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NEW BOUNDS FOR SOMBOR INDEX

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Abstract. The Sombor index $SO(G)$, which is defined as the sum over all pairs of neighboring vertices, is a vertex-degree based graph invariant. The degrees, vertices and edges of different boundaries for the Sombor index are investigated in this paper. In addition, Sombor energy inequalities related to the eigenvalues of the Sombor index are found.

1. Introduction

The Sombor index, which Gutman discovered in 2021 [**8**], is a molecular structure named after the Serbian city of Sombor. Graphs containing (linked) molecular graphs, chemical trees, and hexagonal systems are categorized in terms of the Sombor index.

Sombor index is described as [**9**]

$$SO(G) = \sum_{i\sim j} \sqrt{d_i^2 + d_j^2}$$

where the degree d_i of vertex $i \in V(G)$ is equal to the number of vertices adjacent to i. It is written ij (or ji) if there is an edge connecting vertex i to vertex j.

The Sombor index, which is mostly functional in the molecular structure of atoms, is a fairly new and popular index. The number of edges emerging from the graph's points determines the degrees needed to find the Sombor index.

The chemical significance of the Sombor index is investigated in [**6**] and it is shown that this index is effective in accurately predicting physicochemical properties compared with other well-known and frequently used indices. In [**15**], molecular

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trees are defined in terms of the Sombor index and boundaries are found. The defining characteristics of Sombor index and Reduced Sombor index are investigated. Using graph properties and maximum-minimum degrees, some lower and upper bounds on the Sombor index of graphs are reported in [**4**]. Additionally, there are several relations between the first and second Zagreb indices with the Sombor index. The Sombor index's graph structure with a few degree based defining relations is examined in [**17**].

This study aims to provide a fresh perspective on the Sombor index and contain significant bounds. In addition, Sombor Energy, which is the absolute sum of eigenvalues of Sombor matrix, is investigated. It is provided some important definitions and theorems in Section 2 that will be helpful throughout the remainder of the study. Bounds for the Sombor index are provided in terms of degrees, edges and vertices in Section 3. Also, the Sombor index is associated with some known special graphs and indices with the help of defining relations. Finally, a relation is studied between Sombor energy and Sombor matrix. This essay discusses the Sombor's energy and index. For more information on graph theory and the Sombor index, see [**1**–**3**, **7**].

2. Preliminaries

Let G be a connected graph with the vertices set of $V(G) = \{v_1, v_2, \ldots, v_n\}$. The distance d_{ij}, is the length of the shortest path between the vertices v_i and v_j in G. The minimum and maximum degrees of a connected graph are δ and Δ, respectively.

The Sombor matrix $SOM(G)$ is a symmetric matrix, which is described by [**10**]

$$SOM_{ij}(G) = \begin{cases} \sqrt{d_i^2 + d_j^2} & ; \quad \text{if } i \sim j \\ 0 & ; \quad \text{otherwise.} \end{cases}$$

where the degree of G is d_i.

Let the eigenvalues of the Sombor matrix be $\rho_1,\ \rho_2, \ldots,\ \rho_n$. The SOM(G)'s eigenvalues are $\rho_1 \geqslant \rho_2 \geqslant \ldots \geqslant \rho_n$, where ρ_1 is referred to as the Sombor spectral radius of G.

Sombor energy of graphs is determined by the formula $SOE(G) = \sum_{i=1}^{n} |\rho_i|$. See [**5**, **12**, **16**] for graph energy and Sombor energy.

A graph invariant with the definition $F = F(G) = \sum_{i=1}^{n} d_i^3$ that was once known as the forgotten topological index has recently attracted interest. The identities $F = F(G) = \sum_{i\sim j} d_i^2 + d_j^2$ are satisfied by F [**11**].

The following results are important to verify the main results:

LEMMA 2.1. [**13**] *Let G be a graph with n vertex. Let $\sum_{i=1}^{n} p_i = 1$ and $0 < r \leqslant a_i \leqslant R < \infty$. Then,*

$$\sum_{i=1}^{n} p_i a_i + rR \sum_{i=1}^{n} \frac{p_i}{a_i} \leqslant r + R. \tag{2.1}$$

LEMMA 2.2. [**11**] *Let A, a, B, b be positive numbers, $a_i, b_i \in \mathbb{R}^+$ for any $0 < a \leqslant a_i \leqslant A < \infty$ and $0 < b \leqslant b_i \leqslant B < \infty$, $i = 1, 2, ...n$. Then,*

$$\frac{\sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2}{(\sum_{i=1}^n a_i b_i)^2} \leqslant \frac{(ab + AB)^2}{4abAB}. \tag{2.2}$$

LEMMA 2.3. [**13**] *Let G be a graph with n vertex. Let a_i,r,$R \in \mathbb{R}$, $i = 1, 2, ..., n$ and $0 < r \leqslant a_i \leqslant R$. Then,*

$$n\sum_{i=1}^n a_i^2 - (\sum_{i=1}^n a_i)^2 \geqslant \frac{n}{2}(R - r)^2. \tag{2.3}$$

LEMMA 2.4. [**14**] *For positive numbers $x_1, x_2, ..., x_n \in R$,*

$$\frac{n}{\frac{1}{x_1} + \frac{1}{x_2} + ... + \frac{1}{x_n}} \leqslant \sqrt[n]{x_1 x_2 ... x_n}. \tag{2.4}$$

3. Main results

In the articles written about graph theory, which ways are used, which mathematical operations are performed while an equation is found, and which lemmas are used in which equations are examined in detail. It is aimed to finding new inequalities by making use of the observations obtained as a result of the examination. In this section, some new bounds for molecular graphs are obtained by investigating the Sombor matrix, Sombor index and Sombor energy. Throughout Section 3, G is assumed the graph with p pendent vertices are the vertices that have degree 1.

THEOREM 3.1. *Let G be a graph for p pendent vertices. If G is a connected graph of order n, size m with maximum Δ and minimum non pendent vertex degree δ_1, then*

$$SO(G) \leqslant \frac{p(\sqrt{\Delta^2 + 1} - (m - p)(\delta_1^2 + 1))}{p - m + 1} \tag{3.1}$$

if and only if $G \cong K_{1,n-1}$.

PROOF. According to Cauchy-Schwarz inequality,

$$\begin{aligned} SO(G) &= \sum_{i\sim j, d_j=1} \sqrt{d_i^2 + d_j^2} + \sum_{i\sim j, d_i, d_j>1} \sqrt{d_i^2 + d_j^2} \\ &\leqslant p\sqrt{\Delta^2 + 1} + (m - p) \sum_{i\sim j, d_i, d_j>1} \sqrt{d_i^2 + d_j^2} \\ &= p\sqrt{\Delta^2 + 1} + (m - p)(\sum_{i\sim j} \sqrt{d_i^2 + d_j^2} - \sum_{i\sim j, d_i, d_j=1} \sqrt{d_i^2 + d_j^2}) \\ &= p\sqrt{\Delta^2 + 1} + (m - p)(SO(G) - p(\delta_1^2 + 1)). \end{aligned}$$

Hence,

$$SO(G) \leqslant \frac{p(\sqrt{\Delta^2 + 1} - (m - p)(\delta_1^2 + 1))}{p - m + 1}. \tag{3.2}$$

Suppose that the results in (3.1) hold. Thus all the above inequalities must be equal. From the equality in the second inequality of the proof, it is obtained $d_i = \Delta$ and $d_j = 1$ for any pendent edge $i \sim j$. Also, it has $d_i = d_j = \delta_1$ for any non pendent edge $i \sim j$. In addition, $d_i = \delta_1$ and $d_j = 1$ in fourth equality. If every edge of G is pendent edge, $m = p$, then $G \cong K_{1,n-1}$. Conversely, for $K_{1,n-1}$, it is clear that the equality in (3.1). □

Corollary 3.1. *If G is a connected graph with minimum degree δ_1, then*

$$SO(G) \leqslant (m-p)\sqrt{\delta_1^2+1} + p\sqrt{2} \tag{3.3}$$

if and only if $G \cong K_{1,n-1}$.

Proof. Similarly to Theorem 3.1, $SO(G) = \sum_{i\sim j, d_j=1} \sqrt{d_i^2+d_j^2}$ $+ \sum_{i\sim j, d_i, d_j>1} \sqrt{d_i^2+d_j^2}$ where $d_i = 1$ and $d_j = \delta_1$. □

Theorem 3.2. *If G is connected graph with n vertices and m edges then*

$$SO(G) \leqslant p\sqrt{n^2-2n+2} + (m-p)\sqrt{n^2-2n+5} \tag{3.4}$$

if and only if $G \cong K_{1,n-1}$, with equality.

Proof. Let $f(x) = \sqrt{x^2+1}$ be an increasing function for $x \geqslant 1$. After that,

$$\sqrt{d_i^2+d_j^2} \leqslant \sqrt{(n-1)^2+1}$$

for $d_i = n-1$ and $d_j = 1$, with equality. This requires that

$$\sqrt{d_i^2+d_j^2} \leqslant \sqrt{(n-1)^2+4} \tag{3.5}$$

for $d_i = n-1$ and $d_j = 2$ are true, $d_i \geqslant d_j$. Thus,

$$\begin{aligned} SO(G) &= \sum_{i\sim j, d_j=1} \sqrt{d_i^2+d_j^2} + \sum_{i\sim j, d_i, d_j>1} \sqrt{d_i^2+d_j^2} \\ &\leqslant p\sqrt{n^2-2n+2} + (m-p)\sqrt{n^2-2n+5}. \end{aligned}$$

Suppose that the equality in (3.4) holds. Then the above all inequalities in the expression must be equal. Below, without losing generality, assume that $d_i \geqslant d_j$ for each edge $i \sim j$. Firstly, if G has no pendent edge, $p = 0$. This requires G has a common neighbor between the end vertices of each edge of G in inequality (3.5). This implies that G is isomorphic to $K_{1,n-1}$ for $p = m$. Secondly, suppose that $0 < p < m$ and $d_i = n-1$, $d_k = 1$ with $i \sim k$. Then, G has a non-pendent edge $i \sim j$ with $d_j = 2$ as $m > p$. Therefore, the vertices i and j must have a common neighbor l. In addition, $d_l = n-1$ from the inequality in (3.5). Thus, $l \sim k$, which shows that $d_k \geqslant 2$. It is a contradiction. Conversely, the claim of theorem is obvious for a star $G \cong K_{1,n-1}$. □

Corollary 3.2. *Let G be a connected graph with n vertices and m edges, then*

$$SO(G) \leqslant m\sqrt{n^2-2n+5} \tag{3.6}$$

if and only if $G \cong K_{1,n-1}$.

PROOF. If there are no pendent vertices then $p = 0$. $\square$

THEOREM 3.3. *If G is a connected graph with n nodes, m edges then*

$$\frac{\sqrt{2}(\Delta+\delta) - \sqrt{2n^2(\Delta^2+\delta^2)+(4n^2-8)\Delta\delta}}{2} \leqslant SO(G),$$
$$SO(G) \leqslant \frac{\sqrt{2}(\Delta+\delta) + \sqrt{2n^2(\Delta^2+\delta^2)+(4n^2-8)\Delta\delta}}{2}.$$

PROOF. Let $r = \sqrt{2}\delta$, $a_i = \sqrt{d_i^2 + d_j^2}$, $R = \sqrt{2}\Delta$, $p_i = \frac{1}{n}$, $i = 1, 2, ..., n$. The use of Lemma 2.1, it gets,

$$\sum_{i=1}^{n} \frac{1}{n}\sqrt{d_i^2+d_j^2} + 2\delta\Delta\frac{1}{n\sqrt{d_i^2+d_j^2}} \leqslant \sqrt{2}(\delta+\Delta).$$

Since $\sum_{i=1}^{n} \frac{1}{n}\sqrt{d_i^2+d_j^2} \geqslant \sum_{i\sim j} \frac{1}{n}\sqrt{d_i^2+d_j^2}$, it is represented by

$$\frac{SO(G)}{n} + \frac{2\delta\Delta}{n\sum_{i\sim j}\sqrt{d_i^2+d_j^2}} \leqslant \sqrt{2}(\delta+\Delta).$$

By the inequality $\dfrac{SO(G)}{n} + \dfrac{2\delta\Delta}{nSO(G)} \leqslant \sqrt{2}(\delta+\Delta)$, it is obtained that $SO(G)^2 + 2\delta\Delta \leqslant \sqrt{2}n(\delta+\Delta)SO(G)$ and it is implied that $SO(G)^2+2\delta\Delta-\sqrt{2}n(\delta+\Delta)SO(G) \leqslant 0$. Let $SO(G) = x$. Thus, $x^2 + 2\delta\Delta - \sqrt{2}(\delta+\Delta)nx \leqslant 0$. Since the discriminant of the function is $\bigtriangledown = 2n^2(\Delta^2+\delta^2) + (4n^2-8)\Delta\delta$ then $x_1 = \dfrac{\sqrt{2}(\delta+\Delta) - \sqrt{\bigtriangledown}}{2}$, $x_2 = \dfrac{\sqrt{2}(\delta+\Delta) + \sqrt{\bigtriangledown}}{2}$. It gets, $x_1 \leqslant SO(G) \leqslant x_2$. Hence,

$$\frac{\sqrt{2}(\Delta+\delta) - \sqrt{2n^2(\Delta^2+\delta^2)+(4n^2-8)\Delta\delta}}{2} \leqslant SO(G),$$
$$SO(G) \leqslant \frac{\sqrt{2}(\Delta+\delta) + \sqrt{2n^2(\Delta^2+\delta^2)+(4n^2-8)\Delta\delta}}{2}.$$

$\square$

THEOREM 3.4. *If G is a connected graph with the minimum degree δ_1 for non-pendent vertex degrees, then*

$$SO(G) \geqslant \frac{\sqrt{4n\sqrt{2}F(G)(\sqrt{\Delta^2+\delta_1^2})}}{\sqrt{2}+\sqrt{\Delta^2+\delta_1^2}} \tag{3.7}$$

with equality if and only if G is isomorphic to $K_{1,n-1}$.

PROOF. Consider the $a=\sqrt{2}$, $a_i=\sqrt{d_i^2+d_j^2}$ and $A=\sqrt{\Delta^2+\delta_1^2}$, $b=b_i=B=1$ for any non pendent edge $i\sim j$. Using the Polya-Szego inequality, it gets

$$\frac{\sum_{i=1}^{n}(\sqrt{d_i^2+d_j^2})^2\sum_{i=1}^{n}1^2}{(\sum_{i=1}^{n}\sqrt{d_i^2+d_j^2})^2}\leqslant\frac{(\sqrt{2}+\sqrt{\Delta^2+\delta_1^2})^2}{4\sqrt{2}\sqrt{\Delta^2+\delta_1^2}}. \tag{3.8}$$

By the help of definitions of Sombor index and Forgotten index,

$$\frac{nF(G)}{(SO(G))^2}\leqslant\frac{(\sqrt{2}+\sqrt{\Delta^2+\delta_1^2})^2}{4\sqrt{2}\sqrt{\Delta^2+\delta_1^2}}.$$

This requires that

$$SO(G)\geqslant\frac{\sqrt{4n\sqrt{2}F(G)(\sqrt{\Delta^2+\delta_1^2})}}{\sqrt{2}+\sqrt{\Delta^2+\delta_1^2}}.$$

Now suppose that the result holds in (3.7). Thus all inequalities in above proof must be equal. Also, G has $d_i=\Delta, d_j=\delta_1$ in the expression (3.8). Let each one of the edges of G be a pendent edge, then G is isomorphic to $K_{1,n-1}$. Conversely, the claim is obvious in (3.7) for $K_{1,n-1}$. □

THEOREM 3.5. *If G is a connected graph then*

$$SO(G)\leqslant\sqrt{n(F(G)-(\Delta-\delta)^2)} \tag{3.9}$$

with equality if and only if G is isomorphic to K_3.

PROOF. Let $a_i=\sqrt{d_i^2+d_j^2}$, $R=\sqrt{2}\Delta$ and $r=\sqrt{2}\delta$. By the claim of Lemma 2.3,

$$n\sum_{i=1}^{n}(\sqrt{d_i^2+d_j^2})^2-(\sum_{i=1}^{n}\sqrt{d_i^2+d_j^2})^2\geqslant\frac{n}{2}(\sqrt{2}\Delta-\sqrt{2}\delta)^2.$$

By the definitions of $SO(G)$ and $F(G)$, the result becomes

$$nF(G)-n(\Delta-\delta)^2\geqslant SO(G)^2.$$

Hence,

$$SO(G)\leqslant\sqrt{n(F(G)-(\Delta-\delta)^2)}.$$

Now suppose that the equality holds in (3.9). Then the above all inequalities of expression must be equal. This means that G is isomorphic to K_3. Conversely, the equality holds in (3.9) for a complete graph K_3. □

THEOREM 3.6. *Let G be a connected graph with n nodes and m edges where $|SOM(G)|$ is the determinant of the Sombor matrix. Also, let $SOM(G)$ and $SOE(G)$ be Sombor matrix and Sombor energy of G, respectively. Then*

$$SOE(G)\leqslant n\sqrt[n]{|SOM(G)|}.$$

Proof. Let $p_1 = p_2 = ... = p_n = \frac{1}{n}$, $r = |\rho_n|$, $a_i = |\rho_i|$, $R = |\rho_1|$. By Lemma 2.1,

$$\sum_{i=1}^{n} \frac{1}{n}|\rho_i| + |\rho_n||\rho_1| \sum_{i=1}^{n} \frac{1}{n|\rho_i|} \leqslant |\rho_n| + |\rho_1|.$$

Let $|\rho_n| = x$ and $|\rho_1| = y$. It follows easily that,

$$\frac{SOE(G)}{n} \leqslant x + y - xy\frac{1}{n}\left(\frac{1}{|\rho_1|} + \frac{1}{|\rho_2|} + ... + \frac{1}{|\rho_n|}\right).$$

Also, by Lemma 2.4, the inequality requires that

$$\begin{aligned} \frac{SOE(G)}{n} &\leqslant x + y - \frac{xy}{\sqrt[n]{|\rho_1||\rho_2|...|\rho_n|}} \\ \frac{SOE(G)}{n} &\leqslant x + y - \frac{xy}{\sqrt[n]{|SOM(G)|}}. \end{aligned}$$

Let $x + y - \frac{xy}{\sqrt[n]{|SOM(G)|}} = f(x, y)$ and $\frac{1}{\sqrt[n]{|SOM(G)|}} = k$. This means that, $SOE(G) \leqslant nf(x, y) = n(x + y - xyk)$. Since, $f(x, y) = x + y - xyk$ then $f_x(x, y) = 1 - yk$, $f_y(x, y) = 1 - xk$, $f_{xx}(x, y) = 0$, $f_{yy}(x, y) = 0$. Also, $f_x(x, y) = f_y(x, y) = 0$ and $x = y = \frac{1}{k}$. This implies, $f(x, y) = \frac{1}{k}$. Hence,

$$SOE(G) \leqslant n\sqrt[n]{|SOM(G)|}.$$

□

References

1. F. R. K. Chung, *Spectral Graph Theory*, CBMS Lecture Notes, Providence, (1997).
2. R. Cruz, I. Gutman, and J. Rada, Sombor index of chemical graphs, *Appl. Math. Comp.* **399**(2021), 126018.
3. R. Cruz and J. Rada, Extremal values of the Sombor index in unicyclic and bicyclic graphs,*J. Math. Chem.* **59**(2021), 1098—1116.
4. K.C. Das, A.S. Çevik, I.N. Cangul, and Y. Shang, On Sombor index, *Symmetry* **13**(2021), 140.
5. K. Das and S. Mojallal, Upper bounds for the energy of graphs,*MATCH Commun. Math. Comput. Chem.* **70**(2013), 657—662.
6. H. Deng, Z. Tang, and R. Wu, Molecular trees with extremal values of Sombor indices, *Int. J. Quantum. Chem.* (2021).
7. D. Cvetković, M. Doob, and H. Sachs, *Spectra of Graphs*, Academic press, New York, 1980.
8. I. Gutman, Some basic properties of Sombor indices, *Open J. Discr. Appl. Math.* **4**(2021), 1—3.
9. I. Gutman, Geometric approach to degree based topological indices, *MATCH Commun. Math. Comput. Chem.* **86**(2021), 11—16.
10. I. Gutman, Spectrum and energy of the Sombor matrix, *Vojnotehni Cki Glasnik/ Military Technical Courier* **69**(3)(2021), 551–561.
11. I. Gutman and N. Trinajstic, Graph theory and molecular orbitals, Total electron energy of alternant, hydrocarbons, *Chem. Phys. Lett.* **17**(1972), 535-538.
12. X. Li, Y. Shi, and I. Gutman, Graph Energy, *Springer*, New York, (2012).
13. D.S. Mitrinović and P.M. Vasić, Analytic Inequalities, *Springer*, Berlin, (1970).

14. N.J. Rad, A. Jahanbani, and I. Gutman, Zagreb energy and Zagreb Estrada index of graphs, *MATCH Commun. Math. Comput. Chem.* **79**(2018), 371-386.
15. I. Redzepović, Chemical applicability of Sombor indices, *J. Serb. Chem. Soc.*, in press. **86**(5)(2021).
16. A. Ülker, A. Gürsoy, and G.N. Kırcalı, The Energy and Sombor Index of Graphs, *MATCH Commun. Math. Comput. Chem.* **87**(2022), 51-58.
17. Z. Wang, Y. Mao Li, and B. Furtula, On relations between Sombor and other degree–based indices, *J. Appl. Math. Comput.*, in press. https://doi.org/10.1007/s12190-021-01516-x.

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