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# On the inverse sum indeg index ($ISI$), spectral radius of $ISI$ matrix and $ISI$ energy

**Özge Çolakoğlu Havare**

Mersin University, Science and Arts Faculty Mathematics Department, 33343, Mersin-Turkey; ozgeeclkgl@gmail.com

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**Abstract:** The inverse sum indeg index $ISI(G)$ of a graph is equal to the sum over all edges $uv \in E(G)$ of weights $\frac{d_u d_v}{d_u+d_v}$. This paper presents the relation between the inverse sum indeg index and the chromatic number. The bounds for the spectral radius of the inverse sum indeg matrix and the inverse sum indeg energy are obtained. Additionally, the Nordhaus-Gaddum-type results for the inverse sum indeg index, the inverse sum indeg energy and the spectral radius of the inverse sum index matrix are given.

**Keywords:** Inverse sum indeg index; Inverse sum indeg energy; Spectral radius, Chromatic number; Nordhaus-Gaddum-type result.

**MSC:** 05C07; 05C15; 05C50.

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## 1. Introduction

Let $G$ be a simple connected graph with a vertex set $V(G)$ and edge set $E(G)$. The vertex set and edge set elements are defined by $n$ and $m$, respectively. An edge of $G$ connects the vertices $u$ and $v$ and it is written as $e = uv$. The degree of a vertex $u$ is defined by $d_u$. This paper follows ref. [1] for standard terminology and notations.

Topological indices are real numbers of a molecular structure obtained via a molecular graph $G$ whose vertices and edges represent the atoms and the bonds, respectively. These graph invariants help us to predict certain physicochemical properties such as boiling point, enthalpy of vaporization, stability, and also are used for studying the properties of molecules such as the structure-property relationship (QSPR), the structure-activity relationship (QSAR), and the structural design in chemistry, nanotechnology, and pharmacology [2,3].

The first topological index is the Wiener index. In 1947, Wiener introduced this index which was used to determine physical properties of paraffin [4]. Topological indices can be classified according to the structural characteristics of the graph, such as the degree of vertices, the distances between vertices, the matching, the spectrum, etc. The best-known topological indices are the Wiener index which is based on the distance, the Zagreb and the Randić indices based on degree, the Estrada index, which is based on the spectrum of a graph, the Hosaya index, which is based on the matching. In addition, there is a bond-additive index, which is a measure of peripherality in graphs.

Gutman and Trinajstić defined first Zagreb index [5] as

$$M_1(G) = \sum_{u\in V(G)} d_u^2 = \sum_{uv\in E(G)} d_u + d_v.$$

In 2010, Vukičević and Gašperov introduced Adriatic indices that are obtained by the analysis of the well-known indices such as the Randić and the Wiener index [6]. The discrete Adriatic descriptors, which consist of 148 descriptors have excellent predictive properties. Thus many scientists studied these indices [7,8]. The inverse sum indeg index which is one of the discrete Adriatic descriptors is defined as

$$ISI(G) = \sum_{uv\in E(G)} \frac{1}{\frac{1}{d_u}+\frac{1}{d_v}} = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u+d_v},$$

where $d_u$ is denoted as the degree of vertex $u$ [6].

The inverse sum indeg index gives a significant predictor of the total surface area of octane isomers. Nezhad *et al.*, studied several sharp upper and lower bounds on the inverse sum indeg index [9]. Nezhad *et al.*, computed the inverse sum indeg index of some nanotubes [10]. Sedlar *et al.*, Presented extremal values of this index across several graph classes such as trees and chemical trees [11]. Chen and Deng presented some bounds for the inverse sum indeg index in terms of some graph parameters [12].

This study proves the relation between the inverse sum indeg index and the chromatic number by removing a vertex of a minimum degree on the inverse sum indeg index. The bounds for the spectral radius of the inverse sum indeg adjacent matrix and the inverse sum indeg energy are given, and also the Nordhaus-Gaddum-type results for the inverse sum indeg index, spectral radius of its matrix, and the inverse sum indeg energy are obtained.

## 2. On the inverse sum indeg index and the chromatic number

Hansen and Vukičević proved a result relating the Randić index and the chromatic number that $\chi(G) \leq 2R(G)$ [13]. Deng *et al.*, proved the relationship between the harmonic index and the chromatic number that $\chi(G) \leq 2H(G)$ [14]. The chromatic number $\chi(G)$ of $G$ is the smallest number of colors needed to color all vertices of $G$ in such a way that no pair of adjacent vertices get the same color [1].

This section considers the relation between the inverse sum indeg index $ISI(G)$ and the chromatic number $\chi(G)$, and will prove that $\chi(G) \leq \frac{4}{\delta^2} ISI(G)$ by using the result of removal of a minimum degree vertex on the inverse sum indeg index.

**Theorem 1.** *Let $G$ be a simple graph with the inverse sum indeg index $ISI(G)$ and the minimum degree $\delta \geq 1$. Let $v$ be a vertex of $G$ with degree equal to $\delta$. Then*

$$ISI(G) - ISI(G-v) > 0.$$

**Proof.** First, it is noted that for $x, y \geq 2$

$$\frac{xy}{x+y} - \frac{(x-1)y}{x+y-1} = \frac{y^2}{(x+y)(x+y-1)} > 0 \tag{1}$$

and

$$\frac{xy}{x+y} - \frac{(x-1)(y-1)}{x+y-2} = \frac{x(x-1)+y(y-1)}{(x+y)(x+y-2)} > 0. \tag{2}$$

Let $N(v) = \{v_1, v_2, ..., v_k\}$ be the set of vertices adjacent to vertex $v \in V(G)$. Then,

$$\begin{aligned} ISI(G) - ISI(G-v) &= \sum_{pq \in E(G)} \frac{d_p d_q}{d_p + d_q} - \sum_{p'q' \in E(G-v)} \frac{d_{p'} d_{q'}}{d_{p'} + d_{q'}} \\ &= \sum_{pv \in E(G)} \frac{d_p d_v}{d_p + d_v} + \left( \sum_{pq \in E(G), q \in N(v)} \frac{d_p d_q}{d_p + d_q} - \sum_{pq \in E(G), q \in N(v)} \frac{d_p (d_q - 1)}{d_p + d_q - 1} \right) \\ &\quad + \left( \sum_{pq \in E(G), p,q \in N(v)} \frac{d_p d_q}{d_p + d_q} - \sum_{pq \in E(G), p,q \in N(v)} \frac{(d_p - 1)(d_q - 1)}{d_p + d_q - 2} \right). \end{aligned}$$

From Eqs. (1) and (2), the proof is completed. □

**Theorem 2.** *Let $G$ be a simple graph with chromatic number $\chi(G)$. Then*

$$\chi(G) \leq \frac{4}{\delta^2} ISI(G)$$

*with equality if $G$ is a complete graph.*

**Proof.** If $G$ is a complete graph then $\chi(G) = \frac{4}{\delta^2} ISI(G)$.

Suppose that $\chi(G) > \frac{4}{\delta^2} ISI(G)$, $G$ is not a complete graph and $\chi(G) > 1$. Among all such graphs, let $G$ be chosen in such a way that:

i). There is no simple graph $G'$ such that

$$ISI(G') < \frac{\delta^2}{4}\chi(G')$$

and

$$\chi(G') < \chi(G).$$

ii). There is no proper subgraph $G''$ of $G$ such that

$$\frac{4}{\delta^2}ISI(G'') < \chi(G'').$$

Our proof is written based on the Claim in the proof of the Theorem 4 in [14] and the proofs of Lemma 3 in [13].

**Lemma 1.** [13,14] *Let G be a simple graph with chromatic number $\chi(G)$ then we have $\chi(G) \leq \delta(G) + 1$.*

**Proof.** Suppose that $\delta(G) < \chi(G) - 1$. Let $v$ be a vertex with $d_v(G) = \delta$. Note that $\chi(G - v) < \chi(G)$, otherwise, using Theorem 1,

$$ISI(G - v) < ISI(G) \leq \frac{\delta^2}{4}\chi(G) = \frac{\delta^2}{4}\chi(G - v),$$

which contradicts the minimality of $G$.

Hence all the vertices of $G - v$ can be regularly colored with $\chi(G) - 1$ colors. Since, $d_v(G) < \chi(G) - 1$, it follows that $v$ is not adjacent to any vertex of one of these $\chi(G) - 1$ colors, but then $v$ can be colored with that color. This implies that $G$ can be regularly colored with $\chi(G) - 1$ colors, which is a contradiction. □

Three cases for the proof of the Theorem 2 are distinguished.

**Case 1:** If $\chi(G) = 2$, then

$$ISI(G) = \sum_{pq\in E}\frac{d_p d_q}{d_p + d_q} < \frac{\delta^2}{4}\chi(G) = \frac{\delta^2}{2} = \sum_{pq\in E}\frac{\delta\delta}{\delta + \delta},$$

which $m = \delta$, $d_p, d_q = \delta$. Since all degrees are greater than or equal to $m$ of $G$, this is a contradiction.

**Case 2**: Let $pq$ be an edge which has the smallest weight of $\frac{d_p d_q}{d_p+d_q}$ for $pq \in E$. If $\chi(G) = 3$, then

$$\frac{\chi(G)\delta^2}{4} = \frac{3\delta^2}{4} > ISI(G) \geq m\frac{d_p d_q}{d_p + d_q} \geq (d_p + d_q - 1)\frac{d_p d_q}{d_p + d_q} = d_p d_q - \frac{d_p d_q}{d_p + d_q} \geq \delta^2 - \frac{d_p d_q}{d_p + d_q},$$

which implies $\frac{d_p d_q}{d_p+d_q} \geq \frac{\delta^2}{4}$. From $\frac{3\delta^2}{4} > ISI(G) \geq m\frac{d_p d_q}{d_p+d_q} \geq m\frac{\delta^2}{4}$, we obtain that $m < 3$. This is a contradiction since $\chi(G) = 3$.

**Case 3:** Let $\chi(G) \geq 4$. Again let $pq$ be an edge which has the smallest weight. Observe the graph $G - p - q$ and let $d'_i = d_{G-p-q}(i)$ for $i \in V(G)\backslash\{p, q\}$. From the minimality of $G$, it follows that

$$ISI(G - p - q) \geq \frac{\delta^2}{4}\chi(G - p - q) \geq \frac{\delta^2}{4}\left(\chi(G) - 2\right). \tag{3}$$

We have

$$\begin{aligned} ISI(G) &= \sum_{uv\in E}\frac{d_u d_v}{d_u + d_v} \geq (d_p + d_q - 1)\frac{d_p d_q}{d_p + d_q} + \sum_{uv\in E(G-p-q)}\frac{d_u d_v}{d_u + d_v} \\ &= d_p d_q - \frac{d_p d_q}{d_p + d_q} + \sum_{uv\in E(G-p-q)}\frac{d_{u'} d_{v'}}{d_{u'} + d_{v'}}\left(\frac{\frac{d_{u'}+d_{v'}}{d_{u'}d_{v'}}}{\frac{d_u+d_v}{d_u d_v}}\right) \\ &\geq d_p d_q - \frac{d_p d_q}{d_p + d_q} + \sum_{uv\in E(G-p-q)}\frac{d_{u'} d_{v'}}{d_{u'} + d_{v'}}\left(\frac{\frac{d_u-2+d_v-2}{(d_u-2)(d_v-2)}}{\frac{d_u+d_v}{d_u d_v}}\right) \\ &\geq d_p d_q - \frac{d_p d_q}{d_p + d_q} + \sum_{uv\in E(G-p-q)}\frac{d_{u'} d_{v'}}{d_{u'} + d_{v'}}\left(\frac{\frac{d_u-2+d_v-2}{d_u d_v}}{\frac{d_u+d_v}{d_u d_v}}\right) \end{aligned}$$

$$\geq \delta^2 - \frac{d_p d_q}{d_p + d_q} + \sum_{uv \in E(G-p-q)} \frac{d_{u'} d_{v'}}{d_{u'} + d_{v'}} \left(1 - \frac{2}{\delta}\right).$$

From Lemma 1, we have

$$ISI(G) \geq \delta^2 - \frac{d_p d_q}{d_p + d_q} + \left(1 - \frac{2}{\chi(G) - 1}\right) ISI(G - p - q).$$

Using Eq. (3), one has

$$\begin{aligned} ISI(G) &\geq \delta^2 - \frac{d_p d_q}{d_p + d_q} + \left(1 - \frac{2}{\chi(G) - 1}\right) \frac{\delta^2}{4} (\chi(G) - 2) \\ &= \delta^2 - \frac{d_p d_q}{d_p + d_q} + \frac{\delta^2}{4}\chi(G) + \frac{\delta^2}{\chi(G) - 1} - \frac{\delta^2}{2} - \frac{\chi(G)\delta^2}{2(\chi(G) - 1)}. \end{aligned}$$

Since $ISI(G) < \frac{\delta^2}{4}\chi(G)$, we obtain

$$\begin{aligned} &\frac{\delta^2}{4}\chi(G) > -\frac{d_p d_q}{d_p + d_q} + \frac{\delta^2}{4}\chi(G) + \frac{\delta^2}{2} + \frac{2\delta^2 - \chi(G)\delta^2}{2(\chi(G) - 1)}, \\ &\frac{d_p d_q}{d_p + d_q} > \frac{\delta^2}{2(\chi(G) - 1)}. \end{aligned}$$

We have

$$\frac{\delta^2}{4}\chi(G) > ISI(G) \geq m\frac{d_p d_q}{d_p + d_q} > m\left(\frac{\delta^2}{2(\chi(G) - 1)}\right).$$

It follows that $m < \frac{\chi(G)(\chi(G)-1)}{2}$. Note that each class has to contain at least one vertex of degree $\chi(G) - 1$. Hence, this is a contradiction. Therefore, $m \geq \frac{\chi(G)(\chi(G)-1)}{2}$. Hence $m = \frac{\chi(G)(\chi(G)-1)}{2}$ and $G$ contains a complete graph. □

**Corollary 3.** *For a simple graph $G$ with chromatic index $\chi(G)$, we have*

$$\chi(G) - ISI(G) \leq \left(1 - \frac{\delta^2}{4}\right) n$$

*with equality if only if for $K_n$.*

## 3. The inverse sum indeg energy and spectral radius

The adjacency matrix $A(G)$ of $G$ is an $n \times n$ matrix with the $(i, j)$-entry equal to 1 if vertices $v_i$ and $v_j$ are adjacent and 0 otherwise [15].

Define the inverse sum indeg adjacency matrix $ISI$ to be a matrix with entries $s_{ij}$ as follows [16,17]:

$$s_{ij} = \begin{cases} \frac{d_i d_j}{d_i + d_j}, & ij \in E(G); \\ 0, & \text{otherwise.} \end{cases}.$$

Let $s_1 \geq s_2 \geq \cdots \geq s_n$ be the eigenvalues of the matrix $ISI$. It is elementary to show that

$$tr(ISI) = \sum_{i=1}^{n} s_i = 0 \tag{4}$$

and

$$tr((ISI)^2) = \sum_{i=1}^{n} s_i^2 = 2\sum_{i \sim j}^{n} s_{ij}^2, \tag{5}$$

where $tr(ISI)$ and $tr((ISI)^2)$ are traces of $ISI$ and $(ISI)^2$, respectively [16,17]. The energy of the $ISI$ adjacency matrix is defined in [16,17] as

$$ISIE = \sum_{i=1}^{n} |s_i|. \tag{6}$$

**Lemma 2.** [18]*(**Rayleigh-Ritz**) If $B$ is a real symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$, then for any $x \in R^n$, such that $x \neq 0$,*

$$x^T Bx \leq \lambda_1 x^T x.$$

**Lemma 3.** [19] *Let $B$ be a real symmetric matrix of order $n$, and let $B_k$ be its leading $k \times k$ submatrix. Then, for $i = 1, 2, ..., k$,*

$$\lambda_{n-i+1}(B) \leq \lambda_{k-i+1}(B_k) \leq \lambda_{k-i+1}(B).$$

**Lemma 4.** [20] *Let $B = (b_{ij})$ and $C = (c_{ij})$ are nonnegative symmetric matrices of order $n$. If $B \geq C$, then $\xi_1(B) \geq \xi_1(C)$ which $\xi_1(B), \xi_1(C)$ are the largest eigenvalue $B, C$, respectively.*

**Lemma 5.** [21] *Let $G$ be a connected graph of order $n$ with $m$ edges. If $\lambda_1$ is the largest eigenvalue of the adjacency matrix $A(G)$, then*

$$\lambda_1 \leq \sqrt{2m - n + 1},$$

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

Jahanbani *et al.*, studied a relation between spectral radius of harmonic matrix and chromatic number [22]. Hafeez and Farooq gave the $ISI$ energy formula of some graph classes and some bounds for $ISI$ energy of graphs [23]. Gök proved the inequalities involving the eigenvalues, the graph energy, the matching energy and the graph incidence energy [24]. Bozkurt *et al.*, studied the Randić matrix and the Randić energy [25].

This section proves the inverse sum indeg energy, spectral radius and chromatic index related results. Furthermore, the bounds for spectral radius of the inverse sum indeg adjacency matrix and the inverse sum indeg energy are obtained.

**Theorem 4.** *Let $G$ be an $n$-vertex graph with $s_1$ spectral radius. Then*

$$\frac{2ISI(G)}{n} \leq s_1.$$

**Proof.** Since

$$\begin{aligned} X^T ISIX &= \left( \sum_{j,j\sim 1}^{n} x_j s_{j1}, \sum_{j,j\sim 2}^{n} x_j s_{j2}, ..., \sum_{j,j\sim n}^{n} x_j s_{jn} \right)^T X \\ &= 2\sum_{i\sim j} s_{ij} x_i x_j \end{aligned}$$

for any vector $X = (x_1, x_2, ..., x_n)^T$ and

$$X^T X = \sum_{i=1}^{n} x_i^2. \tag{7}$$

So, from Lemma 2, we have

$$2\sum_{ij\in E} s_{ij} x_i x_j \leq s_1 \sum_{i=1}^{n} x_i^2. \tag{8}$$

Since Eq. (8) is true for any vector $X$, for $X = (1, 1, ..., 1)^T$, we obtain

$$\frac{2ISI(G)}{n} \leq s_1.$$

□

From Theorem 4 and Theorem 2, we obtain following corollary:

**Corollary 5.** *Let $G$ be a graph with $\chi(G)$ chromatic number and $s_1$ spectral radius. Then*

$$\frac{\delta^2}{2n}\chi(G) \leq s_1.$$

**Theorem 6.** *Let G be an n-vertex graph of size m with the maximum degree Δ and minimum degree δ. Then*

$$s_1 \geq \frac{\delta^2 m}{\Delta n}.$$

**Proof.** Let $x = (x_1, x_2, ..., x_n)^T$ be any unit vector in $R^n$. Then

$$XISIX^T = 2\sum_{ij\in E} \frac{d_i d_j}{d_i + d_j} x_i x_j \geq 2\frac{\delta^2}{2\Delta} \sum_{ij\in E} x_i x_j.$$

Putting $X = (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, ..., \frac{1}{\sqrt{n}})^T$ in the Eq. (7), we have

$$XISIX^T \geq \frac{\delta^2}{\Delta n} m.$$

From Lemma 2, this proof is completed. □

**Theorem 7.** *Let G be an n-vertex graph of size m with the maximum degree Δ. Then*

$$s_1 \leq \frac{\Delta}{2}\sqrt{2m - n + 1}.$$

**Proof.** For any edge $v_i v_j \in E$,

$$\frac{1}{d_i} + \frac{1}{d_j} \geq \frac{2}{\Delta}$$

and

$$\frac{1}{\frac{1}{d_i} + \frac{1}{d_j}} \leq \frac{\Delta}{2} \leq \frac{n-1}{2}. \tag{9}$$

If $\xi_1$ is the spectral radius of the matrix $\frac{\Delta}{2}A(G)$, then by Lemma 4, $s_1 \leq \xi_1$. From Lemma 5, we have

$$s_1 \leq \frac{\Delta}{2}\lambda_1 \leq \frac{\Delta}{2}\sqrt{2m - n + 1}.$$

□

Since $f(x) = \frac{x}{2}$ is an increasing function, so by Theorem 7 and the Eq. (9), we obtain the following corollary:

**Corollary 8.** *Let G be an n-vertex graph of size m. Then*

$$s_1 \leq \frac{n-1}{2}\sqrt{2m - n + 1}.$$

**Theorem 9.** *Let G be an n-vertex graph of size m with the maximum degree Δ and minimum degree δ. Then*

$$ISIE \leq \frac{\Delta^2}{2\delta}\sqrt{2nm}.$$

**Proof.** From the Cauchy-Schwarz inequality, we have

$$\left(\sum_{i=1}^{n} |s_i|\right)^2 \leq \left(\sum_{i=1}^{n} |s_i|^2\right)\left(\sum_{i=1}^{n} 1^2\right).$$

Using Eq. (5), we have

$$\sum_{i=1}^{n} |s_i| \leq \left(2\sum_{ij\in E}\left(\frac{d_i d_j}{d_i + d_j}\right)^2\right)^{\frac{1}{2}} \sqrt{n} \leq \left(2m\left(\frac{\Delta^2}{2\delta}\right)^2\right)^{\frac{1}{2}} \sqrt{n}. \tag{10}$$

From Eq. (6), the proof is completed. □

From Eqs. (9) and (10), we obtain the following theorem:

**Theorem 10.** *Let G be an n-vertex graph of size m . Then*

$$ISIE \leq \frac{n-1}{2}\sqrt{2mn}.$$

**Theorem 11.** *Let G be an n-vertex graph of size m. Then*

$$ISIE \geq \left(\frac{2}{m}\right)^{\frac{1}{2}} ISI(G).$$

**Proof.** We have

$$\left(\sum_{i=1}^{n}|s_i|\right)^2 = \sum_{i=1}^{n}s_i^2 + 2\sum_{i,j=1}^{n}|s_i|\,|s_j| \geq \sum_{i=1}^{n}s_i^2 = 2\sum_{ij\in E}\left(\frac{d_id_j}{d_i+d_j}\right)^2$$

By the Cauchy-Schwarz inequality,

$$\begin{aligned}\left(\sum_{i=1}^{n}|s_i|\right)^2 &\geq \frac{2}{m}\left(\sum_{ij\in E}\frac{d_id_j}{d_i+d_j}\right)^2,\\ ISIE &\geq \left(\frac{2}{m}\right)^{\frac{1}{2}} ISI(G).\end{aligned}$$

□

From Theorem 11 and Theorem 2, we obtain the following corollary:

**Corollary 12.** *Let G be an n-vertex graph of size m with $\chi(G)$ chromatic number. Then*

$$\frac{\delta^2}{2\sqrt{2m}}\chi(G) \leq ISIE.$$

## 4. The Nordhaus Gaddum type results for the inverse sum indeg index (ISI), the ISI energy, and the largest ISI eigenvalue of graph

In 1956, Nordhaus-Gaddum gave lower and upper bounds for the chromatic numbers of a graph $G$ and its complement $\overline{G}$ as follow:

$$2\sqrt{n} \leq \chi(G) + \chi(\overline{G}) \leq n+1.$$

Nikiforov and Yuan studied eigenvalue problems of the Nordhaus-Gaddum-type [26]. Wang *et al.*, obtained bounds, and the Nordhaus-Gaddum-type results for the spectral radius of the extended adjacency matrix, the extended energy of a graph [27]. Ashrafi et al. gave formulas related to the Zagreb index, the Zagreb coindex, and its complements [28]. Zhou and Trinajstić obtained the Nordhaus-Gaddum-type results for reciprocal molecular topological index [29]. Das and Gutman proved the identities and inequalities, including relations between the second Zagreb index and its complement [30]. Ma *et al.*, obtained the Nordhaus-Gaddum-type results for irregularities of a graph [31].

In this section, the Nordhaus-Gaddum-type results for the inverse sum indeg index, spectral radius of inverse sum indeg matrix, and inverse sum the energy of a graph are obtained.

**Lemma 6.** [28,30]*The following identity is hold:*

$$\sum_{uv\notin E(G)}(d_u+d_v) = 2m(n-1) - \sum_{uv\in E(G)}(d_u+d_v).$$

**Theorem 13.** *Let both G and $\overline{G}$ be connected graphs. If G has n vertices and m edges, then*

$$ISI(\overline{G}) + ISI(G) \leq \frac{n-1}{2}(\overline{m}-m) + \frac{M_1(G)}{2}.$$

**Proof.** From the arithmetic and harmonic means relationship, we have

$$\frac{2}{\frac{1}{d_i}+\frac{1}{d_j}} \leq \frac{d_i+d_j}{2}. \tag{11}$$

From Eq. (11), we have

$$ISI(G) = \sum_{ij\in E} \frac{1}{\frac{1}{d_i}+\frac{1}{d_j}} \leq \frac{1}{2}\sum_{ij\in E}\frac{d_i+d_j}{2} = \frac{1}{4}\sum_{ij\in E}(d_i+d_j) \tag{12}$$

and

$$ISI(\overline{G}) = \sum_{ij\in \overline{E}} \frac{1}{\frac{1}{\overline{d_i}}+\frac{1}{\overline{d_j}}} \leq \frac{1}{2}\sum_{ij\in E(\overline{G})}\frac{\overline{d_i}+\overline{d_j}}{2}. \tag{13}$$

Using $\overline{d_i} = n-1-d_i$, Eq. (13) is rewritten as

$$\begin{aligned} ISI(\overline{G}) &\leq \frac{1}{2}\sum_{ij\notin E(G)}\frac{(n-1-d_i)+(n-1-d_j)}{2} \\ ISI(\overline{G}) &\leq \frac{1}{4}\left[2\sum_{ij\notin E(G)}(n-1) - \sum_{ij\notin E(G)}(d_i+d_j)\right] \\ ISI(\overline{G}) &\leq \frac{1}{4}\left[2\overline{m}(n-1) - \sum_{ij\notin E(G)}(d_i+d_j)\right]. \end{aligned} \tag{14}$$

Using Eqs. (12), (14) and Lemma 6, this proof is completed. □

**Theorem 14.** *Let both G and $\overline{G}$ be connected graphs. If G has n vertices and m edges, then*

$$\frac{m^2}{M_1(G)} + \frac{\overline{m}^2}{M_1(G)+2(n-1)(\overline{m}-m)} \leq ISI(G)+ISI(\overline{G}).$$

**Proof.** By the Cauchy-Schwarz inequality, we have

$$\left(\sum_{ij\in E}1\right)^2 \leq \sum_{ij\in E}\frac{1}{d_i+d_j}\sum_{ij\in E}d_i+d_j. \tag{15}$$

Also we have

$$\sum_{ij\in E}\frac{1}{d_i+d_j} \leq \sum_{ij\in E}\frac{d_id_j}{d_i+d_j}. \tag{16}$$

From Eqs. (15) and (16), we have

$$\frac{m^2}{\sum_{ij\in E}(d_i+d_j)} \leq ISI(G) \tag{17}$$

and

$$\frac{\overline{m}^2}{\sum_{ij\in \overline{E}}\left(\overline{d_i}+\overline{d_j}\right)} \leq ISI(\overline{G}). \tag{18}$$

Using $\overline{d_i} = n-1-d_i$, Eqs. (17) and (18), we obtain

$$\frac{m^2}{\sum_{ij\in E}(d_i+d_j)} + \frac{\overline{m}^2}{\sum_{ij\notin E}2(n-1) - \sum_{ij\notin E}(d_i+d_j)} \leq ISI(G)+ISI(\overline{G}). \tag{19}$$

The proof is completed using Eq. (19) and Lemma 6. □

**Theorem 15.** *Let both $G$ and $\overline{G}$ be connected graphs. If $G$ has $n$ vertices and $m$ edges, then*

$$\frac{2}{n}\left(\frac{m^2}{M_1(G)}+\frac{\overline{m}^2}{M_1(G)+2(n-1)(\overline{m}-m)}\right)\leq s_1+\overline{s_1}\leq\frac{n-1}{2}\left(\sqrt{2m-n+1}+\sqrt{2\overline{m}-n+1}\right).$$

**Proof.** From Theorem 4, we have

$$\frac{2}{n}\left(ISI(G)+ISI(\overline{G})\right)\leq s_1+\overline{s_1}.$$

By Theorem 14, the lower bound of the proof is completed.

The upper bound of the proof is obtained by Corollary 8. □

**Theorem 16.** *Let both $G$ and $\overline{G}$ be connected graphs. If $G$ has $n$ vertices and $m$ edges, then*

$$\frac{m\sqrt{2m}}{M_1(G)}+\frac{\overline{m}\sqrt{2\overline{m}}}{M_1(G)+2(n-1)(\overline{m}-m)}\leq ISIE+\overline{ISIE}\leq\frac{\sqrt{2n}\,(n-1)}{2}\left(\sqrt{m}+\sqrt{\overline{m}}\right)$$

**Proof.** By the Eqs. (17), (18), and Theorem 11, we obtain

$$\sqrt{\frac{2}{m}}\frac{m^2}{M_1(G)}+\sqrt{\frac{2}{\overline{m}}}\frac{\overline{m}^2}{M_1(G)+2(n-1)(\overline{m}-m)}\leq ISIE+\overline{ISIE},$$

which is the lower bound.

The upper bound is obtained by Theorem 10. □

## 5. Conclusions

The inverse sum index, which can predict well the properties of molecules, is studied. For example, this index gives a significant predictor of the total surface area of octane isomers. In this paper, the relationship between the inverse sum indeg index and the Chromatic number is obtained. Then, it is given bounds for the inverse sum indeg energy and the largest inverse sum indeg eigenvalue of the graph with the first Zagreb index. Finally, the Nordhaus type results for the ISI index, the ISI energy, and the spectral radius are obtained from the lower and upper bounds of the relation with the first Zagreb index.

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