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K-INVARIANT IDENTRIC MEAN LABELING OF SOME GRAPHS AND ANALYSIS OF GEPOTIDACIN

[1]SWATHI M, [2]SAMPATH KUMAR R, [3,†]NAGARAJA K M, [4]SANDEEP KUMAR AND [5]NARASIMHAN G

Abstract. A graph $G = (V, E)$ with p vertices and q edges is said to be K-Invariant identric mean graph, if it is possible to label the vertices $x \in V$ with distinct labels $f(x)$ from $k, k+1, k+2, \cdots, k+q$ in such a way that when each edge $e = uv$ is labeled with an induced mapping $f^* : E(G) \to N$ given by

$$f^*(e) = \left\lceil ef(u)f(v)\left(\frac{f(u)^{f(u)}}{f(v)^{f(v)}}\right)^{\frac{1}{f(v)-f(u)}}\right\rceil \text{ or} f^*(e) = \left\lfloor ef(u)f(v)\left(\frac{f(u)^{f(u)}}{f(v)^{f(v)}}\right)^{\frac{1}{f(v)-f(u)}}\right\rfloor$$

for every $x_ix_j \in V(G)$ and $x_i \neq x_j$ are not identical. This paper provides K-Invariant identric mean labeling of some graphs and represent the molecular structure of Gepotidacin as a chemical graph and analyze its topological features.

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Keywords and phrases. Graph, Labeling, Invariant identric Mean Graph, Cycle, bipartite, Triangular Graphs, Gepotidacin.

1. Introduction and preliminaries

Georghe Toader and Silvia Toader [17] made significant contributions to the study of Greek means, complementary means, and invariant means, along with several associated results. P. S. Bullen [1] provided an extensive account of different types of means and their wide-ranging applications. The fundamental concepts and terminology of graph theory used in this work are standard and can be found in [2, 3].

In the area of graph labeling, Somasundaram et al. [14] established that the geometric mean admits mean labeling for several classes of graphs, including paths, cycles, combs, and ladder graphs. Subsequent studies [4, 16], extended these results by showing that the harmonic mean satisfies mean labeling for duplication graphs, joint sum graphs, identification graphs, and certain snake graphs. Furthermore, Sampath Kumar R et al. [11], demonstrated that the Heron mean supports mean labeling for crown graphs, PnK1,2 and quadrilateral snake graphs. In [9, 12, 13], they also proved that centroidal means admit mean labeling for triangular snake graphs, double triangular snake graphs, and ladder graphs.

In addition, several researchers [7, 8, 10] have investigated labeling techniques based on the power exponential mean, invariant logarithmic mean, and contra-harmonic mean. Yegnanarayanan et al. [15, 18], further explored diverse applications of graph labeling, highlighting its importance in theoretical and applied contexts.

The invariant identric mean has also attracted attention in the literature. A brief discussion of this mean is provided by Bullen in his well-known work Handbook of

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Means and their Inequalities. For two positive real numbers the invariant identric mean is defined as

$$IIM(a,b) = eab\left(\frac{a^a}{b^b}\right)^{\frac{1}{b-a}}. \tag{1.1}$$

Motivated by earlier contributions in [5, 6, 19, 20], the present study introduces the concept of K-invariant identric mean labeling and develops this notion for certain classes of graphs.

Definition 1.1. [13] A ladder graph, denoted by L_n is a graph consisting of two parallel paths each with n vertices, where corresponding vertices of the two paths are joined by edges. It is isomorphic to the Cartisian product of a path P_n and a complete graph K_2. The ladder graph contains $2n$ vertices and $3n-2$ edges.

Definition 1.2. [13] A triangular ladder graph, denoted by TL_n, is constructed by taking a ladder graph L_n and adding an edge across each rectangular face to form a triangle. Each segment between the rungs of the ladder thus becomes a triangle, yielding a structure composed entirely of adjacent triangular faces. The graph has $2n$ vertices and $3n-1$ edges.

Definition 1.3. [13] A bipartite graph is a graph whose vertex set can be partitioned into two disjoint subsets such that no two vertices within the same subset are adjacent. A complete bipartite graph,denoted by $K_{m,n}$, is a bipartite graph in which each vertex of the first subset is connected to every vertex of the second subset. The graph contains $m+n$ vertices and mn edges.

Definition 1.4. [13] The graph $P_n \bigodot nk$ is the corona of a path graph P_n with nk isolated vertices, where each vertex of P_n is connected to k new pendant(isolated) vertices. This results in a graph where every vertex in the path P_n becomes the center of a star with k leaves.

Definition 1.5. [13] A Graph $G = (V, E)$ with p vertices and q edges is called a K-Invariant mean graph if there exists a vertex $f : V(G) \to N$ that assigns distinct lables from the set $\{k, k+1, k+2, ..., k+q\}$ to the vertices of G, where k is a fixed integer. Additionally, each edge $e = uv \in E(G)$ is assigned a label based on an induced mapping $f^* : E(G) \to N$, satisfying,

$$f^*(e) = \left\lceil ef(u)f(v)\left(\frac{f(u)^{f(u)}}{f(v)^{f(v)}}\right)^{\frac{1}{f(v)-f(u)}}\right\rceil, f^*(e) = \left\lfloor ef(u)f(v)\left(\frac{f(u)^{f(u)}}{f(v)^{f(v)}}\right)^{\frac{1}{f(v)-f(u)}}\right\rfloor$$

are all distinct.

Definition 1.6. [13] Let G be a labeled graph under a labeling L. *The density of a vertex* u, denoted by $L(u)$, is defined as the sum of the labels of all edges incident to u. Formally, $L(u) = \sum_{v \in N(u)} f(uv)$ where $N(u)$ denotes the neighbourhood of u, and $f(uv)$ represents the label assigned to the edge uv under the labeling L. Thus, the density of a vertex quantifies the total weight contributed by its incident edges.

2. K-Invariant identric mean labeling of a graph

In this section the K-Invariant identric mean labeling of a path related graphs like Quadrilateral snake, Ttriangular ladders, and ladder are discussed.

Theorem 2.1. *A ladder graph L_n is a K-invariant identric mean graph.*

Proof. Let $u_1, u_2 \ldots, u_n$ and $v_1, v_2 \ldots, v_2$ be the vertices of two paths P_n, and the ladder graph L_n is a graph obtained by connecting corresponding vertices of the two paths. The vertex set is $V(G) = \{u_k, v_k : 1 \leq k \leq n\}$ and the edge set is $E(G) = \{u_k u_{k+1}, v_k v_{k+1} : 1 \leq k \leq n-1\} \cup \{u_k v_k : 1 \leq k \leq n\}$. So that $|V(G)| = 2n$ and $|E(G)| = 2(n-1) + n = 3n - 2$. Define a function by $f : V(G) \to \{1, 2, \ldots, n\}$ by

$$f(u_i) = k + 6i - 5, \quad \text{and} \quad f(v_i) = k + 6i - 3, \quad 1 \leq i \leq m$$

For every distinct $x_i, x_j \in V(G)$ and $x_i \neq x_j$. The edges $\{x_i, y_j\}$are labeled by,

$$f^*(x_i y_j) = \left\lfloor ef(x_i)f(y_j) \left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}} \right)^{\frac{1}{f(y_j)-f(x_i)}} \right\rfloor, 1 \leq i \leq n-1;$$

or

$$f^*(x_i y_j) = \left\lceil ef(x_i)f(y_j) \left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}} \right)^{\frac{1}{f(y_j)-f(x_i)}} \right\rceil, 1 \leq i \leq n-1;$$

The edge $\{u_i, u_{i+1}\}$ is label by an induced function $f^*(u_i u_{i+1}) = k+6i-3, \quad 1 \leq i \leq n-1$; The edge $\{v_i, v_{i+1}\}$ is label by an induced function $f^*(v_i v_{i+1}) = k+6i-1, \quad 1 \leq i \leq n-1$; The edge $\{u_i, v_i\}$ is label by an induced function $f^*(u_i v_i) = k+6i-5, \quad 1 \leq i \leq n$; The resulting edges are distinct. Hence the Ladder graph L_n admits K-invariant identric mean labeling. Therefore the graph L_n is a K-invariant identric mean graph. □

Illustrations: 2.1 Consider a L_5 with 5 vertices. The 100-invariant identric mean labeling of this graph, along with the corresponding Python implementation and the resulting graphical output, are presented.

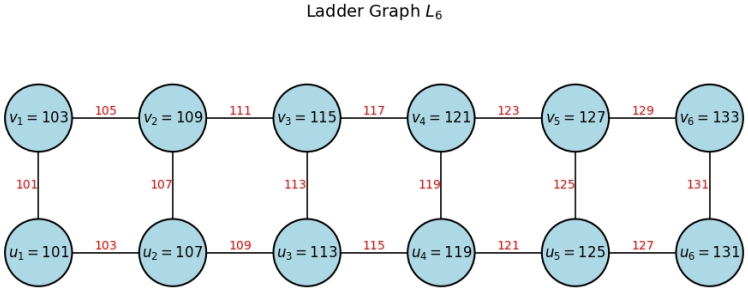


FIGURE 1. Ladder Graph L_6

Density of L_5 at different vertices: $\eta_L(u_1) = 204$, $\eta_L(u_2) = 319$, $\eta_L(u_3) = 337$, $\eta_L(u_4) = 355$, $\eta_L(u_5) = 246$, $\eta_L(v_1) = 206$, $\eta_L(v_2) = 323$, $\eta_L(v_3) = 341$, $\eta_L(v_4) = 359$, $\eta_L(v_5) = 248$.

Theorem 2.2. *A triangular ladder TL_n is an identric K-invariant mean graph.*

Proof. Let $u_1, u_2, u_3 \dots u_n$ and $v_1, v_2, v_3 \dots v_n$ be the vertices of two paths P_n, and the triangular ladder graph TL_n is a graph obtained by connecting the vertices of these two paths with vertical and diagonal edges. The vertex set is $V(G) = \{u_k, v_k : 1 \leq k \leq n\}$ and the edge set is $E(G) = \{u_k u_{k+1}, v_k v_{k+1} : 1 \leq k \leq n-1\} \cup \{u_k v_k : 1 \leq k \leq n\} \cup \{u_{k+1} v_k : 1 \leq k \leq n-1\}$. So that $|V(G)| = 2n$ and $|E(G)| = 2(n-1) + n + (n-1) = 4n-3$. Define a function $f : V(G) \to \{1, 2, \dots, n\}$ by

$$f(u_i) = k + 6i - 1, \quad 1 \leq i \leq n \quad \text{and} \quad f(v_i) = k + 6i - 5, \quad 1 \leq i \leq n$$

For every distinct $x_i, x_j \in V(G)$ and $x_i \neq x_j$. The edges $\{x_i, y_j\}$are labeled by,

$$f^*(x_i y_j) = \left\lfloor ef(x_i)f(y_j) \left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}} \right)^{\frac{1}{f(y_j)-f(x_i)}} \right\rfloor, 1 \leq i \leq n-1;$$

or

$$f^*(x_i y_j) = \left\lceil ef(x_i)f(y_j) \left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}} \right)^{\frac{1}{f(y_j)-f(x_i)}} \right\rceil, 1 \leq i \leq n-1;$$

The edge $\{u_i, u_{i+1}\}$ is label by an induced function $f^*(u_i u_{i+1}) = k+6i-1, \quad 1 \leq i \leq n-1$; The edge $\{v_i, v_{i+1}\}$ is label by an induced function $f^*(v_i v_{i+1}) = k+6i-3, \quad 1 \leq i \leq n-1$; The edge $\{u_i, v_i\}$ is label by an induced function $f^*(u_i v_i) = k+6i-4, \quad 1 \leq i \leq n$; The edge $\{u_i, v_{i+1}\}$ is label by an induced function $f^*(u_i v_{i+1}) = k + 6i - 1, \quad 1 \leq i \leq n-1$; The resulting edges are distinct. Hence the graph TL_n admits K-invariant identric mean labeling. Therefore the graph TL_n is a K-invariant identric mean graph. □

Illustrations: 2.2 Consider a TL_5 with 5 vertices. The 100-invariant identric mean labeling of this graph, along with the corresponding Python implementation and the resulting graphical output, are presented.

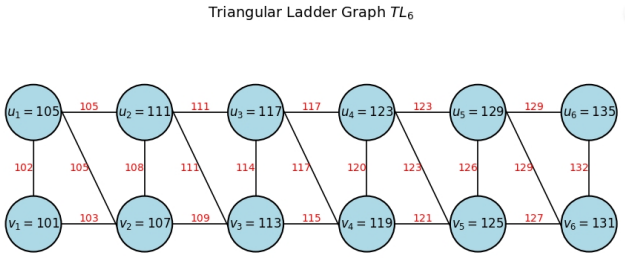


FIGURE 2. Triangular Ladder Graph TL_6

Density of TL_5 at different vertices: $\eta_L(u_1) = 314$, $\eta_L(u_2) = 439$, $\eta_L(u_3) = 463$, $\eta_L(u_4) = 487$, $\eta_L(u_5) = 251$, $\eta_L(v_1) = 205$, $\eta_L(v_2) = 426$, $\eta_L(v_3) = 449$, $\eta_L(v_4) = 473$, $\eta_L(v_5) = 370$.

Theorem 2.3. *A $P_n \bigodot 2k$ is a K-invariant identric mean graph.*

Proof. Let $u_1, u_2, \dots, u_n$ be the vertices of a path P_n. For each vertex u_k, attach two pendant vertices v_k and w_k such that $V(G) = \{u_k, v_k, w_k : 1 \leq k \leq n\}$ and the

edges set is $E(G) = \{u_k u_{k+1} : 1 \leq k \leq n-1\} \cup \{u_k v_k, u_k w_k : 1 \leq k \leq n\}$. Thus, $|V(G)| = 3n$ and $|E(G)| = (n-1) + 2n = 3n - 1$. Define a function $f : V(G) \to \{1, 2, \ldots, n\}$ by

$$f(u_i) = k + 6i - 4, \quad f(v_i) = k + 6i, \quad f(w_i) = k + 6i - 2, \quad 1 \leq i \leq n$$

For every distinct $x_i, x_j \in V(G)$ and $x_i \neq x_j$. The edges $\{x_i, y_j\}$are labeled by,

$$f^*(x_i y_j) = \left\lfloor ef(x_i)f(y_j)\left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}}\right)^{\frac{1}{f(y_j)-f(x_i)}} \right\rfloor, 1 \leq i \leq n-1;$$

or

$$f^*(x_i y_j) = \left\lceil ef(x_i)f(y_j)\left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}}\right)^{\frac{1}{f(y_j)-f(x_i)}} \right\rceil, 1 \leq i \leq n-1;$$

The edge $\{u_i, u_{i+1}\}$ is label by an induced function $f^*(u_i u_{i+1}) = k+6i-2, \quad 1 \leq i \leq n$; The edge $\{u_i, v_i\}$ is label by an induced function $f^*(u_i v_i) = k+6i-3, \quad 1 \leq i \leq n$; The edge $\{u_i w_i\}$ is label by an induced function $f^*(u_i w_i) = k + 6i - 4, \quad 1 \leq i \leq n$; The resulting edges are distinct. Hence the graph $P_n \bigodot 2k$ admits K-invariant identric mean labeling. Therefore, the graph $P_n \bigodot 2k$ is an identric mean graph invariant with K. □

Illustrations: 2.3 Consider a $P_6 \bigodot 2k$ with 6 vertices. The 100-invariant identric mean labeling of this graph, along with the corresponding Python implementation and the resulting graphical output, are presented.

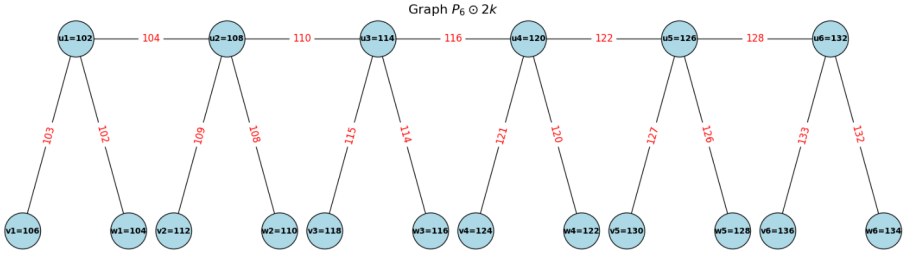


FIGURE 3. Graph $P_6 \bigodot 2k$

Density of $P_6 \bigodot 2(k)$ at different vertices: $\eta_L(u_1) = 309$, $\eta_L(u_2) = 431$, $\eta_L(u_3) = 455$, $\eta_L(u_4) = 479$, $\eta_L(u_5) = 503$, $\eta_L(u_6) = 393$, $\eta_L(v_1) = 103$, $\eta_L(v_2) = 109$, $\eta_L(v_3) = 115$, $\eta_L(v_4) = 121$, $\eta_L(v_5) = 127$, $\eta_L(v_6) = 133$, $\eta_L(w_1) = 102$, $\eta_L(w_2) = 108$, $\eta_L(w_3) = 114$, $\eta_L(w_4) = 120$, $\eta_L(w_5) = 126$, $\eta_L(w_6) = 132$.

Theorem 2.4. *A graph $T_n \bigodot K_1$ is a K-invariant identric mean graph.*

Proof. Let P_n be a path with n vertices $u_1, u_2, \ldots, u_n$ T_n be the triangular snake graph obtained by joining u_k with u_{k+1} and both are connected to the new vertex v_k, *i.e* it forms a cycle C_3 for every edge. Further the path P_n is attached to new vertices w_k *i.e* K_1 is inserted to P_n of all the cycle. The vertex set is defined by $V(G) = \{u_k, v_k, w_k : 1 \leq i \leq n\}$ and the edge set is given by $E(G) = \{u_k u_{k+1} : 1 \leq k \leq n-1\} \cup \{u_k v_k, u_k w_k : 1 \leq k \leq n\}$ so that $|V(G)| = 3n$ and $|E(G)| = 3n - 1$. Define $f : V(G) \to \{1, 2, \ldots, n\}$ by $f(u_i) = k + 5i, \quad 1 \leq i \leq n$; $f(v_i) = k + 5i -$

$1, \quad for \quad 1 \leq i \leq n-1$ and $f(w_i) = k+5i+1 \quad for \quad 1 \leq i \leq n$. For every distinct $x_i, x_j \in V(G)$ and $x_i \neq x_j$. The edges $\{x_i, y_j\}$are labeled by,

$$f^*(x_i y_j) = \left\lfloor ef(x_i)f(y_j)\left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}}\right)^{\frac{1}{f(y_j)-f(x_i)}}\right\rfloor, 1 \leq i \leq n-1; \text{ or}$$

$$f^*(x_i y_j) = \left\lceil ef(x_i)f(y_j)\left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}}\right)^{\frac{1}{f(y_j)-f(x_i)}}\right\rceil, 1 \leq i \leq n-1;$$

The edge $\{u_i, u_{i+1}\}$ is label by an induced function $f^*(u_i u_{i+1}) = k+5i+2, \quad 1 \leq i \leq n-1$; The edge $\{u_i, v_i\}$ is label by an induced function $f^*(u_i v_i) = k+5i-1, \quad 1 \leq i \leq n-1$; The edge $\{u_{i+1} v_i\}$ is label by an induced function $f^*(u_{i+1} v_i) = k+5i+1, \quad 1 \leq i \leq n-1$; The edge $\{u_i, w_i\}$ is label by an induced function $f^*(u_i w_i) = k+5i, \quad 1 \leq i \leq n$; The resulting edges are distinct. Hence the graph $T_n \bigodot K_1$ admits K-invariant identric mean labeling. Therefore the graph $T_n \bigodot K_1$ is a K-invariant identric mean graph. □

Illustrations: 2.4 Consider a $T_5 \bigodot K_1$ with 5 vertices. The 100-invariant identric mean labeling of this graph, along with the corresponding Python implementation and the resulting graphical output, are presented.

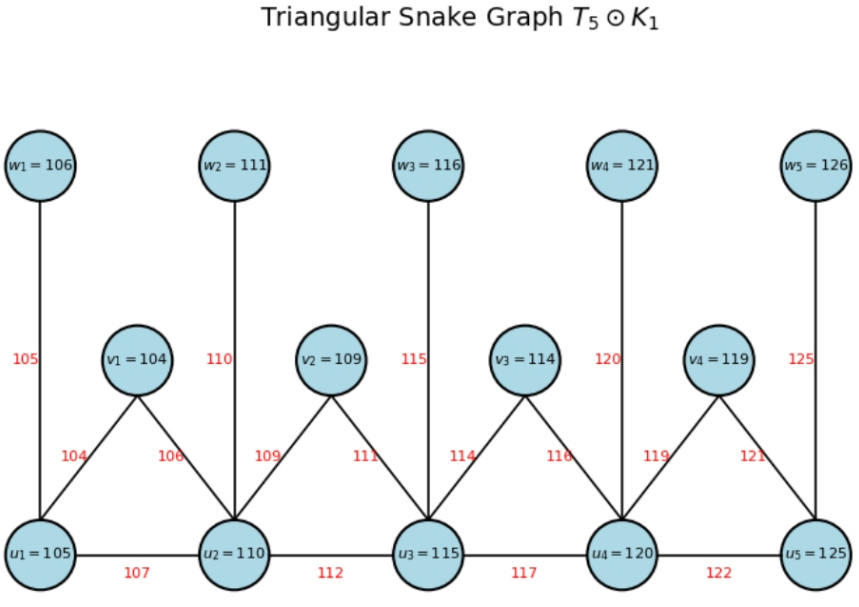


FIGURE 4. Triangular Snake Graph $T_5 \bigodot K_1$

Density of $T_4 \bigodot K_1$ at different vertices: $\eta_L(u_1) = 105$, $\eta_L(u_2) = 110$, $\eta_L(u_3) = 115$, $\eta_L(u_4) = 120$, $\eta_L(u_5) = 125$, $\eta_L(v_1) = 210$, $\eta_L(v_2) = 220$, $\eta_L(v_3) = 230$, $\eta_L(v_4) = 240$, $\eta_L(w_1) = 316$, $\eta_L(w_2) = 544$, $\eta_L(w_3) = 569$, $\eta_L(w_4) = 584$, $\eta_L(w_5) = 368$.

Theorem 2.5. *The $k_{m,n}$ graph is a K-invariant identric mean graph.*

Proof. Let $u_1, u_2, \ldots, u_m$ and $v_1, v_2, \ldots, v_n$ be the vertices of the two disjoint sets of a complete bipartite graph $K_{m,n}$. The vertex set is $V(G) = \{u_i, v_j : 1 \leq i \leq m, 1 \leq j \leq n\}$ and the edge set is $E(G) = \{u_i v_j : 1 \leq i \leq m, 1 \leq j \leq n\}$ so that $|V(G)| = m + n$ and $|E(G)| = mn$. Define $f : V(G) \to \{1, 2, \ldots, (m+n)\}$ as $f(u_i) = k + 4i \quad$ where $i = \{1, 8, 16, \ldots, 7m - 6\}$, $f(v_i) = k + 4i + 10, \quad 1 \leq i \leq n$. For every distinct $x_i, x_j \in V(G)$ and $x_i \neq x_j$. The edges $\{x_i, y_j\}$are labeled by,

$$f^*(x_i y_j) = \left\lfloor ef(x_i)f(y_j)\left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}}\right)^{\frac{1}{f(y_j)-f(x_i)}} \right\rfloor, 1 \leq i \leq n-1;$$

or

$$f^*(x_i y_j) = \left\lceil ef(x_i)f(y_j)\left(\frac{f(x_i)^{f(x_i)}}{f(y_j)^{f(y_j)}}\right)^{\frac{1}{f(y_j)-f(x_i)}} \right\rceil, 1 \leq i \leq n-1;$$

The edge $\{u_i, v_j\}$ is label by an induced function: $f^*(u_i v_j) = \begin{cases} k + 2j + 6, if & i = 1 \\ k + 2j + 21, if & i = 2 \end{cases}$ for $1 \leq j \leq n$;

The resulting edges are distinct. Hence the $K_{m,n}$-graph admits K-invariant identric mean labeling. Therefore the complete bipartite graph $K_{m,n}$ is a K-invariant identric mean graph. □

Illustrations: 2.5 Consider a complete bipartite graph $K_{2,4}$. The 100-invariant identric mean labeling of this graph, along with the corresponding Python implementation and the resulting graphical output, are presented.

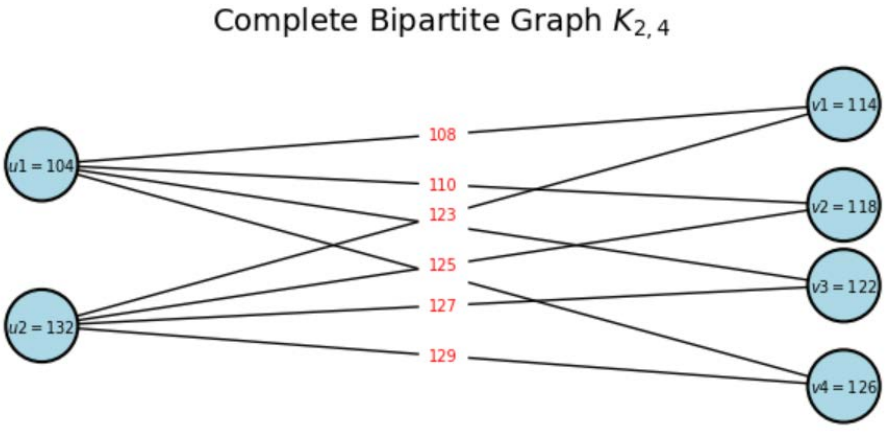


FIGURE 5. complete bipartite graph $K_{2,4}$

Density for $K_{2,4}$ at different vertices: $\eta_L(u_1) = 915$, $\eta_L(u_2) = 1040$, $\eta_L(v_1) = 231$, $\eta_L(v_2) = 235$, $\eta_L(v_3) = 239$, $\eta_L(v_4) = 243$, $\eta_L(v_5) = 246$, $\eta_L(v_6) = 250$, $\eta_L(v_7) = 254$, $\eta_L(v_8) = 257$.

3. Topological Indices

In this section degree based topological indices like Squared Index, Sum Index,Product Index and Nirmala Index of the above discussed graphs are projected.

Graph(G)	Squared Index(SQ)	Product Index(PI)	Sum Index(SI)	Nirmala Index(NI)
Ladder Graph(L_n)	$9n-20$	$\frac{27n}{2}-22$	$9n-8$	$\sqrt{9n-8}$
Triangular ladder(TL_n)	$16n-38$	$32n-52$	$16n-14$	$\sqrt{16n-14}$
$P_n \bigodot 2k$	$9n-14$	$12n-12$	$9n+4$	$\sqrt{9n+4}$
$T_5 \bigodot k1$	$\frac{39n}{2}-54$	$25n-32$	$15n-12$	$\sqrt{15n-12}$
$K_{2,4}$	$8m+2n$	$4mn$	$2m+n$	$\sqrt{2m+n}$

Table 1. Topological Indices

3.1. **Topological Index Analysis of Gepotidacin.** Gepotidacin (PubChem CID: 9805498) is a novel, first-in-class antibacterial agent belonging to the triazaacenaphthylene class. It exhibits a distinctive mechanism of action by selectively inhibiting bacterial DNA gyrase and topoisomerase IV, thereby differentiating it from conventional fluoroquinolone antibiotics. Owing to this unique mode of action, Gepotidacin has shown promising activity against a range of pathogens, including multidrug-resistant bacterial strains.

Currently, Gepotidacin is under investigation for the treatment of uncomplicated urinary tract infections (UTIs) and other bacterial infections. As of 2023, it has successfully completed Phase III clinical trials and has received regulatory recognition from the U.S. Food and Drug Administration under the Qualified Infectious Disease Product (QIDP) designation, although full regulatory approval is still pending.

In the present study, the molecular structure of Gepotidacin is modeled as a chemical graph, where atoms are represented as vertices and bonds as edges. A graph-theoretical approach is employed to examine its structural properties through the computation of several topological indices, including the Sum Index, Squared Index, Product Index, and Nirmala Index. These indices provide quantitative measures of molecular structure, offering insights into the complexity and potential biological activity of the compound.

Graph(G)	Squared Index(SQ)	Product Index(PI)	Sum Index(SI)	Nirmala Index(NI)
Gepotidacin	93	112.5	93	9.644

Table 2. Topological Indices of Gepotidacin

The calculated topological indices of Gepotidacin (Table 2) namely the Squared Index, Product Index, Sum Index and Nirmala Index numerically represent the structural complexity and molecular connectivity of the compound. Such indices can aid in virtual screening, molecular comparison, and rational drug design.

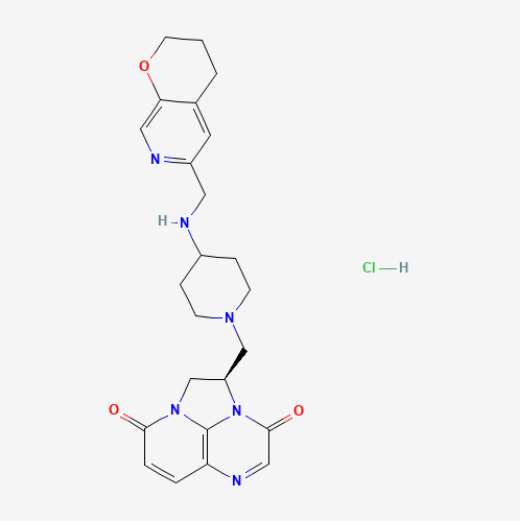


FIGURE 6. Gepotidacin

4. Conclusion

This paper presents a systematic investigation of the structural and topological characteristics of K-invariant identric graphs. By analyzing graph density alongside prominent topological descriptors such as the Sum Index, Squared Index, Product Index, and Nirmala Index, a foundational framework has been established for understanding their mathematical properties. These indices serve as effective quantitative measures, offering deeper insight into the intrinsic structure and behavior of such graphs.

To highlight the practical applicability of these concepts, the developed methodology was applied to the molecular graph of Gepotidacin, a recently investigated antibacterial agent. This application demonstrates the usefulness of topological indices in chemical graph analysis and underscores the potential of linking abstract graph-theoretical constructs with molecular structure characterization.

The present work provides an initial contribution toward the integration of topological graph theory with chemical graph theory. Future studies may extend these techniques to wider classes of molecular structures, enhance predictive approaches for physicochemical and pharmacological properties, and further examine the relationship between graph invariants and biological activity. Consequently, this research opens avenues for interdisciplinary advancements at the interface of mathematics and chemistry.

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[1, 2 & 5] Department of Mathematics, RNS Institute of Technology, Bangalore-560098, India., and affiliated to Visvesvaraya Technological University, Belagavi-590018.
Email address: swathimanjunath.56@gmail.com
Email address: r.sampathkumar1967@gmail.com,
Email address: narasimhan.guru@gmail.com

[3,†], Corresponding Author, Department of Mathematics, JSS Academy of Technical Education, Bangalore-560060, India., and affiliated to Visvesvaraya Technological University, Belagavi-590018.
Email address: nagkmn@gmail.com

[4] Department of Mathematics and Statistics, M S Ramaiah University of Applied Sciences, Bangalore-560058, India.
Email address: skumars1504@gmail.com