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Comparison of the Inverse Degree Index for Certain Transformation Graphs

Rauf Irshad[1,*], Muhammad Hussain[1], Maqsood Ahmad[1]

[1]Department of Mathematics, COMSATS University Islamabad, Pakistan

Abstract. For a molecular graph Λ, the inverse degree index (IDI) is defined by taking the sum over all vertices of the reciprocal degree of each vertex. The IDI is a structurally sensitive topological invariant that emphasizes low-degree vertices, making it effective for analyzing branching, irregularity, and deviations in molecular structures. Graph transformations prove to be an effective tool to construct new chemically meaningful structures. In this work, we study the behavior of IDI under four newly defined graph transformations. We first introduce families of n-vertex networks based on complete graphs of order $l \geq 3$, derive transformed networks, and establish inequalities involving the IDI. We then present extremal results for the transformed graphs and support our findings with computations on several representative examples.

Key words and Phrases: inverse degree index, extremal graph, graph invariants, transformed graphs, complete graph.

1. INTRODUCTION

Graph theory explores the interconnection network designs ranging from social and computer networks to molecular structures and contributes an inclusive understanding of such corresponding matters through their precise structure. The topology of any graph delivers knowledge regarding the techniques through which vertices are attached to the graph. In molecular graphs, vertices are considered to be atoms, and covalent bonds (double or triple) are taken as edges. Graph theory is an effective tool used in various research areas such as chemical graph theory (CGT), mathematical chemistry, and even coding theory [1, 2, 3]. Graph theory is the analysis of associations between various objects. Different graph notations are used to represent graphs, a graph is defined as a combination of a vertex and edge

*Corresponding author: rauf.irshad118@gmail.com

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set $V(\Lambda)$ and $E(\Lambda)$, respectively. There are various types of graphs, such as path, cycle, bipartite, complete, star, wheel graph, and many others. In this study, we work with simple connected graphs that are without multiple, directed, or weighted edges, and self-loops. In this paper, we are working with families of complete, star, cycle, and path graphs. A complete graph is a k-regular graph, where every vertex is connected to all other vertices. A star graph is a class of graphs in which only one vertex has degree $n-1$ and $n-1$ vertices have degree one. A cycle graph is denoted as C_n $(n \geq 3)$ and every vertex has degree 2. Path graph P_n having exactly two vertices of degree one and all the others having degree 2.

Transformation graphs, akin to graph operations, help us in the development of new, complex, and important structures of our own choice. Transformation graphs hold the complete knowledge from the actual graph into a new transformed system. Therefore, if it is feasible to discover the provided graph from the transformed graph, then such a process may be utilized to figure out the structural properties of the initial graph, considering the transformation graphs for details, see [4]. In distinct mathematical literature, several graph transformations have been evaluated where the vertex set of the transformed graph is equal to $V(\Lambda) \cup E(\Lambda)$. The most prominent classification of such graphs is the total graph. The total graph $T(\Lambda)$ of a graph Λ is the graph whose vertex set is $V(\Lambda) \cup E(\Lambda)$ and any two vertices of $T(\Lambda)$ are adjacent if and only if they are either incident or adjacent in Λ [5].

A topological index (TI) transforms a molecular graph into a real number by involving different graph parameters like degrees, distances, and eigenvalues. Among these parameters, the connectivity or degree-related TIs are extensively investigated due to their close correlation with certain physicochemical properties of chemical species. Zagreb indices and their transformations are useful to anticipate about π-elctron energy of alternant hydrocarbons. TIs in certain combinations take part in the design of new drugs by participating in the analysis of quantitative activity and structure-property relationships. The analysis of TIs becomes very interesting for various research areas in the present era, particularly TIs impact on chemistry amongst the theoretical molecular descriptors, due to the prediction capability about physicochemical characteristics of various chemical substances. Some essential TIs of distinct networks were formerly computed in [6, 7, 8]. A chemist, Harold Wiener, initiated the idea of the pioneer distance-related index while working on boiling points of paraffins and named it after his name, the Wiener index [9]. Gutman and Trinajestić [10, 11], were the pioneers who provided the idea of degree-related indices while studying pi-electron energy of saturated hydrocarbons, and defined as follows:

$$M_1(\Lambda) = \sum_{w \in V(\Lambda)} d_\Lambda^2(w) = \sum_{vw \in E(\Lambda)} [d_\Lambda(v) + d_\Lambda(w)]$$

$$M_2(\Lambda) = \sum_{vw \in E(\Lambda)} d_\Lambda(v) \cdot d_\Lambda(w)$$

Later on, the analysis of Zagreb indices discovered many applications in QSPR and QSAR investigations [12, 13]. Chemical applications and mathematical effects of Zagreb indices can be analyzed from [14, 15, 16]. The Zagreb indices have been manipulated to explore molecular complexity, chirality, ZE-isomorphism and hetero-systems. The specific modification of the Zagreb indices is defined with a variable parameter as, $\alpha \in \mathbb{R}$,

$$M_1^{(\alpha)}(\Lambda) = \sum_{w \in V(\Lambda)} (d_\Lambda(w))^\alpha$$

$$M_2^{(\alpha)}(\Lambda) = \sum_{vw \in E(\Lambda)} [d_\Lambda(v) \cdot d_\Lambda(w)]^\alpha$$

These conceptions of the Zagreb indices appear to be preferably evaluated by Li et al[17, 18]. There are some unique cases α, if $\alpha = 2$ then it is the first Zagreb index. For $\alpha = -1$ is the inverse degree index (IDI) described as,

$$IDI(\Lambda) = \sum_{w \in V(\Lambda)} \frac{1}{d_\Lambda(w)}$$

The name of this index was first introduced in (2005) and is also known as the modified total adjacency index [19]. For $\alpha = \dfrac{-1}{2}$ we obtained $({}^0R_{\frac{-1}{2}}(\Lambda))$ zeroth-order connectivity R.I defined as,

$${}^0R_{\frac{-1}{2}}(\Lambda) = \sum_{w \in V(\Lambda)} \frac{1}{\sqrt{d_\Lambda(w)}}$$

For $\alpha = 3$ then,

$$F(\Lambda) = \sum_{w \in V(\Lambda)} (d_\Lambda(w))^3$$

this topological index is called the F index or forgotten index.

The IDI initially appeared in the software Graffiti [20, 21] that generates conjectures and proved to be a promising predictor for various compounds in CGT, such as in discovering the physicochemical characteristics of various kinds of compounds like octane isomers, polychlorobiphenyls, and polyaromatic hydrocarbons [22, 23, 24]. Xu & Das [25] and Das et al. [26] sort out extremal results regarding IDI in terms of graph parameters and the relation of IDI with Randić and harmonic index, respectively. Based upon the idea of the semi-total line & point graphs initiated by Sampathkumar [27] along with the idea of the total graph, Wu and Meng [4] introduced the general transformation graphs Λ^{abc}, where a, b, $c \in \{-, +\}$. Wang et al. [28] computed the tight bounds for the general sum-connectivity index regarding transformation graphs Λ^{abc}. Mohanappriya et al. [29] obtained the expressions for the inverse sum and symmetric division degree indices for graph transformations Λ^{ab}, where a, $b \in \{-, +\}$. Romero et al. [30] ascertained a relation between the inverse degree of a graph and other significant indices while applying them to a particular chemical structure.

Rodríguez et al. [31] worked out various inequalities for IDI in terms of those indices that are useful for QSPR/QSAR analysis and also determined extremal graphs regarding IDI. Asif et al. [32] computed exact values of IDI for some unicyclic graphs and settled bounds for families for $n-$vertex connected graphs with the pendent path of fixed length under the effect of transformations. Manian et al. [33] introduced transformations like pendant-path, contraction to path, contraction to star, and star-translation to obtain extremal values of inverse degree and forgotten indices for a family of unicyclic graphs. Molina et al. [34] applied IDI and e^{IDI} to investigate the properties of octane isomers, such as acentric factor, standard enthalpy of formation, heat capacity at constant pressure, enthalpy of vaporization, entropy, and standard enthalpy of vaporization.

In [35], Molina et al. (2024) explored the IDI, deriving new inequalities, examining its extremal properties, and demonstrating its effectiveness in predicting the structural behavior of diverse molecular graph families. Similarly, in 2024, Granados et al. [36] established sharp bounds for variable topological indices, including those based on inverse degrees. They identified the graphs that achieve these bounds, strengthening the theoretical framework for molecular descriptor analysis. In 2025, Irshad et al. [37] investigated the atom–bond connectivity index under various graph transformations, highlighting how structural modifications impact the topological properties and predictive capacity of molecular graphs. In this article, we discuss various families of n-vertex networks by applying new transformations and established inequalities for IDI regarding these transformations. Also, we employ our formulas on diverse examples to check their precision and validity.

2. Motivation and Applications

The motivation for comparing transformed graphs arises from the fact that graph transformations often alter key structural properties of molecular graphs, which directly affect topological indices like the inverse degree index (IDI). By studying how IDI behaves under different transformations, we can learn about structural sensitivity, characterize extremal properties, develop inequalities to establish general mathematical relationships, and interpret them, which are valuable in chemical graph theory.

IDI can help predict molecular stability, reactivity, and potential reaction sites. Transformations that optimize IDI may guide the design of polymers, nanotubes, or other nanostructures with desired properties. Understanding how transformations affect IDI supports computational methods in cheminformatics. These comparison provide a theoretical aid and insight for molecular graphs akin to transformed graphs in QSPR/QSAR studies.

3. MAIN RESULTS

In this section, before addressing the main problem, we present some transformations of complete graphs attached to the graph. These transformations have solid outcomes over the increase and decrease of $IDI(\Lambda)$. Throughout in this paper, assume the graph $\Lambda_{n,m}^{k,l}$ comprises on n-vertices and m-edges simple graph Λ together with k number complete graphs of order l, $(l \geq 3)$ connected with $v \in \Lambda$ of degree $d_v \geq 1$. $n + k(l-1)$ be the order of $\Lambda_{n,m}^{k,l}$, $\dfrac{2m + kl(l-1)}{2}$ will be the size and $d_1 = \delta_\Lambda \leq d_2 \leq d_3 \leq ... \leq \Delta_\Lambda + (l-1)$ be its degree sequence.

3.1. **Transformations of Graph.**

Suppose $H(\Lambda) \subset E(\Lambda)$, the $\Lambda^{'} = \Lambda - H$ becomes the other graph developed by eliminating edge set $H(\Lambda)$ and $\Lambda'' = \Lambda - V_1(\Lambda)$ becomes new graph constructed by deleting vertex set $V_1(\Lambda) \subset V(\Lambda)$. We will use the next coming transformations like those used in [32]. These transformations have solid effects on IDI of $\Lambda_{n,m}^{k,l}$.

Proposition 3.1. *The IDI of some known graphs are,*

(1) *If Λ is a complete graph of order r and size $s = \dfrac{r(r-1)}{2}$ then* $IDI(\Lambda) = \dfrac{r}{(r-1)} = \dfrac{2s}{(r-1)^2}$
(2) *Consider Λ_r be star graph of order $r+1$ and size $s = r$ then* $IDI(\Lambda_r) = \dfrac{r^2+1}{r} = \dfrac{s^2+1}{s}$
(3) *Let Λ be a path graph of order r and size $s = r-1$ then* $IDI(\Lambda) = \dfrac{r+2}{2} = \dfrac{s+3}{2}$
(4) *Let W_r denotes the wheel graph of order $r+1$ and size $s = 2r$ then*
$IDI(\Lambda) = IDI(W_r) = \dfrac{r^2+3}{3r} = \dfrac{s^2+6}{3s}$
(5) *Let $\Lambda_{n,m} = P_n \times P_m$ is a grid graph of order $r = nm$ and size $s = (2nm - n - m)$ then*
$IDI(\Lambda_{n,m}) = \dfrac{3nm + 2(n+m) + 4}{12}$
(6) *For cylinder graph $\Lambda_{n,m} = C_n \times P_m$ of order $r = nm$ and size $s = n(2m-1)$ then*
$IDI(\Lambda_{n,m}) = \dfrac{n(3m+2)}{12}$.

Transformation A

Let Λ be any simple graph with order and size is n, m respectively. Let $w_i \in V(\Lambda), d_{w_i} \geq 1$ for $1 \leq i \leq k \leq n$ and complete graph at w_i of the form,

$$(w_iu_i^1, w_iu_i^2, w_iu_i^3, ..., w_iu_i^{l-1}), (u_i^1u_i^2, u_i^1u_i^3, ..., u_i^1u_i^{l-1}), (u_i^2u_i^3, ..., u_i^2u_i^{l-1}), ..., (u_i^{l-2}u_i^{l-1})$$

comprises $\Lambda_{n,m}^{k,l}$. Then

$$A(\Lambda_{n,m}^{k,l}) = \Lambda + \sum_{j=1}^{k}\{(w_iu_i^1, w_iu_i^2, w_iu_i^3, ..., w_iu_i^{l-1}) + (u_i^1u_i^2, u_i^1u_i^3, ..., u_i^1u_i^{l-1}) + (u_i^2u_i^3, ..., u_i^2u_i^{l-1}) + ... + (u_i^{l-2}u_i^{l-1})\}$$

The order and size of graph $A(\Lambda_{n,m}^{k,l})$ are $n + k(l-1)$ and $\frac{2m+kl(l-1)}{2}$, respectively. Figure 1 illustrates the Transformation A.

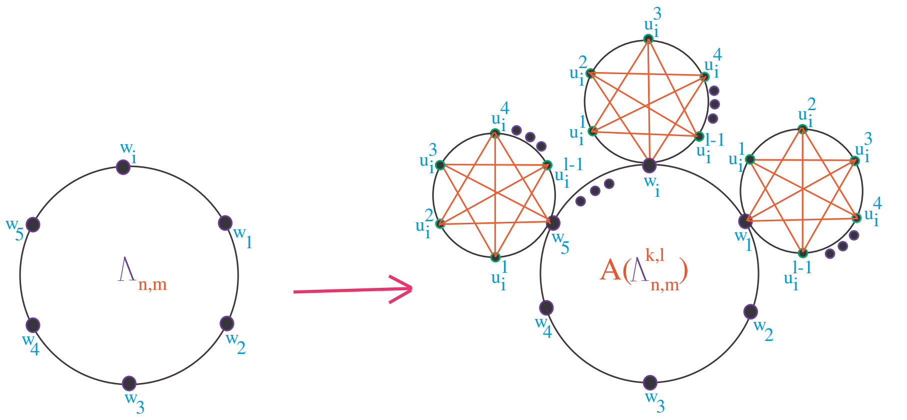

FIGURE 1. Transformation A

Transformation B

Let $A(\Lambda_{n,m}^{k,l})$ be a graph with k number of complete graphs of order l $(l \geq 3)$. Let $w_i \in V(\Lambda_{n,m}^{k,l})$ and form of w_i is,

$$(w_iu_i^1, w_iu_i^2, w_iu_i^3, ..., w_iu_i^{l-1}), (u_i^1u_i^2, u_i^1u_i^3, ..., u_i^1u_i^{l-1}), (u_i^2u_i^3, ..., u_i^2u_i^{l-1}), ..., (u_i^{l-2}u_i^{l-1})$$

In transformation **B** complete graph will be changed into Star graph and form of w_i will becomes,

$$\{w_iu_i^1, w_iu_i^2, w_iu_i^3, ..., w_iu_i^{l-1}\}$$

And

$$(\Lambda_{n,m}^{k,l}) = A(\Lambda_{n,m}^{k,l}) - \sum_{j=1}^{k}\{(u_i^1u_i^2, u_i^1u_i^3, ..., u_i^1u_i^{l-1}) + (u_i^2u_i^3, ..., u_i^2u_i^{l-1}) + ... + (u_i^{l-2}u_i^{l-1})\}$$

The order and size of graph $B(\Lambda_{n,m}^{k,l})$ are $\frac{2n+kl(l-1)}{2}$ and $\frac{2m+kl(l-1)}{2}$, respectively. Transformation B depicted in Figure 2.

If you want to cite or refer to your definition, lemma, proposition, or theorem later in the text, write it down using the following.

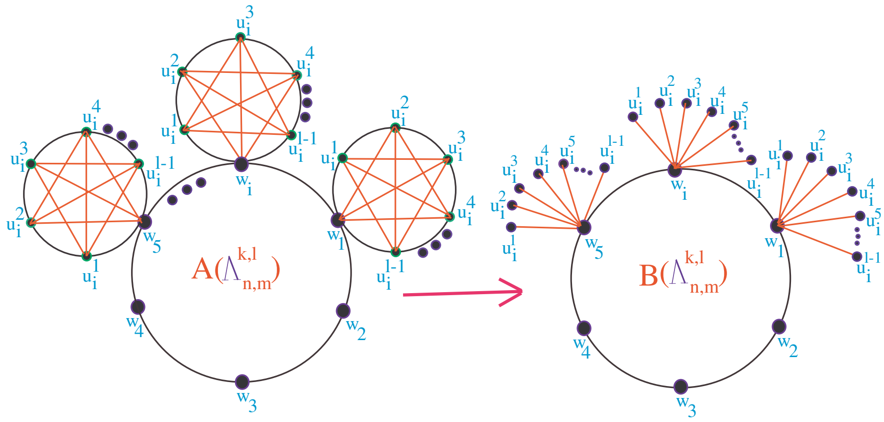

FIGURE 2. Transformation B

Theorem 3.2. *Let Λ be the simple graph of order n and size m. Let Δ and δ be its maximum and minimum degrees, respectively. And $A(\Lambda_{n,m}^{k,l})$ be the graph having k number of complete graphs attached to the fully connected vertices. Then*

$$IDI\{A(\Lambda_{n,m}^{k,l})\} \leq IDI\{B(\Lambda_{n,m}^{k,l})\}$$

Proof. The transformation A transforms Λ into $\Lambda_{n,m}^{k,l}$ be a graph having k number of complete graphs of order l $(l \geq 3)$. Then the construction of $A(\Lambda_{n,m}^{k,l})$ $(l \geq 3)$ proposes

$$|O\{A(\Lambda_{n,m}^{k,l})\}| = n + k(l-1) \text{ and } |E\{A(\Lambda_{n,m}^{k,l})\}| = \frac{2m + kl(l-1)}{2}.$$

In transformation $A(\Lambda_{n,m}^{k,l})$ the number of vertices having degree d_v, k and $k(l-1)$ are $(n-k)$, $(d_v + l - 1)$ and $(l-1)$, respectively. By applying the definition of IDI on $A(\Lambda_{n,m}^{k,l})$ we get,

$$IDI\{A(\Lambda_{n,m}^{k,l})\} = \sum_{v \in A(\Lambda_{n,m}^{k,l}), v=1}^{n-k} \frac{1}{d_v} + \sum_{v \in A(\Lambda_{n,m}^{k,l}), v=1}^{k} \frac{1}{d_v + (l-1)} + k(l-1)\frac{1}{(l-1)}$$

$$IDI\{A(\Lambda_{n,m}^{k,l})\} = \frac{(n-k)}{d_v} + \frac{k}{d_v + (l-1)} + k \tag{1}$$

The transformation $A(\Lambda_{n,m}^{k,l})$ transformed into $B(\Lambda_{n,m}^{k,l})$, be a graph having k number of star graphs attached to the fully connected vertices. Then the establishment of $B(\Lambda_{n,m}^{k,l})$ presnts,

$$|O\{B(\Lambda_{n,m}^{k,l})\}| = \frac{2n + kl(l-1)}{2} \text{ and } |E\{B(\Lambda_{n,m}^{k,l})\}| = \frac{2m + kl(l-1)}{2}.$$

So, there exists k vertices of degree $\left(d_v + \dfrac{l(l-1)}{2}\right)$, vertices with degree $(n-k)$ are d_v and $\frac{kl(l-1)}{2}$ vertices having degree 1. We get $IDI\{B(\Lambda_{n,m}^{k,l})\}$ as,

$$IDI\{B(\Lambda_{n,m}^{k,l})\} = \sum_{v\in B(\Lambda_{n,m}^{k,l}),v=1}^{n-k} \frac{1}{d_v} + \sum_{v\in B(\Lambda_{n,m}^{k,l}),v=1}^{k} \frac{1}{d_v + \frac{l(l-1)}{2}} + \frac{kl(l-1)}{2}$$

$$IDI\{B(\Lambda_{n,m}^{k,l})\} = \frac{(n-k)}{d_v} + \frac{2k}{2d_v + l(l-1)} + \frac{kl(l-1)}{2} \tag{2}$$

From Equations (1) and (2), we get

$$\begin{aligned} IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{B(\Lambda_{n,m}^{k,l})\} &= \frac{(n-k)}{d_v} + \frac{k}{d_v + (l-1)} + k - \frac{(n-k)}{d_v} \\ &\quad - \frac{2k}{2d_v + l(l-1)} - \frac{kl(l-1)}{2} \end{aligned}$$

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{B(\Lambda_{n,m}^{k,l})\} = k\left[\frac{1}{d_v + (l-1)} - \frac{l(l-1)}{2} - \frac{2}{2d_v + l(l-1)} + 1\right] \tag{3}$$

Replace d_v with maximum degree Δ to minimize the Equation (3) which implies,

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{B(\Lambda_{n,m}^{k,l})\} = k\left[\frac{1}{\Delta_\Lambda + (l-1)} - \frac{l(l-1)}{2} - \frac{2}{2\Delta_\Lambda + l(l-1)} + 1\right] \leq 0 \tag{4}$$

It is clear from Equation (4) that,

$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{B(\Lambda_{n,m}^{k,l})\} \leq 0$ which implies $IDI\{A(\Lambda_{n,m}^{k,l})\} \leq IDI\{B(\Lambda_{n,m}^{k,l})\}$.

□

Figure 3 and 4 are helpful in checking result derived in throughout the paper.

Example 3.3. *Let $\Lambda = C_6$ be a cycle graph. The order and size of this graph are $n = m = 6$ with the smallest and the largest degrees being $\delta = \Delta = 2$. Take two copies $k = 2$ of the complete graph of order $l = 4$. After applying transformation A to $\Lambda = C_6$, we obtain 6 vertices of degree 3, 2 vertices of degree 5, and 4 vertices of degree 2. Therefore, $|O\{A(\Lambda_{n,m}^{k,l})\}| = |O\{A(\Lambda_{6,6}^{2,4})\}| = n + k(l-1) = 6 + 2(3) = 12$ and $|E\{A(\Lambda_{n,m}^{k,l})\}| = |E\{A(\Lambda_{6,6}^{2,4})\}| = \dfrac{2m + kl(l-1)}{2} = \dfrac{2(6) + 2(4)(3)}{2} = 18$. Now $IDI\{A(\Lambda_{n,m}^{k,l})\} = IDI\{A(\Lambda_{6,6}^{2,4})\} = 6\left(\dfrac{1}{3}\right) + 2\left(\dfrac{1}{5}\right) + 4\left(\dfrac{1}{2}\right) = 4.4$. In transformation B, the complete graph is converted into a star graph. Thus, we obtain 2 vertices of degree 8, 4 vertices of degree 2, and 12 vertices of degree 1. Hence, for transformation B we have, $|O\{B(\Lambda_{n,m}^{k,l})\}| = |O\{B(\Lambda_{6,6}^{2,4})\}| = \dfrac{2n + kl(l-1)}{2} = \dfrac{2(6) + 2(4)(3)}{2} = 18$ and $|E\{B(\Lambda_{n,m}^{k,l})\}| = |E\{B(\Lambda_{6,6}^{2,4})\}| = \dfrac{2m + kl(l-1)}{2} = \dfrac{2(6) + 2(4)(3)}{2} =$*

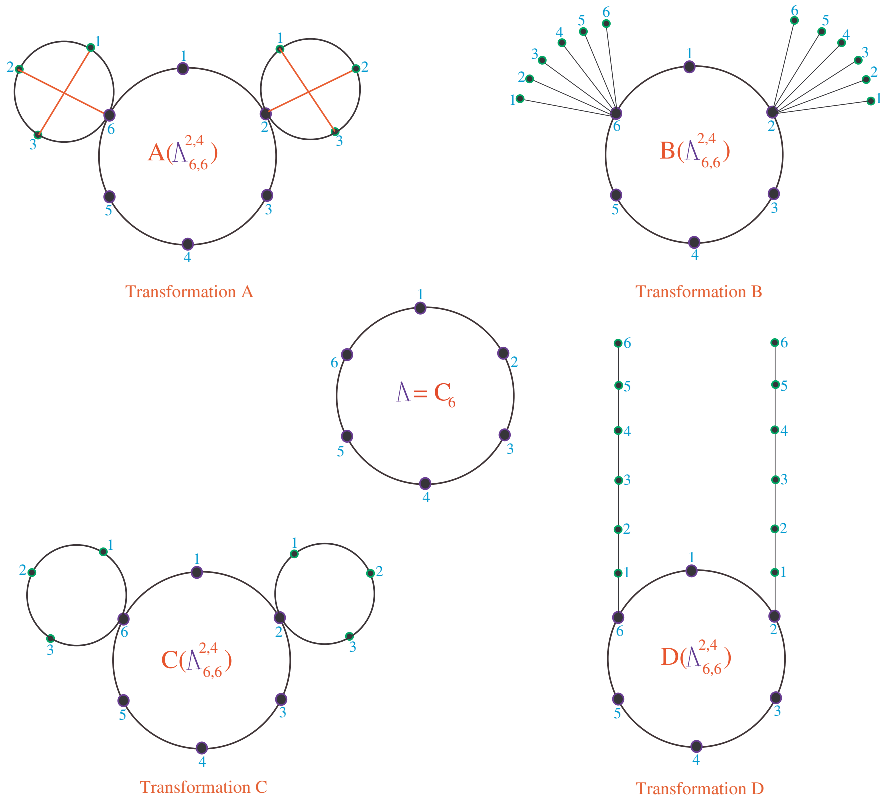

FIGURE 3. Transformation A, B, C and D for C_6

18. *And IDI for transformation B is,* $IDI\{B(\Lambda_{n,m}^{k,l})\} = IDI\{B(\Lambda_{6,6}^{2,4})\} = 2\left(\frac{1}{8}\right) + 4\left(\frac{1}{2}\right) + 12 = 14.25$. *It is easy to verify that* $IDI\{A(\Lambda_{n,m}^{k,l})\} \leq IDI\{B(\Lambda_{n,m}^{k,l})\}$. *The result obtained from Theorem 3.2, is given as*

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{B(\Lambda_{n,m}^{k,l})\} = k\left[\frac{1}{\Delta\Lambda + (l-1)} - \frac{l(l-1)}{2} - \frac{2}{2\Delta\Lambda + l(l-1)} + 1\right]$$

$$= 2\left[\frac{1}{2+(4-1)} - \frac{4(4-1)}{2} - \frac{2}{2 \times 2 + 4(4-1)} + 1\right] = -9.85 \leq 0$$

which is consistent with the aforementioned computations. For further details, see Figure 3. For further details, see Figure (3).

Example 3.4. *Let* $\Lambda = P_5$ *be a path graph containing* $n = 5$, $m = 4$ *vertices and edges, respectively. In* $\Lambda = P_5$ *minimum degree is* $\delta = 1$ *and maximum degree* $\Delta = 2$. *Consider* $k = 3$ *and* $l = 5$. *So* $|O\{A(\Lambda_{n,m}^{k,l})\}| = |O\{A(\Lambda_{5,4}^{3,5})\}| = n + k(l-1) = 5+$

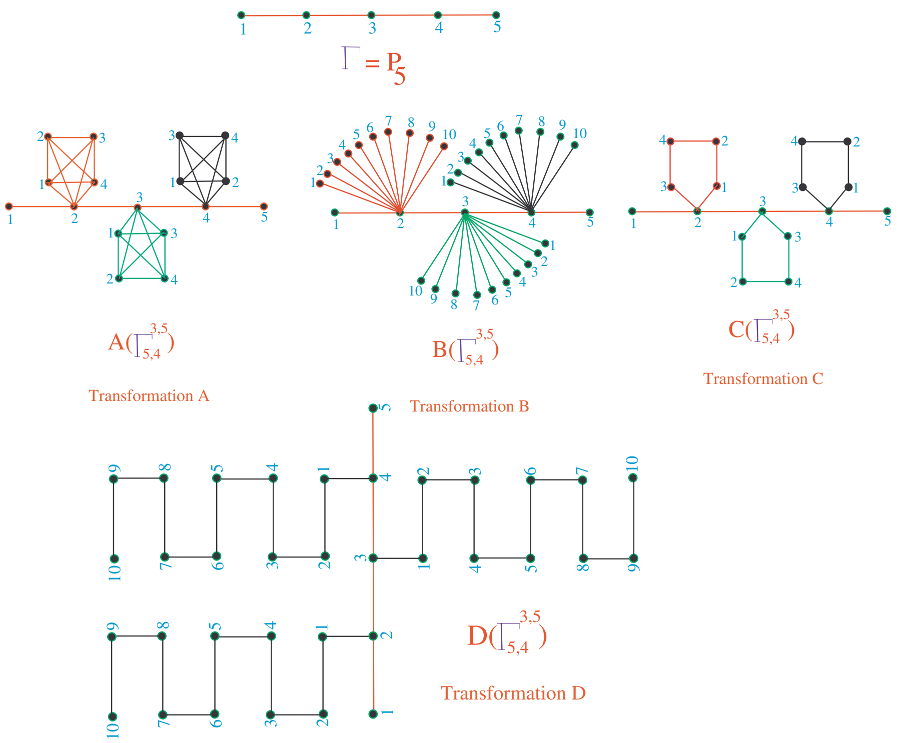

FIGURE 4. Transformation A, B, C and D for P_5

$3(4) = 17$ *and* $|E\{A(\Lambda^{k,l}_{n,m})\}| = |E\{A(\Lambda^{3,5}_{5,4})\}| = \dfrac{2m + kl(l-1)}{2} = \dfrac{2(4) + 3(5)(4)}{2} = 34$. *Now* $IDI\{A(\Lambda^{k,l}_{n,m})\} = IDI\{A(\Lambda^{3,5}_{5,4})\} = 12\left(\dfrac{1}{4}\right) + 3\left(\dfrac{1}{6}\right) + 2 = 5.5$. *For transformation B,* $|O\{B(\Lambda^{k,l}_{n,m})\}| = |O\{B(\Lambda^{3,5}_{5,4})\}| = \dfrac{2n + kl(l-1)}{2} = \dfrac{2(5) + 3(5)(4)}{2} = 35$ *and* $|E\{B(\Lambda^{k,l}_{n,m})\}| = |E\{B(\Lambda^{3,5}_{5,4})\}| = \dfrac{2m + kl(l-1)}{2} = \dfrac{2(4) + 3(5)(4)}{2} = 34$. *IDI for transformation B is,*
$IDI\{B(\Lambda^{k,l}_{n,m})\} = IDI\{B(\Lambda^{3,5}_{5,4})\} = 3\left(\dfrac{1}{12}\right) + 32 = 32.25$. *One can verified very easily that* $IDI\{A(\Lambda^{k,l}_{n,m})\} \leq IDI\{B(\Lambda^{k,l}_{n,m})\}$. *On the other hand result from Theorem (3.2) is* $-26.875 \leq 0$ *also satisfied.*

Transformation C

Let $A(\Lambda^{k,l}_{n,m})$ be a graph with k number of complete graphs of order l $(l \geq 3)$. Let $w_i \in V(\Lambda^{k,l}_{n,m})$ and form of w_i is,

$$\{(w_iu_i^1, w_iu_i^2, w_iu_i^3, ..., w_iu_i^{l-1}), (u_i^1u_i^2, u_i^1u_i^3, ..., u_i^1u_i^{l-1}), (u_i^2u_i^3, ..., u_i^2u_i^{l-1})$$

$$, ..., (u_i^{l-2}u_i^{l-1})\}$$

In transformation **C** complete graph will be replaced with Cycle graph and form of w_i will becomes,

$$\{w_iu_i^1, u_i^1u_i^2, u_i^2u_i^3, ..., u_i^{l-3}u_i^{l-2}, u_i^{l-2}u_i^{l-1}, u_i^{l-1}w_i\}$$

And

$$C(\Lambda_{n,m}^{k,l}) = A(\Lambda_{n,m}^{k,l}) + \sum_{j=1}^{k}\{w_iu_i^1, u_i^1u_i^2, u_i^2u_i^3, ..., u_i^{l-3}u_i^{l-2}, u_i^{l-2}u_i^{l-1}, u_i^{l-1}w_i\}$$

$$-\sum_{j=1}^{k}\{(u_i^1u_i^2, u_i^1u_i^3, ..., u_i^1u_i^{l-1}) + (w_iu_i^1, w_iu_i^2, w_iu_i^3, ..., w_iu_i^{l-1}) + (u_i^2u_i^3, ..., u_i^2u_i^{l-1})$$

$$+ ... + (u_i^{l-2}u_i^{l-1})\}$$

The cardinality of vertex and edge set of $C(\Lambda_{n,m}^{k,l})$ is $n + k(l-1)$ and $m + kl$, respectively.
Figure 5 presents the Transformation C.

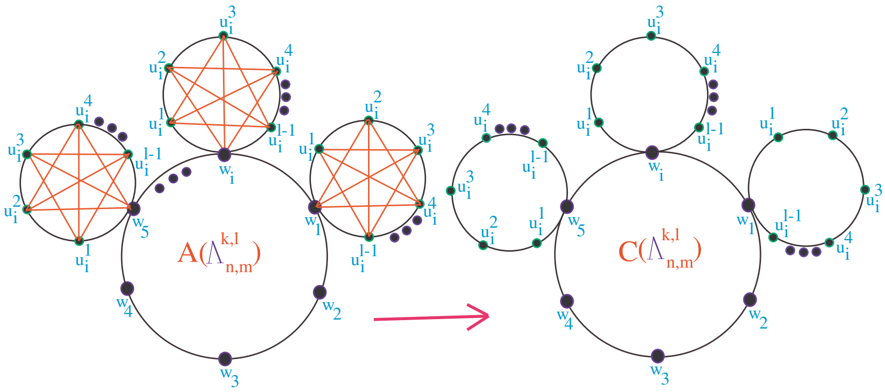

FIGURE 5. Transformation C

Theorem 3.5. *Let n, m be order and size of simple graph Λ, respectively. Let Δ and δ be its maximum and minimum degrees. And $A(\Lambda_{n,m}^{k,l})$ be the graph having k number of complete graphs attached to the fully connected vertices. Then*

$$IDI\{A(\Lambda_{n,m}^{k,l})\} \leq IDI\{C(\Lambda_{n,m}^{k,l})\}$$

Proof. We start the proof from Equation (1) presented below

$$IDI\{A(\Lambda_{n,m}^{k,l})\} = \frac{(n-k)}{d_v} + \frac{k}{d_v + (l-1)} + k$$

The transformation $A(\Lambda_{n,m}^{k,l})$ transformed into $C(\Lambda_{n,m}^{k,l})$ be a graph having k number of cycle graphs attached to the fully connected vertices. Then the setting up of $C(\Lambda_{n,m}^{k,l})$ provides,

$$|O\{C(\Lambda_{n,m}^{k,l})\}| = n + k(l-1) \text{ and } |E\{C(\Lambda_{n,m}^{k,l})\}| = m + kl.$$

The transformation $C(\Lambda_{n,m}^{k,l})$ exactly contained $(n-k)$ vertices of degree d_v, k vertices of degree (d_v+2) and vertices with degree 2 are $k(l-1)$. By definition of ID index,

$$IDI\{C(\Lambda_{n,m}^{k,l})\} = \sum_{v\in C(\Lambda_{n,m}^{k,l}),v=1}^{n-k} \frac{1}{d_v} + \sum_{v\in C(\Lambda_{n,m}^{k,l}),v=1}^{k} \frac{1}{d_v+2} + k(l-1)\frac{1}{2}$$

$$IDI\{C(\Lambda_{n,m}^{k,l})\} = \frac{(n-k)}{d_v} + \frac{k}{d_v+2} + \frac{k(l-1)}{2} \tag{5}$$

Subtracting Equation (5) from Equation (1) we have,

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{C(\Lambda_{n,m}^{k,l})\} = \frac{(n-k)}{d_v} + \frac{k}{d_v+(l-1)} + k - \frac{(n-k)}{d_v} - \frac{k}{d_v+2} - \frac{k(l-1)}{2}$$

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{C(\Lambda_{n,m}^{k,l})\} = k\left[\frac{1}{d_v+(l-1)} - \frac{1}{d_v+2} - \frac{(l-1)}{2} + 1\right] \tag{6}$$

Return to d_v as maximum degree Δ to minimize the relation in Equation (6),

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{C(\Lambda_{n,m}^{k,l})\} = k\left[\frac{1}{\Delta_\Lambda+(l-1)} - \frac{1}{\Delta_\Lambda+2} - \frac{(l-1)}{2} + 1\right] \leq 0 \tag{7}$$

Clearly, from Equation (7), we observe
$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{C(\Lambda_{n,m}^{k,l})\} \leq 0$ which implies $IDI\{A(\Lambda_{n,m}^{k,l})\} \leq IDI\{C(\Lambda_{n,m}^{k,l})\}$.

□

Example 3.6. *Let $\Lambda = C_6$ be a cycle graph. Here is $n = 6$, $m = 6$ and $\delta = \Delta = 2$. Consider $k = 2$ and $l = 4$. Clearly $|O\{A(\Lambda_{n,m}^{k,l})\}| = |O\{A(\Lambda_{6,6}^{2,4})\}| = n+k(l-1) = 6+2(3) = 12$ and $|E\{A(\Lambda_{n,m}^{k,l})\}| = |E\{A(\Lambda_{6,6}^{2,4})\}| = \frac{2m+kl(l-1)}{2} = \frac{2(6)+2(4)(3)}{2} = 18$. Now $IDI\{A(\Lambda_{n,m}^{k,l})\} = IDI\{A(\Lambda_{6,6}^{2,4})\} = 6\left(\frac{1}{3}\right) + 2\left(\frac{1}{5}\right) + 4\left(\frac{1}{2}\right) = 4.4$. For transformation C, $|O\{C(\Lambda_{n,m}^{k,l})\}| = |O\{C(\Lambda_{6,6}^{2,4})\}| = n+k(l-1) = 6+2(3) = 12$ and $|E\{C(\Lambda_{n,m}^{k,l})\}| = |E\{C(\Lambda_{6,6}^{2,4})\}| = m+kl = 6+2(4) = 14$. And IDI for transformation C is, $IDI\{C(\Lambda_{n,m}^{k,l})\} = IDI\{C(\Lambda_{6,6}^{2,4})\} = 10\left(\frac{1}{2}\right) + 2\left(\frac{1}{4}\right) = 5.5$. It is easy to verify that $IDI\{A(\Lambda_{n,m}^{k,l})\} \leq IDI\{C(\Lambda_{n,m}^{k,l})\}$. Whereas the result* *obtained from Theorem (3.5) is* $-1.1 \leq 0$ *also satisfied. For further information, see Figure (3).*

Example 3.7. *Let* $\Lambda = P_5$ *be a path graph containing* $n = 5$, $m = 4$ *vertices and edges, respectively. In* $\Lambda = P_5$ *minimum degree is* $\delta = 1$ *and maximum degree* $\Delta = 2$. *Consider* $k = 3$ *and* $l = 5$. *So* $|O\{A(\Lambda^{k,l}_{n,m})\}| = |O\{A(\Lambda^{3,5}_{5,4})\}| = n+k(l-1) = 5+3(4) = 17$ *and* $|E\{A(\Lambda^{k,l}_{n,m})\}| = |E\{A(\Lambda^{3,5}_{5,4})\}| = \dfrac{2m+kl(l-1)}{2} = \dfrac{2(4)+3(5)(4)}{2} = 34$. *Now* $IDI\{A(\Lambda^{k,l}_{n,m})\} = IDI\{A(\Lambda^{3,5}_{5,4})\} = 12\left(\dfrac{1}{4}\right) + 3\left(\dfrac{1}{6}\right) + 2 = 5.5$. *For transformation C,* $|O\{C(\Lambda^{k,l}_{n,m})\}| = |O\{C(\Lambda^{3,5}_{5,4})\}| = n+k(l-1) = 5+3(4) = 17$ *and* $|E\{C(\Lambda^{k,l}_{n,m})\}| = |E\{C(\Lambda^{3,5}_{5,4})\}| = m+kl = 4+3(5) = 19$. *The IDI for transformation C is,*
$IDI\{C(\Lambda^{k,l}_{n,m})\} = IDI\{C(\Lambda^{3,5}_{5,4})\} = 3\left(\dfrac{1}{4}\right)+2+6 = 8.75$. *One can verified very easily that* $IDI\{A(\Lambda^{k,l}_{n,m})\} \leq IDI\{C(\Lambda^{k,l}_{n,m})\}$. *On the other hand result from Theorem (3.5) is* $-3.375 \leq 0$ *also satisfied. For detailed information, see Figure (4).*

Transformation D
Let $A(\Lambda^{k,l}_{n,m})$ be a graph with k number of complete graphs of order l ($l \geq 3$). Let $w_i \in V(\Lambda^{k,l}_{n,m})$ and form of w_i is,

$$\{(w_iu_i^1, w_iu_i^2, w_iu_i^3, ..., w_iu_i^{l-1}), (u_i^1u_i^2, u_i^1u_i^3, ..., u_i^1u_i^{l-1}), (u_i^2u_i^3, ..., u_i^2u_i^{l-1}) \\ , ..., (u_i^{l-2}u_i^{l-1})\}$$

In transformation **D** complete graph will be converted into Path graph and form of w_i will becomes, $\{w_iu_i^1, u_i^1u_i^2, u_i^2u_i^3, ..., u_i^{l-3}u_i^{l-2}, u_i^{l-2}u_i^{l-1}\}$. We have,

$$\begin{aligned} D(\Lambda^{k,l}_{n,m}) =& A(\Lambda^{k,l}_{n,m}) + \sum_{j=1}^{k}\{w_iu_i^1, u_i^1u_i^2, u_i^2u_i^3, ..., u_i^{l-3}u_i^{l-2}, u_i^{l-2}u_i^{l-1}\} \\ & - \sum_{j=1}^{k}\{(w_iu_i^1, w_iu_i^2, w_iu_i^3, ..., w_iu_i^{l-1}) + (u_i^1u_i^2, u_i^1u_i^3, ..., u_i^1u_i^{l-1}) \\ & + (u_i^2u_i^3, ..., u_i^2u_i^{l-1}) + ... + (u_i^{l-2}u_i^{l-1})\} \end{aligned}$$

The set of vertex transformations D has cardinality $\dfrac{2n+kl(l-1)}{2}$ and size of D is $\dfrac{2m+kl(l-1)}{2}$, respectively.
Transformation D is described in Figure 6.

Theorem 3.8. *Let* Λ *be the simple graph on n vertices and m edges. Let* Δ *and* δ *be its maximum and minimum degrees, respectively. And* $A(\Lambda^{k,l}_{n,m})$ *be the graph that has k number of complete graphs attached to the fully connected vertices. Then*

$$IDI\{A(\Lambda^{k,l}_{n,m})\} \leq IDI\{D(\Lambda^{k,l}_{n,m})\}$$

Proof. Again, starting from Equation (1) as restated here,

$$IDI\{A(\Lambda_{n,m}^{k,l})\} = \frac{(n-k)}{d_v} + \frac{k}{d_v + (l-1)} + k \tag{8}$$

The transformation $A(\Lambda_{n,m}^{k,l})$ transformed into $D(\Lambda_{n,m}^{k,l})$ be a graph having k number of path graphs attached to the vertices. Then a lay out of $D(\Lambda_{n,m}^{k,l})$ produces,

$$|O\{D(\Lambda_{n,m}^{k,l})\}| = \frac{2n + kl(l-1)}{2} \text{ and } |E\{D(\Lambda_{n,m}^{k,l})\}| = \frac{2m + kl(l-1)}{2}.$$

The transformation $D(\Lambda_{n,m}^{k,l})$ consists of $(n-k)$ and k vertices of degrees d_v and $d_v + 1$, respectively. There exist at least k vertices of degree 1 and number of vertices having degree 2 are $k\left(\frac{l(l-1)}{2} - 1\right)$. We have,

$$IDI\{D(\Lambda_{n,m}^{k,l})\} = \sum_{v \in C(\Lambda_{n,m}^{k,l}), v=1}^{n-k} \frac{1}{d_v} + \sum_{v \in C(\Lambda_{n,m}^{k,l}), v=1}^{k} \frac{1}{d_v + 1} + k\left(\frac{\frac{l(l-1)}{2} - 1}{2}\right) + k$$

$$IDI\{D(\Lambda_{n,m}^{k,l})\} = \frac{(n-k)}{d_v} + \frac{k}{d_v + 1} + k\left(\frac{l(l-1) - 2}{4}\right) + k \tag{9}$$

Solving Equations (8) and (9) simultaneously, we get

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{D(\Lambda_{n,m}^{k,l})\} = \frac{(n-k)}{d_v} + \frac{k}{d_v + (l-1)} + k - \frac{(n-k)}{d_v} - \frac{k}{d_v + 1}$$
$$- k\left(\frac{l(l-1) - 2}{4}\right) - k$$

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{D(\Lambda_{n,m}^{k,l})\} = k\left[\frac{1}{d_v + (l-1)} - \frac{1}{d_v + 1} - \frac{l(l-1) - 2}{4}\right] \tag{10}$$

Put back d_v with maximum degree Δ Equation (10) to get the required result,

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{D(\Lambda_{n,m}^{k,l})\} = k\left[\frac{1}{\Delta_\Lambda + (l-1)} - \frac{1}{\Delta_\Lambda + 1} - \frac{l(l-1) - 2}{4}\right] \leq 0 \tag{11}$$

From Equation (11), We get

$$IDI\{A(\Lambda_{n,m}^{k,l})\} - IDI\{D(\Lambda_{n,m}^{k,l})\} \leq 0$$

which implies

$$IDI\{A(\Lambda_{n,m}^{k,l})\} \leq IDI\{D(\Lambda_{n,m}^{k,l})\}.$$

□

Example 3.9. *Let* $\Lambda = C_6$ *be a cycle graph. Here is* $n = 6$, $m = 6$ *and* $\delta = \Delta = 2$. *Consider* $k = 2$ *and* $l = 4$. *Clearly* $|O\{A(\Lambda_{n,m}^{k,l})\}| = |O\{A(\Lambda_{6,6}^{2,4})\}| = n + k(l-1) = 6 + 2(3) = 12$ *and* $|E\{A(\Lambda_{n,m}^{k,l})\}| = |E\{A(\Lambda_{6,6}^{2,4})\}| = \dfrac{2m + kl(l-1)}{2} =$

$\dfrac{2(6)+2(4)(3)}{2} = 18$. *Now* $IDI\{A(\Lambda^{k,l}_{n,m})\} = IDI\{A(\Lambda^{2,4}_{6,6})\} = 6\left(\dfrac{1}{3}\right) + 2\left(\dfrac{1}{5}\right) + 4\left(\dfrac{1}{2}\right) = 4.4$. *For transformation D,* $|O\{D(\Lambda^{k,l}_{n,m})\}| = |O\{D(\Lambda^{2,4}_{6,6})\}| = \dfrac{2n+kl(l-1)}{2} = \dfrac{2(6)+2(4)(3)}{2} = 18$ *and* $|E\{D(\Lambda^{k,l}_{n,m})\}| = |E\{D(\Lambda^{2,4}_{6,6})\}| = \dfrac{2m+kl(l-1)}{2} = \dfrac{2(6)+2(4)(3)}{2} = 18$. *And IDI for transformation D is,* $IDI\{D(\Lambda^{k,l}_{n,m})\} = IDI\{D(\Lambda^{2,4}_{6,6})\} = 14\left(\dfrac{1}{2}\right)+2\left(\dfrac{1}{3}\right)+2 = 9.6$. *It is easy to verify that* $IDI\{A(\Lambda^{k,l}_{n,m})\} \leq IDI\{D(\Lambda^{k,l}_{n,m})\}$. *Where as the result obtained from Theorem (3.8) is* $-5.2 \leq 0$ *also satisfied.*

For further information, see Figure (3).

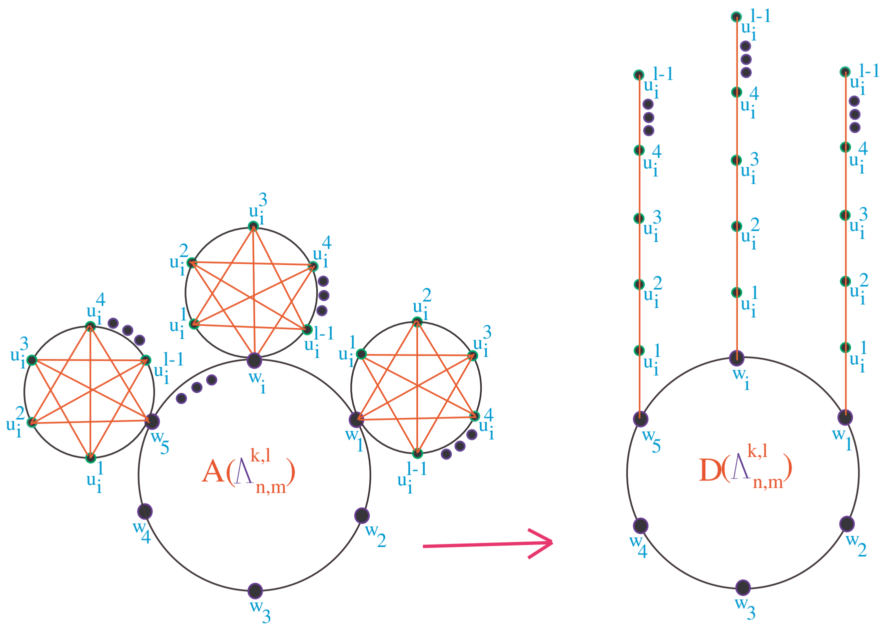

FIGURE 6. Transformation D

Example 3.10. *Let* $\Lambda = P_5$ *be a path graph containing* $n = 5$, $m = 4$ *vertices and edges, respectively. In* $\Lambda = P_5$ *minimum degree is* $\delta = 1$ *and maximum degree* $\Delta = 2$. *Consider* $k = 3$ *and* $l = 5$. *So* $|O\{A(\Lambda^{k,l}_{n,m})\}| = |O\{A(\Lambda^{3,5}_{5,4})\}| = n+k(l-1) = 5+3(4) = 17$ *and* $|E\{A(\Lambda^{k,l}_{n,m})\}| = |E\{A(\Lambda^{3,5}_{5,4})\}| = \dfrac{2m+kl(l-1)}{2} = \dfrac{2(4)+3(5)(4)}{2} =$

34. *Now* $IDI\{A(\Lambda_{n,m}^{k,l})\} = IDI\{A(\Lambda_{5,4}^{3,5})\} = 12\left(\frac{1}{4}\right) + 3\left(\frac{1}{6}\right) + 2 = 5.5$. *For transformation D,* $|O\{D(\Lambda_{n,m}^{k,l})\}| = |O\{D(\Lambda_{5,4}^{3,5})\}| = \frac{2n + kl(l-1)}{2} = \frac{2(5)+3(5)(4)}{2} = 35$ *and* $|E\{D(\Lambda_{n,m}^{k,l})\}| = |E\{D(\Lambda_{5,4}^{3,5})\}| = \frac{2m + kl(l-1)}{2} = \frac{2(4)+3(5)(4)}{2} = 34$. *The IDI for transformation D is,* $IDI\{D(\Lambda_{n,m}^{k,l})\} = IDI\{D(\Lambda_{5,4}^{3,5})\} = 27\left(\frac{1}{2}\right) + 3\left(\frac{1}{3}\right) + 5\left(\frac{1}{2}\right) = 17$. *One can verified very easily that* $IDI\{A(\Lambda_{n,m}^{k,l})\} \leq IDI\{D(\Lambda_{n,m}^{k,l})\}$. *On the other hand result from Theorem (3.8) is* $-14.125 \leq 0$ *also satisfied.*

Corollary 3.11. *Let* Λ *be the simple graph on* n *vertices and* m *edges and* $A(\Lambda_{n,m}^{k,l})$, $B(\Lambda_{n,m}^{k,l})$, $C(\Lambda_{n,m}^{k,l})$ *and* $D(\Lambda_{n,m}^{k,l})$ *are transformed graphs.Then*

$$IDI\{B(\Lambda_{n,m}^{k,l})\} \geq IDI\{C(\Lambda_{n,m}^{k,l})\}$$
$$IDI\{B(\Lambda_{n,m}^{k,l})\} \geq IDI\{D(\Lambda_{n,m}^{k,l})\}$$

Proof. Subtracting Equation (5) from Equation (2) we have,

$$IDI\{B(\Lambda_{n,m}^{k,l})\} - IDI\{C(\Lambda_{n,m}^{k,l})\} = k\left[\frac{2}{2d_v + l(l-1)} + \frac{l(l-1)}{2} - \frac{1}{d_v+2} - \frac{(l-1)}{2}\right] \tag{12}$$

Replace d_v with maximum degree Δ we get,

$$IDI\{B(\Lambda_{n,m}^{k,l})\} \geq IDI\{C(\Lambda_{n,m}^{k,l})\}.$$

Solving Equations (2) and (9) simultaneously,

$$IDI\{B(\Lambda_{n,m}^{k,l})\} - IDI\{D(\Lambda_{n,m}^{k,l})\} = k\left[\frac{2}{2d_v + l(l-1)} + \frac{l(l-1)}{2} - \frac{1}{d_v+1} - \left(\frac{l(l-1)-2}{4}\right) - 1\right] \tag{13}$$

By replacing d_v with Δ we get the required result,

$$IDI\{B(\Lambda_{n,m}^{k,l})\} \geq IDI\{D(\Lambda_{n,m}^{k,l})\}.$$

□

4. CONCLUDING REMARKS

The analysis of mathematical aspects involving topological indices is a partly open issue that "for which member from a family of graphs, a particular index, has extremal value?" In this paper, we probed the impact of IDI that drew attention through myriad conjectures produced by the software Graffiti concerning four new graph transformations. These transformations enable us to create new molecular structures, and IDI, being a good predictor of certain properties of octane isomers, can be used to study those properties for new complicated molecules. We provided a relation among IDI for four graph transformations namely A, B, C, and D. In particular, we concluded that the value of IDI remains lesser for transformation A as compared to transformations B, C, and D. Moreover, the value of IDI for transformation B will remain greater than both transformations C and D. Furthermore, result established are tested and evaluated on specific examples to check their accuracy. The analysis IDI indicates that graph A exhibits a higher structural contribution, branching, complexity, and connectivity compared to its transformations B, C, and D, while among the transformed graphs, B consistently maintains a greater IDI than both C and D. This ordering highlights the effect of different graph transformations on structural properties captured by the IDI and can guide the identification of extremal or structurally significant graphs.

Competing interests

The authors declare no conflict of interest.

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