

Analytical Study of Distance-Based Topological Indices for the Cluster Product of K_m and P_n

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ABSTRACT

A topological index is an analytically derived numerical quantity that characterizes the structural properties of a graph. These indices play a crucial role in chemical graph theory and quantitative structure–property/activity relationship (QSPR/QSAR) studies. In this paper, we investigate several distance-based topological indices and clusters, including the Wiener index (W), Hyper-Wiener index (WW), Harary index (H), Reciprocal Complementary Wiener index (RCW), Sum Connectivity Index (SCI), Batschelet Index (B), Reverse Wiener index (Λ), Reciprocal Reverse Wiener index ($R\Lambda(G)$).

Keywords: Wiener index, Hyper-Wiener Index, Harary Index, Reciprocal Complementary Wiener Index, Sum Connectivity Index, Batschelet Index, Reverse Wiener Index, Reciprocal Reverse Wiener Index and Cluster Product.

Mathematics Subject Classification (MSC) 2020: 05C76, 05C10, 05C38.

1. Introduction

Graph theory, a fundamental area of mathematics, is extensively applied in many scientific and engineering fields. Basically, a graph $G(V, E)$ consists of vertices connected by edges, where vertices represent nodes and edges denote the links between them [1,2]. Edges connected to a vertex are called the degree of the vertex and the shortest length of a connected series of vertices forming a path is called the distance of the graph and is denoted by $d(u, v)$. Topological indices, which are numerical values associated with chemical graphs, correlate with the biological activities and various physical properties of the molecules they represent. [3]. Distance-based topological indices, which incorporate the notion of distance between vertices in a network, are among these indices that are essential for comprehending the structural characteristics of chemical compounds. Total graphs provide a holistic view of chemical network analysis by including both vertex and edge components in a single framework [4].

The fields of graph theory develop various applications in the field of chemistry by using incident or adjacent matrices. In the respective years of 2001 [5] and 2002 [6], Dobrynin and Bonchek studied Wiener index for predicting the molecular ability of a chemical structure. Hosoya and Harary polynomials for graphs are studied by Chen et al. and others for targeting a powerful tool for proving modeling and analyzing molecular structures [7, 8]. [9] contributed to the field with research on distance-based indices in Parikh word representable graphs, while Malik et al. [10, 11] highlighted these indices and related graph entropies in fractal-like molecular graphs.

Comparative study of topological indices for total graphs based on distance offers important new information about the fundamental characteristics of chemical structures. This paper explores a number of well-known distance-based indices,

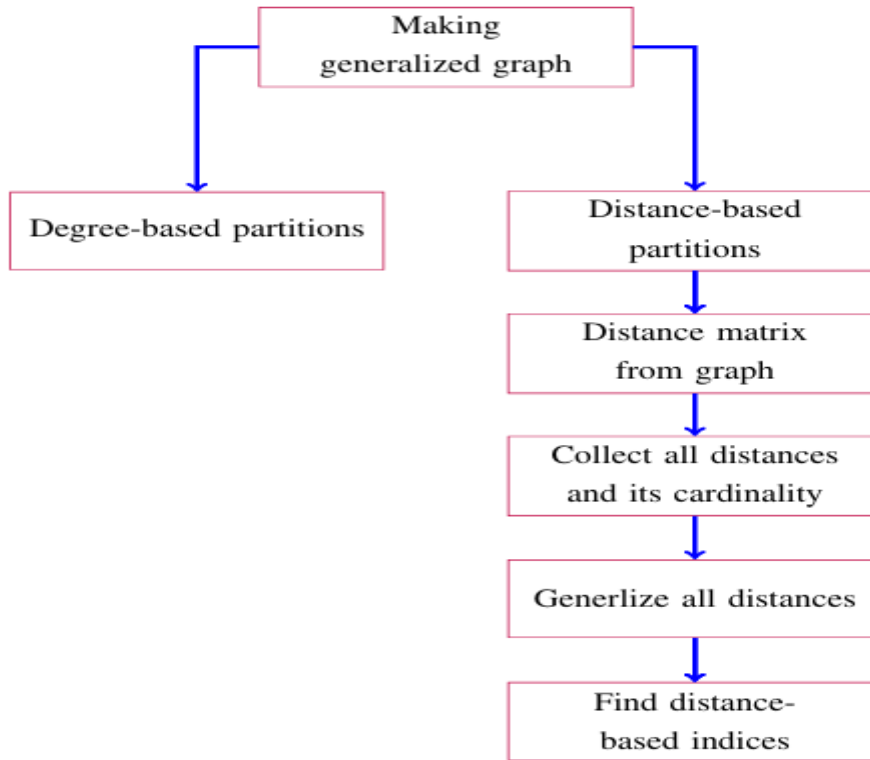
such as the hyper-Wiener index, the Harary index, and the Wiener index [12, 13]. In-depth comparisons of these indices are provided in this research, along with information on their advantages, disadvantages, and suitability for various kinds of chemical networks. Our goal in doing this study is to advance the field of chemical graph theory by offering a solid foundation for the use of distance-based topological indices in complete graph analysis. On sequent, this facilitates the forecasting and enhancement of molecular characteristics for many scientific and industrial uses. We compute the following distance-based topological indices shown in Table 1. In this methodology, we first obtain the desired generalized graph where structure of the graph is in accordance with the required size of the graph. After the graph is created, it is necessary to calculate distance matrix which contains the shortest path distance between each pair of identified vertices. Then we create a vector with all possible distances in it and find their frequencies, that is, the number of times each distinct distance appears in the matrix. This step is generalized according to the size of the graph to ensure scalability for any degree of the graph. These collected distances are organized in the tabular form for easier reference as well as for purpose of further computation of the cardinalities. Employing the table of generalized distances, we calculate various distance-based topological indices including the Wiener index, hyper-Wiener index, Harary index, etc. For every index, the distances and the count of the units are substituted in the formulas equal to the indices chosen. This approach gives a method of quantifying the graph through distance-based features in a consistent and generalized manner irrespective of the size of the graph. The flowchart of the methodology is shown in Figure 1.

Only finite, undirected, connected and simple graphs are examined in this study. The numbers of vertices and edges in a graph $G = (V, E)$ are represented by $|V(G)|$ and $|E(G)|$, respectively. If there is no ambiguity in the graph under discussion, we simply denote it by $d(u, v)$. If $u, v \in V(G)$, the length of the shortest distance between u and v in G is given by $dG(u, v)$. A vertex u in a graph G has eccentricity $e(u) = \max\{d(u, v) : v \in V(G)\}$. $r = rad(G) = \min\{e(v) : v \in V(G)\}$ is the radius (or, more accurately, the diameter) of G (resp. $d = diam(G) = \max\{e(v) : v \in V(G)\}$).

Topological indices derive from graph theory, which represents molecules as graphs. Atoms correspond to vertices, whereas bonds correspond to edges. Distance based topological indices are topological indices that are calculated from the distances between vertices (atoms) in a molecular network. These indices concentrate on the graph structure by measuring the distance between atoms, which can offer information about numerous chemical characteristics and behaviors.

Table 1: Distance-based indices

| Indices | Notations | Formula |
|--|---------------|---|
| Wiener index [14] | $W(G)$ | $W(G) = \sum_{\{u,v \in V(G)\}} d(u, v)$ |
| Hyper-Wiener index [15] | $WW(G)$ | $WW(G) = \frac{1}{2} \sum_{\{u,v \in V(G)\}} d(u, v) + d(u, v)^2$ |
| Harary index [16] | $H(G)$ | $H(G) = \sum_{\{u,v \in V(G)\}} \frac{1}{d(u, v)}$ |
| Reciprocal Complementary Wiener index [17] | $RCW(G)$ | $RCW(G) = \sum_{\{u,v \in V(G)\}} \frac{1}{(d + 1 - d(u, v))}$ |
| Sum Connectivity index [18] | $SCI(G)$ | $SCI(G) = \sum_{\{u,v \in V(G)\}} \frac{1}{(d(u, v) + 1)}$ |
| Batschelet index [19] | $B(G)$ | $B(G) = \sum_{\{u,v \in V(G)\}} d(u, v)^2$ |
| Reverse Wiener index [20] | $\Lambda(G)$ | $\Lambda(G) = \frac{n(n-1)d}{2} - W(G)$ |
| Reciprocal Reverse Wiener index [21] | $R\Lambda(G)$ | $R\Lambda(G) = \sum_{\{u,v \in V(G)\}} \frac{1}{(d - d(u, v))}$ |



A graph is considered complete when each vertex is connected to every other vertex. A complete graph of r vertices is denoted by K_r .

An open walk that does not revisit any vertex is known as a path, often represented by P . A path graph consisting of s vertices is referred to as P_s . In this paper we calculate $W(G)$, $WW(G)$, $H(G)$, $RCW(G)$, $SCI(G)$, $B(G)$, $\Lambda(G)$ and $R \wedge(G)$ of cluster product of complete with path graphs.

Definition 1.1. [22] *The cluster of $G\{H\}$, formed from two graphs G and H , is defined as the graph constructed by selecting one vertex from G and creating $|V(G)|$ copies of the rooted graph H , with the root of the i^{th} vertex in G connected to every vertex in the j^{th} copy of H .*

See Figure 2

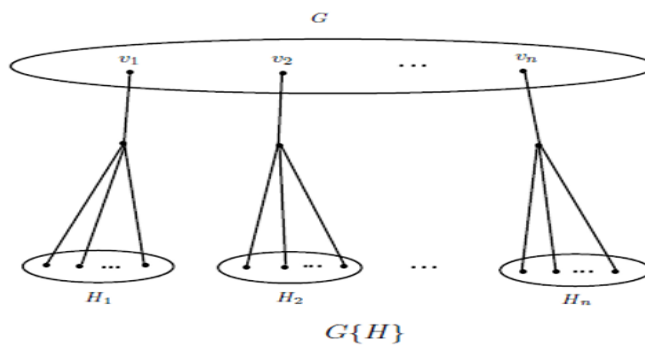


Figure 2: Cluster Product of two graphs G and H

2. Main Results

In this section, we calculate several distance-based topological indices for the cluster product of $K_r\{P_s\}$.

Definition 2.1. The graph that results from taking r vertex of P_s , one vertex of K_r , and linking each vertex in the i^{th} vertex of P_s , to every vertex in the j^{th} vertex of K_r , is known as the cluster product of complete and path graphs, K_r and P_s .

Here $diam(G) = 5$ and the distance between any pair of vertices, from $1, 2, \dots, diam(G)$.

The count of vertex pairs at distance 1 is expressed as $\frac{r(r-1)}{2} + 2rs$.

For distance 2, it is $rs(r-1) + \frac{r(s-1)(s-2)}{2} + rs$.

At distance 3, the count is $\frac{r(r-1)}{2} + rs(r-1)$.

The number of pairs at distance 4 equals $rs(r-1)$.

Lastly, for $r \geq 2$ and $s \geq 2$, the number of vertex pairs at distance 5 is given by $\frac{r(r-1)s^2}{2}$.

These expressions form the basis for deriving subsequent theorems. Then,

Theorem 2.1. Let K_r and P_s be complete and the path graph with $r \geq 2$ and $s \geq 2$. Then

$$(i) W(K_r\{P_s\}) = \left(\frac{r(r-1)}{2}\right) [5s^2 + 14s + 8] + r [s^2 + s + 2]$$

$$(ii) WW(K_r\{P_s\}) = \left(\frac{r(r-1)}{2}\right) [15s^2 + 32s + 13] + r \left[\frac{3s^2 + s + 6}{2}\right]$$

Proof. Let K_r and P_s be complete and the path graph with $r, s \geq 2$, then

(i) By the definition of Wiener index

$$\begin{aligned} W(K_r\{P_s\}) &= \sum d(u, v), \quad u, v \in V(G) \\ &= \left[\frac{r(r-1)}{2} + 2rs\right] (1) + \left[r(r-1) + \frac{r(s-1)(s-2)}{2} + rs\right] (2) \\ &\quad + \left[\frac{r(r-1)(2s+1)}{2}\right] (3) + [rs(r-1)] (4) + \left[\frac{r(r-1)s^2}{2}\right] (5) \\ &= \frac{r(r-1)}{2} + 2rs + 2r(r-1) + r(s-1)(s-2) + 2rs + \frac{3r(r-1)(2s+1)}{2} + 4rs(r-1) \\ &\quad + \frac{5r(r-1)s^2}{2} \\ &= \left(\frac{r(r-1)}{2}\right) [1 + 4 + 3(2s+1) + 8s + 5s^2] + 4rs + r(s^2 - 3s + 2) \\ &= \left(\frac{r(r-1)}{2}\right) [5s^2 + 14s + 8] + r[s^2 + s + 2] \end{aligned}$$

(ii) By the definition of Hyper-Wiener index

$$\begin{aligned} WW(K_r\{P_s\}) &= \frac{1}{2} \sum [d(u, v) + d(u, v)^2], \quad u, v \in V(G) \\ &= \frac{1}{2} \left\{ \left[\frac{r(r-1)}{2} + 2rs\right] (1 + 1^2) + \left[r(r-1) + \frac{r(s-1)(s-2)}{2} + rs\right] (2 + 2^2) \right. \\ &\quad \left. + \left[\frac{r(r-1)(2s+1)}{2}\right] (3 + 3^2) + [rs(r-1)] (4 + 4^2) + \left[\frac{r(r-1)s^2}{2}\right] (5 + 5^2) \right\} \\ &= 1/2 \left\{ \left[\frac{r(r-1)}{2} + 2rs\right] (2) + \left[r(r-1) + \frac{r(s-1)(s-2)}{2} + rs\right] (6) \right. \\ &\quad \left. + \left[\frac{r(r-1)(2s+1)}{2}\right] (12) + [rs(r-1)] (20) + \left[\frac{r(r-1)s^2}{2}\right] (30) \right\} \\ &= \frac{1}{2} \{ r(r-1) + 4rs + 6r(r-1) + 3r(s-1)(s-2) + 6rs + 6r(r-1)(2s+1) + 20rs(r-1) \\ &\quad + 15r(r-1)s^2 \} \\ &= \frac{r(r-1)}{2} + 2rs + 3r(r-1) + \frac{3}{2}r(s-1)(s-2) + 3rs + 3r(r-1)(2s+1) + 10rs(r-1) \\ &\quad + \frac{15}{2}r(r-1)s^2 \\ &= \left(\frac{r(r-1)}{2}\right) [1 + 6 + 6(2s+1) + 20s + 15s^2] + 5rs + \frac{3}{2}r(s^2 - 3s + 2) \\ &= \left(\frac{r(r-1)}{2}\right) [7 + 12s + 6 + 20s + 15s^2] + r \left[5s + \frac{3}{2}(s^2 - 3s + 2)\right] \\ &= \left(\frac{r(r-1)}{2}\right) [15s^2 + 32s + 13] + r \left[\frac{(3s^2 + s + 6)}{2}\right] \end{aligned}$$

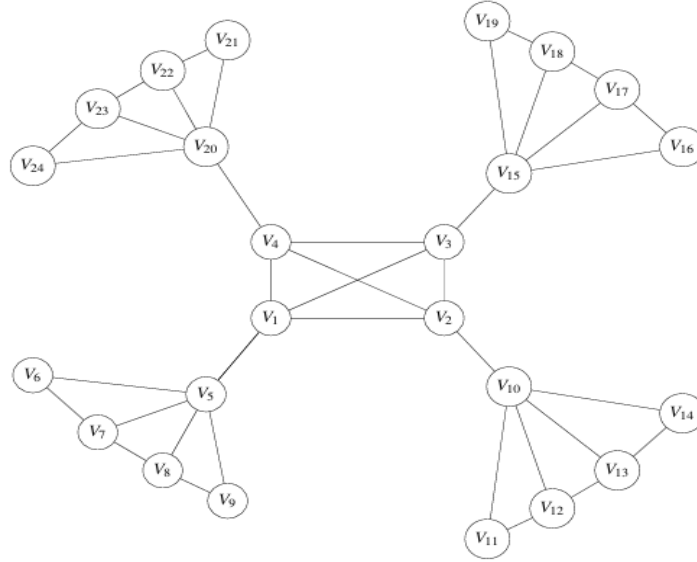


Figure 3: $K_r\{P_s\}$

Theorem 2.2. Let K_r and P_s be complete and the path graph with $r \geq 2$ and $s \geq 2$. Then

$$(i) H(K_r\{P_s\}) = \left(\frac{r(r-1)}{2}\right) \left[\frac{(6s^2 + 35s + 70)}{30}\right] + r \left[\frac{(s^2 + 7s + 2)}{4}\right]$$

$$(ii) RCW(K_r\{P_s\}) = \left(\frac{r(r-1)}{2}\right) \left[\frac{(30s^2 + 50s + 31)}{30}\right] + r \left[\frac{(5s^2 + 11s + 10)}{40}\right]$$

Proof. Let K_r and P_s be as specified earlier, then

(i) By the definition of Harary index

$$H(K_r\{P_s\}) = \sum_{u,v \in V(G)} \frac{1}{d(u,v)}$$

$$= \left\{ \left[\frac{r(r-1)}{2} + 2rs \right] \left(\frac{1}{1}\right) + \left[r(r-1) + \frac{r(s-1)(s-2)}{2} + rs \right] \left(\frac{1}{2}\right) \right.$$

$$\quad \left. + \left[\frac{r(r-1)(2s+1)}{2} \right] \left(\frac{1}{3}\right) + [rs(r-1)] \left(\frac{1}{4}\right) + \left[\frac{r(r-1)s^2}{2} \right] \left(\frac{1}{5}\right) \right\}$$

$$= \frac{r(r-1)}{2} + 2rs + \frac{r(r-1)}{2} + \frac{r(s-1)(s-2)}{4} + \frac{rs}{2} + \frac{r(r-1)(2s+1)}{6}$$

$$\quad + \frac{rs(r-1)}{4} + \frac{r(r-1)s^2}{10}$$

$$= \left(\frac{r(r-1)}{2}\right) \left[1 + 1 + \frac{2s+1}{3} + \frac{s}{2} + \frac{s^2}{5} \right] + r \left[2s + \frac{(s-1)(s-2)}{4} \right]$$

$$= \left(\frac{r(r-1)}{2}\right) \left[\frac{60}{30} + \frac{20s}{30} + \frac{15s}{30} + \frac{6s^2}{30} \right] + r \left[\frac{8s + 2s - s^2 - 3s + 2}{4} \right]$$

$$= \left(\frac{r(r-1)}{2}\right) \left[\frac{6s^2 + 35s + 70}{30} \right] + r \left[\frac{s^2 + 7s + 2}{4} \right]$$

(ii) By the definition Reciprocal Complementary Wiener index

$$RCW(K_r\{P_s\}) = \sum_{u,v \in V(G)} \frac{1}{d+1-d(u,v)}$$

$$= \left\{ \left[\frac{r(r-1)}{2} + 2rs \right] \left(\frac{1}{5}\right) + \left[r(r-1) + \frac{r(s-1)(s-2)}{2} + rs \right] \left(\frac{1}{4}\right) \right.$$

$$\quad \left. + \left[\frac{r(r-1)(2s+1)}{2} \right] \left(\frac{1}{3}\right) + [rs(r-1)] \left(\frac{1}{2}\right) + \left[\frac{r(r-1)s^2}{2} \right] \left(\frac{1}{1}\right) \right\}$$

$$= \frac{r(r-1)}{10} + \frac{2rs}{5} + \frac{r(r-1)}{4} + \frac{r(s-1)(s-2)}{8} + \frac{rs}{4} + \frac{r(r-1)(2s+1)}{6}$$

$$\quad + \frac{rs(r-1)}{2} + \frac{r(r-1)s^2}{2}$$

$$\begin{aligned}
 &= \left(\frac{r(r-1)}{2}\right) \left[\frac{1}{5} + \frac{1}{2} + \frac{2s+1}{3} + s + s^2\right] + r \left[\frac{2s}{5} + \frac{s^2-3s+2}{8} + \frac{s}{4}\right] \\
 &= \left(\frac{r(r-1)}{2}\right) \left[\frac{7}{10} + \frac{2s}{3} + \frac{1}{3} + s + s^2\right] + r \left[\frac{(5s^2+11s+10)}{40}\right] \\
 &= \left(\frac{r(r-1)}{2}\right) \left[\frac{(30s^2+30s+20s+10+21)}{30}\right] + r \left[\frac{(5s^2+11s+10)}{40}\right] \\
 &= \left(\frac{r(r-1)}{2}\right) \left[\frac{(30s^2+50s+31)}{30}\right] + r \left[\frac{(5s^2+11s+10)}{40}\right]
 \end{aligned}$$

Theorem 2.3. Let K_r and P_s be complete and the path graph with $r \geq 2$ and $s \geq 2$. Then

$$(i) \text{SCI}(K_r\{P_s\}) = \left(\frac{r(r-1)}{2}\right) \left[\frac{(10s^2+54s+85)}{60}\right] + r \left[\frac{(s^2+5s+2)}{6}\right]$$

$$(ii) B(K_r\{P_s\}) = \left(\frac{r(r-1)}{2}\right) [25s^2+50s+18] + r [2s^2+4]$$

Proof. Under the assumption that K_r and P_s as specified earlier, then

(i) By the definition of Sum Connectivity index

$$\begin{aligned}
 \text{SCI}(K_r\{P_s\}) &= \sum \frac{1}{d(u,v)+1}, \quad u,v \in V(G) \\
 &= \left\{ \left[\frac{r(r-1)}{2} + 2rs\right] \left(\frac{1}{1+1}\right) + \left[r(r-1) + \frac{r(s-1)(s-2)}{2} + rs\right] \left(\frac{1}{2+1}\right) \right. \\
 &\quad \left. + \left[\frac{r(r-1)(2s+1)}{2}\right] \left(\frac{1}{3+1}\right) + [rs(r-1)] \left(\frac{1}{4+1}\right) + \left[\frac{r(r-1)s^2}{2}\right] \left(\frac{1}{5+1}\right) \right\} \\
 &= \frac{r(r-1)}{4} + rs + \frac{r(r-1)}{3} + \frac{r(s-1)(s-2)}{6} + \frac{rs}{3} + \frac{r(r-1)(2s+1)}{8} \\
 &\quad + \frac{rs(r-1)}{5} + \frac{r(r-1)s^2}{12} \\
 &= \left(\frac{r(r-1)}{2}\right) \left[\frac{1}{2} + \frac{2}{3} + \frac{2s+1}{4} + \frac{2s}{5} + \frac{s^2}{6}\right] + r \left[s + \frac{s}{3} + \frac{s^2-3s+2}{6}\right] \\
 &= \left(\frac{r(r-1)}{2}\right) \left[\frac{(30+40+30s+15+24s+10s^2)}{60}\right] + r \left[\frac{(s^2-3s+2+2s+6s)}{6}\right] \\
 &= \left(\frac{r(r-1)}{2}\right) \left[\frac{(10s^2+54s+85)}{60}\right] + r \left[\frac{(s^2+5s+2)}{6}\right]
 \end{aligned}$$

(ii) By the definition of Batschelet index

$$\begin{aligned}
 B(K_r\{P_s\}) &= \sum d(u,v)^2, \quad u,v \in V(G) \\
 &= \left[\frac{r(r-1)}{2} + 2rs\right] (1^2) + \left[r(r-1) + \frac{r(s-1)(s-2)}{2} + rs\right] (2^2) \\
 &\quad + \left[\frac{r(r-1)(2s+1)}{2}\right] (3^2) + [rs(r-1)] (4^2) + \left[\frac{r(r-1)s^2}{2}\right] (5^2) \\
 &= \frac{r(r-1)}{2} + 2rs + 4r(r-1) + 2r(s-1)(s-2) + 4rs + \frac{9r(r-1)(2s+1)}{2} + 16rs(r-1) \\
 &\quad + \frac{25r(r-1)s^2}{2} \\
 &= \left(\frac{r(r-1)}{2}\right) [1+8+18s+9+32s+25s^2] + r [2s^2+2s-6s+4+4s] \\
 &= \left(\frac{r(r-1)}{2}\right) [25s^2+50s+18] + r [2s^2+4]
 \end{aligned}$$

Theorem 2.4. Let the parameters K_r and P_s be as stated above, then

$$(i) \Lambda(K_r\{P_s\}) = \frac{r}{2} \{5(s+1)[r(s+1)-1] - [(r-1)(5s^2+14s+8) - 2(s^2+s+2)]\}$$

$$(ii) RA(K_r\{P_s\}) = r(r-1)/2 [(36s+17)/12] + r \left[\frac{s^2+2s+2}{6} \right]$$

Proof. Under the assumption that K_r and P_s be as defined above, then

(i) By the definition of Reverse Wiener index,

$$\begin{aligned} \Lambda(K_r\{P_s\}) &= \frac{n(n-1)d}{2} - W(G) \\ &= (r+rs)((r+rs)-1) \cdot \frac{5}{2} - \frac{r(r-1)}{2} (5s^2+14s+8) - r(s^2+s+2) \\ &= \frac{5}{2} [r^2+r^2s-r+r^2s+r^2s^2-rs] - \frac{r(r-1)}{2} (5s^2+14s+8) - r(s^2+s+2) \\ &= 5 \left[\frac{[r^2(1+2s+s^2) - r(s+1)]}{2} \right] - \frac{r(r-1)}{2} (5s^2+14s+8) - r(s^2+s+2) \\ &= \frac{r}{2} \{5[r(s^2+2s+1) - (s+1)] - [(r-1)(5s^2+14s+8) - 2(s^2+s+2)]\} \\ &= \frac{r}{2} \{5(s+1)[r(s+1)-1] - [(r-1)(5s^2+14s+8) - 2(s^2+s+2)]\} \end{aligned}$$

(ii) By the definition of Reciprocal Reverse Wiener index,

$$\begin{aligned} RA(K_r\{P_s\}) &= \sum_{\{u,v \in V(G)\}} \frac{1}{d-d(u,v)} \\ &= \left[\frac{r(r-1)}{2} + 2rs \right] \left(\frac{1}{5-1} \right) + \left[r(r-1) + \frac{r(s-1)(s-2)}{2} + rs \right] \left(\frac{1}{5-2} \right) \\ &\quad + \left[\frac{r(r-1)(2s+1)}{2} \right] \left(\frac{1}{5-3} \right) + [rs(r-1)] \left(\frac{1}{5-4} \right) + \left[\frac{r(r-1)s^2}{2} \right] \left(\frac{1}{5-5} \right) \\ &= \frac{r(r-1)}{8} + \frac{rs}{2} + \frac{r(r-1)}{3} + \frac{r(s-1)(s-2)}{6} + \frac{rs}{3} + \frac{r(r-1)(2s+1)}{4} + rs(r-1) \\ &= \frac{r(r-1)}{2} \left[\frac{1}{4} + \frac{2}{3} + \frac{2s+1}{2} + 2s \right] + r \left[\frac{s}{2} + \frac{s^2-3s+2}{6} + \frac{s}{3} \right] \\ &= \frac{r(r-1)}{2} \left[\frac{36s+17}{12} \right] + r \left[\frac{s^2+2s+2}{6} \right] \end{aligned}$$

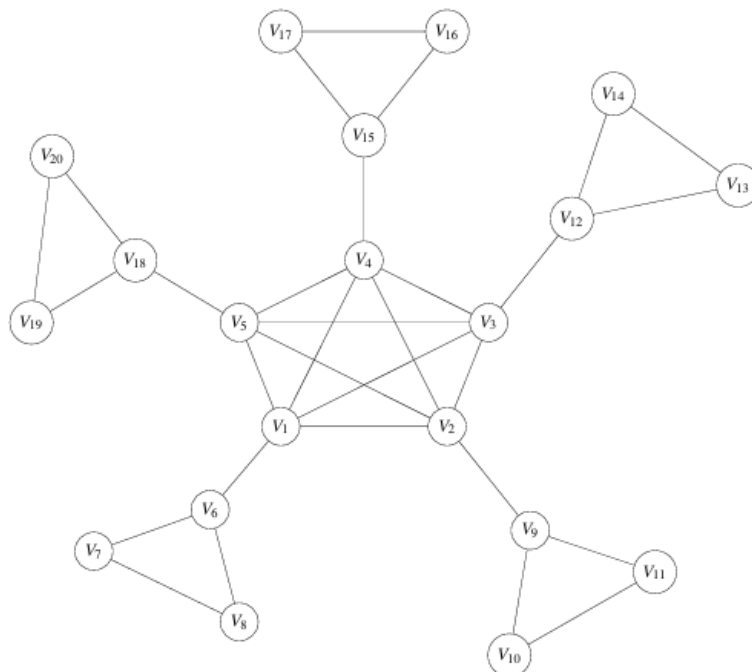


Figure 4: $K_5\{P_2\}$

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