent the eigenvalues of the graph. The energy of graphs has a wide range of applications in science and engineering, such as satellite communications, face recognition, processing of high-resolution satellite images, etc.

The reduced Sombor index is defined as $SO_{red}(G) = \sum\limits_{u_iu_j \in E(G)} \sqrt{(d_i-1)^2+(d_j-1)^2}$. Similarly, we propose the reduced Sombor matrix

$$(S_r(G))_{ij} = \begin{cases} \sqrt{(d_i-1)^2+(d_j-1)^2}, & u_iu_j \in E(G); \\ 0, & others. \end{cases}$$

Let the eigenvalues of $S_r(G)$ be $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$, and $\mu_1(G)$ is the reduced Sombor spectral radius of G. The reduced Sombor energy of G is defined as $E_S(G) = \sum\limits_{i=1}^{n} |\mu_i|$.

Theorem 5.1 *Let G be a simple connected graph with n $(n \geq 3)$ vertices, maximum degree Δ and minimum degree δ. Then*

$$\sqrt{2}(\delta-1)\lambda_1 \leq \mu_1 \leq \sqrt{2}(\Delta-1)\lambda_1,$$

with equality iff G is a connected regular graph.

Proof. (1) Let $X = (x_1, x_2, \cdots, x_n)$ be a unit eigenvector of G corresponding to λ_1. By Rayleigh Quotient, $\mu_1 \geq \frac{X^TS_rX}{X^TX} = X^TS_rX = 2\sum\limits_{u_iu_j \in E(G)} \sqrt{(d_i-1)^2+(d_j-1)^2}x_ix_j \geq 2\sqrt{2}(\delta-1)\sum\limits_{u_iu_j \in E(G)} x_ix_j = \sqrt{2}(\delta-1)X^TAX = \sqrt{2}(\delta-1)\frac{X^TAX}{X^TX} = \sqrt{2}(\delta-1)\lambda_1$, with equality iff $d_i = d_j$ for all $u_iu_j \in E(G)$, i.e., G is a connected regular graph.

(2) Let $Y = (y_1, y_2, \cdots, y_n)$ be a unit eigenvector of G corresponding to μ_1. By Rayleigh Quotient, $\mu_1 = \frac{Y^TS_rY}{Y^TY} = Y^TS_rY = 2\sum\limits_{u_iu_j \in E(G)} \sqrt{(d_i-1)^2+(d_j-1)^2}y_iy_j \leq 2\sqrt{2}(\Delta-1)\sum\limits_{u_iu_j \in E(G)} y_iy_j = \sqrt{2}(\Delta-1)\frac{Y^TAY}{Y^TY} \leq \sqrt{2}(\Delta-1)\lambda_1$, with equality iff $d_i = d_j$ for all $u_iu_j \in E(G)$, i.e., G is a connected regular graph. ■

Theorem 5.2 *Let G be a simple connected graph with n $(n \geq 3)$ vertices, m edges, maximum degree Δ and minimum degree δ. $R(G), Z_g(G)$ are the Randic index and first Zagreb index of G. Then*

(1) $\mu_1 \geq \sqrt{2}(\delta-1)(\overline{d}-\frac{2m}{n})$, *with equality iff G is a $\overline{d}$-regular graph.*

(2) $\mu_1 \geq \frac{\sqrt{2}(\delta-1)}{m}R(G)$, *with equality iff G is a regular graph.*

(3) $(\delta-1)\sqrt{\frac{2Z_g(G)}{n}} \leq \mu_1 \leq \sqrt{2}\Delta(\Delta-1)$, *with equality iff G is a connected regular graph.*

(4) $\frac{2\sqrt{2}m(\delta-1)}{n} \leq \mu_1 \leq (\Delta-1)\sqrt{2(2m-n+1)}$, *with left equality iff G is a connected regular graph, right equality iff $G \cong K_n$.*

(5) $\mu_1 \geq \frac{2\sqrt{2}(\delta-1)(m-\delta)}{n-1}$, *with equality iff G is a regular graph.*

Proof. (1) Since $\lambda_1 \geq \overline{d} - \frac{2m}{n}$, with equality iff G is a $\overline{d}$-regular graph (see [16]). By Theorem 5.1, the result holds.

(2) Since $\lambda_1 \geq \frac{1}{m} \sum\limits_{u_iu_j \in E(G)} \sqrt{d_i d_j} = \frac{R(G)}{m}$, with equality iff G is a regular graph (see [16]). By Theorem 5.1, the result holds.

(3) Since $\sqrt{\frac{Z_g(G)}{n}} \leq \lambda_1 \leq \Delta$, with left equality iff G is a regular or semiregular graph, right equality iff G is a regular graph (see [36]). By Theorem 5.1, the result holds.

(4) Since $\frac{2m}{n} \leq \lambda_1 \leq \sqrt{2m-n+1}$, with left equality iff G is a regular graph, right equality iff $G \cong K_n$ or $G \cong K_{1,n-1}$ (see [21]). By Theorem 5.1, the result holds.

(5) Since $\lambda_1 \geq \frac{2(m-\delta)}{n-1}$ (see [11]). By Theorem 5.1, the result holds. ■

Some of the following properties are similar to some other spectral radius and energy, such as Randić spectral radius and energy, etc. (see [2,38]). For convenience, let $F_r(G) = \sum\limits_{u_iu_j \in E(G)} [(d_i-1)^2+(d_j-1)^2]$. We first obtain the relationship between the reduced Sombor spectral radius μ_1 and F_r.

Theorem 5.3 *Let G be a simple graph with n vertices. Then*

$$\mu_1 \leq \sqrt{\frac{2(n-1)F_r}{n}},$$

with equality iff G is the graph without edges or a complete graph.

Proof. By Cauchy-Schwarz inequality, we have $(\sum\limits_{i=2}^{n} \mu_i)^2 \leq (n-1)(\sum\limits_{i=2}^{n} \mu_i^2)$. Since $\sum\limits_{i=1}^{n} \mu_i = 0$ and $\sum\limits_{i=1}^{n} \mu_i^2 = tr(S_r^2) = 2 \sum\limits_{u_iu_j \in E(G)} [(d_i-1)^2+(d_j-1)^2] = 2F_r$, then $\mu_1^2 \leq (n-1)(2F_r - \mu_1^2)$, so $\mu_1 \leq \sqrt{\frac{2(n-1)F_r}{n}}$, with equality iff $\mu_2 = \mu_3 = \cdots = \mu_n$. i.e., G is the graph without edges or a complete graph (see Proposition 1 of [38]). ■

In the following, we obtain the relationship between the reduced Sombor energy $E_S(G)$ and F_r.

Theorem 5.4 *Let G be a simple graph with n vertices. Then*

(1) $E_S(G) \leq \sqrt{2nF_r}$, *with equality iff G is the graph without edges or all vertices of G have degree one.*

(2) $E_S(G) \geq 2\sqrt{F_r}$, *with equality iff G is the graph without edges or a complete bipartite graph with possibly isolated vertices.*

(3) $E_S(G) \geq \sqrt{n(n-1)\sqrt[n]{D^2} + 2F_r}$, *where* $D = |\mu_1\mu_2\cdots\mu_n| = |det(S_r(G))|$.

(4) $E_S(G) \geq \frac{2F_r + n|\mu_1||\mu_n|}{|\mu_1|+|\mu_n|}$.

(5) $E_S(G) \geq \frac{1}{2}\sqrt{8nF_r - n^2(|\mu_1|-|\mu_n|)^2}$.

(6) $E_S(G) \geq \sqrt{2nF_r - n\lfloor\frac{n}{2}\rfloor(1-\frac{1}{n}\lfloor\frac{n}{2}\rfloor)(|\mu_1|-|\mu_n|)^2}$.

Proof. (1) By Cauchy-Schwarz inequality, $E_S(G) = \sqrt{(\sum_{i=1}^{n}|\mu_i|)^2} \leq \sqrt{\sum_{i=1}^{n}1\sum_{i=1}^{n}|\mu_i|^2} = \sqrt{n\sum_{i=1}^{n}\mu_i^2} = \sqrt{n\times tr(S_r^2)} = \sqrt{2n\sum_{u_iu_j\in E(G)}[(d_i-1)^2+(d_j-1)^2]} = \sqrt{2nF_r}$, with left equality iff $\mu_1 = |\mu_2| = \cdots = |\mu_n|$, i.e., G is the graph without edges or all vertices of G have degree one (see Theorem 4 of [2], Proposition 3 of [38]).

(2) $[E_S(G)]^2 = [\sum_{i=1}^{n}|\mu_i|]^2 = \sum_{i=1}^{n}\mu_i^2 + 2\sum_{1\leq i<j\leq n}|\mu_i||\mu_j| \geq \sum_{i=1}^{n}\mu_i^2 + 2|\sum_{1\leq i<j\leq n}\mu_i\mu_j| = \sum_{i=1}^{n}\mu_i^2 + 2|(-\frac{1}{2}\sum_{i=1}^{n}\mu_i^2)| = 2\sum_{i=1}^{n}\mu_i^2 = 2tr(S_r^2) = 4\sum_{u_iu_j\in E(G)}[(d_i-1)^2+(d_j-1)^2] = 4F_r$, thus $E_S(G) \geq 2\sqrt{F_r}$, with left equality iff G is the graph without edges or a complete bipartite graph with possibly isolated vertices (see Proposition 6 of [38]).

(3) We know the fact that for any $a_i \geq 0$ $(i = 1, 2, \cdots, n)$, then $\frac{a_1+a_2+\cdots+a_n}{n} \geq \sqrt[n]{a_1a_2\cdots a_n}$. Thus $\frac{\sum_{i\neq j}|\mu_i||\mu_j|}{n(n-1)} \geq \sqrt[n(n-1)]{\prod_{i\neq j}|\mu_i||\mu_j|} = \sqrt[n(n-1)]{\prod_{i=1}^{n}|\mu_i|^{2(n-1)}} = \sqrt[n]{\prod_{i=1}^{n}|\mu_i|^2} = \sqrt[n]{D^2}$. Then $\sum_{i\neq j}|\mu_i||\mu_j| \geq n(n-1)\sqrt[n]{D^2}$. By the proof of (2), we have $[E_S(G)]^2 = 2F_r + \sum_{i\neq j}|\mu_i||\mu_j|$, thus we have $E_S(G) \geq \sqrt{n(n-1)\sqrt[n]{D^2} + 2F_r}$.

(4) Since $\sum_{i=1}^{n}a_i^2 + rR\sum_{i=1}^{n}b_i^2 \leq (r+R)(\sum_{i=1}^{n}a_ib_i)$, where $rb_i \leq a_i \leq Rb_i$, a_i, b_i $(1 \leq i \leq n)$ are nonnegative real numbers, r, R are real constants (see [12]). Then $\sum_{i=1}^{n}|\mu_i||\mu_i| + |\mu_1||\mu_n|\sum_{i=1}^{n}1^2 \leq (|\mu_1|+|\mu_n|)(\sum_{i=1}^{n}|\mu_i|\times 1)$. By proof of (2), we have $\sum_{i=1}^{n}|\mu_i|^2 = 2F_r$ and $\sum_{i=1}^{n}|\mu_i| = E_S$. Thus $2F_r + n|\mu_1||\mu_n| \leq (|\mu_1|+|\mu_n|)E_S$, so $E_S(G) \geq \frac{2F_r+n|\mu_1||\mu_n|}{|\mu_1|+|\mu_n|}$.

(5) Since $\sum_{i=1}^{n}a_i^2\sum_{i=1}^{n}b_i^2 - (\sum_{i=1}^{n}a_ib_i)^2 \leq \frac{n^2}{4}(M_1M_2 - m_1m_2)^2$, where a_i, b_i are nonnegative real numbers, $M_1 = max_{1\leq i\leq n}\{a_i\}$; $M_2 = max_{1\leq i\leq n}\{b_i\}$; $m_1 = min_{1\leq i\leq n}\{a_i\}$; $m_2 = min_{1\leq i\leq n}\{b_i\}$ (see [26]). Thus $\sum_{i=1}^{n}1\sum_{i=1}^{n}|\mu_i|^2 - (\sum_{i=1}^{n}|\mu_i|)^2 \leq \frac{n^2}{4}(|\mu_1|-|\mu_n|)^2$, then $2nF_r - E_S^2 \leq$

$\frac{n^2}{4}(|\mu_1|-|\mu_n|)^2$, i.e., $E_S(G)\geq\frac{1}{2}\sqrt{8nF_r-n^2(|\mu_1|-|\mu_n|)^2}$.

(6) Since $|n\sum\limits_{i=1}^{n}a_ib_i-\sum\limits_{i=1}^{n}a_i\sum\limits_{i=1}^{n}b_i|\leq n\lfloor\frac{n}{2}\rfloor(1-\frac{1}{n}\lfloor\frac{n}{2}\rfloor)(A-a)(B-b)$, where $a\leq a_i\leq A$, $b\leq b_i\leq B$, a_i, b_i $(1\leq i\leq n)$ are nonnegative real numbers, a,b,A,B are real constants (see [4]). Thus $|n\sum\limits_{i=1}^{n}|\mu_i||\mu_i|-\sum\limits_{i=1}^{n}|\mu_i|\sum\limits_{i=1}^{n}|\mu_i||\leq n\lfloor\frac{n}{2}\rfloor(1-\frac{1}{n}\lfloor\frac{n}{2}\rfloor)(|\mu_1|-|\mu_n|)(|\mu_1|-|\mu_n|)$. By proof of (2), we have $\sum\limits_{i=1}^{n}|\mu_i|^2=2F_r$ and $\sum\limits_{i=1}^{n}|\mu_i|=E_S$. Thus $|2nF_r-(E_S)^2|\leq n\lfloor\frac{n}{2}\rfloor(1-\frac{1}{n}\lfloor\frac{n}{2}\rfloor)(|\mu_1|-|\mu_n|)^2$. By the conclusion of (1), $2nF_r\geq(E_S)^2$. So $E_S(G)\geq\sqrt{2nF_r-n\lfloor\frac{n}{2}\rfloor(1-\frac{1}{n}\lfloor\frac{n}{2}\rfloor)(|\mu_1|-|\mu_n|)^2}$. ■

5.2 Sombor energy of the splitting graph

Let G be a simple graph, the splitting graph $S'(G)$ (see [30]) is obtained from G by taking a new vertex v' corresponding to each vertex v of G and adding edges between v' and all vertices of G adjacent to v. See Figure 4 for example. Rencently, S. K. Vaidya and K. M. Popat [31] obtained the relationship between the energy of G and the energy of $S'(G)$, which is $E(S'(G))=\sqrt{5}E(G)$. Here, we obtain the relationship between the Sombor energy of G and the Sombor energy of $S'(G)$ in the regular graph, which is $E_S(S'(G))=2E_S(G)$. Without causing confusion, we still denote $E_S(G)$ the Sombor energy of G in this subsection.

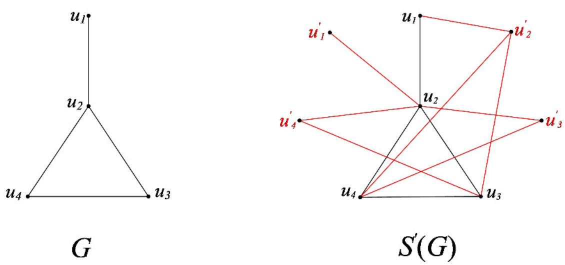


Figure 4: An example for the graph G and its splitting graph $S'(G)$.

Suppose G is a regular graph, then the Sombor matrix $S(G)$ of G is

$$S(G)=\begin{array}{c} \\ u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_n \end{array}\begin{array}{c} \begin{array}{ccccc} u_1 & u_2 & u_3 & \cdots & u_n \end{array} \\ \begin{pmatrix} 0 & \sqrt{d_1^2+d_2^2} & \sqrt{d_1^2+d_3^2} & \cdots & \sqrt{d_1^2+d_n^2} \\ \sqrt{d_2^2+d_1^2} & 0 & \sqrt{d_2^2+d_3^3} & \cdots & \sqrt{d_2^2+d_n^2} \\ \sqrt{d_3^2+d_1^2} & \sqrt{d_3^2+d_2^2} & 0 & \cdots & \sqrt{d_3^2+d_n^2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sqrt{d_n^2+d_1^2} & \sqrt{d_n^2+d_2^2} & \sqrt{d_n^2+d_3^2} & \cdots & 0 \end{pmatrix} \end{array}$$

where d_i is the degree of vertex u_i $(1 \leq i \leq n)$ of G.

The Sombor matrix $S(S'(G))$ of splitting graph $S'(G)$ is

$$\begin{array}{c} \\ u_1 \\ u_2 \\ \vdots \\ u_n \\ u'_1 \\ u'_2 \\ \vdots \\ u'_n \end{array}\begin{array}{c} \begin{array}{cccccccc} u_1 & u_2 & \cdots & u_n & u'_1 & u'_2 & \cdots & u'_n \end{array} \\ \begin{pmatrix} 0 & \sqrt{t_1^2+t_2^2} & \cdots & \sqrt{t_1^2+t_n^2} & 0 & \sqrt{t_1^2+t_2'^2} & \cdots & \sqrt{t_1^2+t_n'^2} \\ \sqrt{t_2^2+t_1^2} & 0 & \cdots & \sqrt{t_2^2+t_n^2} & \sqrt{t_2^2+t_1'^2} & 0 & \cdots & \sqrt{t_2^2+t_n'^2} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \sqrt{t_n^2+t_1^2} & \sqrt{t_n^2+t_2^2} & \cdots & 0 & \sqrt{t_n^2+t_1'^2} & \sqrt{t_n^2+t_2'^2} & \cdots & 0 \\ 0 & \sqrt{t_1'^2+t_2^2} & \cdots & \sqrt{t_1'^2+t_n^2} & 0 & 0 & \cdots & 0 \\ \sqrt{t_2'^2+t_1^2} & 0 & \cdots & \sqrt{t_2'^2+t_n^2} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \sqrt{t_n'^2+t_1^2} & \sqrt{t_n'^2+t_2^2} & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix} \end{array}$$

where $t_i = 2d_i$ is the degree of vertex u_i $(1 \leq i \leq n)$ of $S'(G)$, $t'_i = d'_i$ is the degree of vertex u'_i $(1 \leq i \leq n)$ of $S'(G)$.

Thus,

$$S(S'(G)) = \begin{bmatrix} 2S(G) & \sqrt{\frac{5}{2}}S(G) \\ \sqrt{\frac{5}{2}}S(G) & 0 \end{bmatrix}$$

The Sombor spectrum of $S'(G)$ is

$$\begin{bmatrix} \frac{2+\sqrt{14}}{2}\mu_i & \frac{2-\sqrt{14}}{2}\mu_i \\ n & n \end{bmatrix}$$

where μ_i $(1 \leq i \leq n)$ is the eigenvalue of $S(G)$ and $\frac{2\pm\sqrt{14}}{2}\mu_i$ are the eigenvalue of

$$\begin{bmatrix} 2 & \sqrt{\frac{5}{2}} \\ \sqrt{\frac{5}{2}} & 0 \end{bmatrix}$$

Thus,

$$E_S(S'(G)) = \sum_{i=1}^{n} \left| \frac{2 \pm \sqrt{14}}{2} \mu_i \right| = \sum_{i=1}^{n} |\mu_i| \left(\frac{2+\sqrt{14}}{2} + \frac{2-\sqrt{14}}{2} \right)$$
$$= 2 \sum_{i=1}^{n} |\mu_i| = 2E_S(G) \ .$$

In addition, it is easy to know the relationship between the energy and Sombor energy. If G is a k-regular graph, then $E_S(G) = \sqrt{2}kE(G)$. If G is a (k,t)-semiregular graph, then $E_S(G) = \sqrt{k^2+t^2}E(G)$.

6 Concluding remarks

Owing to the fact that the predictive potential of the reduced Sombor index is slightly better than Sombor index [27], it is more meaningful to study the properties of the reduced Sombor index. In this article, we obtain a large number of important properties of reduced Sombor index. These results could be of some interest to researchers working in chemical applications of graph theory, random graph theory and spectral graph theory. In the following, we propose some novel indices.

The exponential reduced Sombor index is defined as

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

The reduced Sombor coindex is defined as

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

The reduced eccentricity Sombor index is defined as

$$SO_{\varepsilon}(G) = \sum_{\{u,v\} \subseteq V(G)} \sqrt{(\varepsilon_u-1)^2+(\varepsilon_v-1)^2} \,,$$

where ε_u denotes eccentricity rate of vertex u in G.

Similarly, we propose the reduced eccentricity Sombor matrix

$$(S_{\varepsilon}(G))_{ij} = \begin{cases} \sqrt{(\varepsilon_i-1)^2+(\varepsilon_j-1)^2}, & i \neq j; \\ 0, & others. \end{cases}$$

Let the eigenvalues of $S_{\varepsilon}(G)$ be $\nu_1(G) \geq \nu_2(G) \geq \cdots \geq \nu_n(G)$, and $\nu_1(G)$ is the reduced eccentricity Sombor spectral radius of G. The reduced eccentricity Sombor energy of G

is defined as $E_{S\varepsilon}(G) = \sum_{i=1}^{n} |\nu_i|$. Any eccentricity-based descriptor can be viewed as a special case of a eccentricity Sombor-type index. It is, of course, also interesting to consider the properties of these novel indices, we intend to do it in the near future.

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