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On the inverse sum indeg index of some graph operations

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Abstract

Topological indices are the molecular descriptors that describe the structures of chemical compounds. They are used in isomer discrimination, structure-property relationship, and structure-activity relations. The topological indices are used to predict certain physico-chemical properties such as boiling point, enthalpy of vaporization, and stability. In this paper, the inverse sum indeg index is studied. This index ($ISI(G)$) is defined as $\sum \frac{d_u d_v}{d_u+d_v}$. The inverse sum indeg index of some graph operations is computed. These operations are join, sequential join, cartesian product, lexicographic product, and corona operation.

Keywords: Topological index, Inverse sum indeg index, Corona operation, Lexicographic product, Cartesian product

2010 Mathematics Subject Classification: Primary: 05C76; Secondary: 05C07

Introduction

A graph G is a finite nonempty vertex set $V(G)$ together with a edge set E. An edge of G which is e connects the vertices u and v. It writes $e = uv$, says u and v are adjacent. We often use n and m for the order and the size of a graph, respectively [1].

Chemical graph theory is concerned with finding topological indices that are well correlated with the properties of chemical molecules. The edges and the vertices of a graph represent the bonds and the atoms of a molecule, respectively [2].

The topological index which is known as a graph-based molecular descriptor or graph invariant is the real values of the topological structure of a molecule [3].

Topological indices are used for studying the properties of molecules such as structure-property relationship (QSPR), structure-activity relationship (QSAR), and structural design in chemistry, nanotechnology, and pharmacology. Its main role is to work as a numerical molecular descriptor in QSAR/QSPR models [4, 5].

The first topological index is the Wiener index. In 1947, Harold Wiener introduced this index which was used to determine physical properties of paraffin [6]. It was used for the correlation of measured properties of molecules with their structural features by H. Wiener.

Many topological indices were defined. The Zagreb index is the most studied index. The first Zagreb index [7] was defined by Gutman and Trinajstić as

$$M_1(G) = \sum_{u\in V(G)} d_u = \sum_{uv\in E(G)} d_u + d_v. \tag{1}$$

In 2010, D. Vukicevic and M. Gasperov introduced adriatic indices that are obtained by the analyses of well-known indices such as the Randic and the Wiener index. D. Vukicevic and M. Gasperov performed QSAR and QSPR studies of adriatic indices [8]. Three classes of adriatic descriptors are defined. One of these descriptors is the discrete adriatic descriptors which consist of 148 descriptors. These descriptors have very good predictive properties. Thus, many scientists studied these indices. The inverse sum indeg index is one of the discrete adriatic descriptors. The inverse sum indeg index is defined as

$$ISI(G) = \sum_{uv\in E(G)} \frac{1}{\frac{1}{d_u} + \frac{1}{d_v}} = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v}, \tag{2}$$

where d_u is denoted as the degree of vertex u [8].

The inverse sum indeg index gives a significant predictor of total surface area of octane isomers. Nezhad et al. studied several sharp upper and lower bounds on the inverse sum indeg index [9]. Nezdah 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]. Many scientists studied the topological index of graph operations. We encourage to examine the references that are given here [12–15].

Preparation of the manuscript

Throughout this paper, we assume that $G_i = (V_i, E_i)$ where $V_i \cap V_j = \varnothing$ and $E_i \cap E_j = \varnothing, i \neq j$ with $|V_i| = n_i, |E_i| = m_i fori = 1, 2, ..., k$.

Lemma 1 [9] *Let G be a graph of size m. Then,*

$$\sum_{u\in V(G)} d_u = 2m.$$

Definition 1 *Let $x_1, x_2, ..., x_n$ be positive real numbers.*

i The arithmetic mean of $x_1, x_2, ..., x_n$ is equal to

$$AM(x_1, x_2, ..., x_n) = \frac{x_1 + x_2 + ... + x_n}{n}.$$

ii The harmonic mean of $x_1, x_2, ..., x_n$ is equal to

$$HM(x_1, x_2, ..., x_n) = \frac{n}{\frac{1}{x_1} + \frac{1}{x_2} + ... + \frac{1}{x_n}}.$$

Theorem 1 *Let $x_1, x_2, ..., x_n$ be positive real numbers. Then,*
$HM(x_1, x_2, ..., x_n) \leq AM(x_1, x_2, ..., x_n)$ with equality if only if $x_1 = x_2 = ... = x_n$.

Definition 2 *Let x be a vertex* $x \notin V(G_1)$*. Then,* $G_1 + \{x\}$ *is a graph that is obtained from* G_1 *by including the vertex x and joining it to all other vertices of* G_1*. That is,* $G_1 + \{x\} = (V, E)$*, where* $V = V(G_1) \cup \{x\}$ *and* $E = E(G_1) \cup \{ux : u \in V(G_1)\}$ [16]

Definition 3 *The join G=*$G_1 + G_2$ *of* G_1 *and* G_2 *is defined as* $G = (V, E)$ *with* $V = V_1 \cup V_2$ *and where* $E = E_1 \cup E_2 \cup E'$*, where* E' *is the set of all edges joining vertices of* V_1 *with vertices of* V_2 [17].

Definition 4 *For three or more disjoint graphs,* $G_1, G_2, G_3, ..., G_k$*, where* $G_i = (V_i, E_i)$ *and where* $V_i \cap V_j = \varnothing$ *and* $E_i \cap E_j = \varnothing, i \neq j, 1 \leq i, j \leq k$ *the sequential join* $G = G_1 + G_2 + G_3 + ... + G_n = (V, E)$*, where* $V = V_1 \cup V_2 \cup V_3 \cup ... \cup V_k$ *and where* $E = E_1 \cup E_2 \cup ... \cup E_k \cup E'$*, is* $(G_1 + G_2) \cup (G_2 + G_3) \cup ... \cup (G_{k-1} + G_k)$ [17].

Definition 5 *The cartesian product of* G_1 *and* G_2*, denoted* $G_1 \times G_2 = (V, E)$*, is a graph having* $V = V_1 \times V_2$ *and two vertices* (u_1, v_1) *and* (u_2, v_2) *are adjacent if only if either* $u_1 = u_2$ *and* $v_1v_2 \in E_2$ *or* $v_1 = v_2$ *and* $u_1u_2 \in E_1$ [17].

Definition 6 *The composition known as lexicographic product* $G = G_1[G_2]$ *of graphs* G_1 *and* G_2 *is the graph with vertex set* $V = V_1 \times V_2$ *and any two vertices* (u_1, v_1) *and* (u_2, v_2) *are adjacent if only if* $u_1u_2 \in E_1$ *or* $u_1 = u_2$ *and* $v_1v_2 \in E_2$ [16].

Definition 7 *The corona of two graphs was defined in* [16]*, and there have been some results on the corona of two graphs* [12]*. The corona product of two graphs* G_1 *and* G_2*, denoted by* $G_1 \circ G_2$*, is the graph obtained by taking one copy of* G_1 *of order* n_1 *and* n_1 *copies of* G_2*, and then joining by an edge the ith vertex of* G_1 *to every vertex in the ith copy of* G_2*. The corona product is neither associative nor commutative.*

Main results

In this section, it is given sharp bounds on the inverse sum indeg index of above graph operations.

Theorem 2 *Let* $G = G_1 + \{x\}$ *, means that add a new vertex to the graph* G_1*. For* $ISI(G)$*, the following holds*

$$ISI(G) \leq \frac{1}{4}M_1(G) + \frac{m_1}{2} + \frac{n_1^2}{2}.$$

Proof We obtain

$$\begin{aligned} ISI(G) &= \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v} \\ &= \sum_{uv \in E(G_1)} \frac{(d_u + 1)(d_v + 1)}{d_u + 1 + d_v + 1} + \sum_{uv \in E'} \frac{(d_u + 1)n_1}{d_u + 1 + n_1}, \end{aligned} \tag{3}$$

where E' is the set of all edges joining vertices of V_1 with x vertex. By using Theorem 1, we have

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

Let Δ_G be the maximum degree of G. Then,

$$\frac{(d_u+1)n_1}{d_u+1+n_1} \leq \frac{\Delta_G n_1}{\Delta_G+n_1}. \tag{5}$$

Note that $\Delta_G = n_1$. So, Eq. (5) can be rewritten as

$$\frac{(d_u+1)n_1}{d_u+1+n_1} \leq \frac{\Delta_G n_1}{\Delta_G+n_1} = \frac{n_1}{2}. \tag{6}$$

From Eqs. (3), (4), and (6), we have

$$\begin{aligned} ISI(G) &= \sum_{uv\in E(G_1)} \frac{(d_u+1)(d_v+1)}{d_u+1+d_v+1} + \sum_{uv\in E'} \frac{(d_u+1)n_1}{d_u+1+n_1} \\ &\leq \frac{1}{2}\sum_{uv\in E(G_1)} \left(\frac{d_u+d_v}{2}+1\right) + \frac{1}{2}\sum_{uv\in E'} n_1 \end{aligned}$$

or

$$ISI(G) \leq \frac{1}{4}\sum_{uv\in E(G_1)} (d_u+d_v) + \frac{1}{2}\sum_{uv\in E(G_1)} 1 + \frac{n_1}{2}\sum_{uv\in E'} 1.$$

From Eq. (1), we can write

$$ISI(G) \leq \frac{1}{4}M_1(G) + \frac{m_1}{2} + \frac{n_1}{2}n_1.$$

□

Theorem 3 *Let $G = G_1 + G_2$. Then,*

$$\begin{aligned} ISI(G) \leq\ & \frac{1}{4}\left(M_1(G_1)+M_1(G_2)\right) + \frac{m_1+m_2}{2} + n_1n_2\left(\frac{n_1+n_2}{4}\right) + \\ & \frac{m_2n_1+m_1n_2}{2}. \end{aligned}$$

Proof From Eq. (2) and Definition 3, we have

$$\begin{aligned} ISI(G) =\ & \sum_{uv\in E(G_1)} \frac{(d_u+n_2)(d_v+n_2)}{d_u+n_2+d_v+n_2} + \sum_{uv\in E(G_2)} \frac{(d_u+n_1)(d_v+n_1)}{d_u+n_1+d_v+n_1} + \\ & \sum_{\substack{uv\in E' \\ u\in V(G_2) \\ v\in V(G_1)}} \frac{(d_u+n_2)\,(d_v+n_1)}{d_u+n_2+d_v+n_1}. \end{aligned} \tag{7}$$

From Theorem 1, we have

$$\frac{(d_u+n_2)(d_v+n_2)}{d_u+n_2+d_v+n_2} = \frac{1}{2}\frac{2}{\frac{1}{d_u+n_2}+\frac{1}{d_v+n_2}} \leq \frac{1}{2}\left(\frac{d_u+d_v}{2}+n_2\right), \tag{8}$$

$$\frac{(d_u+n_1)(d_v+n_1)}{d_u+n_1+d_v+n_1} = \frac{1}{2}\frac{2}{\frac{1}{d_u+n_1}+\frac{1}{d_v+n_1}} \leq \frac{1}{2}\left(\frac{d_u+d_v}{2}+n_1\right) \tag{9}$$

and

$$\frac{(d_u+n_1)(d_v+n_2)}{d_u+n_1+d_v+n_2} = \frac{1}{2}\frac{2}{\frac{1}{d_u+n_1}+\frac{1}{d_v+n_2}} \leq \frac{1}{2}\left(\frac{d_u+d_v}{2}+\frac{n_2+n_1}{2}\right). \tag{10}$$

Equation (7) can be rewritten with Eqs. (8), (9), and (10) as

$$
\begin{aligned}
ISI(G) \le\ & \frac{1}{2}\sum_{uv\in E(G_1)}\left(\frac{d_u+d_v}{2}+n_2\right)+\frac{1}{2}\sum_{uv\in E(G_2)}\left(\frac{d_u+d_v}{2}+n_1\right)+\\
& \frac{1}{2}\sum_{\substack{uv\in E' \\ u\in V(G_2) \\ v\in V(G_1)}}\left(\frac{d_u+d_v}{2}+\frac{n_1+n_2}{2}\right).
\end{aligned}
$$

By using Eq. (1), we get

$$
\begin{aligned}
ISI(G) \le\ & \frac{1}{4}M_1(G_1)+\frac{n_2}{2}\sum_{uv\in E(G_1)}1+\frac{1}{4}M_1(G_2)+\frac{n_1}{2}\sum_{uv\in E(G_2)}1+\\
& \frac{1}{2}\sum_{uv\in E'}\left(\frac{d_u+d_v}{2}+\frac{n_1+n_2}{2}\right)
\end{aligned}
$$

or

$$
\begin{aligned}
ISI(G) \le\ & \frac{1}{4}M_1(G_1)+\frac{n_2}{2}m_1+\frac{1}{4}M_1(G_2)+\frac{n_1}{2}m_2+\frac{1}{2}\sum_{uv\in E'}\frac{n_1+n_2}{2}+\\
& \frac{1}{4}\sum_{v\in V(G_1)}d_v+\frac{1}{4}\sum_{u\in V(G_2)}d_u.
\end{aligned}
$$

By Lemma 1, we have

$$
\begin{aligned}
ISI(G) \le\ & \frac{1}{4}M_1(G_1)+\frac{n_2}{2}m_1+\frac{1}{4}M_1(G_2)+\frac{n_1}{2}m_2+\frac{1}{2}\left(\frac{n_1+n_2}{2}\right)n_1n_2+\\
& \frac{1}{4}2m_1+\frac{1}{4}2m_2.
\end{aligned}
$$

□

Theorem 4 *Let* $G=G_1+G_2+\cdots+G_k$*. Then,*

$$
\begin{aligned}
ISI(G) \le\ & \frac{1}{4}\sum_{j=1}^{k}M_1(G_j)+\frac{1}{2}\sum_{j=2}^{k}m_jn_{j-1}+\frac{1}{2}\sum_{j=1}^{k-1}m_jn_{j+1}+\\
& \frac{1}{4}\sum_{j=1}^{k-1}\left(n_j^2n_{j+1}+n_{j+1}^2n_j\right)+\frac{1}{2}\sum_{j=1}^{k-2}n_jn_{j+1}n_{j+2}\\
& +\frac{1}{2}\sum_{j=1}^{k-1}m_j+m_{j+1}.
\end{aligned}
$$

Proof From Eq. (2) and Definition 3, we have

$$
\begin{aligned}
ISI(G) = & \sum_{uv\in E(G_1)} \frac{(d_u+n_2)(d_v+n_2)}{(d_u+n_2+d_v+n_2)} + \\
& \sum_{\substack{uv\in E(G_j)\\ j=\overline{2,k-1}}} \frac{(d_u+n_{(j-1)}+n_{(j+1)})(d_v+n_{(j-1)}+n_{(j+1)})}{d_u+n_{(j-1)}+n_{(j+1)}+d_v+n_{(j-1)}+n_{(j+1)}} + \\
& \sum_{uv\in E(G_k)} \frac{(d_u+n_{k-1})(d_v+n_{k-1})}{d_u+n_{k-1}+d_v+n_{k-1}} + \\
& \sum_{\substack{uv\in E'\\ u\in V(G_1)\\ v\in V(G_2)}} \frac{(d_u+n_2)(d_v+n_1+n_3)}{d_u+n_2+d_v+n_1+n_3} + \\
& \sum_{\substack{uv\in E'\\ u\in V(G_j)\\ v\in V(G_{j+1})\\ j=\overline{2,k-1}}} \frac{(d_u+n_{j-1}+n_{j+1})(d_v+n_j+n_{j+2})}{d_u+n_{j-1}+n_{j+1}+d_v+n_j+n_{j+2}} + \\
& \sum_{\substack{uv\in E'\\ u\in V(G_{k-1})\\ v\in V(G_k)}} \frac{(d_u+n_{k-2}+n_k)(d_v+n_{k-1})}{d_u+n_{k-2}+n_k+d_v+n_{k-1}}.
\end{aligned}
\tag{11}
$$

Equation (11) can be rewritten using Theorem 1:

$$
\begin{aligned}
ISI(G) = & \sum_{uv\in E(G_1)} \frac{1}{4}(d_u+d_v+2n_2) + \sum_{\substack{uv\in E(G_j)\\ j=\overline{2,k-1}}} \frac{1}{4}(d_u+d_v+2n_{j-1}+2n_{j+1}) + \\
& \sum_{uv\in E(G_k)} \frac{1}{4}(d_u+d_v+2n_{k-1}) + \sum_{\substack{uv\in E'\\ u\in V(G_1)\\ v\in V(G_2)}} \frac{1}{4}(d_u+d_v+n_1+n_2+n_3) + \\
& \sum_{\substack{uv\in E'\\ u\in V(G_j)\\ v\in V(G_{j+1})\\ j=\overline{2,k-1}}} \frac{1}{4}(d_u+d_v+n_{j-1}+n_j+n_{j+1}+n_{j+2}) + \\
& \sum_{\substack{uv\in E'\\ u\in V(G_{k-1})\\ v\in V(G_k)}} \frac{1}{4}(d_u+d_v+n_{k-2}+n_{k-1}+n_k).
\end{aligned}
$$

By using Eq. (1), we get

$$
\begin{aligned}
ISI(G) \le\ & \frac{1}{4}\left(M_1(G_1)+2n_2m_1\right)+\\
& \frac{1}{4}\sum_{2\le j\le k-1}\left(M_1(G_j)+m_j(2n_{j-1}+2n_{j+1})\right)+\\
& \frac{1}{4}\left(M_1(G_k)+2n_{k-1}m_k\right)+\frac{1}{4}\left(\sum_{u\in V(G_1)} d_v+\sum_{v\in V(G_2)} d_u\right)+\\
& \frac{n_1n_2}{4}\left(n_1+n_2+n_3\right)+\frac{1}{4}\left(\sum_{\substack{u\in V(G_j)\\ j=\overline{2,k-2}}} d_v+\sum_{\substack{v\in V(G_{j+1})\\ j=\overline{2,k-2}}} d_u\right)+\\
& \frac{n_jn_{j+1}}{4}\left(n_{j-1}+n_j+n_{j+1}+n_{j+2}\right)+\frac{1}{4}\sum_{u\in V(G_{k-1})} d_v+\frac{1}{4}\sum_{v\in V(G_k)} d_u+\\
& \frac{n_{k-1}n_k}{4}\left(n_{k-2}+n_{k-1}+n_k\right).
\end{aligned}
$$

By Lemma 1, the proof is completed as

$$
\begin{aligned}
ISI(G) \le\ & \frac{1}{4}\left(M_1(G_1)+2n_2m_1\right)+\frac{1}{4}\sum_{2\le j\le k-1}\left(M_1(G_j)+m_j(2n_{j-1}+2n_{j+1})\right)+\\
& \frac{1}{4}\left(M_1(G_k)+2n_{k-1}m_k\right)+\frac{1}{4}\left(2m_1+2m_2\right)+\frac{n_1n_2}{4}\left(n_1+n_2+n_3\right)+\\
& \frac{1}{4}\sum_{j=\overline{2,k-2}}\left(2m_j+2m_{j+1}\right)+\frac{n_jn_{j+1}}{4}\left(n_{j-1}+n_j+n_{j+1}+n_{j+2}\right)+\\
& \frac{1}{4}\left(2m_{k-1}+2m_k\right)+\frac{n_{k-1}n_k}{4}\left(n_{k-2}+n_{k-1}+n_k\right).
\end{aligned}
$$

□

Theorem 5 *Let $G=G_1\times G_2$. Then,*

$$ISI(G)\le\frac{1}{4}\left(n_2M_1(G_1)+n_1M_1(G_2)\right)+\frac{m_1n_2\Delta_2+m_2n_1\Delta_1}{2}.$$

Proof Assume that $u_i,u_k\in V(G_1), v_j,v_l\in V(G_2)$. From Definition 3, we can write

$$ISI(G)=\sum_{(u_i,v_j)(u_k,v_l)\in E(G)}\frac{d_ud_v}{d_u+d_v}$$

or

$$ISI(G)=\sum_{\substack{(u_i,v_j)(u_i,v_l)\in E(G)\\ j\neq l}}\frac{1}{\frac{1}{d_{u_i}+d_{v_j}}+\frac{1}{d_{u_i}+d_{v_l}}}+\sum_{(u_i,v_j)(u_k,v_j)\in E(G)}\frac{1}{\frac{1}{d_{u_i}+d_{v_j}}+\frac{1}{d_{u_k}+d_{vj}}}. \tag{12}$$

By using Theorem 1, we get

$$\frac{1}{\frac{1}{d_{u_i}+d_{v_j}}+\frac{1}{d_{u_i}+d_{v_l}}}\le\frac{1}{2}\frac{d_{u_i}+d_{v_j}+d_{u_i}+d_{v_l}}{2}=\frac{d_{u_i}}{2}+\frac{d_{u_i}+d_{v_l}}{4}, \tag{13}$$

$$\frac{1}{\frac{1}{d_{u_i}+d_{v_j}}+\frac{1}{d_{u_k}+d_{vj}}}\le\frac{1}{2}\frac{d_{u_i}+d_{v_j}+d_{u_k}+d_{vj}}{2}=\frac{d_{v_j}}{2}+\frac{d_{u_i}+d_{u_k}}{4}. \tag{14}$$

Equation (12) is rewritten using Eqs. (13) and (14).

$$ISI(G) \leq \sum_{u_i \in V(G_1)} \sum_{(v_j,v_l) \in E(G_2)} \left(\frac{d_{u_i}}{2} + \frac{d_{u_i} + d_{v_l}}{4} \right) + \sum_{v_j \in V(G_2)} \sum_{(u_i,u_k) \in E(G_1)} \left(\frac{d_{v_j}}{2} + \frac{d_{u_i} + d_{u_k}}{4} \right). \tag{15}$$

Let Δ_1, Δ_2 be the maximum degree of G_1, G_2 respectively.

$$\frac{d_{u_i}}{2} + \frac{d_{u_i} + d_{v_l}}{4} \leq \frac{\Delta_1}{2} + \frac{d_{u_i} + d_{v_l}}{4}, \tag{16}$$

$$\frac{d_{v_j}}{2} + \frac{d_{u_i} + d_{u_k}}{4} \leq \frac{\Delta_2}{2} + \frac{d_{u_i} + d_{u_k}}{4}. \tag{17}$$

By Eqs. (16) and (17), we have

$$ISI(G) \leq \sum_{u_i \in V(G_1)} \sum_{(v_j,v_l) \in E(G_2)} \left(\frac{\Delta_1}{2} + \frac{d_{u_i} + d_{v_l}}{4} \right) + \sum_{v_j \in V(G_2)} \sum_{(u_i,u_k) \in E(G)} \left(\frac{\Delta_2}{2} + \frac{d_{u_i} + d_{u_k}}{4} \right).$$

From Eq. (1), we get

$$ISI(G) \leq \sum_{u_i \in V(G_1)} \left(\frac{\Delta_1}{2} + \frac{M_1(G_2)}{4} \right) + \sum_{v_j \in V(G_2)} \left(\frac{\Delta_2}{2} + \frac{M_1(G_1)}{4} \right).$$

The following is obtained:

$$ISI(G) \leq \frac{m_2 n_1 \Delta_1}{2} + \frac{n_1 M_1(G_2)}{4} + \frac{m_1 n_2 \Delta_2}{2} + \frac{n_2 M_1(G_1)}{4}.$$

□

Theorem 6 *Let* $G = G_1[G_2]$. *Then,*

$$ISI(G) \leq n_2 \Delta_1 m_2 + \Delta_2 m_1 + \frac{M_1(G_2)}{2} + \frac{n_2 M_1(G_1)}{2}.$$

Proof Assume that $u_i, u_k \in V(G_1), v_j, v_l \in V(G_2)$. From Definition 4 and $d_{G_1[G_2]} = n_2 d_{G_1}(u) + d_{G_2}(v)$, we get

$$\begin{aligned} ISI(G) &= \sum_{(u_i,v_j)(u_k,v_l) \in E(G)} \frac{d_u d_v}{d_u + d_v} \\ &= \sum_{u_i \in V(G_1)} \sum_{\substack{(v_j,v_l) \in E(G_2) \\ j \neq l}} \frac{1}{\frac{1}{n_2 d_{u_i} + d_{v_j}} + \frac{1}{n_2 d_{u_i} + d_{v_l}}} \\ &+ \sum_{u_j \in V(G_2)} \sum_{v_l \in V(G_2)} \sum_{(u_i,u_k) \in E(G_1)} \frac{1}{\frac{1}{n_2 d_{u_i} + d_{v_j}} + \frac{1}{n_2 d_{u_k} + d_{v_l}}}. \end{aligned} \tag{18}$$

Assume that Δ_1, Δ_2 be the maximum degree of G_1, G_2 respectively. From Theorem 1, we have

$$\frac{1}{2} \frac{2}{\frac{1}{n_2 d_{u_i} + d_{v_j}} + \frac{1}{n_2 d_{u_i} + d_{v_l}}} \leq \frac{n_2 d_{u_i} + d_{v_j} + n_2 d_{u_i} + d_{v_l}}{2} \leq n_2 \Delta_1 + \frac{d_{v_j} + d_{v_l}}{2} \tag{19}$$

and

$$\frac{1}{2}\frac{2}{\frac{1}{n_2 d_{u_i}+d_{v_j}}+\frac{1}{n_2 d_{u_k}+d_{v_l}}} \leq \frac{n_2 d_{u_i}+d_{v_j}+n_2 d_{u_k}+d_{v_l}}{2} \leq \Delta_2+\frac{n_2(d_{u_i}+d_{u_k})}{2}. \qquad (20)$$

Equation (18) is rewritten by Eqs. (19) and (20):

$$ISI(G) \leq \sum_{v_j v_l \in E(G_2)} \left(n_2\Delta_1+\frac{d_{v_j}+d_{v_l}}{2}\right)+\sum_{u_i u_k \in E(G_2)} \left(\Delta_2+\frac{n_2(d_{u_i}+d_{u_k})}{2}\right).$$

By Eq. (1), it is obtained as

$$ISI(G) \leq n_2\Delta_1 m_2+\frac{M_1(G_2)}{2}+\frac{n_2 M_1(G_1)}{2}+\Delta_2 m_1.$$

□

Theorem 7 *Let $G=G_1\circ G_2$. Then,*

$$\begin{aligned} ISI(G) \leq{}& \frac{\Delta_1}{\delta_1+n_2}ISI(G_1)+\frac{n_1\Delta_2}{\delta_2+1}ISI(G_2)+n_2 m_1\frac{2\Delta_1+n_2}{2\delta_1+2n_2}+ \\ & n_1 m_2\frac{2\Delta_2+1}{2\delta_2+2}+\frac{(\Delta_1+n_2)\,(\Delta_2+1)}{\delta_1+\delta_2+n_2+1}n_1 n_2. \end{aligned}$$

Proof From Definition 7, we have

$$\begin{aligned} ISI(G) ={}& \sum_{uv\in E(G_1)}\frac{(d_u+n_2)(d_v+n_2)}{d_u+n_2+d_v+n_2}+n_1\sum_{uv\in E(G_2)}\frac{(d_u+1)(d_v+1)}{d_u+d_v+2}+ \\ & \sum_{\substack{uv\in E' \\ u\in V(G_2) \\ v\in V(G_1)}}\frac{(d_u+n_2)(d_v+1)}{d_u+n_2+d_v+1}. \end{aligned}$$

Note that

$$\begin{aligned} \frac{(d_u+n_2)(d_v+n_2)}{d_u+n_2+d_v+n_2} &= \frac{d_u d_v}{d_u+d_v+2n_2}+\frac{n_2(d_u+d_v)+n_2^2}{d_u+d_v+2n_2} \\ &\leq \frac{d_u d_v}{d_u+d_v}\frac{d_u+d_v}{d_u+d_v+2n_2}+\frac{n_2(d_u+d_v)+n_2^2}{d_u+d_v+2n_2} \end{aligned}$$

and

$$\begin{aligned} \frac{(d_u+1)(d_v+1)}{d_u+d_v+2} &= \frac{d_u d_v}{d_u+d_v+2}+\frac{d_u+d_v+1}{d_u+d_v+2} \\ &\leq \frac{d_u d_v}{d_u+d_v}\frac{d_u+d_v}{d_u+d_v+2}+\frac{d_u+d_v+1}{d_u+d_v+2}. \end{aligned}$$

Then,

$$\begin{aligned} ISI(G) \leq{}& \sum_{uv\in E(G_1)}\frac{d_u d_v}{d_u+d_v}\frac{d_u+d_v}{d_u+d_v+2n_2}+\sum_{uv\in E(G_1)}\frac{n_2(d_u+d_v)+n_2^2}{d_u+d_v+2n_2}+ \\ & n_1\sum_{uv\in E(G_2)}\frac{d_u d_v}{d_u+d_v}\frac{d_u+d_v}{d_u+d_v+2}+n_1\sum_{uv\in E(G_2)}\frac{d_u+d_v+1}{d_u+d_v+2}+ \\ & \sum_{\substack{uv\in E' \\ u\in V(G_2) \\ v\in V(G_1)}}\frac{(d_u+n_2)(d_v+1)}{d_u+n_2+d_v+1}. \end{aligned}$$

Assume that $\Delta_1(\delta_1), \Delta_2(\delta_2)$ be maximum (minimum) degree of G_1, G_2 respectively.

$$\begin{aligned} ISI(G) \leq & \sum_{uv \in E(G_1)} \frac{d_u d_v}{d_u + d_v} \frac{2\Delta_1}{2\delta_1 + 2n_2} + \sum_{uv \in E(G_1)} \frac{n_2 2\Delta_1 + n_2^2}{2\delta_1 + 2n_2} + \\ & n_1 \sum_{uv \in E(G_2)} \frac{d_u d_v}{d_u + d_v} \frac{2\Delta_2}{2\delta_2 + 2} + n_1 \sum_{uv \in E(G_2)} \frac{2\Delta_2 + 1}{2\delta_2 + 2} + \\ & \sum_{\substack{uv \in E' \\ u \in V(G_2) \\ v \in V(G_1)}} \frac{(\Delta_1 + n_2)(\Delta_2 + 1)}{\delta_1 + n_2 + \delta_2 + 1}. \end{aligned}$$

By Eq. (2), we obtain

$$\begin{aligned} ISI(G) \leq & \frac{\Delta_1}{\delta_1 + n_2} ISI(G_1) + \frac{n_1 \Delta_2}{\delta_2 + 1} ISI(G_2) + n_2 m_1 \frac{2\Delta_1 + n_2}{2\delta_1 + 2n_2} + \\ & n_1 m_2 \frac{2\Delta_2 + 1}{2\delta_2 + 2} + \frac{(\Delta_1 + n_2)(\Delta_2 + 1)}{\delta_1 + \delta_2 + n_2 + 1} n_1 n_2. \end{aligned}$$

□

Conclusions

The topological indices are used theoretically to predict the physical-chemical properties of a chemical structure. In particular, they are used to estimate the physical and chemical properties of the new molecular structure without experimentation.

The $ISI(G)$ index which is a significant predictor of the total surface area of octane isomers has been many studied among topological indices. The graph operations play an important role in graph theory. Upper bounds for new graphs that are obtained by graph operations are given. These bounds are based on minimum-maximum degree, vertex-edge numbers. The results of this study may be used as a predictor especially in the chemical graph theory.

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