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Research article

Bounds of modified Sombor index, spectral radius and energy

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Abstract: Let G be a simple graph with edge set $E(G)$. The modified Sombor index is defined as ${}^{m}SO(G) = \sum\limits_{uv\in E(G)} \frac{1}{\sqrt{d_u^2+d_v^2}}$, where d_u (resp. d_v) denotes the degree of vertex u (resp. v). In this paper, we determine some bounds for the modified Sombor indices of graphs with given some parameters (e.g., maximum degree Δ, minimum degree δ, diameter d, girth g) and the Nordhaus-Gaddum-type results. We also obtain the relationship between modified Sombor index and some other indices. At last, we obtain some bounds for the modified spectral radius and energy.

Keywords: modified Sombor index; modified Sombor spectral radius; extremal value
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1. Introduction

Recently, a novel topological index, named as Sombor index [13], was introduced by Gutman, which is defined as

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

The maximum chemical trees with respect to Sombor indices were determined by Deng [10] and Cruz [6], independently. And then, present authors [22] characterized the first fourteen minimum chemical trees, the first four minimum chemical unicyclic graphs, the first three minimum chemical bicyclic graphs, the first seven minimum chemical tricyclic graphs. Chemical applicability of Sombor indices was studied by Redžepović [34]. Milovanović et al. [32] determined relations between Sombor indices and other indices. Other results about Sombor index can be found in [1, 5, 9, 12–14, 18, 21, 23, 24, 35, 38]. Some other results about topological indices can see [30, 31] and so on.

Kulli and Gutman also proposed the modified Sombor index [19], which is defined as

$$^{m}SO(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u^2+d_v^2}}.$$

In this paper, we determine some bounds for the modified Sombor indices of graphs with given some parameters (e.g., maximum degree Δ, minimum degree δ, diameter d, girth g) and the Nordhaus-Gaddum-type results. We also obtain the relationship between modified Sombor index and some other indices. At last, we obtain some bounds for modified Sombor spectral radius and energy. In this paper, all notations and terminologies used but not defined here can refer to Bondy and Murty [4].

2. Bounds for the modified Sombor indices of graphs

Note that the Randic index $R(G)=\sum\limits_{uv\in E(G)}\frac{1}{\sqrt{d_ud_v}}$ (see [25, 27]) and by the definition of modified Sombor index, we have

Theorem 2.1. *Let G be a simple graph with maximum degree Δ, minimum degree δ and Randic index $R(G)$. Then*

$$\frac{R(G)}{\sqrt{\frac{\Delta}{\delta}+\frac{\delta}{\Delta}}}\leq {}^{m}SO(G)\leq\frac{\sqrt{2}}{2}R(G),$$

with equality iff G is a regular graph.

Proof. Since $d_u^2+d_u^2\geq 2d_ud_v$, then $\frac{1}{\sqrt{d_u^2+d_v^2}}\leq\frac{\sqrt{2}}{2}\frac{1}{\sqrt{d_ud_v}}$, and it follows that $^{m}SO(G)\leq\frac{\sqrt{2}}{2}R(G)$, with equality iff $d_u=d_v$ for every edge $uv\in E(G)$, i.e., G is a regular graph.

On the other hand, we have $^{m}SO(G)=\sum\limits_{uv\in E(G)}\frac{1}{\sqrt{d_u^2+d_v^2}}=\sum\limits_{uv\in E(G)}\frac{1}{\sqrt{d_ud_v}}\frac{1}{\sqrt{\frac{d_u^2+d_v^2}{d_ud_v}}}=\sum\limits_{uv\in E(G)}\frac{1}{\sqrt{d_ud_v}}\frac{1}{\sqrt{\frac{d_u}{d_v}+\frac{d_v}{d_u}}}\geq$ $\sum\limits_{uv\in E(G)}\frac{1}{\sqrt{d_ud_v}}\frac{1}{\sqrt{\frac{\Delta}{\delta}+\frac{\delta}{\Delta}}}=\frac{R(G)}{\sqrt{\frac{\Delta}{\delta}+\frac{\delta}{\Delta}}}$, with equality iff G is a regular graph. □

Lemma 2.2. *[3] Let G be a graph with energy $\mathcal{E}(G)$ and Randic index $R(G)$. Then $\mathcal{E}(G)\geq 2R(G)$.*

By Theorem 2.1 and Lemma 2.2, we have

Corollary 2.3. *Let G be a graph with energy $\mathcal{E}(G)$. Then $^{m}SO(G)\leq\frac{\sqrt{2}}{4}\mathcal{E}(G)$.*

It is known that $R(G)\leq\frac{n}{2}$, with equality iff G is a regular graph (see [2,7,39]). by Theorem 2.1, we have

Corollary 2.4. *Let G be a simple graph with n vertices. Then*

$$^{m}SO(G)\leq\frac{\sqrt{2}}{4}n,$$

with equality iff G is a regular graph.

By Corollary 2.4, we determine the maximum unicyclic graphs with respect to modified Sombor index.

Corollary 2.5. *Let G be an unicyclic graph with n vertices. Then*

$$^{m}SO(G) \leq \frac{\sqrt{2}}{4}n,$$

with equality iff $G \cong C_n$.

Denote by $\chi = \sum\limits_{uv\in E(G)} \frac{1}{d_u^2+d_v^2}$.

Theorem 2.6. *Let G be a simple graph with m edges and minimum degree δ. Then*

$$\sqrt{2}\delta\chi \leq {}^{m}SO(G) \leq \sqrt{m\chi},$$

with left equality iff G is a regular graph, right equality iff G is a semiregular graph.

Proof. Since $\sum\limits_{uv\in E(G)} \sqrt{1}\cdot\sqrt{\frac{1}{d_u^2+d_v^2}} \leq \sqrt{\sum\limits_{uv\in E(G)} 1 \sum\limits_{uv\in E(G)} \frac{1}{d_u^2+d_v^2}}$, thus ${}^{m}SO(G) \leq \sqrt{m\chi}$, with equality iff $d_u^2 + d_v^2 = \lambda$ (a constant) for every edge $uv \in E(G)$, i.e., G is a semiregular graph (see [16]).

On the other hand, we have

${}^{m}SO(G) = \sum\limits_{uv\in E(G)} \frac{1}{\sqrt{d_u^2+d_v^2}} = \sum\limits_{uv\in E(G)} \frac{\sqrt{d_u^2+d_v^2}}{d_u^2+d_v^2} \geq \sum\limits_{uv\in E(G)} \frac{\sqrt{2}\delta}{d_u^2+d_v^2} = \sqrt{2}\delta\chi$, with equality iff G is a regular graph. □

It is obvious that $\frac{1}{\sqrt{2}\Delta} \leq \frac{1}{\sqrt{d_u^2+d_v^2}} \leq \frac{1}{\sqrt{2}\delta}$. By the definition of modified Sombor index, we have

Theorem 2.7. *Let G be a simple graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$\frac{\sqrt{2}m}{2\Delta} \leq {}^{m}SO(G) \leq \frac{\sqrt{2}m}{2\delta},$$

with equality iff G is a regular graph.

Corollary 2.8. *Let G be a simple graph with n vertices, maximum degree Δ and minimum degree δ. Then*

$$\frac{\sqrt{2}n\delta}{4\Delta} \leq {}^{m}SO(G) \leq \frac{\sqrt{2}n\Delta}{4\delta},$$

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 by Theorem 2.7, we obtain the results as desired. □

In the following, we discuss the relation between modified Sombor index and general Randic index $R_{-1}(G)$. The general Randic index is defined as $R_{-1}(G) = \sum\limits_{uv\in E(G)} \frac{1}{d_u d_v}$.

Theorem 2.9. *Let G be a simple graph with maximum degree Δ, minimum degree δ and general Randic index $R_{-1}(G)$. Then*

$$\frac{\sqrt{2}\delta}{2}R_{-1}(G) \leq {}^{m}SO(G) \leq \frac{\sqrt{2}\Delta}{2}R_{-1}(G),$$

with equality iff G is a regular graph.

Proof. ${}^{m}SO(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u^2+d_v^2}} = \sum_{uv\in E(G)} \frac{1}{d_u d_v \sqrt{\frac{1}{d_u^2}+\frac{1}{d_v^2}}} \geq \sum_{uv\in E(G)} \frac{1}{d_u d_v \sqrt{\frac{1}{\delta^2}+\frac{1}{\delta^2}}} = \frac{\sqrt{2}\delta}{2} R_{-1}(G)$, with equality iff G is a regular graph. Similarly, we can obtain the corresponding upper bound. □

In the following, we get the relation between modified Sombor index and Harmonic index. The Harmonic index [11] is defined as $H(G) = \sum_{uv\in E(G)} \frac{2}{d_u+d_v}$.

Theorem 2.10. *Let G be a graph with n vertices and the Harmonic index H(G). Then*

$$\frac{1}{2}H(G) \leq {}^{m}SO(G) \leq \frac{\sqrt{2}}{2}H(G),$$

with left equality iff $G \cong \overline{K_n}$*, and right equality iff G is a regular graph.*

Proof. Since $\frac{1}{\sqrt{d_u^2+d_v^2}} \leq \frac{\sqrt{2}}{d_u+d_v}$, with equality iff $d_u = d_v$ for every edge $uv \in E(G)$. Thus ${}^{m}SO(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u^2+d_v^2}} \leq \sqrt{2} \sum_{uv\in E(G)} \frac{1}{d_u+d_v} = \frac{\sqrt{2}}{2}H(G)$, with equality iff G is a regular graph.

On the other hand, we have ${}^{m}SO(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u^2+d_v^2}} = \sum_{uv\in E(G)} \frac{1}{\sqrt{(d_u+d_v)^2-2d_ud_v}} \geq \sum_{uv\in E(G)} \frac{1}{\sqrt{(d_u+d_v)^2}} = \sum_{uv\in E(G)} \frac{1}{d_u+d_v} = \frac{1}{2}H(G)$, with equality iff $G \cong \overline{K_n}$. □

In the following, we obtain the bounds of modified Sombor index with given some parameters.

Corollary 2.11. *Let G be a connected graph with n vertices and diameter D(G).*

(1) ${}^{m}SO(G) \leq \frac{\sqrt{2}}{2}D(G) + \frac{\sqrt{2}}{4}n - \frac{\sqrt{2}}{2}$*, with equality iff* $G \cong K_n$*.*

(2) ${}^{m}SO(G) \leq \frac{\sqrt{2}}{4}nD(G)$*, with equality iff* $G \cong K_n$*.*

Proof. Note that $H(G) \leq D(G) + \frac{n}{2} - 1$ and $H(G) \leq \frac{1}{2}nD(G)$, with equality iff $G \cong K_n$ (see [20]). Combining these with Theorem 2.10, we obtain the desired results. □

Corollary 2.12. *Let G be a connected molecular graph with n vertices and m edges. Then*

$${}^{m}SO(G) \leq \frac{\sqrt{2}}{12}(m+2n),$$

with equality iff $G \cong C_n$*.*

Proof. Notice that $H(G) \leq \frac{m+2n}{6}$, with equality iff $G \cong P_n$ or C_n (see [36]). Combine with Theorem 2.10, we obtain the conclusion. □

Corollary 2.13. *Let G be a connected n-vertices graph with girth g(G) satisfying* $g(G) \geq k \geq 3$*. Then*

(1) ${}^{m}SO(G) \leq \frac{3\sqrt{2}}{4}n - \frac{\sqrt{2}}{2}g(G)$*,*

(2) ${}^{m}SO(G) \leq \frac{\sqrt{2}n^2}{4g(G)}$*,*

(3) ${}^{m}SO(G) \leq \frac{\sqrt{2}}{2}(\frac{n}{2} + g(G) - k)$*,*

(4) ${}^{m}SO(G) \leq \frac{\sqrt{2}ng(G)}{4k}$*,*

(1) and (2) with equalities iff $G \cong C_n$*, (3) and (4) with equalities iff G is a regular graph and* $g(G) = k$*.*

Proof. Since (1) $H(G) \leq \frac{3n}{2} - g(G)$, (2) $H(G) \leq \frac{n^2}{2g(G)}$, (3) $H(G) \leq \frac{n}{2} + g(G) - k$, (4) $H(G) \leq \frac{ng(G)}{2k}$. (1) and (2) with equalities iff $G \cong C_n$. (3) and (4) with equalities iff G is a regular graph and $g(G) = k$ (see [40]). Combine with Theorem 2.10, we obtain the conclusion. □

Corollary 2.14. *Let G be a connected graph with n vertices and m edges. Denote ν_1 the largest eigenvalue of the sum-connectivity matrix $S(G)$. Then*

$$^{m}SO(G) \geq \frac{n}{2(n-1)}\nu_1^2,$$

with equality iff $G \cong \overline{K_n}$.

Proof. Since $H(G) \geq \frac{n}{n-1}\nu_1^2$, with equality iff $G \cong K_n$ or $\overline{K_n}$ (see [43]). Combine with Theorem 2.10, we obtain the conclusion. □

A more precise result for Theorem 2.1 is given as follows.

Corollary 2.15. *Let G be a connected graph with n vertices, m edges and Randic index $R(G)$. Then*

$$^{m}SO(G) \leq \frac{\sqrt{2}}{2}R(G),$$

with equality iff G is a $\frac{2m}{n}$-regular graph.

Proof. Since $H(G) \leq R(G)$, with equality iff G is a $\frac{2m}{n}$-regular graph (see [39]). Combine with Theorem 2.10, we obtain the conclusion. □

Corollary 2.16. *Let G be a connected graph with Randic index $R(G)$ and ABC index $ABC(G)$. Then*

$$^{m}SO(G) \leq \frac{\sqrt{2}}{4}(ABC(G) + 2R(G)),$$

with equality iff $G \cong P_2$.

Proof. Since $H(G) \leq \frac{1}{2}ABC(G) + R(G)$, with equality iff $G \cong P_2$ (see [37]). Combine with Theorem 2.10, we obtain the conclusion. □

Corollary 2.17. *Let G be a connected graph. The minimum degree of G is at least $k \geq 2$. Let $X(G)$ be the sum-connectivity index of G. Then*

(1) $^{m}SO(G) \leq \sqrt{\frac{2}{k}}X(G)$,

(2) $^{m}SO(G) \leq \frac{ABC(G)}{2\sqrt{k-1}}$,

with equality iff G is a k-regular graph.

Proof. Since $H(G) \leq \frac{2}{\sqrt{k}}X(G)$ and $H(G) \leq \frac{ABC(G)}{\sqrt{2k-2}}$ with equality iff G is a k-regular graph (see [41]). Combine with Theorem 2.10, we obtain the conclusion. □

Corollary 2.18. *Let G be a simple graph with minimum degree δ, maximum degree Δ and geometric-arithmetic index $GA(G)$. Then*

$$\frac{GA(G)}{2\Delta} \leq {}^{m}SO(G) \leq \frac{\sqrt{2}GA(G)}{2\delta},$$

with left equality iff $G \cong \overline{K_n}$, right equality iff G is a regular graph.

Proof. Since $\frac{GA(G)}{\Delta} \leq H(G) \leq \frac{GA(G)}{\delta}$ with equality iff G is a regular graph (see [28]). Combine with Theorem 2.10, we obtain the conclusion. □

Corollary 2.19. *Let G be a simple graph with minimum degree δ, maximum degree Δ and geometric-arithmetic index $GA(G)$. Then*

$$\frac{\delta GA(G)^2}{2M_2(G)} \leq {}^mSO(G) \leq \frac{\sqrt{2}GA(G)^2(\delta^2+\Delta^2)^2}{8\delta^2\Delta M_2(G)},$$

with left equality iff $G \cong \overline{K_n}$, right equality iff G is a regular graph.

Proof. Since $\frac{\delta GA(G)^2}{M_2(G)} \leq {}^mSO(G) \leq \frac{GA(G)^2(\delta^2+\Delta^2)^2}{4\delta^2\Delta M_2(G)}$, with equality iff G is a regular graph (see [29]). Combine with Theorem 2.10, we obtain the conclusion. □

Denote the inverse degree by $ID(G) = \sum\limits_{u\in V(G)} \frac{1}{d_u}$.

Corollary 2.20. *Let G be a connected graph with maximum degree Δ and inverse degree $ID(G)$. Then*

$${}^mSO(G) \leq \frac{\sqrt{2}}{4} ID(G)\Delta,$$

with equality iff G is a regular graph.

Proof. Since $H(G) \leq \frac{1}{2} ID(G)\Delta$, with equality iff G is a regular graph (see [8]). Combine with Theorem 2.10, we obtain the conclusion. □

Corollary 2.21. *Let G be a simple graph with m edges, minimum degree δ, maximum degree Δ, the second Zagreb index $M_2(G)$ and inverse sum indeg index $ISI(G)$. Then*

$${}^mSO(G) \leq \frac{\sqrt{2}m(\delta+\Delta)ISI(G)}{2\sqrt{\delta\Delta}M_2(G)},$$

with equality iff G is a regular graph.

Proof. Since $H(G) \leq \frac{m(\delta+\Delta)ISI(G)}{\sqrt{\delta\Delta}M_2(G)}$, with equality iff G is a regular graph (see [33]). Combine with Theorem 2.10, we obtain the conclusion. □

Corollary 2.22. *Let G be a simple graph with minimum degree δ, maximum degree Δ and inverse sum indeg index $ISI(G)$. Then*

$$\frac{ISI(G)}{\Delta^2} \leq {}^mSO(G) \leq \frac{\sqrt{2}ISI(G)}{\delta^2},$$

with left equality iff $G \cong \overline{K_n}$, right equality iff G is a regular graph.

Proof. Since $\frac{2ISI(G)}{\Delta^2} \leq H(G) \leq \frac{2ISI(G)}{\delta^2}$, with equality iff G is a regular graph (see [26]). Combine with Theorem 2.10, we obtain the conclusion. □

In the following, we obtain a Nordhaus-Gaddum-type result with respect to modified Sombor index.

Theorem 2.23. *Let G be a simple graph with n vertices. Then*

$$^{m}SO(G) + {}^{m}SO(\overline{G}) \geq \frac{\sqrt{2}}{4}n,$$

with equality iff $G \cong K_n$ or $G \cong \overline{K_n}$.

Proof. Since $|E(G)| + |E(\overline{G})| = \binom{n}{2}$ and $\frac{1}{\sqrt{d_G(u)^2+d_G(v)^2}} \geq \frac{1}{\sqrt{2}(n-1)}$ for every $uv \in E(G)$. Similarly, $\frac{1}{\sqrt{d_{\overline{G}}(u)^2+d_{\overline{G}}(v)^2}} \geq \frac{1}{\sqrt{2}(n-1)}$ for every $uv \in E(\overline{G})$.

By the definition of modified Sombor index, we have

$^{m}SO(G) + {}^{m}SO(\overline{G}) = \sum\limits_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)^2+d_G(v)^2}} + \sum\limits_{uv\in E(\overline{G})} \frac{1}{\sqrt{d_{\overline{G}}(u)^2+d_{\overline{G}}(v)^2}} \geq \frac{\binom{n}{2}}{\sqrt{2}(n-1)} = \frac{\sqrt{2}}{4}n$, with equality iff $G \cong K_n$ or $G \cong \overline{K_n}$. □

3. Bounds for the modified Sombor spectral radius and energy

Denote by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ the eigenvalues of adjacent matrix $A(G)$ of G. Let $E_A(G) = \sum_{i=1}^{n} |\lambda_i|$ be the energy of G (see [15]).

The modified Sombor matrix can be denoted by

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

Denote by $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$ the eigenvalues of modified Sombor matrix $S(G)$ of G. Let $E_S(G) = \sum_{i=1}^{n} |\lambda_i|$ be the modified Sombor energy of G.

Theorem 3.1. *Let G be a simple connected graph with n ($n \geq 3$) vertices, maximum degree Δ and minimum degree δ. Then*

$$\frac{\sqrt{2}\lambda_1}{2\Delta} \leq \mu_1 \leq \frac{\sqrt{2}\lambda_1}{2\delta},$$

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 theorem, then $\mu_1 \geq \frac{X^TSX}{X^TX} = X^TSX = 2\sum\limits_{u_iu_j\in E(G)} \frac{1}{\sqrt{d_i^2+d_j^2}} x_ix_j \geq \frac{\sqrt{2}}{\Delta} \sum\limits_{u_iu_j\in E(G)} x_ix_j = \frac{\sqrt{2}}{2\Delta}(X^TAX) = \frac{\sqrt{2}}{2\Delta}\frac{X^TAX}{X^TX} = \frac{\sqrt{2}\lambda_1}{2\Delta}$.

(2) Let $Y = (y_1, y_2, \cdots, y_n)$ be a unit eigenvector of G corresponding to μ_1. By Rayleigh theorem, then $\mu_1 = \frac{Y^TSY}{Y^TY} = Y^TSY = 2\sum\limits_{u_iu_j\in E(G)} \frac{1}{\sqrt{d_i^2+d_j^2}} y_iy_j \leq \frac{\sqrt{2}}{\delta} \sum\limits_{u_iu_j\in E(G)} y_iy_j = \frac{\sqrt{2}}{2\delta}\frac{Y^TSY}{Y^TY} \leq \frac{\sqrt{2}\lambda_1}{2\delta}$, with equality iff G is a connected regular graph. □

Corollary 3.2. *Let G be a simple connected graph with n ($n \geq 3$) vertices, maximum degree Δ and minimum degree δ. $Z_1(G)$ is the first Zagreb index. Then*

$$\frac{1}{\Delta}\sqrt{\frac{Z_1(G)}{2n}} \leq \mu_1 \leq \frac{\sqrt{2}\Delta}{2\delta},$$

with equality iff G is a connected regular graph.

Proof. Since $\sqrt{\frac{Z_1(G)}{n}} \leq \lambda_1 \leq \Delta$, with left equality iff G is a regular graph or semiregular graph, with right equality iff G is a regular graph (see [42]). Combine with Theorem 3.1, we obtain the conclusion. $\square$

Corollary 3.3. *Let G be a simple connected graph with n ($n \geq 3$) vertices, m edges, maximum degree Δ and minimum degree δ. Then*

$$\frac{\sqrt{2}m}{\Delta n} \leq \mu_1 \leq \frac{\sqrt{2(2m-n+1)}}{2\delta},$$

with equality iff G is a connected regular graph.

Proof. Since $\frac{2m}{n} \leq \lambda_1 \leq \sqrt{2m-n+1}$, with left equality iff G is a regular graph, with right equality iff $G \cong K_n$ or $G \cong K_{1,n-1}$ (see [17]). Combine with Theorem 3.1, the conclusion holds. $\square$

Denote by $\chi(G) = \sum\limits_{u_iu_j \in E(G)} \frac{1}{d_i^2+d_j^2}$.

Theorem 3.4. *Let G be a simple graph with n vertices. Then*

$$\mu_1 \leq \sqrt{\frac{2(n-1)\chi}{n}}.$$

Proof. Since $(\sum\limits_{i=2}^{n} \mu_i)^2 \leq (n-1)(\sum\limits_{i=2}^{n} \mu_i^2)$, and $\sum\limits_{i=1}^{n} \mu_i^2 = 2 \sum\limits_{u_iu_j \in E(G)} \frac{1}{d_i^2+d_j^2} = 2\chi$, then $\mu_1 \leq \sqrt{\frac{2(n-1)\chi}{n}}$. $\square$

Lemma 3.5. *Let G be a simple graph with n vertices. The modified Sombor matrix of G is $S(G)$ and it's modified Sombor eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. Then*

(1) $tr(S) = \sum\limits_{i=1}^{n} \mu_i = 0$;

(2) $tr(S^2) = \sum\limits_{i=1}^{n} \mu_i^2 = \sum\limits_{i \sim j} \frac{2}{d_i^2+d_j^2}$;

(3) $tr(S^3) = \sum\limits_{i=1}^{n} \mu_i^3 = 2\sum\limits_{i \sim j} \frac{1}{\sqrt{d_i^2+d_j^2}}(\sum\limits_{k \sim i, k \sim j} \frac{1}{\sqrt{(d_i^2+d_k^2)(d_k^2+d_j^2)}})$;

(4) $tr(S^4) = \sum\limits_{i=1}^{n} \mu_i^4 = \sum\limits_{i=1}^{n}(\sum\limits_{i \sim j} \frac{1}{d_i^2+d_j^2})^2 + \sum\limits_{i \neq j}(\sum\limits_{k \sim i, k \sim j} \frac{1}{\sqrt{(d_i^2+d_k^2)(d_k^2+d_j^2)}})^2$;

Proof. (1) It is obvious that $tr(S) = \sum\limits_{i=1}^{n} \mu_i = 0$.

(2) If $i = j$, then $(S^2)_{ii} = \sum\limits_{j=1}^{n} S_{ij}S_{ji} = \sum\limits_{i \sim j}(S_{ij})^2 = \sum\limits_{i \sim j} \frac{1}{d_i^2+d_j^2}$.

If $i \neq j$, then $(S^2)_{ij} = \sum\limits_{k=1}^{n} S_{ik}S_{kj} = S_{ii}S_{ij} + S_{ij}S_{jj} + \sum\limits_{k \sim i, k \sim j} S_{ik}S_{kj} = \sum\limits_{k \sim i, k \sim j} \frac{1}{\sqrt{(d_i^2+d_k^2)(d_k^2+d_j^2)}}$.

Thus, $tr(S^2) = \sum\limits_{i=1}^{n}(\sum\limits_{i \sim j} \frac{1}{d_i^2+d_j^2}) = \sum\limits_{i \sim j} \frac{2}{d_i^2+d_j^2}$.

(3) If $i = j$, then $(S^3)_{ii} = \sum\limits_{j=1}^{n} S_{ij}(S^2)_{ji} = \sum\limits_{i \sim j} \frac{1}{d_i^2+d_j^2}(S^2)_{ji} = \sum\limits_{i \sim j} \frac{1}{\sqrt{d_i^2+d_j^2}}(\sum\limits_{k \sim i, k \sim j} \frac{1}{\sqrt{(d_i^2+d_k^2)(d_k^2+d_j^2)}})$.

Thus, $tr(S^3) = \sum\limits_{i=1}^{n}[\sum\limits_{i\sim j}\frac{1}{\sqrt{d_i^2+d_j^2}}(\sum\limits_{k\sim i,k\sim j}\frac{1}{\sqrt{(d_i^2+d_k^2)(d_k^2+d_j^2)}})] = 2\sum\limits_{i\sim j}\frac{1}{\sqrt{d_i^2+d_j^2}}(\sum\limits_{k\sim i,k\sim j}\frac{1}{\sqrt{(d_i^2+d_k^2)(d_k^2+d_j^2)}})$.

(4) Since $tr(S^4) = \|S^2\|_F^2$, where $\|S^2\|_F$ is the Frobenius norm of S^2. Therefore, $tr(S^4) = \sum\limits_{i,j=1}^{n}|(S^2)_{ij}|^2 = \sum\limits_{i=j}|(S^2)_{ij}|^2 + \sum\limits_{i\neq j}|(S^2)_{ij}|^2 = \sum\limits_{i=1}^{n}(\sum\limits_{i\sim j}\frac{1}{d_i^2+d_j^2})^2 + \sum\limits_{i\neq j}(\sum\limits_{k\sim i,k\sim j}\frac{1}{\sqrt{(d_i^2+d_k^2)(d_k^2+d_j^2)}})^2$. □

Theorem 3.6. *Let G be a simple graph with n vertices, $m \geq 1$ edges. Then*

$$E_S(G) \geq 2\sum_{i\sim j}\frac{1}{d_i^2+d_j^2}\sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_i^2+d_j^2}}{\sum\limits_{i=1}^{n}(\sum\limits_{i\sim j}\frac{1}{d_i^2+d_j^2})^2 + \sum\limits_{i\neq j}(\sum\limits_{k\sim i,k\sim j}\frac{1}{\sqrt{(d_i^2+d_k^2)(d_k^2+d_j^2)}})^2}}.$$

Proof. By discrete Hölder inequality, we have $\sum\limits_{i=1}^{n}|\mu_i|^{\frac{2}{3}}(|\mu_i|^4)^{\frac{1}{3}} \leq (\sum\limits_{i=1}^{n}|\mu_i|)^{\frac{2}{3}}(\sum\limits_{i=1}^{n}|\mu_i|^4)^{\frac{1}{3}}$.

By Lemma 3.5, we have $E_S(G) = \sum\limits_{i=1}^{n}|\mu_i|$, $\sum\limits_{i=1}^{n}\mu_i^2 = tr(S^2) = \sum\limits_{i\sim j}\frac{2}{d_i^2+d_j^2}$, and $\sum\limits_{i=1}^{n}\mu_i^4 = tr(S^4) = \sum\limits_{i=1}^{n}(\sum\limits_{i\sim j}\frac{1}{d_i^2+d_j^2})^2 + \sum\limits_{i\neq j}(\sum\limits_{k\sim i,k\sim j}\frac{1}{\sqrt{(d_i^2+d_k^2)(d_k^2+d_j^2)}})^2$.

So, $tr(S^2) \leq [E_S(G)]^{\frac{2}{3}}[tr(S^4)]^{\frac{1}{3}}$, thus $E_S(G) \geq \sqrt{\frac{[tr(S^2)]^3}{tr(S^4)}}$. This completes the proof. □

4. Concluding remarks

In chemical graph theory, it is important to study the extremal structure of graph with respect to the topological indices, because it provides some useful information to determine the applicability range of the topological indices in QSPR and QSAR. In this paper, we obtain some bounds for modified Sombor indices of graphs with given some parameters and Nordhaus-Gaddum-type results. Then, we obtain some bounds for the modified Sombor spectral radius and energy. It is interesting to consider other properties of modified Sombor index. Therefore, we propose the following problems.

Problem 4.1. *Determine more properties of modified Sombor index.*

Problem 4.2. *Determine the extremal trees, unicyclic graphs, bicyclic graphs with respect to modified Sombor index.*

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Conflict of interest

All authors declare no conflicts of interest in this paper.

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