Iranian Journal of Mathematical Chemistry

IJMC

DOI: 10.22052/ijmc.2026.257236.2033
Vol. 17, No. 4, 2026, pp. 401-414
Research Paper

On the Inverse Sum Indeg Index and its Associated Energy

Slobodan Filipovski [1*], Mirza Redžić[2] and Elvis Baraković[3]

[1]Faculty of Mathematics, Natural Sciences and Information Technologies, University of Primorska, Glagoljaška 8, SI-6000 Koper, Slovenia

[2]Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

[3] Faculty of Natural Sciences and Mathematics, University of Tuzla, Univerzitetska 4, 75000 Tuzla, Bosnia and Herzegovina

Keywords:

Inverse sum indeg index,
ISI energy,
Degree-based topological indices,
Spectral graph theory,
Graph energy

AMS Subject Classification (2020):

05C50; 05C09; 05C92

Article History:

Received: 17 September 2025
Accepted: 30 August 2026

Abstract

Let G be a simple graph with degree sequence $\{d_v\}$. The inverse sum indeg (ISI) matrix S is defined by $s_{uv} = \frac{d_u d_v}{d_u + d_v}$ if $uv \in E(G)$ and 0 otherwise. The ISI energy of G is defined as $\mathcal{E}_{ISI}(G) = \sum_{i=1}^{n} |\tau_i|$, where $\tau_1, \ldots, \tau_n$ are the eigenvalues of S.

In this paper, we establish new upper and lower bounds for the ISI index and ISI energy in terms of classical degree-based graph invariants, including the second Zagreb index, geometric–arithmetic index, harmonic index, Sombor index, and Randić index. Several of these results refine and improve the classical estimate $\mathcal{E}_{ISI}(G) \leq \sqrt{2nB}$, where $B = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v}\right)^2$.

We further derive spectral refinements involving extremal eigenvalues and the variance of the squared eigenvalues, and recall known determinant-based bounds. In addition, we obtain new bounds for the largest eigenvalue of S and establish further relations between ISI energy and structural molecular descriptors.

© 2026 University of Kashan Press. All rights reserved.

1 Introduction

Let G be a simple undirected graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, the neighborhood of v, denoted by $N(v)$, is the set of all vertices adjacent to v, and the degree of v is $d(v) = |N(v)|$. Spectral graph theory plays a central role in mathematical chemistry, particularly through graph energy, introduced by Gutman in [1] as the sum of the absolute values of the eigenvalues of the adjacency matrix. This notion provides a spectral

*Corresponding author
E-mail addresses: slobodan.filipovski@famnit.upr.si (S. Filipovski), mirza.redzic@kit.edu (M. Redžić), elvis.barakovic@untz.ba (E. Baraković)
Academic Editor: Modjtaba Ghorbani

analogue of total π-electron energy in molecular systems, where vertices represent atoms and edges represent chemical bonds.

Motivated by this framework, numerous degree-based topological indices have been introduced to describe structural properties of molecular graphs. Among them, the *inverse sum indeg index (ISI)*, introduced by Vukičević and Gašperov [2], is defined as:

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

This index has been widely studied in the context of QSAR and QSPR analysis due to its ability to capture molecular surface-related properties. Unlike classical degree-based invariants, the ISI index incorporates a nonlinear interaction between endpoint degrees, combining harmonic-type averaging with multiplicative behavior. This makes it naturally comparable with several classical indices such as the Zagreb, harmonic, geometric-arithmetic, and Sombor indices.

A considerable amount of research has been devoted to extremal properties and applications of the ISI index. Sedlar et al. [3] obtained extremal results for several graph classes including trees and chemical graphs, while Falahati-Nezhad et al. [4, 5] derived sharp bounds and explicit computations for special molecular structures such as nanotubes. Further developments introduced a spectral perspective on ISI. In particular, Zangi et al. [6] defined the *ISI matrix* S of a graph G by

$$s_{u,v} = \begin{cases} \frac{d_u d_v}{d_u + d_v}, & uv \in E(G), \\ 0, & \text{otherwise}, \end{cases}$$

and introduced the corresponding *ISI energy*

$$\mathcal{E}_{ISI}(G) = \sum_{i=1}^{n} |\tau_i|,$$

where $\tau_1 \geq \tau_2 \geq \cdots \geq \tau_n$ are the eigenvalues of S. This spectral invariant has been further investigated in [7–10], revealing connections with chemical properties of molecular systems and drug design.

A key structural quantity associated with the ISI matrix is

$$B = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v} \right)^2.$$

In [11] Jamal et al. proved that the sum of the squares of the eigenvalues of the ISI matrix can be expressed using B as:

$$\sum_{i=1}^{n} \tau_i^2 = -2 \sum_{1 \leq i < j \leq n} \tau_i \tau_j = 2 \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v} \right)^2 = 2B.$$

Moreover, they proved the following relation between the ISI energy of graphs and the invariant B.

Lemma 1.1. *([11]). Let G be a graph with n vertices. Then $\mathcal{E}_{ISI}(G) \leq \sqrt{2nB}$.*

Despite significant progress, relatively few results establish sharp relationships between ISI energy and classical graph invariants such as Zagreb-type indices, Sombor index, Randić index, and other molecular descriptors. In particular, refined spectral inequalities that incorporate structural parameters of graphs remain limited in the literature.

1.1 Main contributions

In this paper, we develop new upper and lower bounds for the ISI index and ISI energy in terms of classical topological indices and spectral parameters. The main contributions are summarized as follows:

- We establish new inequalities relating the ISI index to classical molecular descriptors, including the second Zagreb index, the Sombor index, and the geometric-arithmetic index.
- We refine the classical bound
$$\mathcal{E}_{ISI}(G) \leq \sqrt{2nB},$$
by incorporating additional spectral and structural parameters of the ISI matrix, leading to improved estimates.
- We derive new upper bounds for the ISI energy in terms of degree-based indices, including the forgotten index, and investigate refinements based on eigenvalue variance.
- We obtain new estimates for extremal eigenvalues of the ISI matrix in terms of ISI energy and structural graph invariants.
- We further establish connections between ISI energy and classical molecular descriptors, highlighting the interplay between spectral properties and degree-based structure.

The determinant-based bounds in Propositions 3.5 and 4.2 are recalled from Hafeez and Farooq [9]. The remainder of the paper is organized as follows. Section 2 presents new relationships between the ISI index and classical topological invariants. Section 3 establishes the improved upper bounds for ISI energy, while Section 4 provides lower bounds and extremal spectral estimates.

2 Connections between the ISI index and classical topological invariants

The inverse sum indeg (ISI) index is closely related to several classical degree-based topological indices that arise in mathematical chemistry and chemical graph theory. In this section, we establish bounds for the ISI index in terms of well-known invariants, including the second Zagreb index, geometric–arithmetic index, harmonic index, and Sombor index. These results highlight the interplay between harmonic-type averaging and multiplicative degree structure.

For a simple graph G, we recall the following standard degree-based indices:

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}, \qquad H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v},$$

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

We begin with a lower bound for the ISI index in terms of the second Zagreb index.

Proposition 2.1. *Let G be a triangle-free graph on n vertices with at least one edge. Then*

$$ISI(G) \geq \frac{1}{n} M_2(G).$$

Equality holds if and only if G is a complete bipartite graph.

Proof. Since G is triangle-free, for every edge $uv \in E(G)$, the neighborhoods $N(u)$ and $N(v)$ are disjoint. Hence,

$$d_u + d_v \leq n.$$

Therefore,

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v} \geq \frac{1}{n} \sum_{uv \in E(G)} d_u d_v = \frac{1}{n} M_2(G).$$

Equality holds if and only if $d_u + d_v = n$ for every edge $uv \in E(G)$.
Suppose that equality holds and fix an edge uv. Since $N(u) \cap N(v) = \varnothing$ and $d_u + d_v = n$, we have

$$V(G) = N(u) \cup N(v).$$

Set $A = N(v)$ and $B = N(u)$. Since G is triangle-free, both A and B are independent sets. For every $x \in A$, the edge xv and the equality condition give

$$d_x + d_v = n = d_u + d_v,$$

and hence $d_x = d_u = |B|$. Since x has no neighbors in A, it follows that x is adjacent to every vertex of B. Thus, G is complete bipartite.

Conversely, if $G = K_{p,q}$ with $p + q = n$, then every edge joins vertices of degrees q and p, respectively, so $d_u + d_v = n$ for every edge. Hence, equality holds. ■

Next we derive an upper bound for the ISI index in terms of the second Zagreb index.

Proposition 2.2. *Let G be a simple graph with m edges. Then,*

$$ISI(G) \leq \frac{1}{2} \sqrt{m\, M_2(G)}.$$

Equality holds if and only if all nonisolated vertices of G have the same degree.

Proof. We write

$$ISI(G) = \sum_{uv \in E(G)} \sqrt{d_u d_v} \cdot \frac{\sqrt{d_u d_v}}{d_u + d_v}.$$

Applying the Cauchy–Schwarz inequality yields

$$ISI(G)^2 \leq \left(\sum_{uv \in E(G)} d_u d_v \right) \left(\sum_{uv \in E(G)} \frac{d_u d_v}{(d_u + d_v)^2} \right).$$

Since $(d_u + d_v)^2 \geq 4 d_u d_v$, we obtain:

$$\sum_{uv \in E(G)} \frac{d_u d_v}{(d_u + d_v)^2} \leq \frac{m}{4}.$$

Combining the inequalities gives the desired result. Equality holds if and only if equality occurs in both the Cauchy–Schwarz inequality and $(d_u + d_v)^2 \geq 4d_u d_v$. The latter requires $d_u = d_v$ for every edge $uv \in E(G)$. Equality in the Cauchy–Schwarz inequality further requires $d_u + d_v$ to be constant over all edges. Hence, there exists $r \geq 1$ such that $d_u = d_v = r$ for every edge $uv \in E(G)$. Equivalently, all nonisolated vertices of G have the same degree. Conversely, this condition clearly yields equality in both inequalities above. ■

We now establish a lower bound involving the geometric-arithmetic and harmonic indices, showing that the ISI index is controlled by the ratio of two classical mixed-degree measures.

Proposition 2.3. *For any simple graph G with at least one edge,*

$$ISI(G) \geq \frac{GA^2(G)}{2H(G)}.$$

Equality holds if and only if $d_u d_v$ is constant over all edges $uv \in E(G)$.

Proof. Applying the Cauchy–Schwarz inequality, we obtain:

$$\left(\sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{d_u + d_v}\right)^2 \leq \left(\sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v}\right)\left(\sum_{uv\in E(G)} \frac{1}{d_u + d_v}\right).$$

Since

$$\sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{d_u + d_v} = \frac{GA(G)}{2} \quad \text{and} \quad \sum_{uv\in E(G)} \frac{1}{d_u + d_v} = \frac{H(G)}{2},$$

it follows that

$$\frac{GA^2(G)}{4} \leq ISI(G)\frac{H(G)}{2},$$

and therefore,

$$ISI(G) \geq \frac{GA^2(G)}{2H(G)}.$$

Equality in the Cauchy–Schwarz inequality holds if and only if there exists a constant $c > 0$ such that $\sqrt{d_u d_v} = c$ for every $uv \in E(G)$, which is equivalent to $d_u d_v$ being constant over all edges of G. ■

Proposition 2.4. *Let G be a simple graph. Then,*

$$ISI(G) \leq \frac{1}{2\sqrt{2}} SO(G).$$

Equality holds if and only if $d_u = d_v$ for every edge $uv \in E(G)$, or equivalently, every nontrivial connected component of G is regular.

Proof. For every edge $uv \in E(G)$, the arithmetic–geometric mean inequality gives $d_u + d_v \geq 2\sqrt{d_u d_v}$, while $d_u^2 + d_v^2 \geq 2d_u d_v$. Therefore,

$$\frac{d_u d_v}{d_u + d_v} \leq \frac{\sqrt{d_u d_v}}{2} \leq \frac{1}{2\sqrt{2}}\sqrt{d_u^2 + d_v^2}.$$

Summing over all edges yields

$$ISI(G) \leq \frac{1}{2\sqrt{2}} SO(G).$$

Equality holds in both inequalities above if and only if $d_u = d_v$. Hence, equality in the stated bound holds if and only if $d_u = d_v$ for every edge $uv \in E(G)$, which is equivalent to every nontrivial connected component of G being regular. ■

Table 1 illustrates the obtained bounds for several standard graph families and, in particular, shows that equality is attained in several of the above inequalities.

Table 1: Comparison of the ISI index and the bounds obtained in Section 2. The bound $M_2(G)/n$ applies only to triangle-free graphs.

Graph G	$ISI(G)$	$\frac{M_2(G)}{n}$	$\frac{GA^2(G)}{2H(G)}$	$\frac{SO(G)}{2\sqrt{2}}$
P_4	2.333	2.000	2.271	2.581
P_5	3.333	2.400	3.235	3.581
P_6	4.333	2.667	4.212	4.581
$K_{1,3}$	2.250	2.250	2.250	3.354
$K_{1,4}$	3.200	3.200	3.200	5.831
$K_{1,5}$	4.167	4.167	4.167	9.014
C_4	4.000	4.000	4.000	4.000
C_6	6.000	4.000	6.000	6.000
C_8	8.000	4.000	8.000	8.000
K_5	20.000	—	20.000	20.000

3 Upper bounds for the ISI energy

In this section, we derive several upper bounds for the ISI energy $\mathcal{E}_{ISI}(G)$. Our main objective is to refine the classical estimate

$$\mathcal{E}_{ISI}(G) \leq \sqrt{2nB},$$

where

$$B = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v} \right)^2.$$

We first obtain bounds involving structural graph invariants, and then derive sharper spectral refinements based on the determinant and variance of the eigenvalues of the ISI matrix.

Lemma 3.1. *Let $f(x,y) = \frac{xy}{x+y}$ for $x, y > 0$. Then f is increasing in both variables x and y.*

Proof. It suffices to show that the result holds for x and is symmetric for y. Calculating the partial derivative with respect to the variable x, we get:

$$\frac{\partial}{\partial x} f(x,y) = \frac{\partial}{\partial x} \frac{xy}{x+y} = \frac{y^2}{(x+y)^2} \geq 0.$$

■

Proposition 3.2. *Let G be a simple graph without isolated vertices. Then,*

$$\mathcal{E}_{ISI}(G) \leq 4B.$$

Proof. Since G has no isolated vertices, $d_v \geq 1$ for every $v \in V(G)$. By Lemma 3.1, for every edge $uv \in E(G)$,

$$\frac{d_u d_v}{d_u + d_v} \geq \frac{1 \cdot 1}{1+1} = \frac{1}{2}.$$

Consequently,

$$B = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v} \right)^2 \geq \frac{m}{4}.$$

Moreover, since the minimum degree δ satisfies $\delta \geq 1$, we have $2m = \sum_{v \in V(G)} d_v \geq n\delta \geq n$. Thus, $8B \geq 2m \geq n$. Using Lemma 1.1, we obtain:

$$\mathcal{E}_{ISI}(G) \leq \sqrt{2nB} \leq \sqrt{(8B)(2B)} = 4B.$$

■

Proposition 3.3. *Let G be a graph with n vertices, and let $F(G)$ be the forgotten index of the graph. Then,*

$$\mathcal{E}_{ISI}(G) \leq \frac{1}{2}\sqrt{n \cdot F(G)}.$$

Proof. Observe that

$$\left(\frac{d_u d_v}{d_u + d_v} \right)^2 = \left(\frac{1}{\frac{1}{d_u} + \frac{1}{d_v}} \right)^2 = \frac{1}{4} \left(\frac{2}{\frac{1}{d_u} + \frac{1}{d_v}} \right)^2. \tag{1}$$

Now, applying the quadratic-harmonic mean inequality, we obtain the following:

$$\frac{1}{4} \left(\frac{2}{\frac{1}{d_u} + \frac{1}{d_v}} \right)^2 \leq \frac{1}{4} \frac{d_u^2 + d_v^2}{2} = \frac{d_u^2 + d_v^2}{8}. \tag{2}$$

Combining (1) and (2) we derive the following upper bound for B:

$$B = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v} \right)^2 \leq \frac{1}{8} \sum_{uv \in E(G)} (d_u^2 + d_v^2) = \frac{1}{8} \sum_{u \in V(G)} d_u^3 = \frac{F(G)}{8}.$$

By Lemma 1.1, we have that

$$\mathcal{E}_{ISI}(G) \leq \sqrt{2nB} \leq \sqrt{2n \cdot \frac{F(G)}{8}} = \frac{1}{2}\sqrt{n \cdot F(G)}.$$

■

For the next result, we employ the following inequality:

Lemma 3.4. *([12]). Let $a_1, \ldots, a_n$ be non-negative numbers. Then,*

$$n\left(\frac{1}{n} \sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i \right)^{\frac{1}{n}} \right) \leq n \sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n} \sqrt{a_i} \right)^2.$$

Proposition 3.5. *([9]). Let G be a simple graph on n vertices and let $\tau_1, \tau_2, \ldots, \tau_n$ be the eigenvalues of the ISI matrix S. Then,*

$$\mathcal{E}_{ISI}(G) \leq \sqrt{2B(n-1) + n\sqrt[n]{|\det(S)|^2}}.$$

We include a proof for completeness.

Proof. Setting $a_i = \tau_i^2$ in Lemma 3.4, we obtain:

$$n\left(\frac{1}{n}\sum_{i=1}^{n}\tau_i^2 - \left(\prod_{i=1}^{n}\tau_i^2\right)^{\frac{1}{n}}\right) \leq n\sum_{i=1}^{n}\tau_i^2 - \left(\sum_{i=1}^{n}\sqrt{\tau_i^2}\right)^2 \Leftrightarrow$$

$$n\left(\frac{1}{n}\cdot 2B - \left(\left(\prod_{i=1}^{n}|\tau_i|\right)^2\right)^{\frac{1}{n}}\right) \leq n\cdot 2B - \mathcal{E}_{ISI}^2(G) \Leftrightarrow$$

$$\mathcal{E}_{ISI}^2(G) \leq -2B + n\left(|\det(S)|^2\right)^{\frac{1}{n}} + n\cdot 2B \Leftrightarrow$$

$$\mathcal{E}_{ISI}(G) \leq \sqrt{2B(n-1) + n\sqrt[n]{|\det(S)|^2}}.$$

■

Remark 1. From the inequality between arithmetic and geometric mean for the nonnegative numbers $\tau_1^2, \tau_2^2, \ldots, \tau_n^2$, we get:

$$\frac{2B}{n} = \frac{\tau_1^2 + \tau_2^2 + \ldots + \tau_n^2}{n} \geq \sqrt[n]{\tau_1^2\cdots\tau_n^2}.$$

Hence, $2B \geq n\sqrt[n]{|\det(S)|^2}$. From Proposition 3.5, we obtain:

$$\mathcal{E}_{ISI}(G) \leq \sqrt{2B(n-1) + n\sqrt[n]{|\det(S)|^2}} \leq \sqrt{2nB}.$$

We conclude that the bound in the above proposition refines the well-known bound $\mathcal{E}_{ISI}(G) \leq \sqrt{2nB}$.

In the following result, we improve the upper bound $\mathcal{E}_{ISI}(G) \leq \sqrt{2nB}$ by using the obtained refinement of the inequality between the quadratic and arithmetic means published in [13].

Lemma 3.6. *([13]). Let $a_1, \ldots, a_n$ be n nonnegative real numbers such that $a_1^2 + \ldots + a_n^2 \neq 0$. It holds*

$$\sqrt{\frac{a_1^2 + \ldots + a_n^2}{n}} \geq \frac{a_1 + \ldots + a_n}{n} + \frac{1}{4n}\cdot\sum_{i=1}^{n}\frac{(na_i^2 - (a_1^2 + \ldots + a_n^2))^2}{n^2a_i^4 + (a_1^2 + \ldots + a_n^2)^2}a_i.$$

Let σ^2 be the variance of the squared eigenvalues $\tau_1^2, \tau_2^2, \ldots, \tau_n^2$. The above lemma yields the following result.

Proposition 3.7. *Let G be a connected graph on $n \geq 2$ vertices and let $\tau_1, \tau_2, \ldots, \tau_n$ be the eigenvalues of the ISI matrix S such that $|\tau_1| \geq |\tau_2| \geq \cdots \geq |\tau_n|$. If σ^2 is the variance of $\tau_1^2, \tau_2^2, \ldots, \tau_n^2$, then*

$$\mathcal{E}_{ISI}(G) \leq \sqrt{2nB} - \frac{|\tau_n|}{8\tau_1^4}n\sigma^2. \tag{3}$$

Proof. Setting $a_i = |\tau_i|$ in Lemma 3.6, we get:

$$\sqrt{\frac{2B}{n}} = \sqrt{\frac{\tau_1^2 + \ldots + \tau_n^2}{n}} \geq \frac{\mathcal{E}_{ISI}(G)}{n} + \frac{|\tau_n|}{4n}\cdot\sum_{i=1}^{n}\frac{(\tau_i^2 - \frac{2B}{n})^2}{\tau_i^4 + \left(\frac{2B}{n}\right)^2}. \tag{4}$$

Since $\tau_i^4 + \left(\frac{2B}{n}\right)^2 \leq 2\tau_1^4$ for all i, and given that $\sigma^2 = \frac{\sum_{i=1}^{n}\left(\tau_i^2 - \frac{2B}{n}\right)^2}{n}$, we obtain the desired inequality. ■

Remark 2. The correction term

$$\frac{|\tau_n|}{8\tau_1^4} n\sigma^2,$$

is nonnegative. Hence, Proposition 3.7 always refines the classical bound

$$\mathcal{E}_{ISI}(G) \leq \sqrt{2nB}.$$

The refinement is strict whenever $|\tau_n| > 0$ and $\sigma^2 > 0$. Moreover, for fixed extremal eigenvalues, the correction term increases with the variance of the squared eigenvalues.

The next result provides a parametric variation of the well-known bound $\mathcal{E}_{ISI}(G) \leq \sqrt{2nB}$.

Proposition 3.8. *Let G be a simple connected graph on $n \geq 2$ vertices. If $p \geq q > 0$ are two positive real numbers, then*

$$\mathcal{E}_{ISI}(G) \leq (4B)^{\frac{p}{p+q}} \cdot \left(\frac{n}{2}\right)^{\frac{q}{p+q}}.$$

Proof. By Lemma 1.1, we get $\mathcal{E}_{ISI}^2(G) \leq 2nB$, that is, $\frac{2\mathcal{E}_{ISI}}{n} \leq \frac{4B}{\mathcal{E}_{ISI}(G)}$. By Proposition 3.2, we have $\frac{4B}{\mathcal{E}_{ISI}(G)} \geq 1$. Hence, if $x \geq 1$ is a real number, then the following inequalities hold:

$$\left(\frac{4B}{\mathcal{E}_{ISI}(G)}\right)^x \geq \frac{4B}{\mathcal{E}_{ISI}(G)} \geq \frac{2 \cdot \mathcal{E}_{ISI}(G)}{n} \Leftrightarrow n \cdot (4B)^x \geq 2 \cdot \mathcal{E}_{ISI}^{x+1}(G)$$

$$\Leftrightarrow \mathcal{E}_{ISI}(G) \leq \left(\frac{n}{2}\right)^{\frac{1}{x+1}} \cdot (4B)^{\frac{x}{x+1}}.$$

To conclude the proof, we let $x = \frac{p}{q}$ to obtain the following.

$$\mathcal{E}_{ISI}(G) \leq \left(\frac{n}{2}\right)^{\frac{1}{\frac{p+q}{q}}} (4B)^{\frac{\frac{p}{q}}{\frac{p+q}{q}}} \Leftrightarrow \mathcal{E}_{ISI}(G) \leq \left(\frac{n}{2}\right)^{\frac{q}{p+q}} (4B)^{\frac{p}{p+q}}.$$

■

The next result provides an estimate for the spectral radius of the ISI matrix in terms of the ISI energy and the invariant B.

Proposition 3.9. *Let G be a simple graph on $n \geq 2$ vertices and let $\tau_1, \ldots, \tau_n$ be the eigenvalues of the ISI matrix of G, such that $\tau_1 \geq \tau_2 \geq \cdots \geq \tau_n$. It holds*

$$\tau_1 \leq \frac{\mathcal{E}_{ISI}(G)}{n} + \frac{n-1}{n}\sqrt{\frac{2nB - \mathcal{E}_{ISI}^2(G)}{n-1}}. \tag{5}$$

Proof. Since the ISI matrix S is a symmetric nonnegative matrix, its largest eigenvalue τ_1 is nonnegative. Moreover,

$$\mathcal{E}_{ISI}(G) - \tau_1 = \sum_{i=2}^{n} |\tau_i|.$$

By the Cauchy–Schwarz inequality,

$$(\mathcal{E}_{ISI}(G) - \tau_1)^2 \leq (n-1)\sum_{i=2}^{n} \tau_i^2. \tag{6}$$

Using $\sum_{i=1}^{n} \tau_i^2 = 2B$, inequality (6) gives

$$(\mathcal{E}_{ISI}(G) - \tau_1)^2 \leq (n-1)(2B - \tau_1^2).$$

Expanding and rearranging, we obtain

$$n\tau_1^2 - 2\mathcal{E}_{ISI}(G)\tau_1 + \mathcal{E}_{ISI}^2(G) - 2B(n-1) \leq 0. \tag{7}$$

Solving the quadratic inequality (7) with respect to τ_1 yields

$$\tau_1 \leq \frac{\mathcal{E}_{ISI}(G) + \sqrt{(n-1)\left(2nB - \mathcal{E}_{ISI}^2(G)\right)}}{n}. \tag{8}$$

Finally, rewriting (8), we obtain:

$$\tau_1 \leq \frac{\mathcal{E}_{ISI}(G)}{n} + \frac{n-1}{n}\sqrt{\frac{2nB - \mathcal{E}_{ISI}^2(G)}{n-1}},$$

which proves the result. ■

To illustrate the effectiveness of the determinant-based refinement, we compare it numerically with the classical bound $\mathcal{E}_{ISI}(G) \leq \sqrt{2nB}$ for several standard graphs. The results are presented in Table 2.

Table 2: Comparison of the ISI energy with the classical bound $\sqrt{2nB}$ and the determinant-based refinement.

Graph G	$\mathcal{E}_{ISI}(G)$	$\sqrt{2nB}$	$\sqrt{2B(n-1) + n\lvert\det(S)\rvert^{2/n}}$
P_4	3.333	3.887	3.621
P_5	4.460	5.375	4.807
P_6	5.870	6.831	6.510
$K_{1,3}$	2.598	3.674	3.182
$K_{1,4}$	3.200	5.060	4.525
$K_{1,5}$	3.727	6.455	5.893
C_4	4.000	5.657	4.899
C_6	8.000	8.485	8.338
C_8	9.657	11.314	10.583
K_5	16.000	20.000	18.837

4 Lower bounds for the ISI energy

In this section, we establish several lower bounds for the inverse sum indeg energy $\mathcal{E}_{ISI}(G)$ in terms of structural and spectral parameters of graphs. While upper bounds for $\mathcal{E}_{ISI}(G)$ are typically obtained via the second moment quantity B, the derivation of lower bounds requires more delicate analysis of the extremal behavior of the eigenvalues of the ISI matrix.

We first present bounds that depend on the extreme eigenvalues of the ISI matrix and on classical spectral invariants such as the determinant. Subsequently, we relate the ISI energy to well-known degree-based indices, including the second Zagreb index and the Randić index. These results illustrate how the distribution of vertex degrees influences the lower spectral energy of the ISI matrix.

Proposition 4.1. *Let G be a simple graph with at least one edge, and let $\tau_1, \ldots, \tau_n$ be the eigenvalues of its ISI matrix, ordered so that*

$$|\tau_1| \geq |\tau_2| \geq \cdots \geq |\tau_n|.$$

Then,

$$\mathcal{E}_{ISI}(G) \geq \frac{n|\tau_1\tau_n| + 2B}{|\tau_1| + |\tau_n|}.$$

Proof. For every $i = 1, \ldots, n$, we have $|\tau_n| \leq |\tau_i| \leq |\tau_1|$, and hence

$$(|\tau_1| - |\tau_i|)(|\tau_n| - |\tau_i|) \leq 0. \tag{9}$$

Expanding (9), we obtain:

$$|\tau_1\tau_n| - (|\tau_1| + |\tau_n|)|\tau_i| + \tau_i^2 \leq 0.$$

Summing over $i = 1, \ldots, n$ gives

$$n|\tau_1\tau_n| - (|\tau_1| + |\tau_n|)\sum_{i=1}^{n} |\tau_i| + \sum_{i=1}^{n} \tau_i^2 \leq 0.$$

Using

$$\sum_{i=1}^{n} |\tau_i| = \mathcal{E}_{ISI}(G) \quad \text{and} \quad \sum_{i=1}^{n} \tau_i^2 = 2B,$$

we obtain:

$$n|\tau_1\tau_n| - (|\tau_1| + |\tau_n|)\mathcal{E}_{ISI}(G) + 2B \leq 0.$$

Therefore,

$$\mathcal{E}_{ISI}(G) \geq \frac{n|\tau_1\tau_n| + 2B}{|\tau_1| + |\tau_n|},$$

as required. ■

Remark 3. Equality holds if and only if

$$|\tau_i| \in \{|\tau_1|, |\tau_n|\},$$

for every $i = 1, \ldots, n$.

Proposition 4.2. *([9]). Let G be a simple graph on $n \geq 2$ vertices, and let S be its ISI matrix. Then,*

$$\mathcal{E}_{ISI}(G) \geq \sqrt{2B + n(n-1)|\det S|^{2/n}}.$$

We include a proof for completeness.

Proof. We have

$$\mathcal{E}_{ISI}^2(G) = \left(\sum_{i=1}^{n} |\tau_i|\right)^2 = \sum_{i=1}^{n} \tau_i^2 + 2\sum_{1 \leq i < j \leq n} |\tau_i\tau_j|.$$

Since $\sum_{i=1}^{n} \tau_i^2 = 2B$, it remains to estimate the second term.

By the arithmetic–geometric mean inequality applied to the $\binom{n}{2}$ nonnegative numbers $|\tau_i\tau_j|$, $1 \leq i < j \leq n$, we obtain:

$$\sum_{1\leq i<j\leq n} |\tau_i\tau_j| \geq \frac{n(n-1)}{2} \left(\prod_{1\leq i<j\leq n} |\tau_i\tau_j| \right)^{\frac{2}{n(n-1)}}.$$

Each $|\tau_i|$ occurs exactly $n-1$ times in the above product, so

$$\prod_{1\leq i<j\leq n} |\tau_i\tau_j| = \left(\prod_{i=1}^{n} |\tau_i| \right)^{n-1} = |\det S|^{n-1}.$$

Therefore,

$$\sum_{1\leq i<j\leq n} |\tau_i\tau_j| \geq \frac{n(n-1)}{2} |\det S|^{2/n}.$$

Hence,

$$\mathcal{E}_{ISI}^2(G) \geq 2B + n(n-1)|\det S|^{2/n},$$

which gives the desired bound. ■

The proof of the next result follows the same argument as that of Proposition 2 in [14], and is therefore omitted.

Proposition 4.3. *Let G be a simple graph on n vertices with at least one edge. Let S be its ISI matrix. If τ_1 is the largest eigenvalue of S, then*

$$\mathcal{E}_{ISI}(G) \geq \tau_1 + \frac{(n-1)^2|\det S|^{2/n}}{(n-2)|\det S|^{1/n} + \tau_1}. \tag{10}$$

In the next result, we use the Randić index $R(G)$, defined by

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

Since $d_u d_v \geq 1$ for every edge $uv \in E(G)$, we have $R(G) \leq m$.

Proposition 4.4. *Let G be a connected graph on n vertices with minimum degree δ. Then,*

$$\mathcal{E}_{ISI}(G) \geq \frac{2\delta}{n} R(G).$$

Proof. By Lemma 3.1, for every edge $uv \in E(G)$, $\frac{d_u d_v}{d_u + d_v} \geq \frac{\delta}{2}$. Summing over all edges, we obtain:

$$ISI(G) \geq \frac{m\delta}{2}. \tag{11}$$

On the other hand, the known bound [11]

$$\mathcal{E}_{ISI}(G) \geq \frac{4}{n} ISI(G), \tag{12}$$

together with (11) yields

$$\mathcal{E}_{ISI}(G) \geq \frac{2m\delta}{n}.$$

Finally, since $R(G) \leq m$, we obtain:

$$\mathcal{E}_{ISI}(G) \geq \frac{2\delta}{n} R(G),$$

which completes the proof. ■

We conclude this section with a lower bound for the ISI energy of triangle-free graphs in terms of the second Zagreb index. Combining Proposition 2.1 with

$$\mathcal{E}_{ISI}(G) \geq \frac{4}{n} ISI(G),$$

we immediately obtain the following result.

Proposition 4.5. *Let G be a connected triangle-free graph on n vertices. Then,*

$$\mathcal{E}_{ISI}(G) \geq \frac{4}{n^2} M_2(G).$$

To illustrate the lower bounds obtained above, we compare them with the exact ISI energy for several standard graphs. The results are presented in the following table.

Table 3: Comparison of lower bounds for the ISI energy. The bound $4M_2(G)/n^2$ applies only to triangle-free graphs.

Graph G	$\mathcal{E}_{ISI}(G)$	$\frac{4M_2(G)}{n^2}$	$\frac{2\delta}{n} R(G)$
P_4	3.333	2.000	0.957
P_5	4.460	1.920	0.966
P_6	5.870	1.778	0.971
$K_{1,3}$	2.598	2.250	0.866
$K_{1,4}$	3.200	2.560	0.800
$K_{1,5}$	3.727	2.778	0.745
C_4	4.000	4.000	2.000
C_6	8.000	2.667	2.000
C_8	9.657	2.000	2.000
K_5	16.000	—	4.000

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

References

[1] I. Gutman, The energy of a graph, *Ber. Math.-Statist. Sekt. Forschungsz. Graz.* **103** (1978) 1–22.

[2] D. Vukičević and M. Gašperov, Bond additive modeling 1. Adriatic indices, *Croat. Chem. Acta* **83** (2010) 243–260.

[3] J. Sedlar, D. Stevanović and A. Vasilyev, On the inverse sum indeg index, *Discrete Appl. Math.* **184** (2015) 202–212, https://doi.org/10.1016/j.dam.2014.11.013.

[4] F. Falahati-Nezhad and M. Azari, The inverse sum indeg index of some nanotubes, *Stud. Univ. Babeş-Bolyai Chem.* **61** (2016) 63–70.

[5] F. Falahati-Nezhad, M. Azari and T. Došlić, Sharp bounds on the inverse sum indeg index, *Discrete Appl. Math.* **217** (2017) 185–195, https://doi.org/10.1016/j.dam.2016.09.014.

[6] S. Zangi, M. Ghorbani and M. Eslampour, On the eigenvalues of some matrices based on vertex degree, *Iranian J. Math. Chem.* **9** (2018) 149–156, https://doi.org/10.22052/ijmc.2017.93637.1303.

[7] A. Altassan, B. A. Rather and M. Imran, Inverse sum indeg index (energy) with applications to anticancer drugs, *Mathematics* **10** (2022) #4749, https://doi.org/10.3390/math10244749.

[8] A. Bharali, A. Mahanta, I. J. Gogoi and A. Doley, Inverse sum indeg index and ISI matrix of graphs, *J. Discrete Math. Sci. Cryptogr.* **23** (2020) 1315–1333, https://doi.org/10.1080/09720529.2020.1815340.

[9] S. Hafeez and R. Farooq, Inverse sum indeg energy of graphs, *IEEE Access* **7** (2019) 100860–100866, https://doi.org/10.1109/ACCESS.2019.2929528.

[10] Ö. Çolakoğlu Havare, The inverse sum indeg index (ISI) and ISI energy of Hyaluronic Acid-Paclitaxel molecules used in anticancer drugs, *Open J. Discret. Appl. Math.* **4** (2021) 72–81, https://doi.org/10.30538/psrp-odam2021.0065.

[11] F. Jamal, M. Imran and B. A. Rather, On inverse sum indeg energy of graphs, *Spec. Matrices* **11** (2023) #20220175, https://doi.org/10.1515/spma-2022-0175.

[12] B. Zhou, I. Gutman and T. Aleksić, A note on Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 441–446.

[13] S. Filipovski, Improved Cauchy–Schwarz inequality and its applications, *Turkish J. Ineq.* **3** (2019) 8–12.

[14] S. Filipovski and R. Jajcay, Bounds for the energy of graphs, *Mathematics* **9** (2021) #1687, https://doi.org/10.3390/math9141687.